Full wwPDB EM Validation Report

Oct 21, 2023 – 09:54 am BST

PDB ID	:	8BHF
EMDB ID	:	EMD-16052
Title	:	Cryo-EM structure of stalled rabbit 80S ribosomes in complex with human CCR4-NOT and CNOT4
Authors	:	Absmeier, E.; Chandrasekaran, V.; O'Reilly, F.J.; Stowell, J.A.W.; Rappsilber, J.; Passmore, L.A.
Deposited on	:	2022-10-31
Resolution	:	3.10 Å(reported)

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

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

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

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

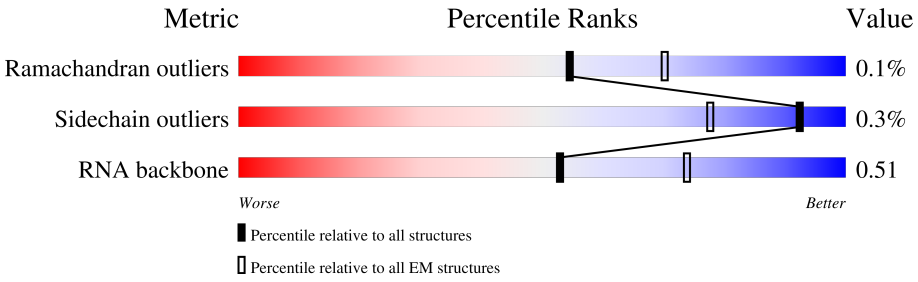
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A1	203	99%
2	B1	199	100%
3	C1	153	99%
4	D1	187	98%
5	E1	180	16% 99%
6	F1	176	100%
7	G1	159	99%
8	H1	99	12% 100%

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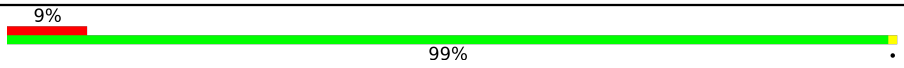
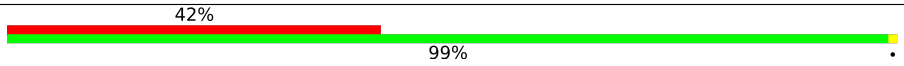
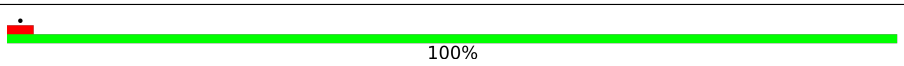
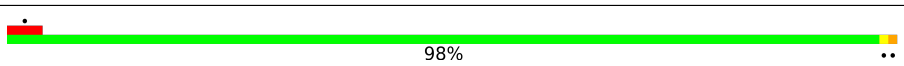
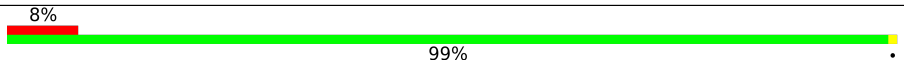
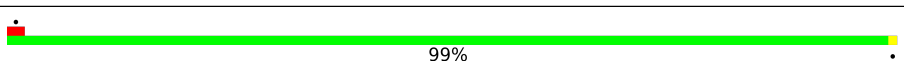
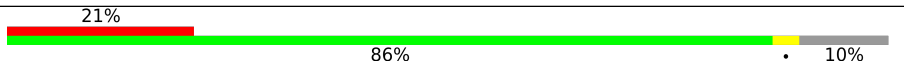
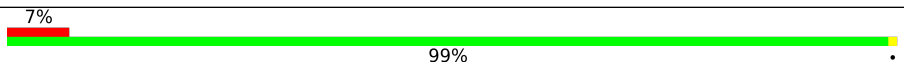
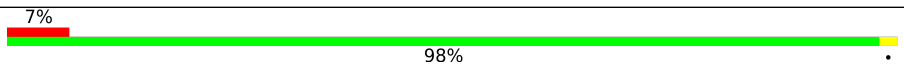
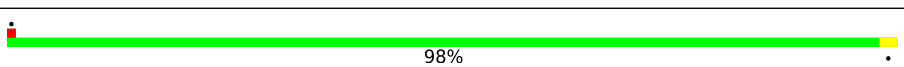
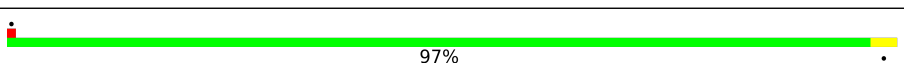
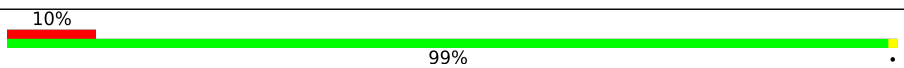
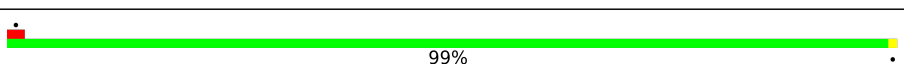
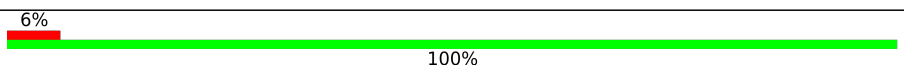
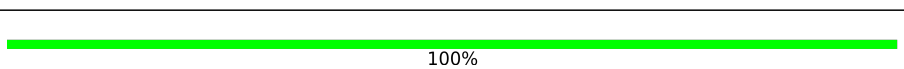
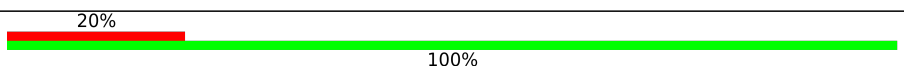
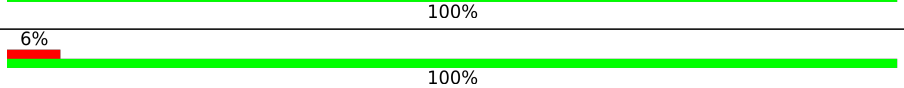
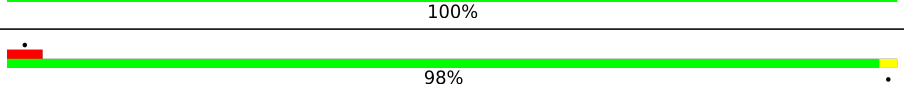
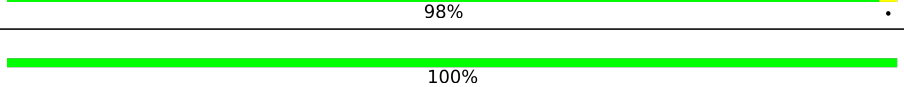
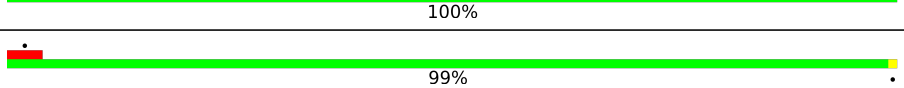
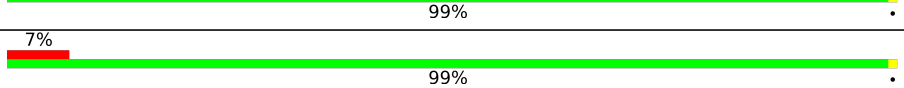
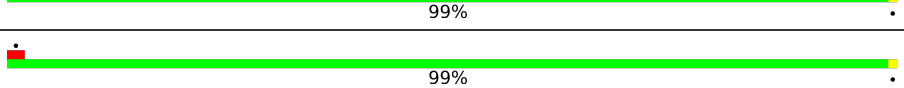
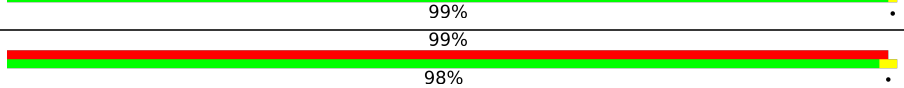
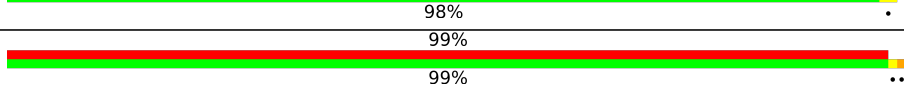
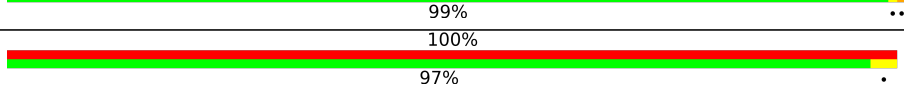
Mol	Chain	Length	Quality of chain
9	I1	139	
10	J1	106	
11	K1	118	
12	L1	134	
13	M1	135	
14	N1	147	
15	O1	116	
16	P1	98	
17	Q1	107	
18	R1	128	
19	S1	109	
20	T1	114	
21	U1	122	
22	V1	102	
23	W1	86	
24	X1	69	
25	Y1	50	
26	Z1	52	
27	a1	25	
28	b1	104	
29	c1	91	
30	d1	124	
31	e1	196	
32	f1	153	
33	l1	206	

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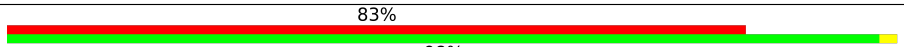
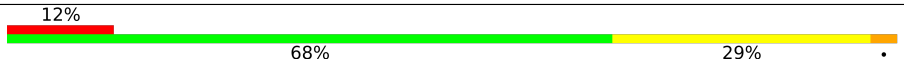
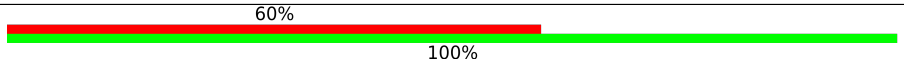
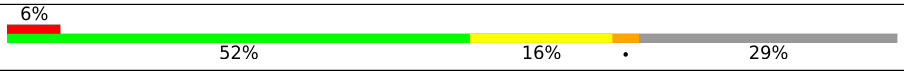
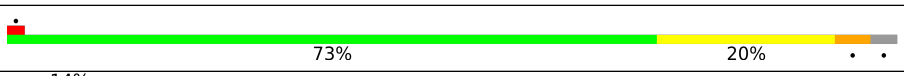
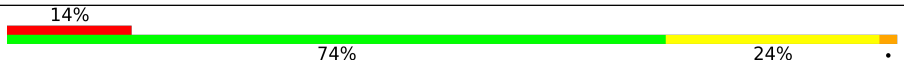
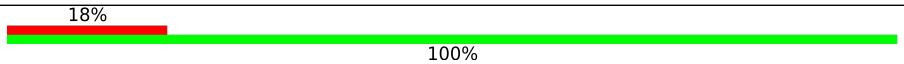
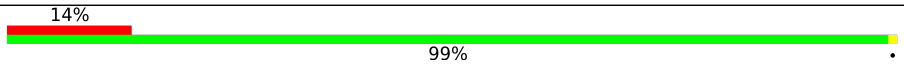
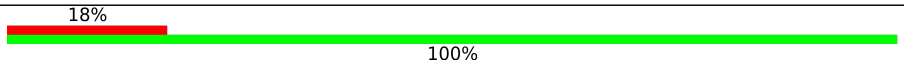
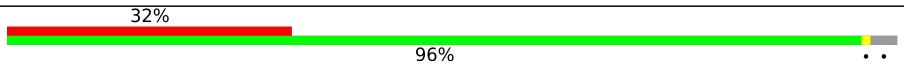
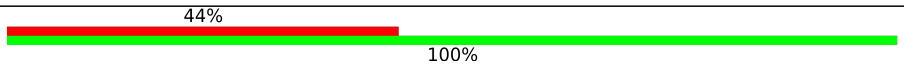
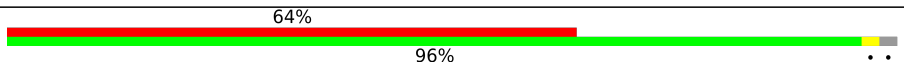
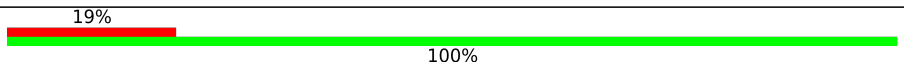
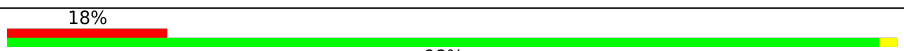
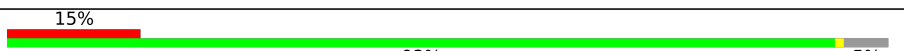
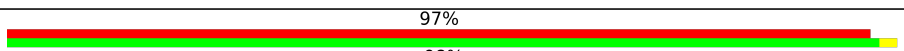
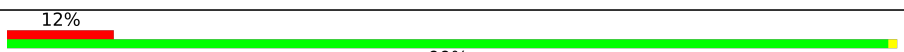
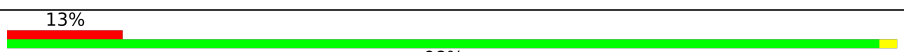
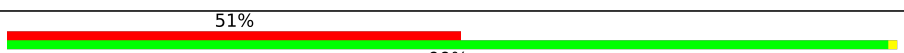
Mol	Chain	Length	Quality of chain
34	m1	3	
35	n1	236	
36	21	76	
37	11	5	
38	A2	5051	
39	B2	119	
40	C2	156	
41	A3	1697	
42	B3	217	
43	C3	213	
44	D3	221	
45	E3	228	
46	F3	262	
47	G3	191	
48	H3	237	
49	I3	189	
50	J3	206	
51	K3	185	
52	L3	96	
53	M3	151	
54	N3	117	
55	O3	149	
56	P3	136	
57	Q3	129	
58	R3	142	

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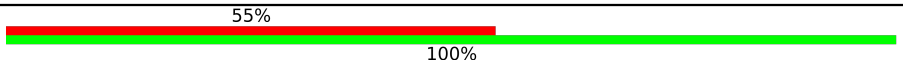
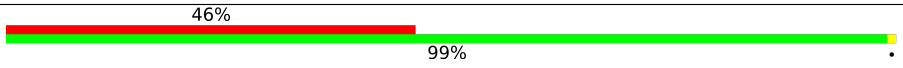
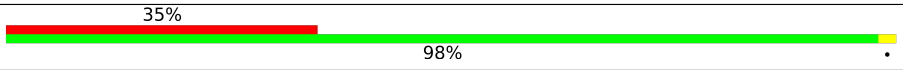
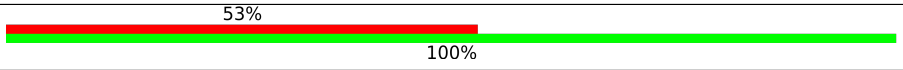
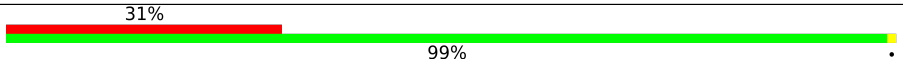
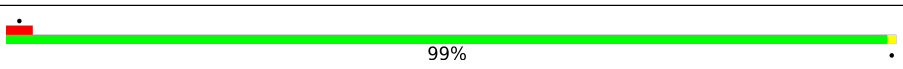
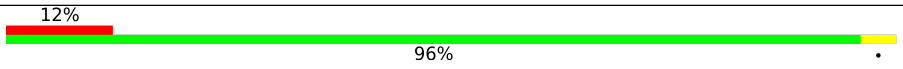
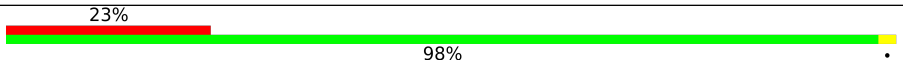
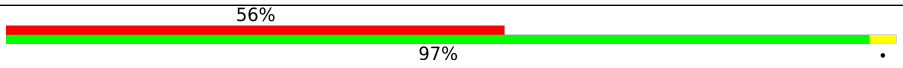
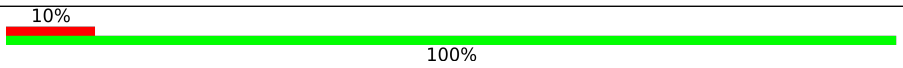
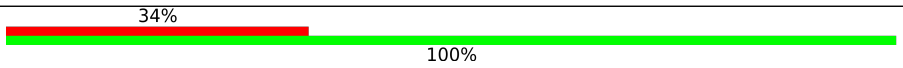
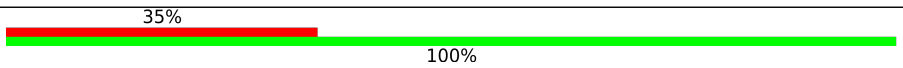
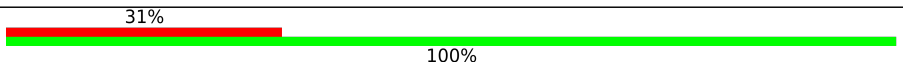
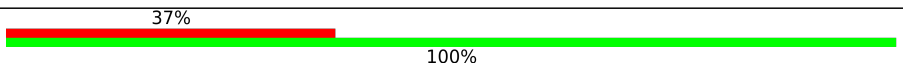
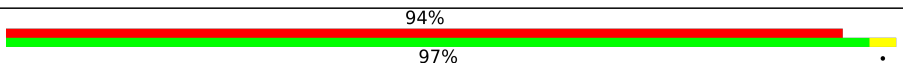
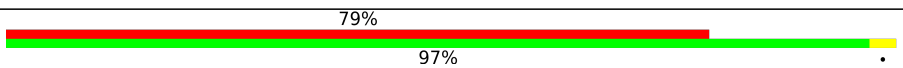
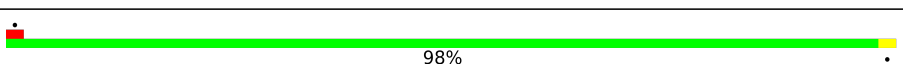
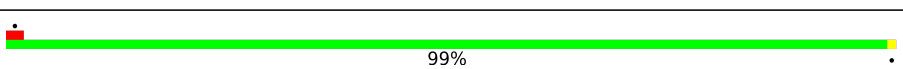
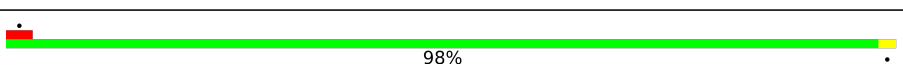
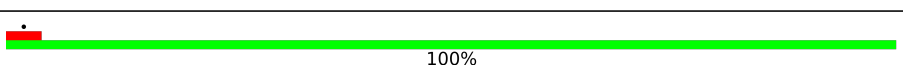
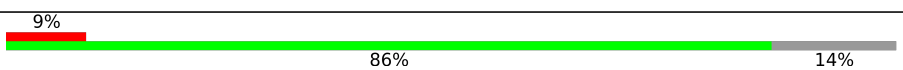
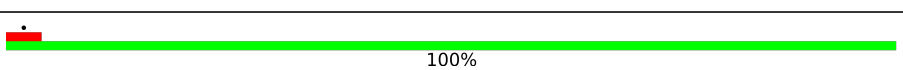
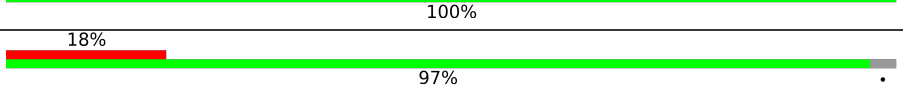
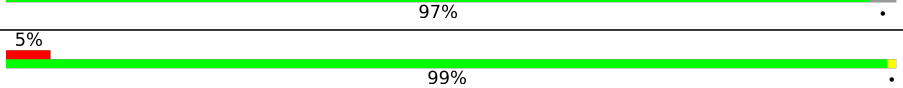
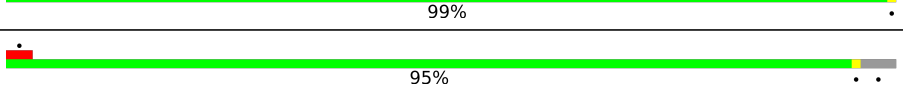
Mol	Chain	Length	Quality of chain
59	S3	132	
60	T3	144	
61	U3	141	
62	V3	100	
63	W3	83	
64	X3	129	
65	Y3	141	
66	Z3	124	
67	a3	75	
68	b3	101	
69	c3	83	
70	d3	62	
71	e3	55	
72	f3	57	
73	g3	68	
74	h3	313	
75	j3	248	
76	k3	394	
77	l3	362	
78	m3	293	
79	n3	251	
80	o3	225	
81	p3	240	
82	q3	190	
83	r3	213	

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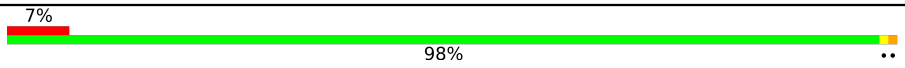
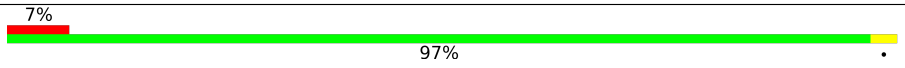
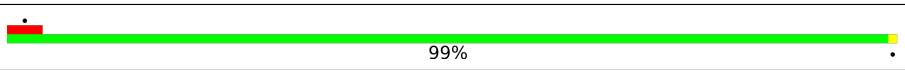
Mol	Chain	Length	Quality of chain
84	s3	170	
85	t3	210	
86	u3	138	

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 219017 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 protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A1	203	1701	1072	359	266	4	0	0

- Molecule 2 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B1	199	1630	1051	319	255	5	0	0

- Molecule 3 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C1	153	1242	777	241	215	9	0	0

- Molecule 4 is a protein called Ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D1	187	1515	946	315	250	4	0	0

- Molecule 5 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E1	180	1508	933	328	238	9	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E1	38	ARG	HIS	conflict	UNP G1TYL6
E1	151	ARG	HIS	conflict	UNP G1TYL6

- Molecule 6 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F1	176	Total	C	N	O	S	0	0
			1462	930	285	236	11		

- Molecule 7 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G1	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 8 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H1	99	Total	C	N	O	S	0	0
			809	519	141	147	2		

- Molecule 9 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I1	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 10 is a protein called TRASH domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J1	106	Total	C	N	O	S	0	0
			860	538	174	144	4		

- Molecule 11 is a protein called Ribosomal protein L23/L25 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K1	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 12 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L1	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 13 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M1	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 14 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N1	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 15 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O1	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 16 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P1	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 17 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q1	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 18 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R1	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 19 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S1	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 20 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T1	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 21 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U1	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 22 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V1	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V1	31	GLY	ARG	conflict	UNP G1TBH2
V1	58	MET	ILE	conflict	UNP G1TBH2

- Molecule 23 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W1	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 24 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X1	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X1	24	LYS	ASN	conflict	UNP G1U001

- Molecule 25 is a protein called 60S ribosomal protein L39-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y1	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 26 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z1	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 27 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a1	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 28 is a protein called Ribosomal protein L36a like.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b1	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 29 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c1	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 30 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d1	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 31 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e1	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 32 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f1	153	Total	C	N	O	S	0	0
			1160	722	218	217	3		

- Molecule 33 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	l1	206	Total	C	N	O	S	0	0
			1654	1058	297	291	8		

- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	m1	3	Total	C	N	O	P	0	0
			62	28	9	22	3		

- Molecule 35 is a protein called CCR4-NOT transcription complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	n1	236	Total	C	N	O	S	0	0
			1948	1209	346	387	6		

- Molecule 36 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	21	76	Total	C	N	O	P	0	0
			1620	723	287	534	76		

- Molecule 37 is a protein called nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	11	5	Total	C	N	O	0	0
			34	23	5	6		

- Molecule 38 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A2	3603	Total	C	N	O	P	0	0
			77264	34409	14151	25101	3603		

- Molecule 39 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	B2	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

- Molecule 40 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	C2	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 41 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	A3	1697	Total	C	N	O	P	0	0
			36229	16171	6507	11855	1696		

- Molecule 42 is a protein called 40S_SA_C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	B3	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

- Molecule 43 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	C3	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 44 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	D3	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 45 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	E3	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 46 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	F3	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F3	25	GLY	SER	conflict	UNP G1TK17
F3	51	ARG	LYS	conflict	UNP G1TK17
F3	78	THR	ALA	conflict	UNP G1TK17
F3	156	VAL	MET	conflict	UNP G1TK17

- Molecule 47 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	G3	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 48 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	H3	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 49 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	I3	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 50 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	J3	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J3	47	ARG	GLY	variant	UNP G1TJW1

- Molecule 51 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
51	K3	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 52 is a protein called Plectin/S10 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	L3	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 53 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	M3	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 54 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	N3	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 55 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	O3	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 56 is a protein called Ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	P3	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 57 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Q3	129	Total	C	N	O	S	0	0
			1058	670	201	180	7		

- Molecule 58 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	R3	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 59 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	S3	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 60 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	T3	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 61 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	U3	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U3	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 62 is a protein called Ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	V3	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 63 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	W3	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 64 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	X3	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 65 is a protein called Ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Y3	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 66 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Z3	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 67 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	a3	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 68 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	b3	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 69 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	c3	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 70 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	d3	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 71 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	e3	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 72 is a protein called Ubiquitin-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	f3	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 73 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	g3	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 74 is a protein called Ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	h3	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 75 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	j3	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 76 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	k3	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

- Molecule 77 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	l3	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

- Molecule 78 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	m3	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

- Molecule 79 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	n3	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 80 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	o3	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

- Molecule 81 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	p3	233	Total	C	N	O	S	0	0
			1879	1199	361	315	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p3	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 82 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	q3	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 83 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	r3	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 84 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	s3	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 85 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	t3	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
t3	74	ARG	HIS	conflict	UNP G1TKB3
t3	190	ARG	HIS	conflict	UNP G1TKB3

- Molecule 86 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	u3	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	C1	1	Total	Mg	0
			1	1	
87	I1	1	Total	Mg	0
			1	1	
87	N1	1	Total	Mg	0
			1	1	
87	T1	1	Total	Mg	0
			1	1	
87	A2	189	Total	Mg	0
			189	189	
87	B2	6	Total	Mg	0
			6	6	
87	C2	4	Total	Mg	0
			4	4	
87	A3	69	Total	Mg	0
			69	69	
87	M3	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
87	j3	1	Total Mg 1 1	0
87	r3	1	Total Mg 1 1	0

- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

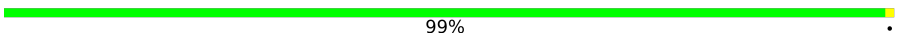
Mol	Chain	Residues	Atoms	AltConf
88	T1	1	Total Zn 1 1	0
88	W1	1	Total Zn 1 1	0
88	Z1	1	Total Zn 1 1	0
88	b1	1	Total Zn 1 1	0
88	c1	1	Total Zn 1 1	0
88	b3	1	Total Zn 1 1	0
88	e3	1	Total Zn 1 1	0

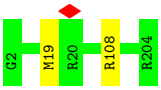
3 Residue-property plots (i)

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

• Molecule 1: Ribosomal protein L15

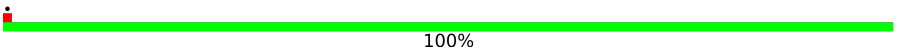
Chain A1:





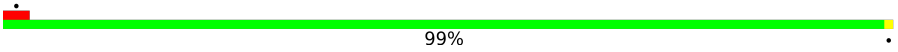
• Molecule 2: 60S ribosomal protein L13a

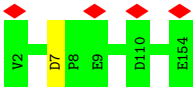
Chain B1:



• Molecule 3: 60S ribosomal protein L17

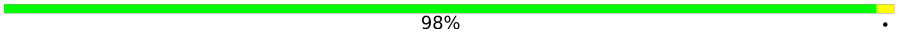
Chain C1:

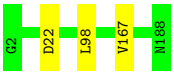




• Molecule 4: Ribosomal protein L18

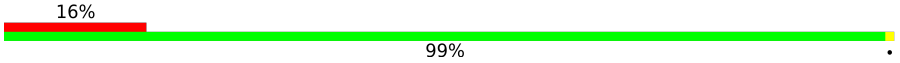
Chain D1:

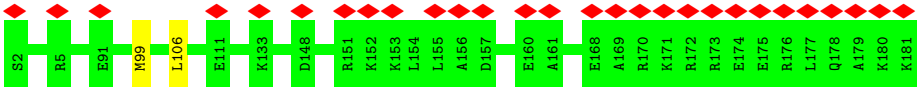




• Molecule 5: Ribosomal protein L19

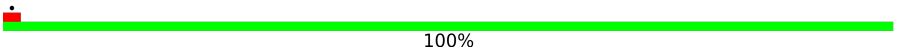
Chain E1:

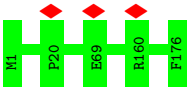




• Molecule 6: 60S ribosomal protein L18a

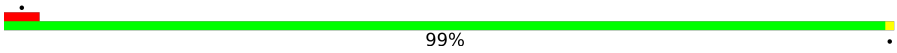
Chain F1:

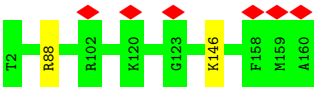




• Molecule 7: 60S ribosomal protein L21

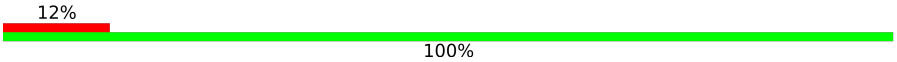
Chain G1:

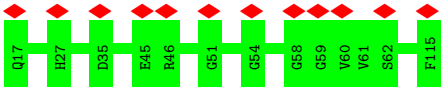




• Molecule 8: 60S ribosomal protein L22

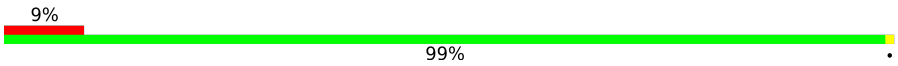
Chain H1:

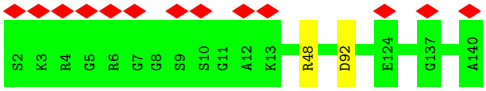




• Molecule 9: 60S ribosomal protein L23

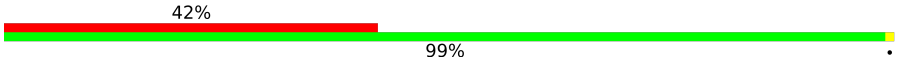
Chain I1:

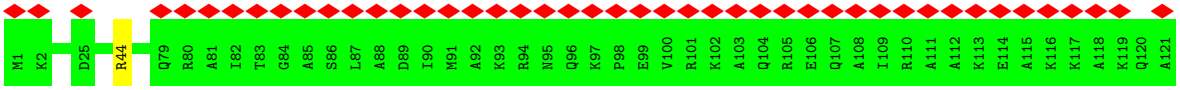




• Molecule 10: TRASH domain-containing protein

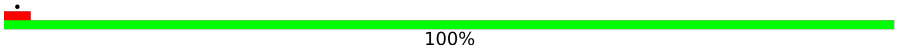
Chain J1:

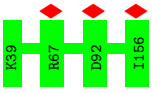




• Molecule 11: Ribosomal protein L23/L25 N-terminal domain-containing protein

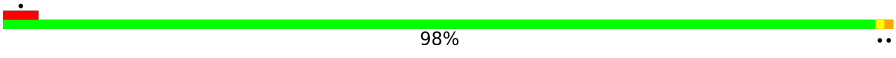
Chain K1:

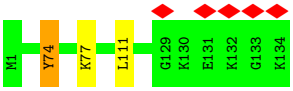




• Molecule 12: Ribosomal protein L26

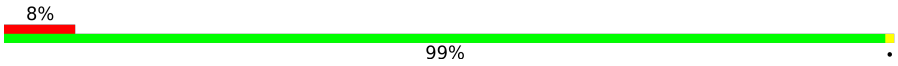
Chain L1:

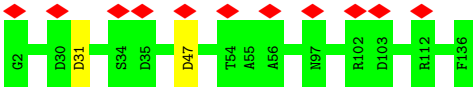




• Molecule 13: 60S ribosomal protein L27

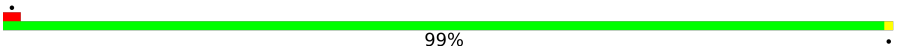
Chain M1:

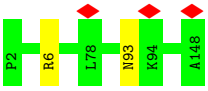




• Molecule 14: 60S ribosomal protein L27a

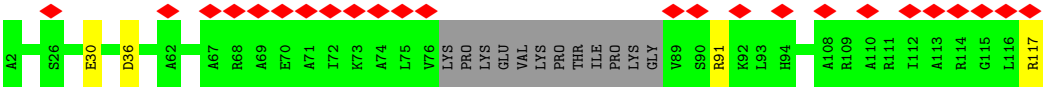
Chain N1:





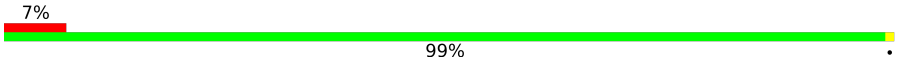
• Molecule 15: 60S ribosomal protein L29

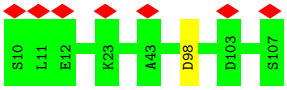
Chain O1:



• Molecule 16: 60S ribosomal protein L30

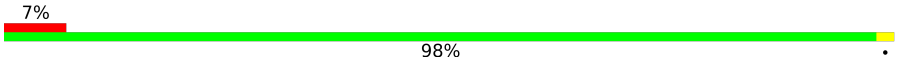
Chain P1:

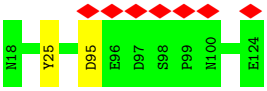




• Molecule 17: 60S ribosomal protein L31

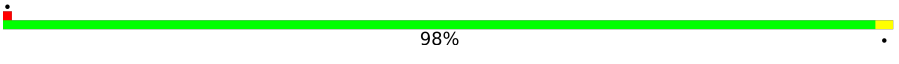
Chain Q1:

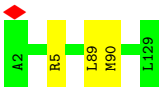




• Molecule 18: Ribosomal protein L32

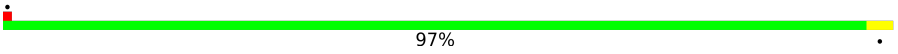
Chain R1:

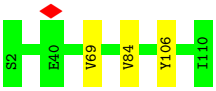




• Molecule 19: 60S ribosomal protein L35a

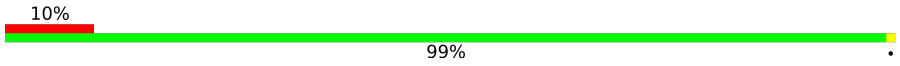
Chain S1:

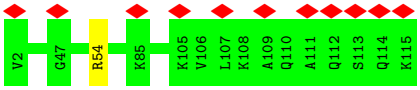




• Molecule 20: 60S ribosomal protein L34

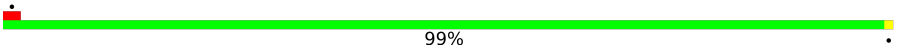
Chain T1:

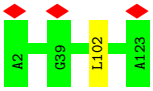




• Molecule 21: 60S ribosomal protein L35

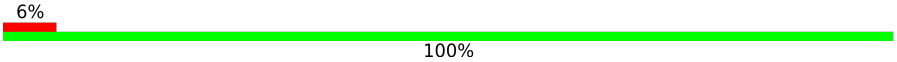
Chain U1:

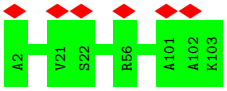




• Molecule 22: 60S ribosomal protein L36

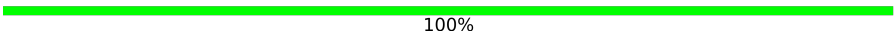
Chain V1:





• Molecule 23: Ribosomal protein L37

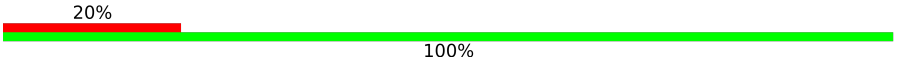
Chain W1:

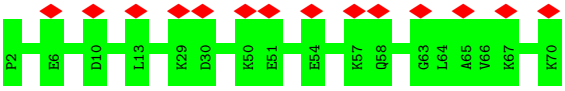


There are no outlier residues recorded for this chain.

• Molecule 24: 60S ribosomal protein L38

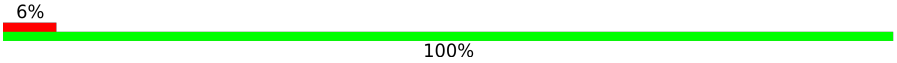
Chain X1:

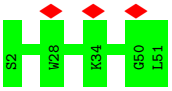




• Molecule 25: 60S ribosomal protein L39-like

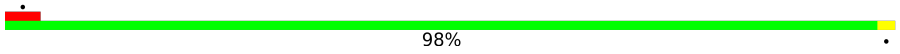
Chain Y1:

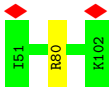




• Molecule 26: Ubiquitin-60S ribosomal protein L40

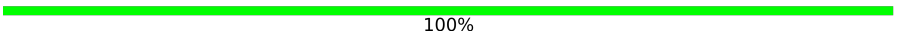
Chain Z1:





• Molecule 27: 60S ribosomal protein L41

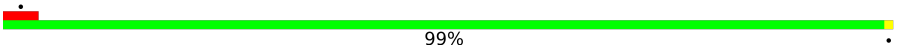
Chain a1:

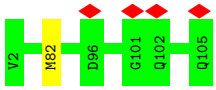


There are no outlier residues recorded for this chain.

• Molecule 28: Ribosomal protein L36a like

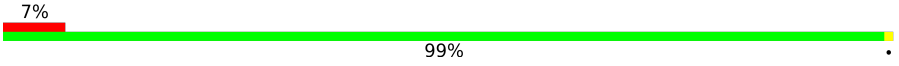
Chain b1:

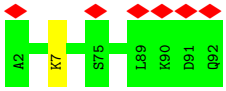




• Molecule 29: 60S ribosomal protein L37a

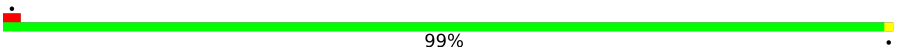
Chain c1:

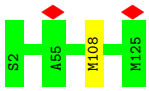




• Molecule 30: 60S ribosomal protein L28

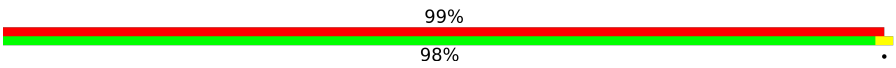
Chain d1:

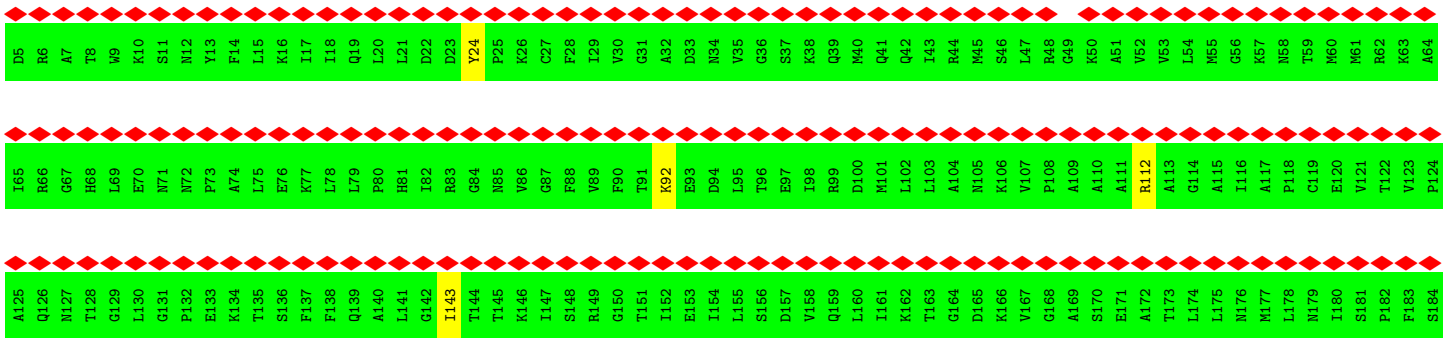




• Molecule 31: 60S acidic ribosomal protein P0

Chain e1:





F185 G186 L187 I188 I189 Q190 Q191 V192 F193 D194 N195 G196 S197 I198 Y199 N200

• Molecule 32: 60S ribosomal protein L12

Chain f1: 99% 99%

E9 I10 K11 V12 V13 Y14 L15 R16 C17 T18 G19 G20 E21 V22 G23 A24 T25 S26 A27 L28 A29 P30 K31 I32 G33 P34 L35 G36 L37 S38 P39 K40 K41 V42 G43 D44 D45 I46 A47 K48 A49 T50 G51 D52 W53 K54 G55 L56 R57 I58 T59 V60 K61 L62 T63 I64 Q65 N66 R67 Q68

A69 Q70 I71 E72 V73 V74 P75 S76 A77 S78 A79 L80 I81 I82 K83 A84 L85 K86 E87 P88 P89 R90 D91 R92 K93 K94 Q95 K96 N97 I98 K99 H100 S101 G102 N103 I104 T105 F106 D107 E108 I109 V110 N111 I112 A113 R114 Q115 M116 R117 H118 R119 S120 L121 A122 R123 E124 L125 S126 G127 T128

I129 K130 E131 I132 L133 G134 T135 A136 Q137 S138 V139 G140 C141 N142 V143 D144 G145 R146 H147 P148 H149 D150 I151 I152 D153 D154 I155 N156 S157 G158 A159 V160 E161

• Molecule 33: 60S ribosomal protein L10a

Chain l1: 100% 97%

V5 S6 R7 D8 T9 L10 Y11 E12 A13 V14 R15 E16 V17 L18 H19 G20 N21 Q22 R23 K24 R25 R26 K27 F28 L29 E30 T31 V32 E33 L34 Q35 I36 S37 L38 K39 N40 Y41 D42 P43 Q44 K45 D46 K47 R48 F49 S50 G51 T52 V53 R54 L55 K56 S57 T58 P59 R60 P61 K62 F63 S64

V65 C66 V67 L68 G69 D70 Q71 Q72 H73 C74 D75 E76 A77 K78 A79 V80 D81 I82 P83 H84 M85 D86 I87 E88 A89 L90 K91 K92 L93 N94 K95 N96 K97 K98 L99 V100 K101 K102 L103 A104 K105 K106 Y107 D108 A109 F110 L111 A112 S113 E114 S115 L116 I117 K118 Q119 I120 P121 R122 I123 L124

G125 P126 G127 L128 N129 K130 A131 G132 K133 F134 P135 S136 L137 L138 T139 H140 N141 E142 N143 M144 V145 A146 K147 V148 D149 E150 V151 K152 S153 T154 I155 K156 F157 Q158 M159 K160 K161 V162 L163 C164 L165 A166 V167 A168 V169 G170 H171 V172 K173 M174 T175 D176 D177 E178 L179 V180 Y181 N182 I183 H184

L185 A186 V187 N188 F189 L190 V191 S192 L193 L194 K195 K196 N197 W198 Q199 N200 V201 R202 A203 L204 Y205 I206 K207 S208 T209 M210

• Molecule 34: mRNA

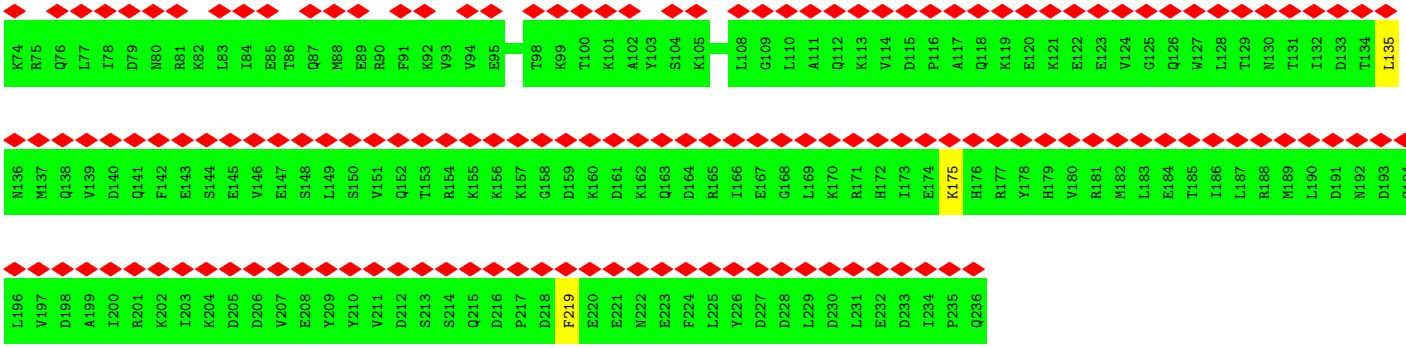
Chain m1: 67% 33%

U36 U37 A38

• Molecule 35: CCR4-NOT transcription complex subunit 3

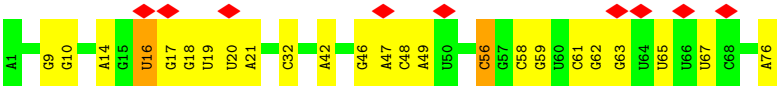
Chain n1: 83% 98%

M1 A2 D3 L7 Q8 G9 D12 R13 K16 E20 G21 V22 E23 Q24 F25 E26 D27 I28 W29 H33 N34 A35 A36 N37 A38 N39 Q40 K41 E42 K43 Y44 E45 A46 D47 L48 K49 K50 K54 L55 Q56 R57 L58 R59 D60 Q61 I62 K63 S68 N69 E70 I71 K72 D73



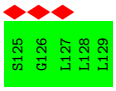
• Molecule 36: P-site tRNA

Chain 21:



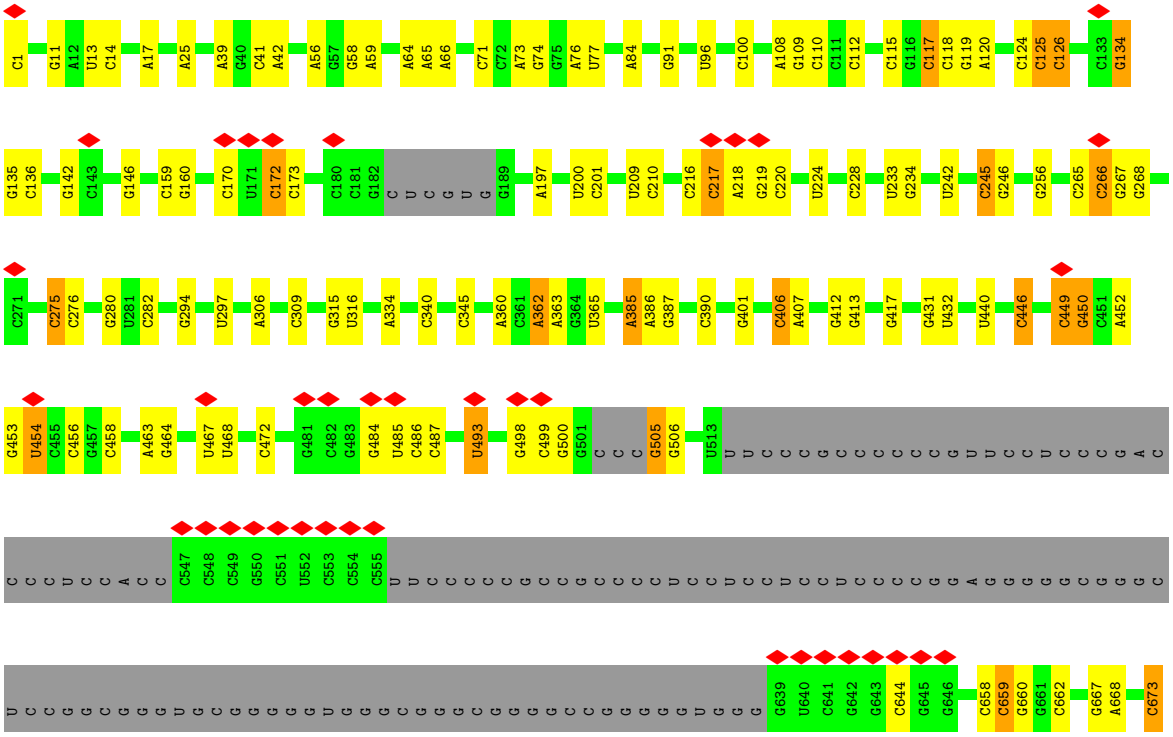
• Molecule 37: nascent chain

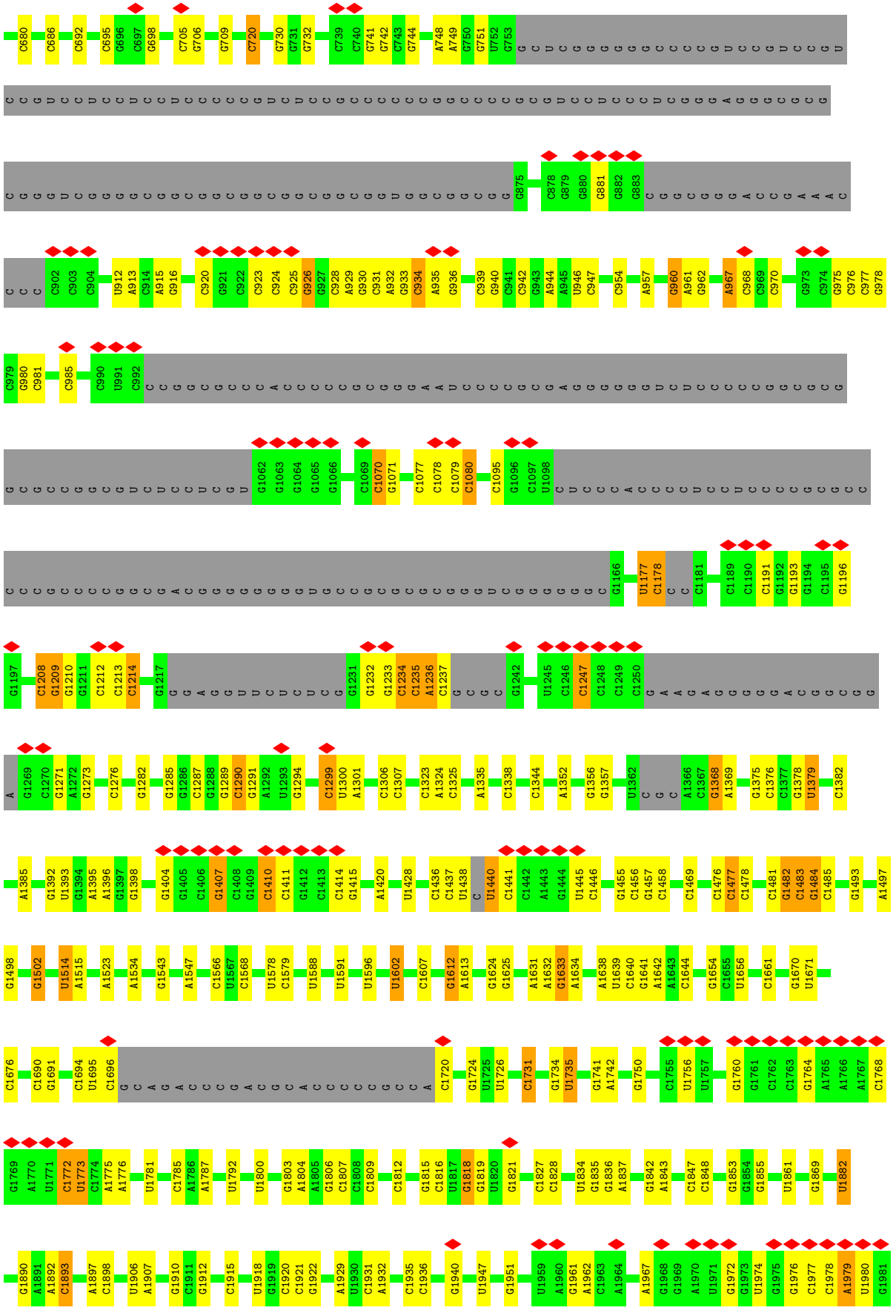
Chain 11:

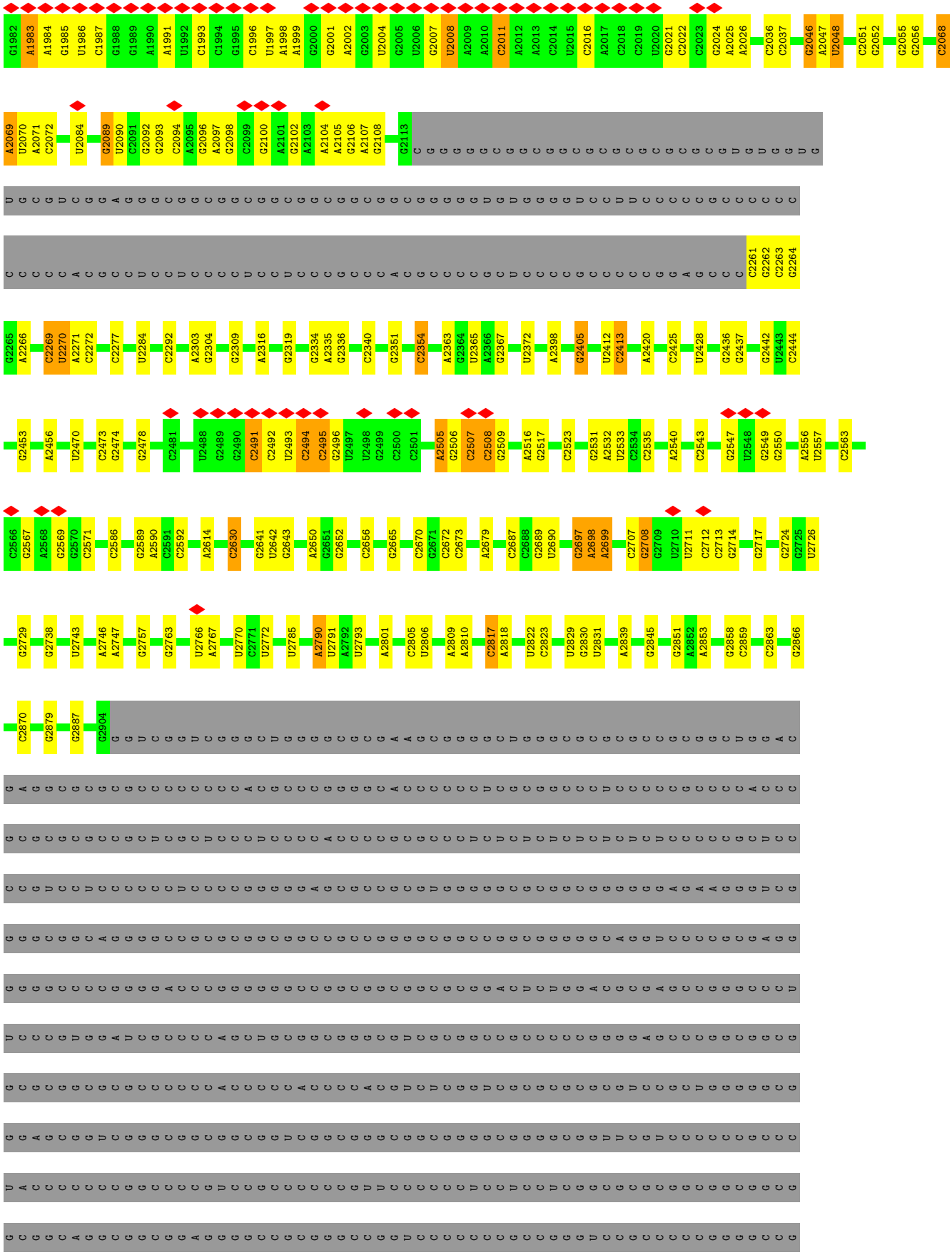


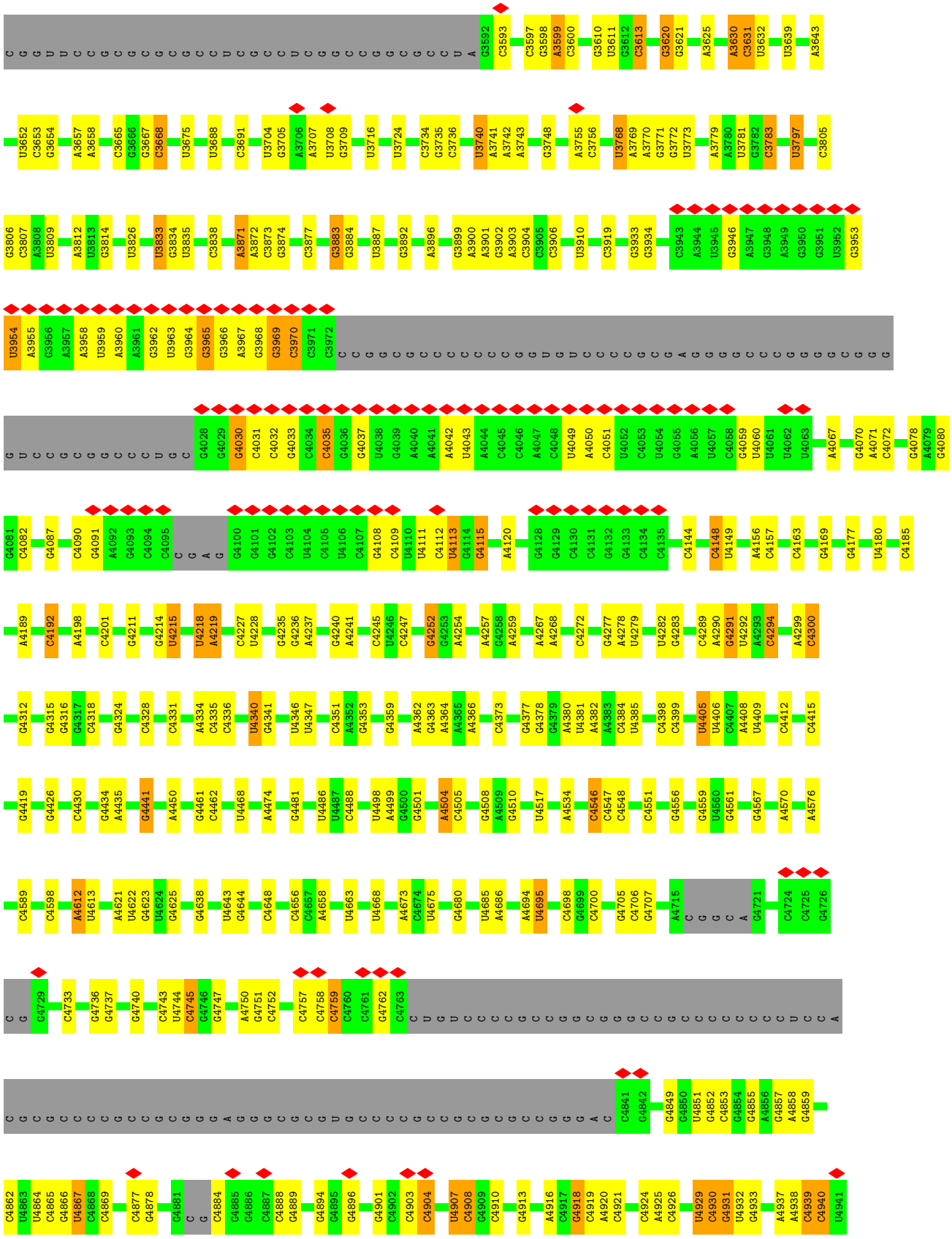
• Molecule 38: 28S ribosomal RNA

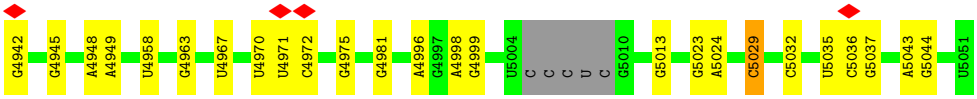
Chain A2:





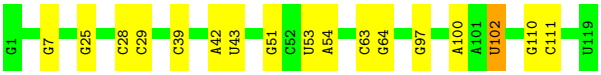






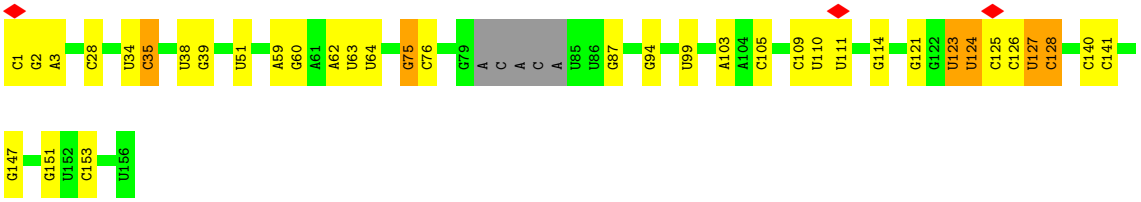
• Molecule 39: 5S ribosomal RNA

Chain B2:



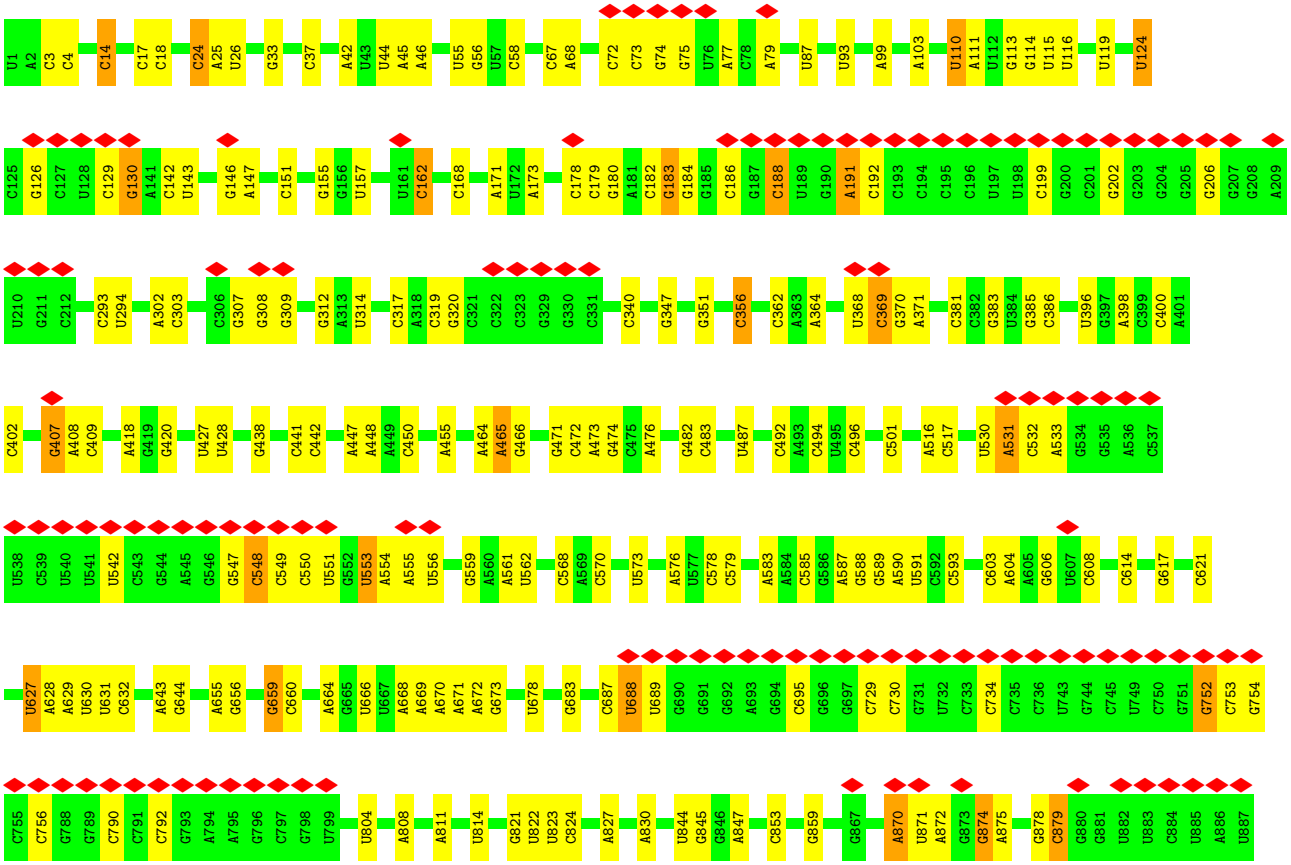
• Molecule 40: 5.8S ribosomal RNA

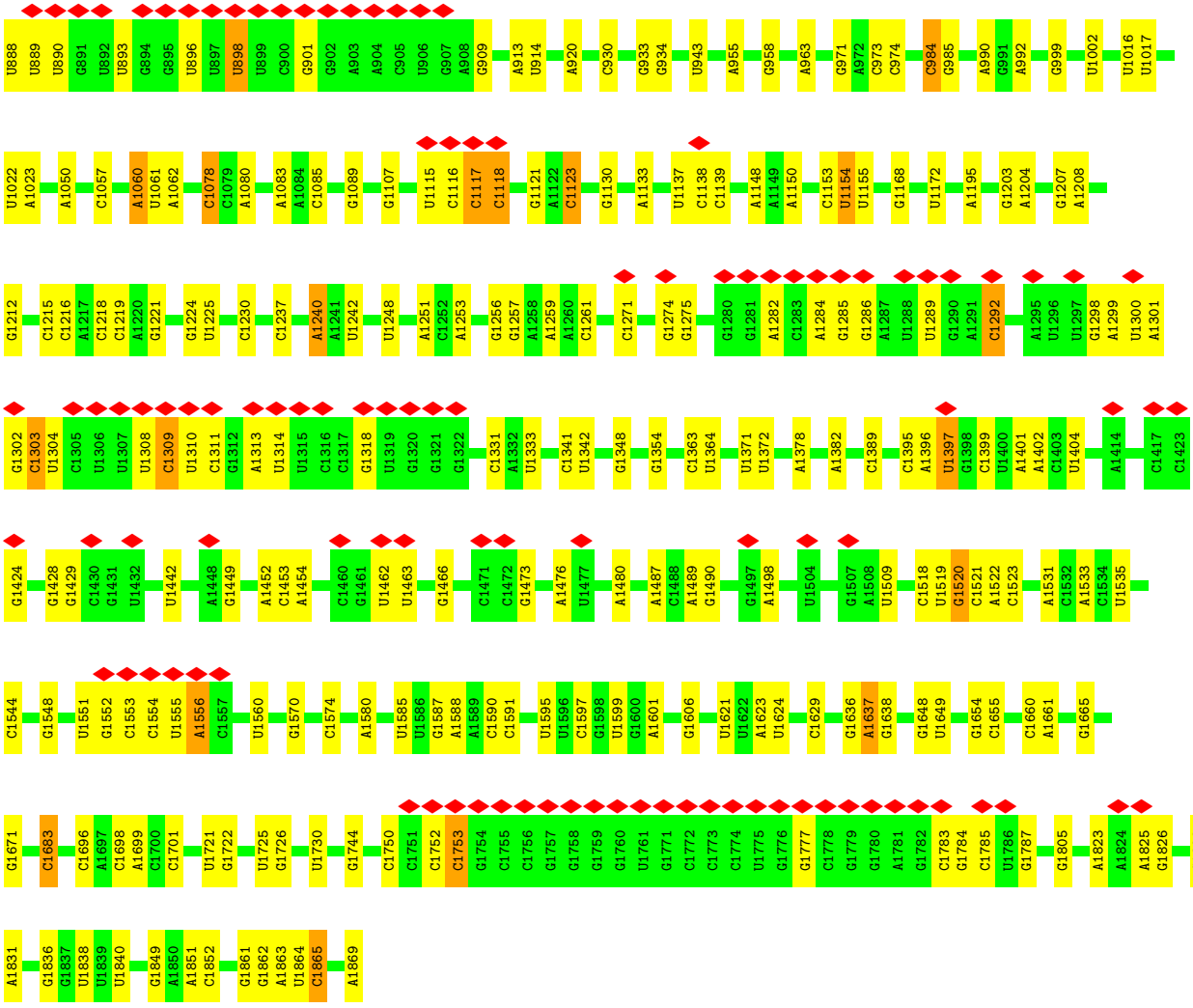
Chain C2:



• Molecule 41: 18S ribosomal RNA

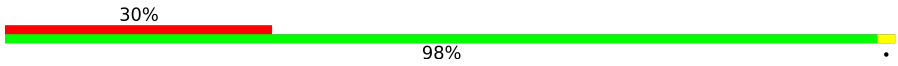
Chain A3:

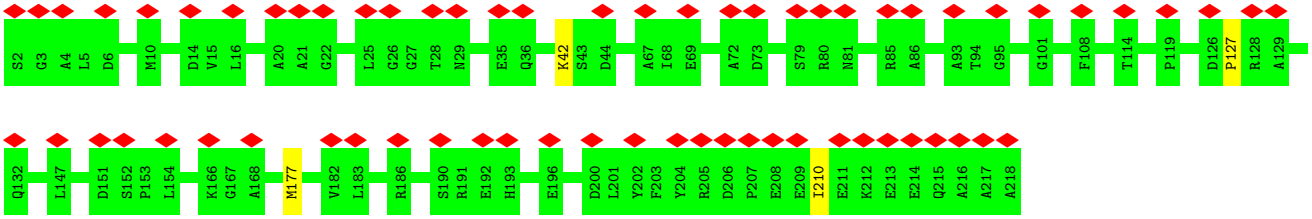




• Molecule 42: 40S_SA_C domain-containing protein

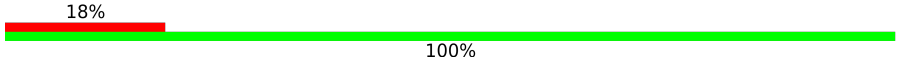
Chain B3:

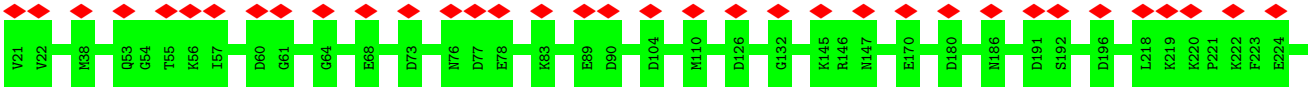


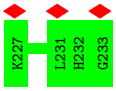


• Molecule 43: 40S ribosomal protein S3a

Chain C3:

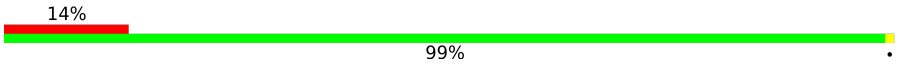


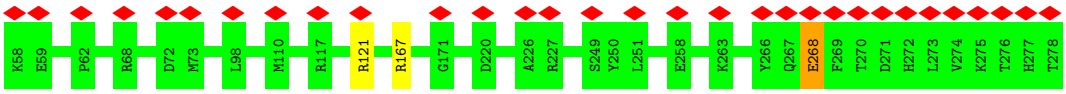




• Molecule 44: 40S ribosomal protein S2

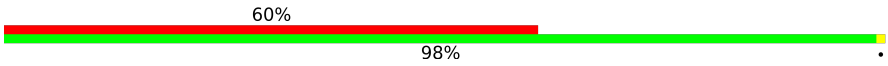
Chain D3:

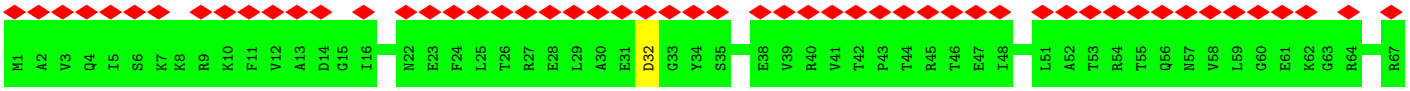


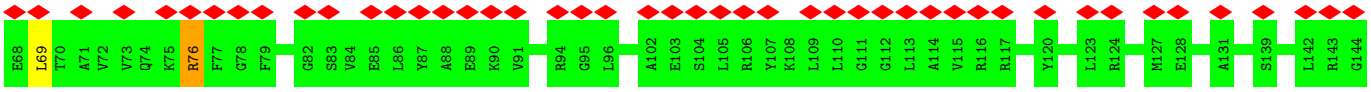


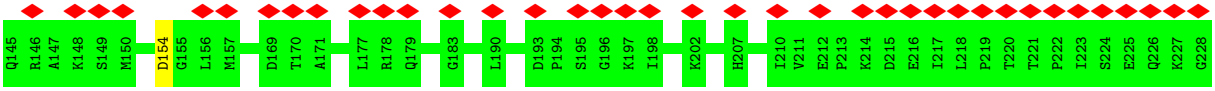
• Molecule 45: Ribosomal protein S3

Chain E3:



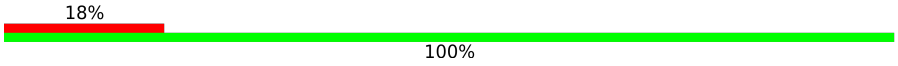


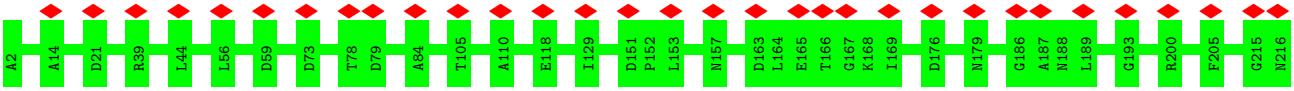


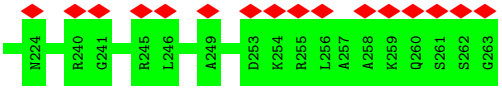


• Molecule 46: 40S ribosomal protein S4

Chain F3:

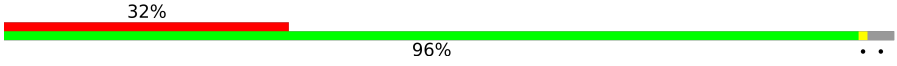


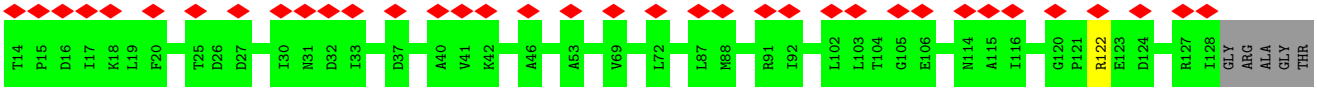


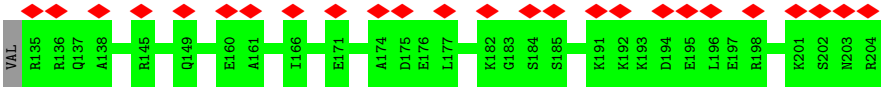


• Molecule 47: Ribosomal protein S5

Chain G3:

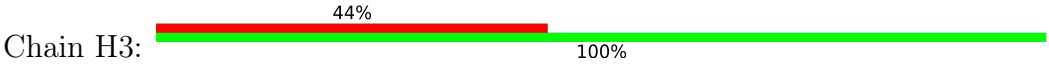


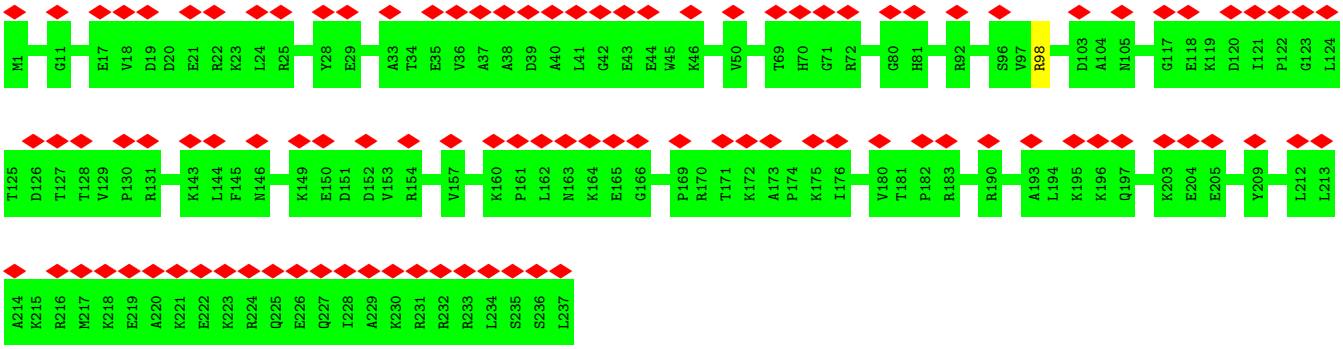




• Molecule 48: 40S ribosomal protein S6

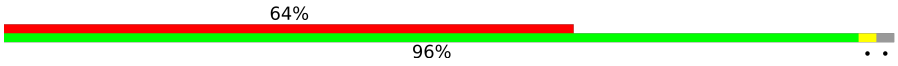
Chain H3:

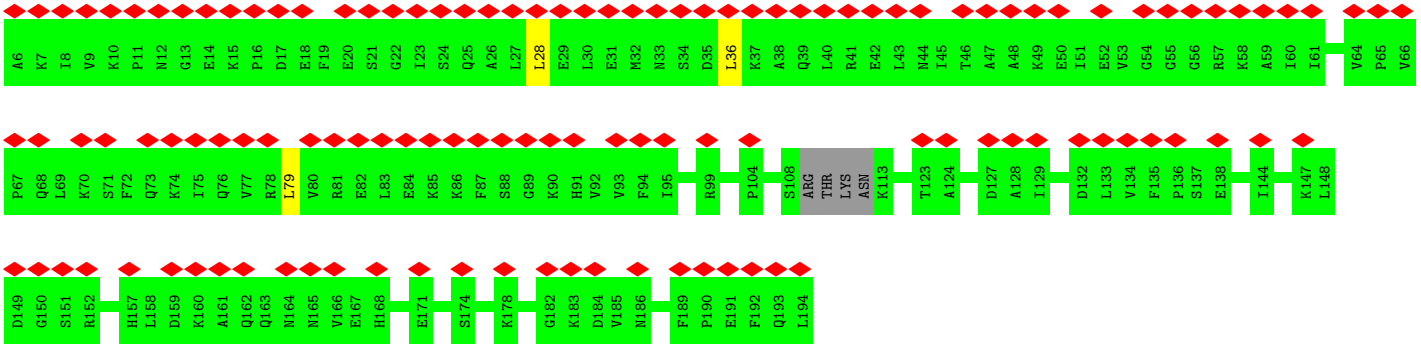




• Molecule 49: 40S ribosomal protein S7

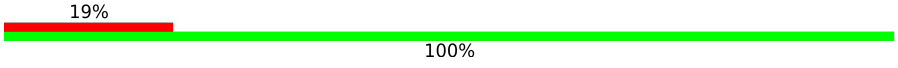
Chain I3:

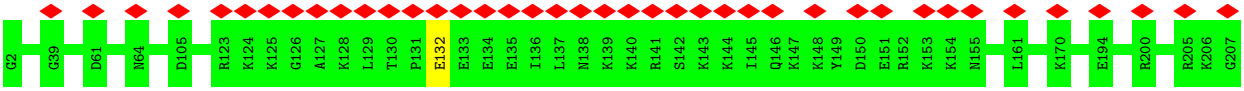




• Molecule 50: 40S ribosomal protein S8

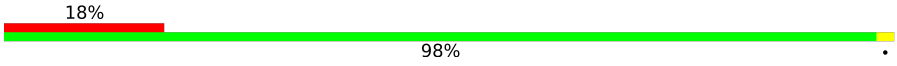
Chain J3:

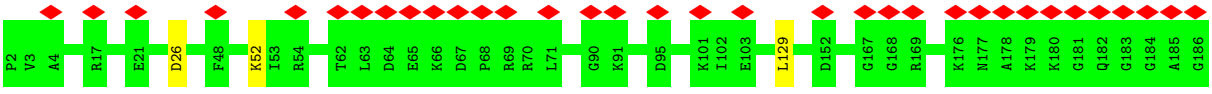




• Molecule 51: Ribosomal protein S9 (Predicted)

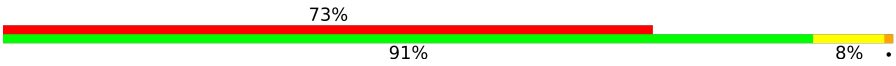
Chain K3:

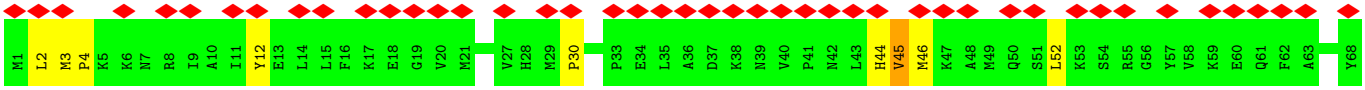


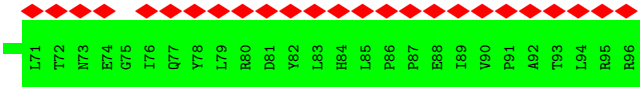


• Molecule 52: Plectin/S10 N-terminal domain-containing protein

Chain L3:

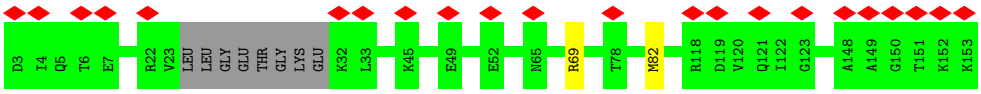






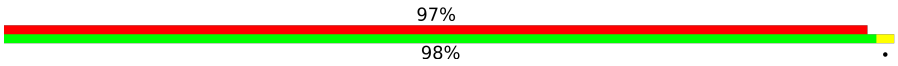
• Molecule 53: 40S ribosomal protein S11

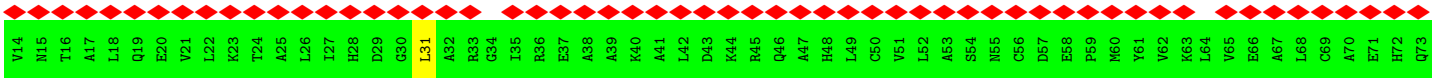
Chain M3:

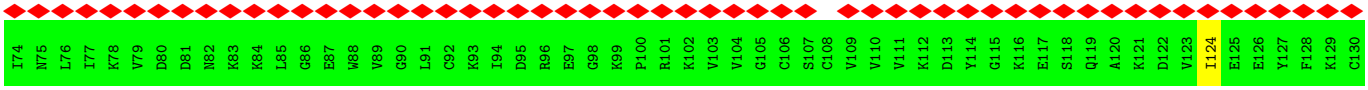


• Molecule 54: 40S ribosomal protein S12

Chain N3:

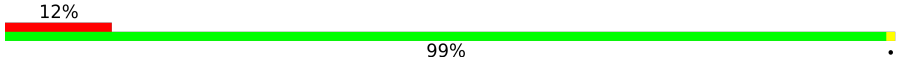


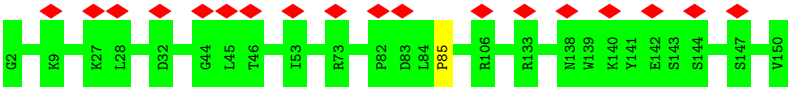




• Molecule 55: ribosomal protein uS15

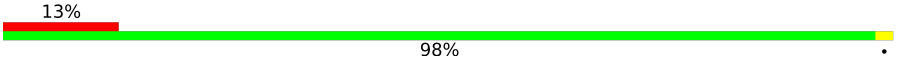
Chain O3:

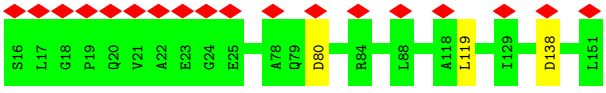




• Molecule 56: Ribosomal protein S14

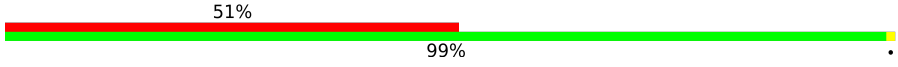
Chain P3:

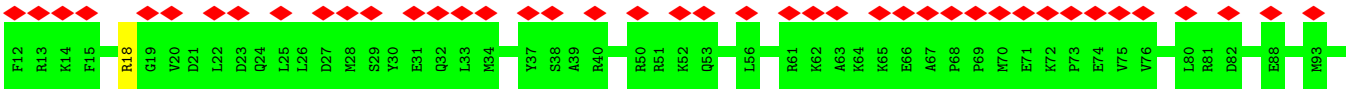


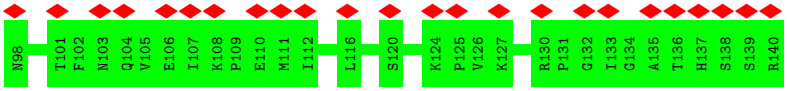


• Molecule 57: 40S ribosomal protein S15

Chain Q3:

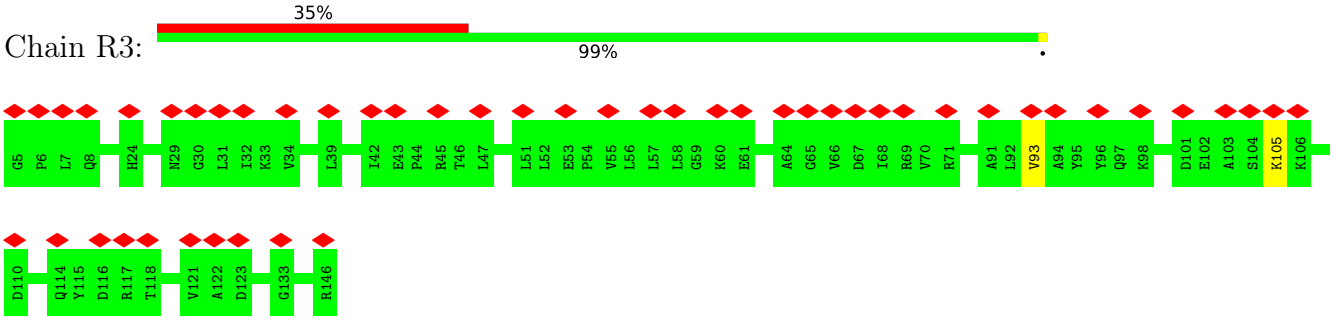






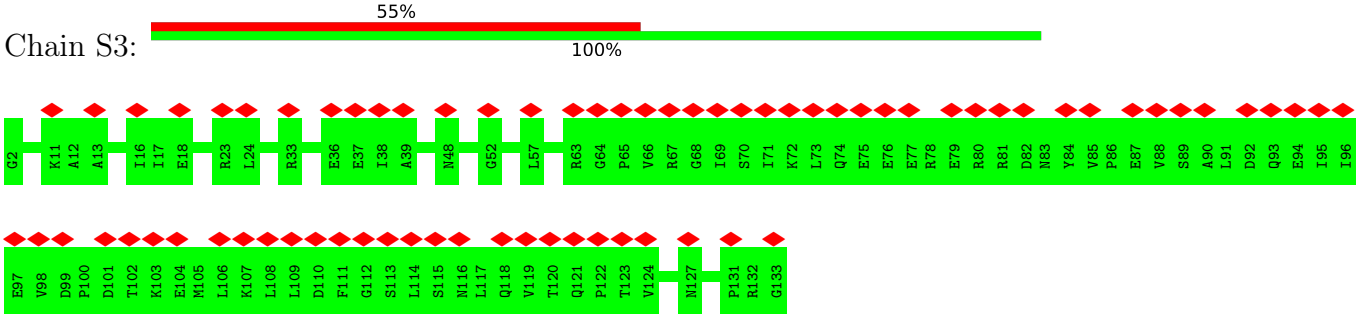
• Molecule 58: Ribosomal protein S16

Chain R3:



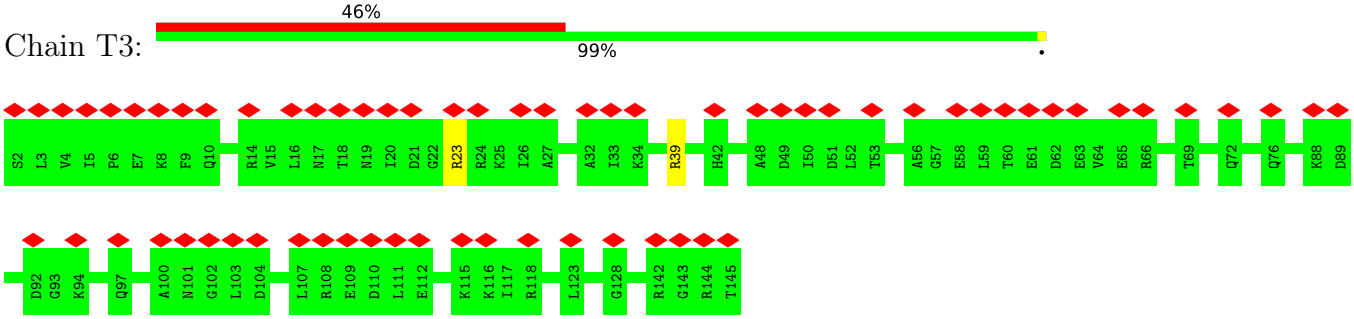
• Molecule 59: 40S ribosomal protein S17

Chain S3:



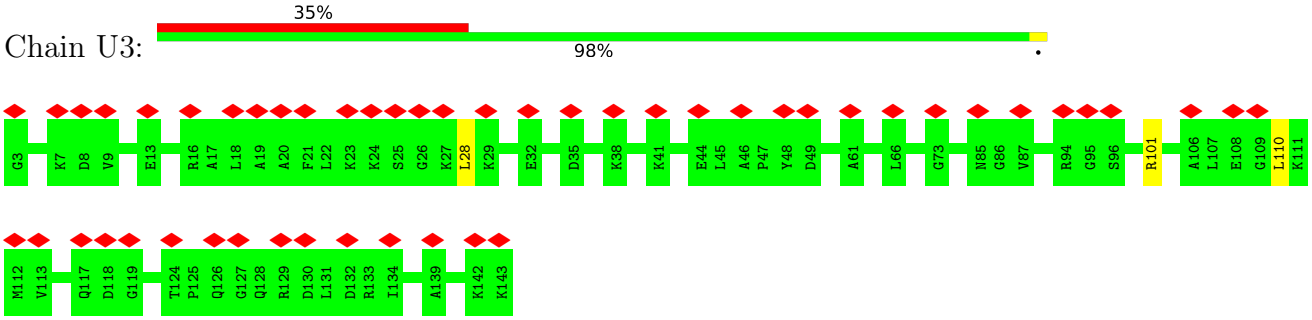
• Molecule 60: 40S ribosomal protein S18

Chain T3:



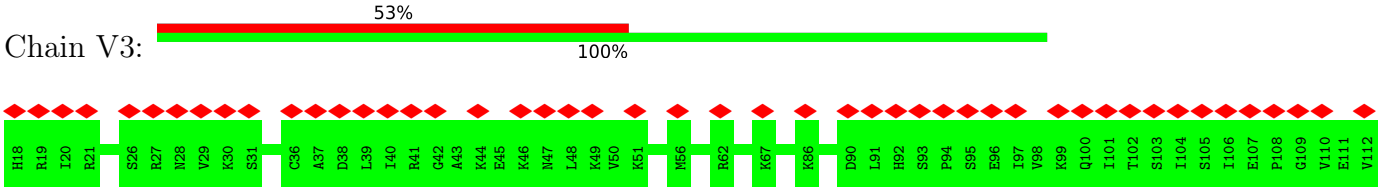
• Molecule 61: 40S ribosomal protein S19

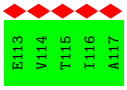
Chain U3:



• Molecule 62: Ribosomal protein S20

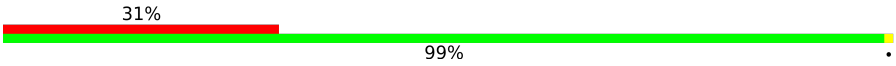
Chain V3:

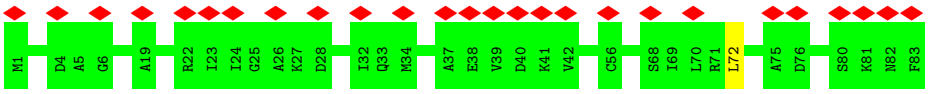




• Molecule 63: 40S ribosomal protein S21

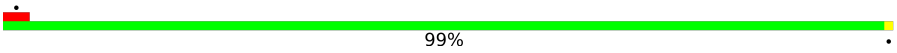
Chain W3:

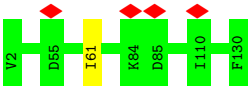




• Molecule 64: Ribosomal protein S15a

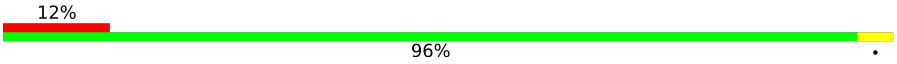
Chain X3:

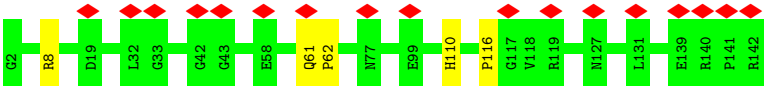




• Molecule 65: Ribosomal protein S23

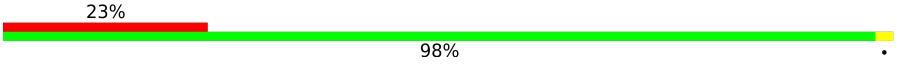
Chain Y3:

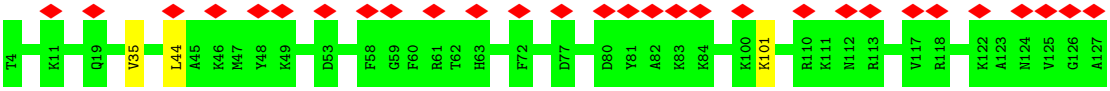




• Molecule 66: 40S ribosomal protein S24

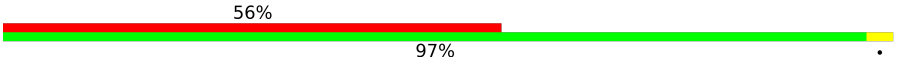
Chain Z3:

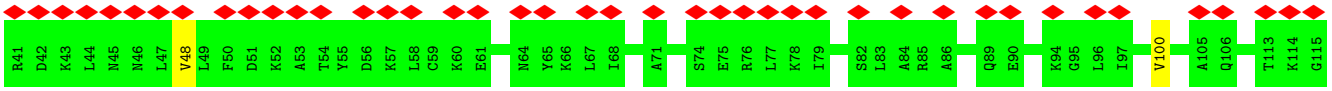




• Molecule 67: 40S ribosomal protein S25

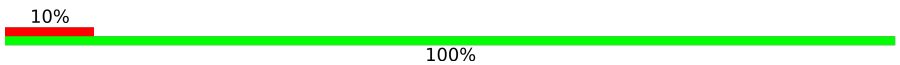
Chain a3:

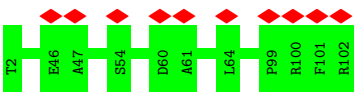




• Molecule 68: 40S ribosomal protein S26

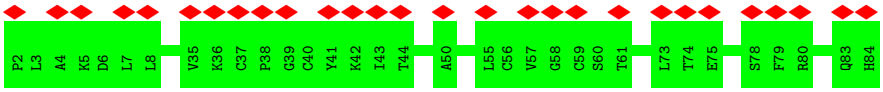
Chain b3:





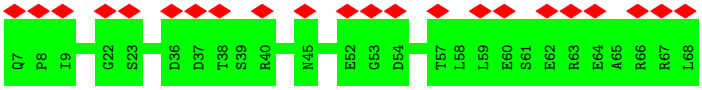
• Molecule 69: 40S ribosomal protein S27

Chain c3:



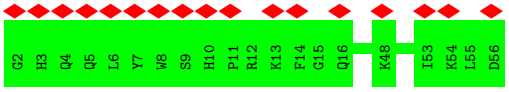
• Molecule 70: Ribosomal protein S28

Chain d3:



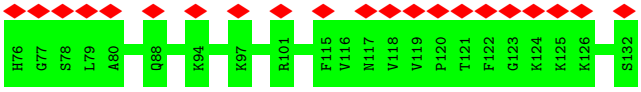
• Molecule 71: 40S ribosomal protein S29

Chain e3:



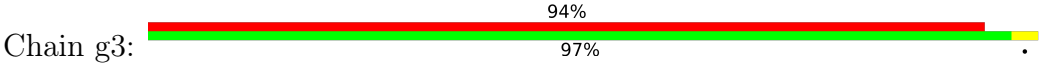
• Molecule 72: Ubiquitin-like domain-containing protein

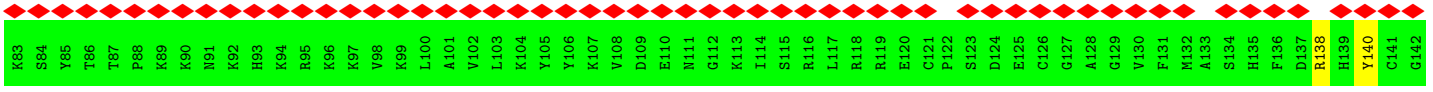
Chain f3:

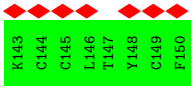


• Molecule 73: Ubiquitin-40S ribosomal protein S27a

Chain g3:

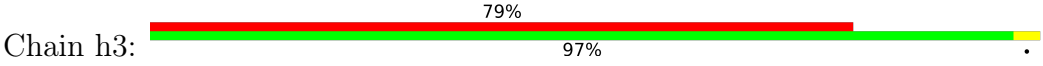


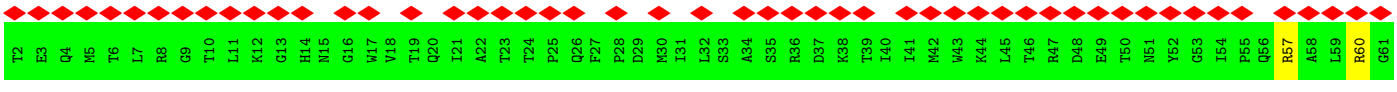


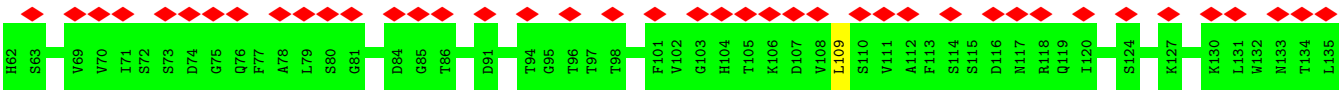


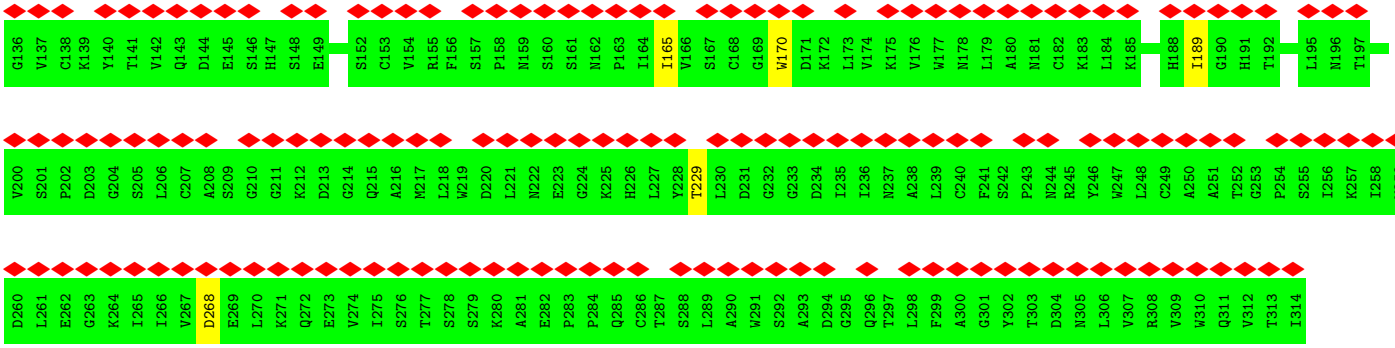
• Molecule 74: Ribosomal protein RACK1

Chain h3:



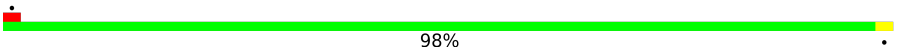






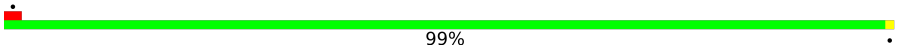
• Molecule 75: 60S ribosomal protein L8

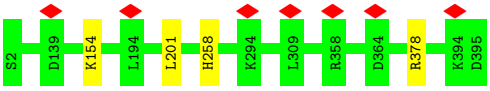
Chain j3:



• Molecule 76: Ribosomal protein L3

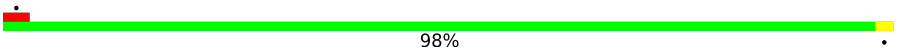
Chain k3:

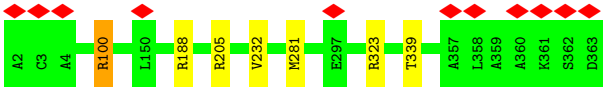




• Molecule 77: 60S ribosomal protein L4

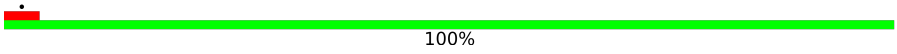
Chain l3:

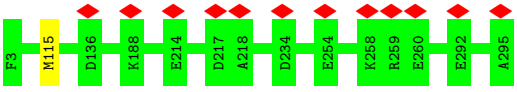




• Molecule 78: 60S ribosomal protein L5

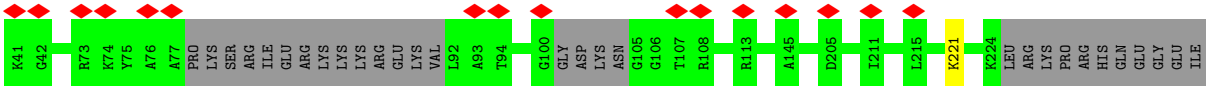
Chain m3:

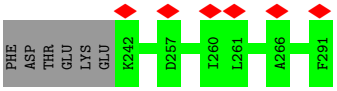




• Molecule 79: 60S ribosomal protein L6

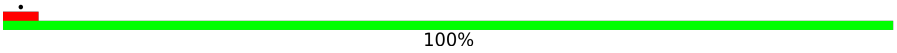
Chain n3:

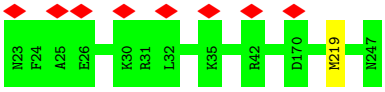




• Molecule 80: 60S ribosomal protein L7

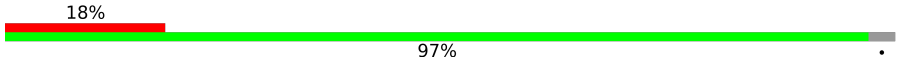
Chain o3:

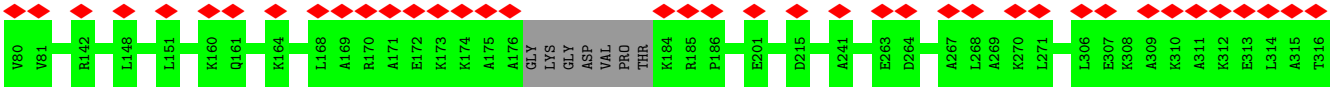




• Molecule 81: 60S ribosomal protein L7a

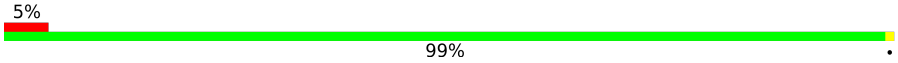
Chain p3:

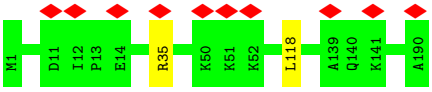




• Molecule 82: 60S ribosomal protein L9

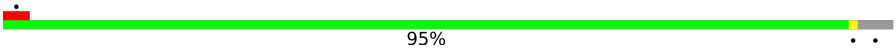
Chain q3:

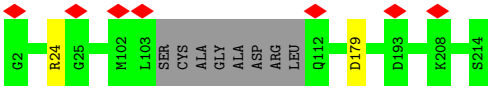




• Molecule 83: Ribosomal protein L10

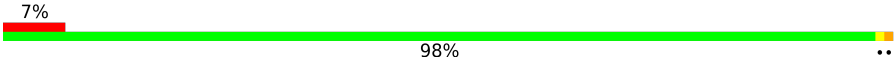
Chain r3:

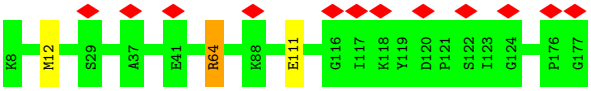




• Molecule 84: 60S ribosomal protein L11

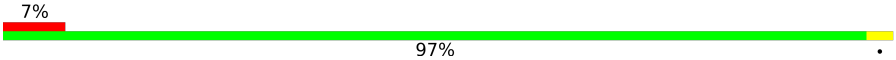
Chain s3:

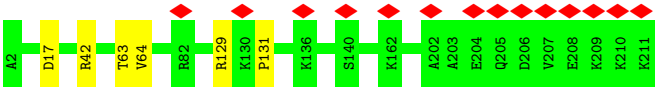




• Molecule 85: 60S ribosomal protein L13

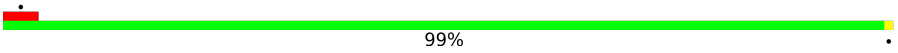
Chain t3:

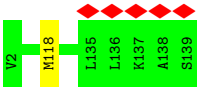




• Molecule 86: 60S ribosomal protein L14

Chain u3:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19437	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	47.5	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	414.5, 414.5, 414.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A1	0.46	0/1746	0.72	1/2338 (0.0%)
2	B1	0.43	0/1662	0.71	0/2222
3	C1	0.45	0/1268	0.74	1/1700 (0.1%)
4	D1	0.48	1/1539 (0.1%)	0.79	2/2054 (0.1%)
5	E1	0.37	0/1524	0.73	2/2013 (0.1%)
6	F1	0.44	0/1501	0.71	0/2012
7	G1	0.46	0/1326	0.71	1/1770 (0.1%)
8	H1	0.39	0/823	0.72	0/1104
9	I1	0.42	0/1048	0.70	1/1402 (0.1%)
10	J1	0.42	0/873	0.71	1/1158 (0.1%)
11	K1	0.37	0/984	0.68	0/1323
12	L1	0.52	2/1132 (0.2%)	0.81	3/1504 (0.2%)
13	M1	0.40	0/1130	0.69	2/1507 (0.1%)
14	N1	0.44	0/1191	0.68	0/1590
15	O1	0.42	1/861 (0.1%)	0.76	1/1138 (0.1%)
16	P1	0.49	0/771	0.76	1/1034 (0.1%)
17	Q1	0.51	1/903 (0.1%)	0.72	0/1216
18	R1	0.44	0/1071	0.72	3/1429 (0.2%)
19	S1	0.51	1/895 (0.1%)	0.74	1/1198 (0.1%)
20	T1	0.46	0/916	0.69	0/1220
21	U1	0.35	0/1021	0.71	1/1348 (0.1%)
22	V1	0.33	0/841	0.69	0/1112
23	W1	0.42	0/720	0.71	0/952
24	X1	0.40	0/575	0.72	0/761
25	Y1	0.43	0/459	0.71	0/608
26	Z1	0.39	0/435	0.66	0/575
27	a1	0.44	0/240	0.86	0/305
28	b1	0.43	0/864	0.71	1/1140 (0.1%)
29	c1	0.42	0/718	0.72	0/953
30	d1	0.41	0/1010	0.74	1/1354 (0.1%)
31	e1	0.54	3/1530 (0.2%)	0.84	8/2064 (0.4%)
32	f1	0.34	0/1174	0.77	1/1582 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	l1	0.43	0/1680	0.81	2/2255 (0.1%)
34	m1	0.50	0/68	1.33	2/103 (1.9%)
35	n1	0.47	1/1971 (0.1%)	0.74	5/2639 (0.2%)
36	21	0.50	0/1810	1.16	13/2819 (0.5%)
37	11	0.28	0/33	0.89	0/43
38	A2	1.58	15/86400 (0.0%)	1.18	693/134684 (0.5%)
39	B2	0.65	0/2836	1.08	13/4421 (0.3%)
40	C2	0.71	0/3581	1.16	32/5577 (0.6%)
41	A3	0.52	1/40502 (0.0%)	1.16	345/63100 (0.5%)
42	B3	0.39	0/1747	0.73	3/2374 (0.1%)
43	C3	0.35	0/1756	0.66	0/2350
44	D3	0.45	2/1753 (0.1%)	0.69	1/2369 (0.0%)
45	E3	0.43	0/1796	0.82	5/2417 (0.2%)
46	F3	0.34	0/2118	0.67	0/2849
47	G3	0.34	0/1492	0.67	0/2005
48	H3	0.36	0/1946	0.72	0/2590
49	I3	0.34	0/1510	0.76	3/2022 (0.1%)
50	J3	0.36	0/1715	0.70	1/2287 (0.0%)
51	K3	0.35	0/1550	0.74	3/2069 (0.1%)
52	L3	1.07	3/834 (0.4%)	1.45	11/1125 (1.0%)
53	M3	0.39	0/1195	0.66	1/1597 (0.1%)
54	N3	0.36	0/918	0.76	2/1233 (0.2%)
55	O3	0.76	1/1226 (0.1%)	1.02	3/1649 (0.2%)
56	P3	0.39	0/1029	0.76	3/1380 (0.2%)
57	Q3	0.39	0/1079	0.74	0/1441
58	R3	0.42	1/1146 (0.1%)	0.77	3/1534 (0.2%)
59	S3	0.36	0/1082	0.74	0/1452
60	T3	0.40	0/1208	0.84	1/1618 (0.1%)
61	U3	0.36	0/1115	0.75	3/1493 (0.2%)
62	V3	0.33	0/805	0.78	0/1081
63	W3	0.36	0/643	0.68	1/860 (0.1%)
64	X3	0.42	0/1051	0.72	1/1406 (0.1%)
65	Y3	0.35	0/1116	0.67	1/1490 (0.1%)
66	Z3	0.44	1/1028 (0.1%)	0.72	1/1366 (0.1%)
67	a3	0.41	1/604 (0.2%)	0.82	1/810 (0.1%)
68	b3	0.35	0/828	0.71	0/1109
69	c3	0.31	0/665	0.65	0/891
70	d3	0.33	0/490	0.64	0/656
71	e3	0.35	0/470	0.69	0/623
72	f3	0.36	0/462	0.69	0/607
73	g3	0.62	2/567 (0.4%)	0.83	1/753 (0.1%)
74	h3	0.44	2/2493 (0.1%)	0.83	6/3394 (0.2%)
75	j3	0.44	0/1936	0.74	3/2596 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	k3	0.45	0/3240	0.71	1/4339 (0.0%)
77	l3	0.43	1/2937 (0.0%)	0.71	3/3946 (0.1%)
78	m3	0.39	0/2437	0.65	1/3264 (0.0%)
79	n3	0.35	0/1762	0.66	1/2362 (0.0%)
80	o3	0.42	0/1911	0.69	1/2549 (0.0%)
81	p3	0.38	0/1910	0.70	0/2569
82	q3	0.42	0/1535	0.76	1/2063 (0.0%)
83	r3	0.45	0/1702	0.73	1/2272 (0.0%)
84	s3	0.45	1/1385 (0.1%)	0.76	3/1852 (0.2%)
85	t3	0.54	2/1733 (0.1%)	1.00	5/2316 (0.2%)
86	u3	0.41	0/1158	0.73	1/1547 (0.1%)
All	All	1.03	43/234715 (0.0%)	1.03	1213/343902 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A1	0	1
12	L1	0	1
14	N1	0	1
17	Q1	0	1
19	S1	0	1
33	l1	0	2
42	B3	0	1
44	D3	0	2
52	L3	0	2
61	U3	0	1
65	Y3	0	1
76	k3	0	1
77	l3	0	3
82	q3	0	1
84	s3	0	1
85	t3	0	3
All	All	0	23

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A2	935	A	N7-C5	203.95	2.61	1.39
38	A2	935	A	N9-C4	197.60	2.56	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A2	935	A	C8-N7	167.52	2.48	1.31
38	A2	935	A	N9-C8	160.18	2.65	1.37
38	A2	935	A	C5-C4	146.96	2.41	1.38
38	A2	936	G	C5'-C4'	118.73	2.93	1.51
52	L3	4	PRO	CG-CD	-23.01	0.74	1.50
55	O3	85	PRO	CG-CD	-22.53	0.76	1.50
52	L3	4	PRO	CB-CG	11.65	2.08	1.50
85	t3	131	PRO	CG-CD	-8.62	1.22	1.50
31	e1	24	TYR	CG-CD1	-8.27	1.28	1.39
73	g3	140	TYR	CD1-CE1	-8.27	1.26	1.39
17	Q1	25	TYR	CD2-CE2	-8.16	1.27	1.39
85	t3	131	PRO	CB-CG	-8.02	1.09	1.50
31	e1	24	TYR	CD1-CE1	-7.86	1.27	1.39
12	L1	74	TYR	CD2-CE2	-7.45	1.28	1.39
38	A2	936	G	C4'-C3'	7.17	1.61	1.53
31	e1	24	TYR	CE1-CZ	-7.12	1.29	1.38
66	Z3	35	VAL	CB-CG1	-6.75	1.38	1.52
44	D3	268	GLU	CD-OE2	-6.67	1.18	1.25
4	D1	167	VAL	CB-CG1	-6.60	1.39	1.52
44	D3	268	GLU	CG-CD	-6.44	1.42	1.51
12	L1	74	TYR	CE2-CZ	-6.37	1.30	1.38
74	h3	229	THR	CB-CG2	-6.07	1.32	1.52
19	S1	84	VAL	CB-CG1	-5.95	1.40	1.52
38	A2	978	G	N7-C5	-5.86	1.35	1.39
52	L3	4	PRO	N-CD	5.80	1.55	1.47
41	A3	656	G	C6-N1	-5.76	1.35	1.39
35	n1	219	PHE	CB-CG	-5.49	1.42	1.51
38	A2	4504	A	N9-C8	-5.38	1.33	1.37
38	A2	3653	C	O3'-P	-5.35	1.54	1.61
84	s3	64	ARG	CG-CD	-5.34	1.38	1.51
67	a3	48	VAL	CB-CG2	-5.30	1.41	1.52
58	R3	105	LYS	CB-CG	-5.29	1.38	1.52
38	A2	4115	G	N3-C4	-5.27	1.31	1.35
38	A2	980	G	N9-C4	-5.24	1.33	1.38
73	g3	140	TYR	CE1-CZ	-5.24	1.31	1.38
38	A2	4291	G	C2-N3	-5.21	1.28	1.32
77	l3	232	VAL	CB-CG1	-5.18	1.42	1.52
38	A2	2699	A	N9-C4	-5.17	1.34	1.37
74	h3	170	TRP	CB-CG	-5.14	1.41	1.50
15	O1	30	GLU	CB-CG	-5.11	1.42	1.52
38	A2	493	U	C5-C6	-5.09	1.29	1.34

All (1213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	L3	4	PRO	N-CD-CG	-29.06	59.62	103.20
38	A2	935	A	N1-C2-N3	24.68	141.64	129.30
38	A2	935	A	N7-C8-N9	-23.29	102.16	113.80
38	A2	935	A	C6-N1-C2	21.66	131.59	118.60
85	t3	131	PRO	N-CD-CG	-21.39	71.12	103.20
38	A2	935	A	C4-C5-C6	-20.53	106.73	117.00
52	L3	4	PRO	CA-CB-CG	-19.83	66.32	104.00
85	t3	131	PRO	CA-CB-CG	-19.71	66.55	104.00
38	A2	935	A	C6-C5-N7	18.99	145.59	132.30
55	O3	85	PRO	N-CD-CG	-18.88	74.88	103.20
55	O3	85	PRO	CB-CG-CD	18.83	179.95	106.50
38	A2	935	A	N3-C4-C5	-17.47	114.57	126.80
38	A2	935	A	C5-N7-C8	16.18	111.99	103.90
38	A2	4504	A	O5'-P-OP2	-15.83	91.46	105.70
55	O3	85	PRO	CA-CB-CG	-14.22	76.98	104.00
38	A2	172	C	C6-N1-C2	13.53	125.71	120.30
41	A3	1117	C	N1-C2-O2	12.66	126.49	118.90
38	A2	935	A	N3-C4-N9	12.43	137.35	127.40
38	A2	936	G	C5'-C4'-C3'	12.18	135.50	116.00
38	A2	2261	C	N1-C2-O2	12.06	126.13	118.90
41	A3	656	G	N3-C2-N2	12.03	128.32	119.90
38	A2	2839	A	C8-N9-C4	11.85	110.54	105.80
38	A2	4115	G	N9-C4-C5	11.84	110.13	105.40
38	A2	362	A	N1-C6-N6	-11.69	111.59	118.60
41	A3	1453	C	N1-C2-O2	11.33	125.70	118.90
41	A3	293	C	N1-C2-O2	11.06	125.53	118.90
41	A3	501	C	N1-C2-O2	10.95	125.47	118.90
38	A2	2839	A	N9-C4-C5	-10.80	101.48	105.80
38	A2	935	A	C8-N9-C4	10.74	110.09	105.80
38	A2	4035	C	N1-C2-O2	10.73	125.34	118.90
41	A3	656	G	N1-C2-N2	-10.62	106.64	116.20
38	A2	4405	U	N1-C2-O2	10.49	130.14	122.80
41	A3	1453	C	C2-N1-C1'	10.49	130.34	118.80
38	A2	2261	C	N3-C2-O2	-10.47	114.57	121.90
38	A2	2261	C	C2-N1-C1'	10.23	130.06	118.80
41	A3	501	C	C2-N1-C1'	10.16	129.98	118.80
41	A3	1397	U	N1-C2-O2	10.08	129.86	122.80
38	A2	100	C	C2-N1-C1'	10.01	129.81	118.80
41	A3	1397	U	N3-C2-O2	-9.87	115.29	122.20
38	A2	2630	C	N1-C2-O2	9.83	124.80	118.90
38	A2	4940	C	N1-C2-O2	9.82	124.79	118.90
74	h3	165	ILE	CG1-CB-CG2	-9.76	89.93	111.40
41	A3	183	G	C2-N3-C4	9.74	116.77	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	A3	853	C	N1-C2-O2	9.71	124.72	118.90
38	A2	4405	U	N3-C2-O2	-9.65	115.45	122.20
41	A3	183	G	N3-C2-N2	-9.62	113.16	119.90
38	A2	936	G	O5'-C5'-C4'	9.61	129.95	111.70
67	a3	100	VAL	CG1-CB-CG2	-9.60	95.53	110.90
38	A2	4115	G	N3-C2-N2	-9.58	113.19	119.90
28	b1	82	MET	CG-SD-CE	-9.52	84.97	100.20
41	A3	823	U	N3-C2-O2	-9.52	115.54	122.20
38	A2	3768	U	O5'-P-OP1	-9.51	97.14	105.70
41	A3	1117	C	C2-N1-C1'	9.48	129.23	118.80
40	C2	64	U	N3-C2-O2	-9.47	115.57	122.20
52	L3	30	PRO	CA-N-CD	-9.41	98.32	111.50
41	A3	356	C	N1-C2-O2	9.40	124.54	118.90
41	A3	1117	C	N3-C2-O2	-9.35	115.35	121.90
38	A2	115	C	N1-C2-O2	9.28	124.47	118.90
38	A2	1612	G	N3-C4-N9	9.28	131.57	126.00
41	A3	293	C	C2-N1-C1'	9.28	129.01	118.80
41	A3	853	C	C2-N1-C1'	9.24	128.96	118.80
38	A2	978	G	C5-C6-O6	9.24	134.14	128.60
38	A2	4862	C	N1-C2-O2	9.20	124.42	118.90
41	A3	356	C	C2-N1-C1'	9.18	128.89	118.80
38	A2	4115	G	C4-C5-N7	-9.17	107.13	110.80
38	A2	1485	C	N1-C2-O2	9.16	124.39	118.90
41	A3	1139	C	N1-C2-O2	9.06	124.34	118.90
38	A2	980	G	N3-C4-N9	-9.04	120.58	126.00
41	A3	293	C	N3-C2-O2	-9.03	115.58	121.90
38	A2	4035	C	N3-C2-O2	-9.02	115.59	121.90
38	A2	4908	C	C2-N1-C1'	9.00	128.70	118.80
41	A3	1303	C	N1-C2-O2	8.97	124.28	118.90
41	A3	1389	C	C2-N1-C1'	8.96	128.65	118.80
38	A2	3654	G	O5'-P-OP1	8.90	121.38	110.70
38	A2	4035	C	C6-N1-C2	-8.89	116.74	120.30
41	A3	1139	C	C2-N1-C1'	8.89	128.58	118.80
38	A2	2261	C	C6-N1-C2	-8.88	116.75	120.30
38	A2	4289	C	N1-C2-O2	8.79	124.17	118.90
38	A2	936	G	C5'-C4'-O4'	8.76	119.62	109.10
38	A2	172	C	N3-C4-C5	8.74	125.40	121.90
38	A2	4291	G	N3-C2-N2	-8.73	113.79	119.90
38	A2	4745	C	C2-N1-C1'	8.73	128.40	118.80
38	A2	4289	C	C2-N1-C1'	8.70	128.37	118.80
38	A2	1080	C	N1-C2-O2	8.69	124.11	118.90
41	A3	178	C	N1-C2-O2	8.68	124.11	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A2	4862	C	C2-N1-C1'	8.62	128.28	118.80
41	A3	501	C	N3-C2-O2	-8.62	115.87	121.90
41	A3	823	U	N1-C2-O2	8.62	128.83	122.80
38	A2	4405	U	C2-N1-C1'	8.61	128.03	117.70
38	A2	4406	U	N1-C2-O2	8.60	128.82	122.80
41	A3	1060	A	O4'-C1'-N9	8.57	115.05	108.20
38	A2	2823	C	N1-C2-O2	8.56	124.03	118.90
38	A2	100	C	N1-C2-O2	8.53	124.02	118.90
74	h3	229	THR	CA-CB-CG2	-8.53	100.46	112.40
38	A2	3965	G	O4'-C1'-N9	8.53	115.02	108.20
38	A2	4406	U	N3-C2-O2	-8.50	116.25	122.20
38	A2	115	C	C2-N1-C1'	8.46	128.11	118.80
38	A2	1639	U	C2-N1-C1'	8.46	127.85	117.70
41	A3	183	G	N3-C4-C5	-8.45	124.38	128.60
41	A3	1303	C	C2-N1-C1'	8.44	128.08	118.80
38	A2	2630	C	C2-N1-C1'	8.41	128.05	118.80
38	A2	1323	C	N3-C2-O2	-8.40	116.02	121.90
21	U1	102	LEU	CB-CG-CD2	-8.36	96.79	111.00
38	A2	1379	U	C2-N1-C1'	8.36	127.73	117.70
38	A2	77	U	N3-C2-O2	-8.31	116.38	122.20
38	A2	454	U	N3-C2-O2	-8.31	116.39	122.20
41	A3	1750	C	N1-C2-O2	8.30	123.88	118.90
41	A3	879	C	C2-N1-C1'	8.30	127.93	118.80
84	s3	12	MET	CG-SD-CE	-8.30	86.92	100.20
38	A2	978	G	N7-C8-N9	8.29	117.25	113.10
85	t3	17	ASP	CB-CG-OD2	-8.25	110.87	118.30
41	A3	1624	U	C2-N1-C1'	8.25	127.60	117.70
38	A2	3631	C	N3-C2-O2	-8.24	116.13	121.90
45	E3	32	ASP	CB-CG-OD1	8.23	125.70	118.30
38	A2	4115	G	N1-C2-N2	8.21	123.59	116.20
41	A3	1520	G	C4-N9-C1'	8.21	137.17	126.50
41	A3	1453	C	N3-C2-O2	-8.20	116.16	121.90
38	A2	1410	C	C5-C6-N1	8.17	125.08	121.00
41	A3	853	C	N3-C2-O2	-8.16	116.18	121.90
41	A3	501	C	C6-N1-C2	-8.16	117.03	120.30
41	A3	1364	U	C2-N1-C1'	8.16	127.50	117.70
38	A2	4289	C	N3-C2-O2	-8.16	116.19	121.90
30	d1	108	MET	CG-SD-CE	-8.15	87.15	100.20
41	A3	1022	U	C2-N1-C1'	8.15	127.48	117.70
52	L3	4	PRO	N-CA-CB	-8.15	93.52	103.30
38	A2	1483	C	C6-N1-C2	-8.15	117.04	120.30
38	A2	2011	C	N1-C2-O2	8.13	123.78	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	q3	118	LEU	CB-CG-CD2	-8.05	97.31	111.00
38	A2	4115	G	C8-N9-C4	-8.05	103.18	106.40
38	A2	100	C	N3-C2-O2	-8.04	116.27	121.90
38	A2	4851	U	C2-N1-C1'	8.01	127.32	117.70
41	A3	1535	U	C2-N1-C1'	8.00	127.30	117.70
42	B3	210	ILE	CG1-CB-CG2	-7.99	93.82	111.40
41	A3	1389	C	N1-C2-O2	7.98	123.69	118.90
38	A2	4409	U	N3-C2-O2	-7.98	116.61	122.20
38	A2	2507	C	C6-N1-C2	-7.96	117.11	120.30
38	A2	2494	C	C6-N1-C2	-7.96	117.12	120.30
38	A2	4910	C	C6-N1-C2	-7.96	117.12	120.30
40	C2	75	G	C8-N9-C4	7.94	109.58	106.40
40	C2	76	C	C5-C6-N1	7.93	124.97	121.00
38	A2	980	G	C4-N9-C1'	-7.92	116.20	126.50
38	A2	4406	U	C2-N1-C1'	7.92	127.20	117.70
41	A3	183	G	C8-N9-C4	-7.91	103.24	106.40
41	A3	1364	U	N1-C2-O2	7.90	128.33	122.80
38	A2	4331	C	C6-N1-C2	-7.89	117.14	120.30
38	A2	4148	C	N1-C2-O2	7.86	123.61	118.90
41	A3	55	U	C2-N1-C1'	7.86	127.13	117.70
38	A2	4745	C	N1-C2-O2	7.84	123.61	118.90
38	A2	978	G	C8-N9-C4	-7.83	103.27	106.40
41	A3	1523	C	C6-N1-C2	-7.82	117.17	120.30
38	A2	1639	U	N1-C2-O2	7.81	128.27	122.80
38	A2	1484	G	N3-C4-N9	7.80	130.68	126.00
41	A3	1591	C	N1-C2-O2	7.80	123.58	118.90
38	A2	1234	C	C6-N1-C2	-7.80	117.18	120.30
41	A3	1139	C	N3-C2-O2	-7.80	116.44	121.90
41	A3	1865	C	C6-N1-C2	-7.80	117.18	120.30
40	C2	75	G	N9-C1'-C2'	-7.78	103.44	112.00
38	A2	1999	A	O5'-P-OP1	-7.77	98.71	105.70
38	A2	2630	C	N3-C2-O2	-7.77	116.46	121.90
77	l3	281	MET	CG-SD-CE	-7.77	87.77	100.20
45	E3	32	ASP	CB-CG-OD2	-7.76	111.31	118.30
41	A3	898	U	N1-C2-O2	7.76	128.23	122.80
41	A3	630	U	C2-N1-C1'	7.75	127.00	117.70
41	A3	898	U	C2-N1-C1'	7.74	126.99	117.70
38	A2	4252	G	N3-C4-C5	-7.73	124.74	128.60
38	A2	4908	C	N1-C2-O2	7.70	123.52	118.90
38	A2	4862	C	N3-C2-O2	-7.69	116.52	121.90
74	h3	229	THR	OG1-CB-CG2	-7.66	92.37	110.00
41	A3	1636	G	N3-C4-N9	7.65	130.59	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A2	1485	C	N3-C2-O2	-7.64	116.55	121.90
41	A3	752	G	N3-C4-N9	-7.62	121.42	126.00
38	A2	4940	C	N3-C2-O2	-7.62	116.57	121.90
41	A3	356	C	N3-C2-O2	-7.59	116.59	121.90
78	m3	115	MET	CG-SD-CE	-7.58	88.07	100.20
38	A2	4744	U	C2-N1-C1'	7.58	126.79	117.70
41	A3	199	C	N1-C2-O2	7.57	123.44	118.90
31	e1	24	TYR	OH-CZ-CE2	7.56	140.51	120.10
38	A2	4291	G	N1-C2-N2	7.56	123.00	116.20
41	A3	1453	C	C5-C6-N1	7.55	124.78	121.00
41	A3	823	U	C2-N1-C1'	7.54	126.75	117.70
38	A2	4940	C	C2-N1-C1'	7.53	127.09	118.80
41	A3	1453	C	C6-N1-C2	-7.53	117.29	120.30
16	P1	98	ASP	CB-CG-OD1	7.53	125.07	118.30
38	A2	1484	G	C4-N9-C1'	7.52	136.28	126.50
41	A3	1271	C	N1-C2-O2	7.52	123.41	118.90
38	A2	14	C	C6-N1-C2	-7.51	117.30	120.30
41	A3	1364	U	N3-C2-O2	-7.50	116.95	122.20
38	A2	115	C	N3-C2-O2	-7.50	116.65	121.90
38	A2	2641	G	N3-C4-N9	-7.49	121.51	126.00
38	A2	4939	C	N1-C2-O2	7.49	123.39	118.90
38	A2	417	G	O4'-C1'-N9	7.48	114.19	108.20
41	A3	656	G	N1-C6-O6	-7.47	115.42	119.90
41	A3	659	G	C4-N9-C1'	7.45	136.18	126.50
41	A3	1016	U	N3-C2-O2	-7.44	116.99	122.20
45	E3	154	ASP	CB-CG-OD1	7.44	125.00	118.30
36	21	56	C	C2-N1-C1'	7.43	126.97	118.80
38	A2	4399	C	C2-N1-C1'	7.42	126.96	118.80
41	A3	1016	U	N1-C2-O2	7.41	127.98	122.80
38	A2	4115	G	N3-C4-N9	-7.40	121.56	126.00
38	A2	4907	U	OP2-P-O3'	7.40	121.47	105.20
41	A3	188	C	N1-C2-O2	7.40	123.34	118.90
18	R1	90	MET	CG-SD-CE	-7.39	88.37	100.20
38	A2	4752	C	C6-N1-C2	-7.39	117.34	120.30
41	A3	1219	C	N1-C2-O2	7.39	123.33	118.90
40	C2	128	C	N1-C2-O2	7.38	123.33	118.90
41	A3	1057	C	C2-N1-C1'	7.38	126.92	118.80
38	A2	4744	U	N3-C2-O2	-7.37	117.04	122.20
38	A2	978	G	N1-C2-N2	-7.37	109.57	116.20
41	A3	630	U	N1-C2-O2	7.35	127.94	122.80
38	A2	1407	G	C4-N9-C1'	7.35	136.05	126.50
38	A2	4744	U	N1-C2-O2	7.34	127.94	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	A3	1551	U	C2-N1-C1'	7.34	126.51	117.70
38	A2	1484	G	N3-C4-C5	-7.33	124.94	128.60
41	A3	1016	U	C2-N1-C1'	7.33	126.49	117.70
41	A3	55	U	N1-C2-O2	7.32	127.92	122.80
41	A3	1261	C	N1-C2-O2	7.32	123.29	118.90
38	A2	980	G	N3-C4-C5	7.31	132.25	128.60
38	A2	4399	C	N1-C2-O2	7.28	123.27	118.90
74	h3	189	ILE	CG1-CB-CG2	-7.28	95.37	111.40
38	A2	1276	C	N3-C2-O2	-7.28	116.81	121.90
41	A3	1750	C	N3-C2-O2	-7.26	116.81	121.90
38	A2	1344	C	C6-N1-C2	-7.26	117.40	120.30
41	A3	656	G	C5-C6-O6	7.23	132.94	128.60
41	A3	632	C	C2-N1-C1'	7.22	126.74	118.80
38	A2	1070	C	P-O3'-C3'	7.21	128.35	119.70
38	A2	980	G	O4'-C1'-N9	7.20	113.96	108.20
38	A2	1178	C	C2-N1-C1'	7.19	126.71	118.80
39	B2	29	C	C6-N1-C2	-7.19	117.42	120.30
41	A3	317	C	N1-C2-O2	7.19	123.22	118.90
38	A2	4695	U	N1-C2-O2	7.19	127.83	122.80
38	A2	1485	C	C2-N1-C1'	7.18	126.70	118.80
38	A2	362	A	C5-C6-N6	7.18	129.44	123.70
38	A2	2531	G	C4-N9-C1'	7.17	135.82	126.50
38	A2	1612	G	C4-N9-C1'	7.17	135.82	126.50
85	t3	131	PRO	CB-CG-CD	7.16	134.42	106.50
75	j3	122	ASP	CB-CG-OD2	7.16	124.74	118.30
38	A2	4252	G	C4-N9-C1'	7.15	135.80	126.50
41	A3	1636	G	N3-C4-C5	-7.15	125.03	128.60
38	A2	4384	C	N1-C2-O2	7.14	123.19	118.90
41	A3	178	C	C2-N1-C1'	7.14	126.65	118.80
31	e1	24	TYR	CE1-CZ-OH	-7.12	100.87	120.10
41	A3	1750	C	C6-N1-C2	-7.12	117.45	120.30
38	A2	1671	U	N1-C2-O2	7.12	127.78	122.80
38	A2	2413	C	C2-N1-C1'	7.12	126.63	118.80
38	A2	2494	C	C5-C6-N1	7.12	124.56	121.00
38	A2	4409	U	C2-N1-C1'	7.12	126.24	117.70
41	A3	1397	U	C2-N1-C1'	7.12	126.24	117.70
38	A2	1773	U	C2-N1-C1'	7.10	126.22	117.70
44	D3	268	GLU	CG-CD-OE2	-7.10	104.11	118.30
38	A2	1410	C	C6-N1-C2	-7.09	117.46	120.30
38	A2	2022	C	N3-C2-O2	-7.09	116.94	121.90
38	A2	3904	C	C6-N1-C2	-7.09	117.47	120.30
41	A3	1303	C	N3-C2-O2	-7.09	116.94	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A2	1612	G	N3-C4-C5	-7.08	125.06	128.60
38	A2	1404	G	C4-N9-C1'	7.07	135.70	126.50
41	A3	501	C	C5-C6-N1	7.07	124.53	121.00
38	A2	3734	C	C2-N1-C1'	7.06	126.56	118.80
38	A2	4851	U	N3-C2-O2	-7.05	117.27	122.20
41	A3	898	U	N3-C2-O2	-7.04	117.27	122.20
41	A3	1520	G	C8-N9-C1'	-7.04	117.84	127.00
38	A2	2261	C	OP1-P-O3'	7.04	120.69	105.20
41	A3	1310	U	N1-C2-O2	7.04	127.73	122.80
52	L3	30	PRO	N-CD-CG	-7.03	92.65	103.20
41	A3	183	G	N1-C2-N2	7.03	122.52	116.20
41	A3	1453	C	C6-N1-C1'	-7.03	112.37	120.80
83	r3	179	ASP	CB-CG-OD2	7.02	124.62	118.30
39	B2	28	C	C6-N1-C2	-7.02	117.49	120.30
38	A2	77	U	N1-C2-O2	7.01	127.71	122.80
41	A3	178	C	N3-C2-O2	-7.01	116.99	121.90
12	L1	111	LEU	CA-CB-CG	7.01	131.42	115.30
38	A2	450	G	O5'-P-OP2	-7.00	99.40	105.70
38	A2	1483	C	C5-C6-N1	7.00	124.50	121.00
38	A2	978	G	C2-N3-C4	-7.00	108.40	111.90
38	A2	4215	U	N3-C2-O2	-7.00	117.30	122.20
38	A2	1080	C	N3-C2-O2	-6.99	117.01	121.90
73	g3	140	TYR	CB-CG-CD1	-6.99	116.81	121.00
38	A2	2046	G	P-O3'-C3'	6.98	128.07	119.70
41	A3	1518	C	N3-C2-O2	-6.97	117.02	121.90
41	A3	427	U	C2-N1-C1'	6.97	126.06	117.70
40	C2	1	C	N1-C2-O2	6.97	123.08	118.90
38	A2	100	C	C6-N1-C1'	-6.97	112.44	120.80
38	A2	1407	G	N3-C4-C5	-6.96	125.12	128.60
36	21	32	C	N1-C2-O2	6.95	123.07	118.90
38	A2	3630	A	N1-C6-N6	6.95	122.77	118.60
38	A2	976	C	N3-C2-O2	-6.95	117.04	121.90
38	A2	4695	U	N3-C2-O2	-6.94	117.34	122.20
38	A2	3906	C	C5-C6-N1	6.93	124.47	121.00
38	A2	126	C	C5-C6-N1	6.93	124.46	121.00
38	A2	1882	U	C5-C4-O4	-6.93	121.74	125.90
38	A2	1639	U	N3-C2-O2	-6.92	117.36	122.20
41	A3	1310	U	N3-C2-O2	-6.92	117.36	122.20
41	A3	1518	C	N1-C2-O2	6.92	123.05	118.90
38	A2	1379	U	N1-C2-O2	6.91	127.64	122.80
36	21	16	U	N3-C2-O2	-6.91	117.36	122.20
38	A2	4888	C	C2-N1-C1'	6.91	126.40	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	A3	1624	U	N1-C2-O2	6.91	127.64	122.80
38	A2	4180	U	N3-C2-O2	-6.90	117.37	122.20
74	h3	109	LEU	CB-CG-CD2	-6.90	99.27	111.00
41	A3	1551	U	N3-C2-O2	-6.90	117.37	122.20
41	A3	752	G	C4-N9-C1'	-6.89	117.55	126.50
41	A3	124	U	N1-C2-O2	6.89	127.62	122.80
41	A3	1389	C	C6-N1-C2	-6.88	117.55	120.30
41	A3	630	U	N3-C2-O2	-6.87	117.39	122.20
38	A2	1816	C	C6-N1-C2	-6.87	117.55	120.30
38	A2	928	C	N1-C2-O2	6.86	123.02	118.90
38	A2	2823	C	N3-C2-O2	-6.86	117.10	121.90
38	A2	3773	U	N3-C2-O2	-6.86	117.40	122.20
41	A3	752	G	C8-N9-C1'	6.86	135.92	127.00
38	A2	3954	U	P-O3'-C3'	6.85	127.92	119.70
38	A2	4215	U	N1-C2-O2	6.85	127.59	122.80
38	A2	1612	G	C8-N9-C1'	-6.84	118.11	127.00
38	A2	3631	C	C6-N1-C2	-6.84	117.56	120.30
38	A2	4409	U	N1-C2-O2	6.84	127.59	122.80
41	A3	570	C	C6-N1-C2	-6.84	117.56	120.30
49	I3	36	LEU	CA-CB-CG	6.84	131.03	115.30
41	A3	178	C	C6-N1-C2	-6.82	117.57	120.30
38	A2	4648	C	C6-N1-C2	-6.82	117.57	120.30
41	A3	879	C	C5-C6-N1	6.82	124.41	121.00
38	A2	4148	C	C2-N1-C1'	6.81	126.30	118.80
38	A2	4752	C	C2-N1-C1'	6.80	126.28	118.80
38	A2	1428	U	N1-C2-O2	6.80	127.56	122.80
38	A2	692	C	C2-N1-C1'	6.80	126.28	118.80
38	A2	3906	C	C6-N1-C2	-6.80	117.58	120.30
38	A2	4504	A	C8-N9-C4	6.78	108.51	105.80
41	A3	752	G	P-O3'-C3'	6.78	127.84	119.70
41	A3	553	U	P-O3'-C3'	6.78	127.83	119.70
38	A2	1323	C	C6-N1-C2	-6.77	117.59	120.30
38	A2	920	C	N1-C2-O2	6.77	122.96	118.90
38	A2	3632	U	N3-C2-O2	-6.76	117.47	122.20
41	A3	627	U	P-O3'-C3'	6.76	127.81	119.70
40	C2	64	U	N1-C2-O2	6.76	127.53	122.80
38	A2	659	C	N1-C2-O2	6.76	122.95	118.90
40	C2	128	C	N3-C2-O2	-6.76	117.17	121.90
40	C2	127	U	N3-C2-O2	-6.75	117.47	122.20
10	J1	44	ARG	CG-CD-NE	6.75	125.98	111.80
41	A3	188	C	C2-N1-C1'	6.75	126.23	118.80
41	A3	973	C	N1-C2-O2	6.75	122.95	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A2	1407	G	N3-C4-N9	6.75	130.05	126.00
38	A2	4851	U	N1-C2-O2	6.75	127.53	122.80
41	A3	1518	C	C2-N1-C1'	6.74	126.22	118.80
38	A2	3965	G	N3-C4-N9	6.74	130.04	126.00
38	A2	4340	U	P-O3'-C3'	6.74	127.78	119.70
41	A3	688	U	P-O3'-C3'	6.74	127.78	119.70
41	A3	1117	C	C6-N1-C2	-6.73	117.61	120.30
38	A2	1306	C	C6-N1-C2	-6.73	117.61	120.30
38	A2	3773	U	N1-C2-O2	6.73	127.51	122.80
38	A2	3631	C	N1-C2-O2	6.72	122.93	118.90
38	A2	4930	C	C2-N1-C1'	6.72	126.19	118.80
53	M3	82	MET	CG-SD-CE	-6.72	89.45	100.20
41	A3	303	C	N1-C2-O2	6.71	122.93	118.90
38	A2	4907	U	P-O3'-C3'	6.71	127.75	119.70
38	A2	2413	C	C5-C6-N1	6.70	124.35	121.00
40	C2	75	G	N9-C4-C5	-6.69	102.72	105.40
3	C1	7	ASP	CB-CG-OD2	6.69	124.32	118.30
41	A3	317	C	N3-C2-O2	-6.69	117.22	121.90
38	A2	2016	C	N1-C2-O2	6.68	122.91	118.90
38	A2	3871	A	P-O3'-C3'	6.68	127.71	119.70
38	A2	1208	C	N1-C2-O2	6.67	122.90	118.90
38	A2	662	C	N1-C2-O2	6.66	122.90	118.90
38	A2	4745	C	N3-C2-O2	-6.66	117.24	121.90
65	Y3	116	PRO	CA-N-CD	-6.66	102.18	111.50
41	A3	1636	G	C4-N9-C1'	6.65	135.14	126.50
41	A3	853	C	C6-N1-C1'	-6.65	112.83	120.80
41	A3	1314	U	C2-N1-C1'	6.63	125.66	117.70
38	A2	2698	A	P-O3'-C3'	6.63	127.66	119.70
52	L3	45	VAL	CG1-CB-CG2	6.63	121.51	110.90
38	A2	3783	C	N1-C2-O2	6.62	122.87	118.90
41	A3	958	G	O4'-C1'-N9	6.62	113.50	108.20
41	A3	1752	C	N1-C2-O2	6.61	122.87	118.90
38	A2	96	U	N3-C2-O2	-6.61	117.58	122.20
38	A2	4148	C	N3-C2-O2	-6.60	117.28	121.90
38	A2	1834	U	C2-N1-C1'	6.60	125.62	117.70
41	A3	1523	C	O5'-P-OP2	-6.59	99.77	105.70
38	A2	1818	G	O4'-C1'-N9	6.59	113.47	108.20
41	A3	1624	U	N3-C2-O2	-6.59	117.58	122.20
38	A2	2089	G	P-O3'-C3'	6.58	127.60	119.70
41	A3	501	C	C6-N1-C1'	-6.58	112.91	120.80
38	A2	112	C	C2-N1-C1'	6.58	126.03	118.80
41	A3	293	C	C6-N1-C2	-6.58	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A2	4353	G	N1-C2-N3	6.57	127.84	123.90
40	C2	51	U	N1-C2-O2	6.56	127.39	122.80
38	A2	4384	C	N3-C2-O2	-6.55	117.32	121.90
41	A3	124	U	N3-C2-O2	-6.55	117.62	122.20
36	21	16	U	N1-C2-O2	6.54	127.38	122.80
38	A2	117	C	N1-C2-O2	6.53	122.82	118.90
38	A2	1772	C	C2-N1-C1'	6.53	125.99	118.80
38	A2	4462	C	C2-N1-C1'	6.53	125.98	118.80
38	A2	1483	C	N1-C2-O2	6.53	122.82	118.90
41	A3	1535	U	N1-C2-O2	6.53	127.37	122.80
38	A2	2563	C	C2-N1-C1'	6.52	125.98	118.80
38	A2	3736	C	N3-C2-O2	-6.52	117.33	121.90
61	U3	28	LEU	CB-CG-CD2	6.52	122.08	111.00
77	l3	205	ARG	NE-CZ-NH2	-6.52	117.04	120.30
40	C2	99	U	N3-C2-O2	-6.51	117.64	122.20
38	A2	1344	C	C5-C6-N1	6.51	124.25	121.00
38	A2	2543	C	C5-C6-N1	6.51	124.25	121.00
38	A2	3630	A	C5-C6-N6	-6.51	118.49	123.70
38	A2	1816	C	C5-C6-N1	6.51	124.25	121.00
41	A3	1551	U	N1-C2-O2	6.50	127.35	122.80
38	A2	1834	U	N3-C2-O2	-6.50	117.65	122.20
13	M1	47	ASP	CB-CG-OD1	6.49	124.14	118.30
41	A3	1556	A	C2-N3-C4	6.49	113.84	110.60
38	A2	1323	C	N1-C2-O2	6.48	122.79	118.90
38	A2	2859	C	N1-C2-O2	6.48	122.79	118.90
41	A3	356	C	C6-N1-C1'	-6.48	113.03	120.80
51	K3	52	LYS	CD-CE-NZ	-6.47	96.82	111.70
38	A2	4252	G	N3-C4-N9	6.47	129.88	126.00
1	A1	19	MET	CG-SD-CE	-6.47	89.85	100.20
41	A3	1520	G	N3-C4-N9	6.47	129.88	126.00
41	A3	1057	C	N1-C2-O2	6.46	122.78	118.90
38	A2	3970	C	C2-N1-C1'	6.46	125.91	118.80
39	B2	102	U	N1-C2-O2	6.46	127.32	122.80
80	o3	219	MET	CG-SD-CE	6.46	110.53	100.20
41	A3	1314	U	N3-C2-O2	-6.46	117.68	122.20
38	A2	100	C	C6-N1-C2	-6.45	117.72	120.30
38	A2	4745	C	C6-N1-C2	-6.45	117.72	120.30
38	A2	2543	C	C6-N1-C2	-6.45	117.72	120.30
38	A2	14	C	C2-N1-C1'	6.44	125.89	118.80
38	A2	1671	U	N3-C2-O2	-6.44	117.69	122.20
38	A2	1338	C	C5-C6-N1	6.44	124.22	121.00
31	e1	24	TYR	CB-CG-CD1	-6.43	117.14	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A2	3773	U	C2-N1-C1'	6.43	125.42	117.70
38	A2	978	G	C6-C5-N7	-6.43	126.55	130.40
38	A2	2507	C	C5-C6-N1	6.42	124.21	121.00
38	A2	3770	A	N7-C8-N9	6.42	117.01	113.80
38	A2	2022	C	N1-C2-O2	6.42	122.75	118.90
38	A2	4908	C	N3-C2-O2	-6.42	117.41	121.90
38	A2	1469	C	C6-N1-C2	-6.42	117.73	120.30
38	A2	976	C	N1-C2-O2	6.41	122.75	118.90
38	A2	1484	G	C8-N9-C1'	-6.41	118.67	127.00
38	A2	446	C	C6-N1-C2	-6.41	117.74	120.30
38	A2	4227	C	C2-N1-C1'	6.40	125.84	118.80
41	A3	1261	C	N3-C2-O2	-6.40	117.42	121.90
41	A3	1117	C	C6-N1-C1'	-6.40	113.12	120.80
41	A3	1022	U	N1-C2-O2	6.39	127.28	122.80
41	A3	1216	C	N1-C2-O2	6.39	122.73	118.90
38	A2	4733	C	C2-N1-C1'	6.39	125.83	118.80
38	A2	1602	U	N3-C2-O2	-6.39	117.73	122.20
38	A2	2261	C	C6-N1-C1'	-6.38	113.14	120.80
39	B2	39	C	N1-C2-O2	6.38	122.73	118.90
38	A2	266	C	O5'-P-OP2	-6.37	99.97	105.70
38	A2	4346	U	N3-C2-O2	-6.37	117.74	122.20
38	A2	1208	C	C2-N1-C1'	6.36	125.80	118.80
38	A2	2531	G	N3-C4-C5	-6.36	125.42	128.60
31	e1	92	LYS	CA-CB-CG	6.36	127.38	113.40
38	A2	1307	C	C6-N1-C2	-6.35	117.76	120.30
38	A2	2571	C	C2-N1-C1'	6.35	125.79	118.80
38	A2	4218	U	P-O3'-C3'	6.35	127.32	119.70
38	A2	1996	C	C6-N1-C2	-6.34	117.76	120.30
40	C2	127	U	N1-C2-O2	6.34	127.24	122.80
41	A3	199	C	N3-C2-O2	-6.34	117.46	121.90
38	A2	2011	C	N3-C2-O2	-6.34	117.46	121.90
38	A2	2535	C	C2-N1-C1'	6.34	125.77	118.80
35	n1	27	ASP	CB-CG-OD1	6.33	124.00	118.30
36	21	56	C	N1-C2-O2	6.33	122.70	118.90
38	A2	1178	C	N1-C2-O2	6.33	122.69	118.90
38	A2	4910	C	C2-N1-C1'	6.33	125.76	118.80
38	A2	4279	U	N3-C2-O2	-6.32	117.78	122.20
41	A3	1660	C	C2-N1-C1'	6.32	125.75	118.80
38	A2	4462	C	N3-C2-O2	-6.32	117.48	121.90
38	A2	1411	C	C5-C6-N1	6.32	124.16	121.00
51	K3	26	ASP	CB-CG-OD1	6.32	123.98	118.30
38	A2	2839	A	O4'-C1'-N9	6.31	113.25	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	A3	1753	C	C6-N1-C2	-6.31	117.78	120.30
38	A2	1404	G	N3-C4-C5	-6.31	125.45	128.60
41	A3	1397	U	C5-C6-N1	6.31	125.85	122.70
38	A2	385	A	OP1-P-O3'	6.30	119.06	105.20
38	A2	928	C	C2-N1-C1'	6.30	125.73	118.80
41	A3	974	C	C6-N1-C2	-6.29	117.78	120.30
41	A3	879	C	C6-N1-C2	-6.29	117.78	120.30
41	A3	1753	C	C2-N1-C1'	6.28	125.71	118.80
41	A3	371	A	O5'-P-OP2	-6.28	100.05	105.70
54	N3	31	LEU	CA-CB-CG	6.28	129.74	115.30
38	A2	2531	G	N3-C4-N9	6.27	129.76	126.00
41	A3	442	C	C5-C6-N1	6.27	124.14	121.00
38	A2	4245	C	C5-C6-N1	6.27	124.14	121.00
38	A2	4300	C	N1-C2-O2	6.27	122.66	118.90
38	A2	4668	U	N3-C2-O2	-6.26	117.81	122.20
40	C2	51	U	N3-C2-O2	-6.26	117.81	122.20
41	A3	1725	U	N3-C2-O2	-6.26	117.82	122.20
38	A2	100	C	O4'-C1'-N1	6.26	113.20	108.20
38	A2	1379	U	C6-N1-C1'	-6.25	112.44	121.20
38	A2	4035	C	C5-C6-N1	6.25	124.13	121.00
38	A2	1079	C	N1-C2-O2	6.25	122.65	118.90
38	A2	446	C	C2-N1-C1'	6.25	125.67	118.80
75	j3	241	ARG	CG-CD-NE	6.25	124.92	111.80
38	A2	115	C	C6-N1-C1'	-6.24	113.31	120.80
38	A2	1890	G	N3-C4-N9	-6.24	122.25	126.00
41	A3	659	G	C8-N9-C1'	-6.24	118.89	127.00
38	A2	13	U	N1-C2-O2	6.24	127.17	122.80
38	A2	4908	C	C6-N1-C2	-6.24	117.80	120.30
38	A2	1890	G	N3-C4-C5	6.24	131.72	128.60
41	A3	293	C	C6-N1-C1'	-6.24	113.32	120.80
49	I3	28	LEU	CA-CB-CG	6.23	129.62	115.30
41	A3	1637	A	P-O3'-C3'	6.22	127.17	119.70
41	A3	814	U	N3-C2-O2	-6.22	117.85	122.20
41	A3	1057	C	N3-C2-O2	-6.22	117.55	121.90
41	A3	1314	U	N1-C2-O2	6.22	127.15	122.80
38	A2	980	G	C8-N9-C1'	6.22	135.08	127.00
38	A2	4399	C	N3-C2-O2	-6.22	117.55	121.90
38	A2	4441	G	O5'-P-OP1	6.21	118.15	110.70
41	A3	1389	C	N3-C2-O2	-6.20	117.56	121.90
38	A2	4289	C	C6-N1-C1'	-6.20	113.36	120.80
38	A2	2531	G	C8-N9-C1'	-6.19	118.95	127.00
38	A2	282	C	N3-C2-O2	-6.19	117.57	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	A3	579	C	N1-C2-O2	6.19	122.61	118.90
38	A2	282	C	C6-N1-C2	-6.18	117.83	120.30
38	A2	1482	G	O4'-C1'-N9	6.18	113.15	108.20
38	A2	4504	A	OP1-P-OP2	6.18	128.87	119.60
40	C2	76	C	C6-N1-C2	-6.18	117.83	120.30
41	A3	427	U	N3-C2-O2	-6.18	117.87	122.20
38	A2	1410	C	C2-N1-C1'	6.18	125.60	118.80
38	A2	41	C	C5-C6-N1	6.18	124.09	121.00
41	A3	804	U	C5-C6-N1	6.18	125.79	122.70
41	A3	1683	C	N1-C2-O2	6.18	122.61	118.90
38	A2	4908	C	C6-N1-C1'	-6.17	113.40	120.80
40	C2	124	U	P-O3'-C3'	6.17	127.10	119.70
41	A3	1139	C	C6-N1-C1'	-6.17	113.40	120.80
40	C2	141	C	C5-C6-N1	6.16	124.08	121.00
38	A2	1773	U	N1-C2-O2	6.16	127.11	122.80
38	A2	3704	U	C2-N1-C1'	6.16	125.09	117.70
41	A3	494	C	N1-C2-O2	6.16	122.59	118.90
38	A2	695	C	N3-C2-O2	-6.15	117.59	121.90
38	A2	2641	G	C4-N9-C1'	-6.15	118.51	126.50
38	A2	456	C	C6-N1-C2	-6.14	117.84	120.30
41	A3	55	U	N3-C2-O2	-6.14	117.90	122.20
41	A3	585	C	C6-N1-C2	-6.14	117.84	120.30
38	A2	4504	A	O5'-P-OP1	6.14	118.06	110.70
38	A2	4353	G	C5-C6-O6	6.13	132.28	128.60
38	A2	3599	A	N7-C8-N9	6.13	116.86	113.80
38	A2	3736	C	N1-C2-O2	6.13	122.58	118.90
41	A3	1535	U	C6-N1-C1'	-6.12	112.64	121.20
40	C2	99	U	N1-C2-O2	6.12	127.08	122.80
38	A2	1607	C	N3-C2-O2	-6.11	117.62	121.90
38	A2	406	C	P-O3'-C3'	6.11	127.03	119.70
56	P3	80	ASP	CB-CG-OD1	6.11	123.80	118.30
38	A2	2491	C	N1-C2-O2	6.11	122.56	118.90
38	A2	4862	C	C6-N1-C1'	-6.11	113.47	120.80
41	A3	1271	C	C6-N1-C2	-6.11	117.86	120.30
38	A2	1807	C	C2-N1-C1'	6.11	125.52	118.80
38	A2	4219	A	O5'-P-OP1	-6.11	100.20	105.70
38	A2	4910	C	N3-C2-O2	-6.11	117.63	121.90
31	e1	143	ILE	CG1-CB-CG2	-6.10	97.99	111.40
38	A2	1632	A	C2-N3-C4	6.10	113.65	110.60
38	A2	4918	G	P-O3'-C3'	6.09	127.01	119.70
38	A2	2630	C	C6-N1-C2	-6.09	117.86	120.30
38	A2	2270	U	C2-N1-C1'	6.09	125.01	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A2	4752	C	C5-C6-N1	6.09	124.05	121.00
41	A3	1219	C	N3-C2-O2	-6.09	117.64	121.90
36	21	56	C	C6-N1-C1'	-6.09	113.49	120.80
38	A2	217	C	C2-N1-C1'	6.09	125.50	118.80
41	A3	119	U	N3-C2-O2	-6.09	117.94	122.20
41	A3	1261	C	C6-N1-C2	-6.09	117.87	120.30
38	A2	4939	C	C2-N1-C1'	6.08	125.49	118.80
41	A3	656	G	N3-C4-N9	6.08	129.65	126.00
38	A2	1299	C	C6-N1-C2	-6.08	117.87	120.30
38	A2	934	C	N1-C2-O2	6.08	122.55	118.90
38	A2	695	C	N1-C2-O2	6.07	122.54	118.90
38	A2	923	C	C6-N1-C2	-6.07	117.87	120.30
38	A2	2068	C	OP1-P-O3'	6.07	118.56	105.20
38	A2	1414	C	N1-C2-O2	6.07	122.54	118.90
41	A3	1261	C	C2-N1-C1'	6.07	125.47	118.80
38	A2	2016	C	N3-C2-O2	-6.07	117.65	121.90
38	A2	2413	C	C6-N1-C2	-6.06	117.87	120.30
41	A3	1591	C	N3-C2-O2	-6.06	117.66	121.90
38	A2	1407	G	C8-N9-C1'	-6.06	119.12	127.00
41	A3	870	A	P-O3'-C3'	6.05	126.96	119.70
38	A2	2069	A	O5'-P-OP1	-6.05	100.25	105.70
38	A2	935	A	C4-C5-N7	-6.05	107.68	110.70
38	A2	1772	C	C5-C6-N1	6.05	124.02	121.00
38	A2	2261	C	C5-C6-N1	6.05	124.02	121.00
41	A3	151	C	C2-N1-C1'	6.04	125.45	118.80
38	A2	2708	G	N3-C4-N9	6.04	129.62	126.00
38	A2	4399	C	C6-N1-C1'	-6.04	113.56	120.80
38	A2	4695	U	C2-N1-C1'	6.03	124.94	117.70
41	A3	632	C	C5-C6-N1	6.03	124.01	121.00
38	A2	3969	G	P-O3'-C3'	6.03	126.93	119.70
38	A2	1080	C	C2-N1-C1'	6.03	125.43	118.80
38	A2	1393	U	N3-C2-O2	-6.02	117.99	122.20
38	A2	1800	U	N3-C2-O2	-6.02	117.99	122.20
38	A2	2495	C	C2-N1-C1'	6.02	125.42	118.80
41	A3	427	U	N1-C2-O2	6.02	127.01	122.80
38	A2	4294	C	N1-C2-O2	6.02	122.51	118.90
41	A3	119	U	N1-C2-O2	6.02	127.01	122.80
41	A3	1649	U	N1-C2-O2	6.01	127.01	122.80
39	B2	29	C	C2-N1-C1'	6.01	125.41	118.80
38	A2	1633	G	P-O3'-C3'	6.01	126.91	119.70
38	A2	1848	C	C6-N1-C2	-6.01	117.90	120.30
41	A3	1840	U	C5-C6-N1	6.00	125.70	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	A3	179	C	N1-C2-O2	6.00	122.50	118.90
38	A2	662	C	C2-N1-C1'	5.99	125.39	118.80
38	A2	1731	C	C2-N1-C1'	5.99	125.39	118.80
38	A2	2354	C	C2-N1-C1'	5.99	125.39	118.80
38	A2	4668	U	N1-C2-O2	5.99	126.99	122.80
38	A2	2641	G	C8-N9-C1'	5.99	134.79	127.00
40	C2	128	C	C2-N1-C1'	5.99	125.39	118.80
36	21	32	C	C2-N1-C1'	5.98	125.38	118.80
36	21	65	U	N1-C2-O2	5.98	126.99	122.80
38	A2	2707	C	C2-N1-C1'	5.98	125.38	118.80
41	A3	369	C	C2-N1-C1'	5.98	125.38	118.80
52	L3	52	LEU	CB-CG-CD1	-5.98	100.83	111.00
41	A3	1303	C	C6-N1-C1'	-5.97	113.63	120.80
38	A2	2822	U	N3-C2-O2	-5.97	118.02	122.20
41	A3	984	C	C6-N1-C2	-5.97	117.91	120.30
38	A2	4908	C	O4'-C1'-N1	5.96	112.97	108.20
38	A2	977	C	C6-N1-C2	-5.96	117.92	120.30
41	A3	879	C	N1-C2-O2	5.96	122.48	118.90
49	I3	79	LEU	CB-CG-CD1	5.96	121.13	111.00
38	A2	2340	C	C6-N1-C2	-5.96	117.92	120.30
33	l1	28	PHE	N-CA-CB	5.96	121.33	110.60
38	A2	245	C	P-O3'-C3'	5.96	126.85	119.70
41	A3	1696	C	C2-N1-C1'	5.96	125.35	118.80
38	A2	2817	C	N1-C2-O2	5.95	122.47	118.90
38	A2	4385	U	N3-C2-O2	-5.95	118.04	122.20
41	A3	465	A	P-O3'-C3'	5.94	126.83	119.70
38	A2	1428	U	N3-C2-O2	-5.94	118.04	122.20
38	A2	458	C	O5'-P-OP2	-5.94	100.36	105.70
38	A2	659	C	N3-C2-O2	-5.93	117.75	121.90
42	B3	127	PRO	N-CD-CG	-5.93	94.30	103.20
38	A2	1477	C	C6-N1-C2	-5.93	117.93	120.30
41	A3	1271	C	N3-C2-O2	-5.93	117.75	121.90
41	A3	1304	U	N1-C2-O2	5.93	126.95	122.80
38	A2	3968	G	C5'-C4'-C3'	5.92	125.47	116.00
38	A2	1214	C	C6-N1-C2	-5.91	117.94	120.30
41	A3	199	C	C2-N1-C1'	5.91	125.30	118.80
41	A3	824	C	N1-C2-O2	5.90	122.44	118.90
41	A3	1389	C	C6-N1-C1'	-5.90	113.72	120.80
38	A2	1983	A	P-O3'-C3'	5.90	126.78	119.70
41	A3	124	U	C2-N1-C1'	5.90	124.78	117.70
38	A2	3632	U	N1-C2-O2	5.89	126.92	122.80
40	C2	1	C	N3-C2-O2	-5.89	117.78	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	A3	1289	U	N1-C2-O2	5.89	126.92	122.80
35	n1	175	LYS	CD-CE-NZ	5.88	125.24	111.70
38	A2	1404	G	N3-C4-N9	5.88	129.53	126.00
41	A3	1117	C	C5-C6-N1	5.88	123.94	121.00
38	A2	2870	C	C2-N1-C1'	5.88	125.27	118.80
38	A2	2269	C	P-O3'-C3'	5.88	126.75	119.70
50	J3	132	GLU	CA-CB-CG	5.88	126.33	113.40
41	A3	930	C	N1-C2-O2	5.87	122.42	118.90
38	A2	1915	C	N3-C2-O2	-5.87	117.79	121.90
38	A2	3783	C	C2-N1-C1'	5.87	125.25	118.80
38	A2	217	C	N1-C2-O2	5.86	122.42	118.90
41	A3	119	U	C2-N1-C1'	5.86	124.73	117.70
85	t3	131	PRO	CA-N-CD	-5.85	103.31	111.50
86	u3	118	MET	CB-CG-SD	5.85	129.95	112.40
40	C2	75	G	N7-C8-N9	-5.85	110.18	113.10
56	P3	119	LEU	CA-CB-CG	5.85	128.75	115.30
41	A3	1520	G	N3-C4-C5	-5.84	125.68	128.60
38	A2	1834	U	N1-C2-O2	5.84	126.89	122.80
38	A2	4468	U	N1-C2-O2	5.84	126.89	122.80
13	M1	31	ASP	CB-CG-OD1	5.84	123.56	118.30
36	21	65	U	C2-N1-C1'	5.84	124.71	117.70
38	A2	1290	C	C5-C6-N1	5.84	123.92	121.00
38	A2	1481	C	C2-N1-C1'	5.83	125.22	118.80
38	A2	4030	G	P-O3'-C3'	5.83	126.70	119.70
38	A2	4745	C	C6-N1-C1'	-5.83	113.80	120.80
41	A3	814	U	N1-C2-O2	5.83	126.88	122.80
38	A2	4247	C	C5-C6-N1	5.83	123.91	121.00
41	A3	687	C	N1-C2-O2	5.83	122.40	118.90
38	A2	1936	C	N1-C2-O2	5.83	122.40	118.90
38	A2	1079	C	N3-C2-O2	-5.82	117.82	121.90
38	A2	220	C	C2-N1-C1'	5.82	125.20	118.80
38	A2	1979	A	P-O3'-C3'	5.81	126.68	119.70
31	e1	24	TYR	CD1-CE1-CZ	5.81	125.03	119.80
38	A2	1579	C	C6-N1-C2	-5.81	117.98	120.30
38	A2	960	G	P-O3'-C3'	5.81	126.67	119.70
38	A2	1812	C	N1-C2-O2	5.80	122.38	118.90
38	A2	446	C	C5-C6-N1	5.80	123.90	121.00
34	m1	37	U	N3-C2-O2	-5.80	118.14	122.20
38	A2	2016	C	C6-N1-C2	-5.80	117.98	120.30
40	C2	38	U	N3-C2-O2	-5.80	118.14	122.20
41	A3	1590	C	C6-N1-C2	-5.80	117.98	120.30
38	A2	1177	U	N3-C2-O2	-5.80	118.14	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A2	1853	G	C4-N9-C1'	5.80	134.03	126.50
38	A2	1656	U	N3-C2-O2	-5.79	118.14	122.20
38	A2	4113	U	O5'-P-OP1	-5.79	100.49	105.70
38	A2	1178	C	N3-C2-O2	-5.79	117.85	121.90
38	A2	4192	C	C5-C6-N1	5.79	123.89	121.00
41	A3	1139	C	C6-N1-C2	-5.79	117.98	120.30
38	A2	112	C	C6-N1-C2	-5.78	117.99	120.30
41	A3	792	C	N3-C2-O2	-5.78	117.86	121.90
38	A2	1079	C	C2-N1-C1'	5.78	125.15	118.80
38	A2	1440	U	N1-C2-O2	5.77	126.84	122.80
41	A3	666	U	C2-N1-C1'	5.77	124.62	117.70
36	21	32	C	N3-C2-O2	-5.77	117.86	121.90
38	A2	41	C	C6-N1-C2	-5.77	117.99	120.30
38	A2	1906	U	N1-C2-O2	5.77	126.84	122.80
36	21	65	U	N3-C2-O2	-5.77	118.16	122.20
52	L3	12	TYR	CB-CG-CD2	-5.77	117.54	121.00
45	E3	76	ARG	CG-CD-NE	5.76	123.91	111.80
63	W3	72	LEU	CB-CG-CD1	5.76	120.80	111.00
38	A2	4245	C	C6-N1-C2	-5.76	118.00	120.30
38	A2	4675	U	C5-C6-N1	5.75	125.58	122.70
38	A2	4546	C	N3-C2-O2	-5.75	117.87	121.90
41	A3	1591	C	C6-N1-C2	-5.75	118.00	120.30
38	A2	2072	C	C5-C6-N1	5.75	123.87	121.00
41	A3	26	U	C5-C6-N1	5.74	125.57	122.70
38	A2	1483	C	N3-C2-O2	-5.74	117.88	121.90
38	A2	3783	C	N3-C2-O2	-5.74	117.88	121.90
41	A3	752	G	O4'-C1'-N9	5.74	112.79	108.20
15	O1	36	ASP	CB-CG-OD2	5.74	123.46	118.30
41	A3	1310	U	C2-N1-C1'	5.73	124.58	117.70
38	A2	1612	G	C6-C5-N7	-5.72	126.97	130.40
41	A3	1022	U	N3-C2-O2	-5.72	118.19	122.20
38	A2	13	U	N3-C2-O2	-5.72	118.19	122.20
38	A2	1379	U	N3-C2-O2	-5.72	118.20	122.20
41	A3	1309	C	C2-N1-C1'	5.71	125.08	118.80
41	A3	1397	U	C6-N1-C2	-5.71	117.57	121.00
38	A2	2354	C	C6-N1-C2	-5.71	118.02	120.30
38	A2	4468	U	N3-C2-O2	-5.71	118.21	122.20
38	A2	1827	C	C2-N1-C1'	5.70	125.07	118.80
38	A2	126	C	C2-N1-C1'	5.70	125.07	118.80
38	A2	4163	C	C6-N1-C2	-5.70	118.02	120.30
41	A3	87	U	N3-C2-O2	-5.70	118.21	122.20
38	A2	4163	C	C5-C6-N1	5.70	123.85	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	A3	1204	A	N7-C8-N9	5.70	116.65	113.80
64	X3	61	ILE	CG1-CB-CG2	-5.70	98.87	111.40
41	A3	199	C	C6-N1-C2	-5.69	118.02	120.30
38	A2	4612	A	O5'-P-OP2	-5.69	100.58	105.70
41	A3	730	C	C2-N1-C1'	5.69	125.06	118.80
41	A3	1752	C	N3-C2-O2	-5.69	117.92	121.90
38	A2	5029	C	N1-C2-O2	5.69	122.31	118.90
41	A3	958	G	C4-N9-C1'	5.69	133.90	126.50
40	C2	141	C	C6-N1-C2	-5.69	118.03	120.30
38	A2	1607	C	N1-C2-O2	5.68	122.31	118.90
41	A3	1752	C	C2-N1-C1'	5.68	125.05	118.80
38	A2	3883	G	P-O3'-C3'	5.68	126.51	119.70
41	A3	1696	C	C6-N1-C2	-5.68	118.03	120.30
38	A2	134	G	P-O3'-C3'	5.67	126.51	119.70
38	A2	4192	C	C6-N1-C2	-5.67	118.03	120.30
41	A3	303	C	N3-C2-O2	-5.67	117.93	121.90
40	C2	140	C	C6-N1-C2	-5.66	118.03	120.30
38	A2	1368	G	P-O3'-C3'	5.66	126.49	119.70
38	A2	935	A	N9-C4-C5	5.66	108.06	105.80
41	A3	37	C	C6-N1-C2	-5.66	118.04	120.30
38	A2	1338	C	C6-N1-C2	-5.66	118.04	120.30
38	A2	2008	U	C2-N1-C1'	5.66	124.49	117.70
38	A2	2473	C	N1-C2-O2	5.66	122.30	118.90
41	A3	55	U	C6-N1-C1'	-5.66	113.28	121.20
41	A3	151	C	C6-N1-C2	-5.66	118.04	120.30
38	A2	4201	C	N1-C2-O2	5.65	122.29	118.90
41	A3	530	U	C2-N1-C1'	5.65	124.48	117.70
38	A2	449	C	P-O3'-C3'	5.65	126.48	119.70
7	G1	88	ARG	NE-CZ-NH2	-5.65	117.48	120.30
38	A2	1307	C	C5-C6-N1	5.65	123.82	121.00
38	A2	2630	C	C6-N1-C1'	-5.65	114.02	120.80
41	A3	1453	C	C2-N3-C4	5.64	122.72	119.90
38	A2	926	G	N7-C8-N9	5.64	115.92	113.10
38	A2	4227	C	N1-C2-O2	5.64	122.28	118.90
38	A2	4384	C	C6-N1-C2	-5.64	118.04	120.30
41	A3	578	C	N1-C2-O2	5.64	122.28	118.90
38	A2	2508	C	C6-N1-C2	-5.63	118.05	120.30
41	A3	142	C	N1-C2-O2	5.63	122.28	118.90
41	A3	14	C	C6-N1-C2	-5.63	118.05	120.30
41	A3	179	C	N3-C2-O2	-5.63	117.96	121.90
38	A2	1177	U	C2-N1-C1'	5.62	124.45	117.70
38	A2	454	U	N1-C2-O2	5.62	126.74	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	A3	1599	U	N3-C2-O2	-5.62	118.26	122.20
41	A3	1230	C	C6-N1-C2	-5.62	118.05	120.30
38	A2	741	G	N1-C6-O6	-5.62	116.53	119.90
38	A2	4668	U	C2-N1-C1'	5.62	124.44	117.70
38	A2	3620	G	P-O3'-C3'	5.62	126.44	119.70
41	A3	1130	G	C4-N9-C1'	5.62	133.80	126.50
38	A2	1639	U	C6-N1-C1'	-5.62	113.34	121.20
38	A2	2442	G	C4-N9-C1'	5.62	133.80	126.50
38	A2	2859	C	N3-C2-O2	-5.61	117.97	121.90
38	A2	2687	C	C6-N1-C2	-5.61	118.06	120.30
38	A2	228	C	C6-N1-C2	-5.61	118.06	120.30
38	A2	658	C	C2-N1-C1'	5.61	124.97	118.80
40	C2	123	U	N1-C2-O2	5.61	126.72	122.80
38	A2	4430	C	N1-C2-O2	5.60	122.26	118.90
38	A2	4430	C	N3-C2-O2	-5.60	117.98	121.90
38	A2	2806	U	N3-C2-O2	-5.60	118.28	122.20
41	A3	1022	U	C6-N1-C1'	-5.60	113.36	121.20
38	A2	3688	U	N1-C2-O2	5.60	126.72	122.80
38	A2	4700	C	N1-C2-O2	5.60	122.26	118.90
41	A3	531	A	C4-N9-C1'	5.60	136.38	126.30
38	A2	1080	C	C6-N1-C2	-5.60	118.06	120.30
38	A2	2051	C	C6-N1-C2	-5.59	118.06	120.30
38	A2	3970	C	C5-C6-N1	5.59	123.80	121.00
41	A3	1725	U	N1-C2-O2	5.59	126.72	122.80
38	A2	4340	U	OP2-P-O3'	5.59	117.50	105.20
41	A3	1218	C	C6-N1-C2	-5.59	118.06	120.30
38	A2	217	C	P-O3'-C3'	5.59	126.41	119.70
40	C2	128	C	C6-N1-C2	-5.59	118.06	120.30
38	A2	1792	U	C2-N1-C1'	5.59	124.41	117.70
41	A3	356	C	C6-N1-C2	-5.59	118.06	120.30
41	A3	1219	C	C2-N1-C1'	5.59	124.94	118.80
41	A3	1399	C	C2-N1-C1'	5.59	124.95	118.80
58	R3	105	LYS	CD-CE-NZ	-5.59	98.85	111.70
4	D1	22	ASP	CB-CG-OD1	5.58	123.32	118.30
41	A3	1649	U	N3-C2-O2	-5.58	118.30	122.20
38	A2	1	C	N1-C2-O2	5.58	122.25	118.90
38	A2	4488	C	C6-N1-C2	-5.58	118.07	120.30
41	A3	1523	C	C5-C6-N1	5.58	123.79	121.00
38	A2	1469	C	C5-C6-N1	5.57	123.79	121.00
38	A2	1726	U	N3-C2-O2	-5.57	118.30	122.20
38	A2	2641	G	N3-C4-C5	5.57	131.39	128.60
38	A2	4759	C	N1-C2-O2	5.57	122.24	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A2	4353	G	C8-N9-C4	-5.57	104.17	106.40
41	A3	659	G	N3-C4-C5	-5.57	125.81	128.60
41	A3	314	U	N3-C2-O2	-5.57	118.30	122.20
38	A2	1235	C	N1-C2-O2	5.57	122.24	118.90
38	A2	4940	C	C6-N1-C2	-5.57	118.07	120.30
41	A3	1852	C	C6-N1-C2	-5.56	118.08	120.30
38	A2	1404	G	C8-N9-C1'	-5.56	119.77	127.00
38	A2	1323	C	C2-N1-C1'	5.56	124.91	118.80
41	A3	1117	C	C2-N3-C4	5.56	122.68	119.90
38	A2	3652	U	N3-C2-O2	-5.55	118.31	122.20
38	A2	4700	C	N3-C2-O2	-5.55	118.01	121.90
41	A3	578	C	N3-C2-O2	-5.55	118.01	121.90
61	U3	110	LEU	CA-CB-CG	5.55	128.07	115.30
41	A3	1624	U	C6-N1-C1'	-5.55	113.44	121.20
38	A2	1290	C	C6-N1-C2	-5.54	118.08	120.30
38	A2	4192	C	C2-N1-C1'	5.54	124.90	118.80
41	A3	1225	U	N3-C2-O2	-5.54	118.32	122.20
38	A2	4551	C	C6-N1-C2	-5.54	118.08	120.30
38	A2	658	C	N1-C2-O2	5.54	122.22	118.90
38	A2	1690	C	C6-N1-C2	-5.54	118.08	120.30
41	A3	162	C	C5-C6-N1	5.54	123.77	121.00
38	A2	1236	A	P-O3'-C3'	5.54	126.34	119.70
38	A2	365	U	N1-C2-O2	5.53	126.67	122.80
41	A3	4	C	C2-N1-C1'	5.53	124.88	118.80
38	A2	2687	C	C5-C6-N1	5.53	123.76	121.00
38	A2	4939	C	N3-C2-O2	-5.53	118.03	121.90
38	A2	2068	C	P-O3'-C3'	5.53	126.33	119.70
54	N3	124	ILE	CG1-CB-CG2	-5.53	99.24	111.40
38	A2	4462	C	C6-N1-C2	-5.52	118.09	120.30
38	A2	1502	G	N3-C4-N9	-5.52	122.69	126.00
41	A3	879	C	C6-N1-C1'	-5.52	114.17	120.80
79	n3	221	LYS	CD-CE-NZ	-5.52	99.00	111.70
38	A2	1785	C	C2-N1-C1'	5.52	124.87	118.80
38	A2	1477	C	P-O3'-C3'	5.52	126.32	119.70
38	A2	4279	U	N1-C2-O2	5.52	126.66	122.80
41	A3	317	C	C2-N1-C1'	5.52	124.87	118.80
38	A2	1882	U	N3-C4-O4	5.51	123.26	119.40
38	A2	3970	C	C6-N1-C1'	-5.51	114.18	120.80
38	A2	1287	C	C6-N1-C2	-5.51	118.09	120.30
41	A3	1389	C	C5-C6-N1	5.51	123.76	121.00
38	A2	4745	C	O4'-C1'-N1	5.51	112.61	108.20
41	A3	183	G	N9-C4-C5	5.51	107.60	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	U3	28	LEU	CB-CG-CD1	-5.51	101.63	111.00
38	A2	1234	C	C5-C6-N1	5.51	123.75	121.00
38	A2	1514	U	N3-C2-O2	-5.51	118.34	122.20
38	A2	1720	C	N1-C2-O2	5.51	122.20	118.90
41	A3	1636	G	C2-N3-C4	5.51	114.65	111.90
41	A3	110	U	P-O3'-C3'	5.50	126.30	119.70
38	A2	282	C	N1-C2-O2	5.50	122.20	118.90
38	A2	2806	U	N1-C2-O2	5.50	126.65	122.80
35	n1	135	LEU	CB-CG-CD1	5.49	120.33	111.00
38	A2	4108	G	N3-C4-N9	-5.49	122.71	126.00
41	A3	530	U	N1-C2-O2	5.49	126.64	122.80
41	A3	1364	U	C5-C6-N1	5.49	125.44	122.70
41	A3	162	C	C6-N1-C2	-5.49	118.11	120.30
41	A3	1636	G	C8-N9-C1'	-5.49	119.87	127.00
41	A3	93	U	N3-C2-O2	-5.49	118.36	122.20
41	A3	183	G	C4-N9-C1'	5.49	133.63	126.50
41	A3	407	G	N3-C4-C5	-5.48	125.86	128.60
41	A3	632	C	C6-N1-C2	-5.48	118.11	120.30
38	A2	4851	U	C6-N1-C1'	-5.48	113.53	121.20
41	A3	579	C	N3-C2-O2	-5.48	118.07	121.90
38	A2	1792	U	N3-C2-O2	-5.47	118.37	122.20
41	A3	188	C	N3-C2-O2	-5.47	118.07	121.90
38	A2	3768	U	OP1-P-OP2	5.47	127.80	119.60
38	A2	2284	U	N1-C2-O2	5.47	126.63	122.80
41	A3	188	C	C6-N1-C2	-5.47	118.11	120.30
41	A3	1852	C	C2-N1-C1'	5.47	124.81	118.80
38	A2	1209	G	P-O3'-C3'	5.46	126.26	119.70
38	A2	4598	C	N1-C2-O2	5.46	122.18	118.90
38	A2	1929	A	C4-N9-C1'	5.46	136.13	126.30
41	A3	1752	C	C6-N1-C2	-5.46	118.12	120.30
38	A2	3704	U	N3-C2-O2	-5.46	118.38	122.20
41	A3	178	C	C5-C6-N1	5.45	123.72	121.00
38	A2	954	C	C6-N1-C2	-5.45	118.12	120.30
38	A2	4291	G	C2-N3-C4	5.45	114.62	111.90
74	h3	268	ASP	CB-CG-OD2	-5.45	113.40	118.30
18	R1	5	ARG	CB-CG-CD	-5.45	97.44	111.60
38	A2	242	U	N3-C2-O2	-5.45	118.39	122.20
38	A2	3613	C	C6-N1-C2	-5.45	118.12	120.30
38	A2	4347	U	N3-C2-O2	-5.45	118.39	122.20
41	A3	1271	C	C2-N1-C1'	5.44	124.78	118.80
58	R3	93	VAL	CA-CB-CG1	5.44	119.06	110.90
38	A2	673	C	C5-C6-N1	5.43	123.72	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A2	4252	G	C8-N9-C4	-5.43	104.23	106.40
38	A2	4382	A	N1-C2-N3	-5.43	126.58	129.30
38	A2	1440	U	N3-C2-O2	-5.43	118.40	122.20
39	B2	39	C	N3-C2-O2	-5.43	118.10	121.90
38	A2	4328	C	C6-N1-C2	-5.43	118.13	120.30
31	e1	24	TYR	CZ-CE2-CD2	-5.42	114.92	119.80
38	A2	4698	C	C6-N1-C2	-5.42	118.13	120.30
38	A2	4215	U	C2-N1-C1'	5.42	124.20	117.70
38	A2	4291	G	C8-N9-C4	-5.42	104.23	106.40
40	C2	127	U	C2-N1-C1'	5.42	124.20	117.70
45	E3	69	LEU	CB-CG-CD2	-5.42	101.79	111.00
38	A2	978	G	C5-C6-N1	-5.42	108.79	111.50
38	A2	4252	G	C8-N9-C1'	-5.41	119.96	127.00
35	n1	55	LEU	CB-CG-CD1	-5.41	101.80	111.00
38	A2	1656	U	N1-C2-O2	5.41	126.59	122.80
38	A2	1893	C	C2-N1-C1'	5.41	124.75	118.80
38	A2	3599	A	C8-N9-C4	-5.41	103.64	105.80
38	A2	3826	U	N1-C2-O2	5.41	126.59	122.80
41	A3	402	C	C6-N1-C2	-5.41	118.14	120.30
38	A2	112	C	C5-C6-N1	5.41	123.70	121.00
38	A2	720	C	C2-N1-C1'	5.41	124.75	118.80
38	A2	3756	C	N1-C2-O2	5.41	122.14	118.90
38	A2	1915	C	N1-C2-O2	5.40	122.14	118.90
38	A2	2405	G	C2-N3-C4	5.40	114.60	111.90
38	A2	2707	C	C5-C6-N1	5.40	123.70	121.00
38	A2	4546	C	C2-N1-C1'	5.40	124.74	118.80
38	A2	4867	U	N3-C2-O2	-5.40	118.42	122.20
38	A2	1671	U	C5-C6-N1	5.40	125.40	122.70
38	A2	1773	U	N3-C2-O2	-5.40	118.42	122.20
38	A2	3826	U	N3-C2-O2	-5.39	118.42	122.20
41	A3	1216	C	N3-C2-O2	-5.39	118.13	121.90
41	A3	1655	C	C6-N1-C2	-5.39	118.14	120.30
52	L3	4	PRO	CA-N-CD	-5.39	103.95	111.50
38	A2	449	C	OP2-P-O3'	5.39	117.06	105.20
38	A2	2563	C	C5-C6-N1	5.39	123.69	121.00
38	A2	2563	C	C6-N1-C2	-5.39	118.14	120.30
38	A2	4929	U	P-O3'-C3'	5.38	126.16	119.70
41	A3	1865	C	C2-N1-C1'	5.38	124.72	118.80
38	A2	4862	C	O4'-C1'-N1	5.38	112.51	108.20
38	A2	920	C	N3-C2-O2	-5.38	118.13	121.90
38	A2	4405	U	C6-N1-C1'	-5.38	113.67	121.20
38	A2	978	G	C5-N7-C8	-5.38	101.61	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A2	1726	U	N1-C2-O2	5.38	126.56	122.80
41	A3	1624	U	O4'-C1'-N1	5.38	112.50	108.20
41	A3	752	G	C6-C5-N7	5.38	133.62	130.40
41	A3	531	A	C8-N9-C1'	-5.37	118.03	127.70
41	A3	442	C	C6-N1-C2	-5.37	118.15	120.30
38	A2	2442	G	C8-N9-C1'	-5.37	120.02	127.00
41	A3	1123	C	C6-N1-C2	-5.37	118.15	120.30
38	A2	365	U	N3-C2-O2	-5.36	118.45	122.20
38	A2	1568	C	C2-N1-C1'	5.36	124.69	118.80
9	I1	92	ASP	CB-CG-OD2	5.36	123.12	118.30
39	B2	102	U	N3-C2-O2	-5.36	118.45	122.20
38	A2	493	U	C2-N1-C1'	5.35	124.12	117.70
38	A2	2412	U	C4-C5-C6	5.35	122.91	119.70
38	A2	4385	U	N1-C2-O2	5.35	126.55	122.80
38	A2	1996	C	C5-C6-N1	5.35	123.67	121.00
38	A2	1382	C	C6-N1-C2	-5.35	118.16	120.30
38	A2	2853	A	C8-N9-C4	-5.35	103.66	105.80
39	B2	39	C	C2-N1-C1'	5.35	124.69	118.80
38	A2	117	C	C2-N1-C1'	5.35	124.68	118.80
75	j3	102	LEU	CA-CB-CG	5.35	127.60	115.30
12	L1	77	LYS	CB-CG-CD	5.35	125.50	111.60
41	A3	790	C	C5-C6-N1	5.34	123.67	121.00
56	P3	138	ASP	CB-CG-OD1	5.34	123.11	118.30
32	f1	123	ARG	CA-CB-CG	5.34	125.15	113.40
41	A3	1649	U	C2-N1-C1'	5.34	124.11	117.70
38	A2	1484	G	C6-C5-N7	-5.34	127.20	130.40
38	A2	3668	C	N1-C2-O2	5.33	122.10	118.90
38	A2	1414	C	N3-C2-O2	-5.33	118.17	121.90
38	A2	3734	C	C6-N1-C2	-5.33	118.17	120.30
38	A2	1809	C	C5-C6-N1	5.33	123.67	121.00
38	A2	4294	C	N3-C2-O2	-5.33	118.17	121.90
39	B2	111	C	C5-C6-N1	5.33	123.67	121.00
38	A2	2535	C	C5-C6-N1	5.33	123.66	121.00
38	A2	390	C	C5-C6-N1	5.33	123.66	121.00
38	A2	2707	C	C6-N1-C2	-5.32	118.17	120.30
41	A3	553	U	OP1-P-O3'	5.32	116.91	105.20
41	A3	1057	C	C6-N1-C1'	-5.32	114.41	120.80
38	A2	2823	C	C2-N1-C1'	5.32	124.65	118.80
38	A2	4430	C	C6-N1-C2	-5.32	118.17	120.30
41	A3	1172	U	N1-C2-O2	5.32	126.52	122.80
38	A2	14	C	C5-C6-N1	5.32	123.66	121.00
38	A2	3877	C	C2-N1-C1'	5.32	124.65	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	L3	4	PRO	CB-CG-CD	-5.32	85.77	106.50
41	A3	1118	C	C2-N1-C1'	5.32	124.65	118.80
38	A2	505	G	P-O3'-C3'	5.31	126.08	119.70
38	A2	913	A	N1-C6-N6	-5.31	115.41	118.60
38	A2	741	G	C6-N1-C2	-5.31	121.91	125.10
38	A2	2853	A	N7-C8-N9	5.31	116.45	113.80
41	A3	24	C	P-O3'-C3'	5.31	126.07	119.70
41	A3	1078	C	C2-N1-C1'	5.31	124.64	118.80
38	A2	2284	U	C2-N1-C1'	5.31	124.07	117.70
38	A2	2708	G	C4-N9-C1'	5.30	133.40	126.50
38	A2	1191	C	C6-N1-C2	-5.30	118.18	120.30
41	A3	687	C	N3-C2-O2	-5.30	118.19	121.90
41	A3	984	C	N1-C2-N3	5.30	122.91	119.20
38	A2	3740	U	N3-C2-O2	-5.30	118.49	122.20
41	A3	293	C	C5-C6-N1	5.30	123.65	121.00
38	A2	96	U	N1-C2-O2	5.30	126.51	122.80
38	A2	1568	C	C5-C6-N1	5.29	123.65	121.00
41	A3	1289	U	C2-N1-C1'	5.29	124.05	117.70
38	A2	2805	C	C6-N1-C2	-5.29	118.18	120.30
41	A3	191	A	OP1-P-O3'	5.29	116.83	105.20
38	A2	4862	C	C6-N1-C2	-5.29	118.19	120.30
40	C2	28	C	C6-N1-C2	-5.29	118.19	120.30
38	A2	1809	C	C6-N1-C2	-5.29	118.19	120.30
38	A2	4913	G	N3-C2-N2	-5.29	116.20	119.90
38	A2	4930	C	N3-C2-O2	-5.28	118.20	121.90
38	A2	4201	C	C6-N1-C2	-5.28	118.19	120.30
38	A2	3904	C	N3-C2-O2	-5.28	118.21	121.90
38	A2	1458	C	N1-C2-O2	5.27	122.06	118.90
38	A2	1485	C	C6-N1-C2	-5.27	118.19	120.30
38	A2	3797	U	C2-N1-C1'	5.27	124.03	117.70
38	A2	3970	C	N1-C2-O2	5.27	122.06	118.90
41	A3	530	U	N3-C2-O2	-5.27	118.51	122.20
41	A3	1172	U	N3-C2-O2	-5.27	118.51	122.20
38	A2	4548	C	C6-N1-C2	-5.27	118.19	120.30
34	m1	37	U	N1-C2-O2	5.27	126.49	122.80
38	A2	390	C	C6-N1-C2	-5.27	118.19	120.30
38	A2	4382	A	C6-N1-C2	5.27	121.76	118.60
38	A2	1481	C	N1-C2-O2	5.27	122.06	118.90
38	A2	3630	A	C4-C5-N7	5.27	113.33	110.70
41	A3	1219	C	C6-N1-C2	-5.27	118.19	120.30
38	A2	1853	G	C8-N9-C1'	-5.26	120.16	127.00
38	A2	3704	U	N1-C2-O2	5.26	126.48	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A2	71	C	C6-N1-C2	-5.26	118.19	120.30
38	A2	1514	U	N1-C2-O2	5.26	126.48	122.80
39	B2	39	C	C6-N1-C2	-5.26	118.20	120.30
41	A3	1292	C	C6-N1-C2	-5.26	118.19	120.30
38	A2	1407	G	C2-N3-C4	5.26	114.53	111.90
38	A2	2641	G	N3-C2-N2	-5.26	116.22	119.90
4	D1	98	LEU	CB-CG-CD1	-5.26	102.06	111.00
38	A2	4918	G	OP1-P-O3'	5.25	116.76	105.20
41	A3	1595	U	N3-C2-O2	-5.25	118.52	122.20
38	A2	124	C	C6-N1-C2	-5.25	118.20	120.30
38	A2	4904	C	C6-N1-C2	-5.25	118.20	120.30
41	A3	752	G	N9-C4-C5	5.25	107.50	105.40
41	A3	1154	U	O4'-C1'-N1	5.25	112.40	108.20
41	A3	303	C	C6-N1-C2	-5.25	118.20	120.30
39	B2	102	U	C2-N1-C1'	5.24	123.99	117.70
41	A3	729	C	C6-N1-C2	-5.24	118.20	120.30
41	A3	1304	U	N3-C2-O2	-5.24	118.53	122.20
38	A2	2630	C	C5-C6-N1	5.24	123.62	121.00
41	A3	930	C	C2-N1-C1'	5.24	124.56	118.80
38	A2	2367	G	N3-C2-N2	-5.24	116.23	119.90
38	A2	4351	C	C6-N1-C2	-5.23	118.21	120.30
38	A2	4462	C	N1-C2-O2	5.23	122.04	118.90
38	A2	1235	C	N3-C2-O2	-5.23	118.24	121.90
38	A2	1807	C	C6-N1-C2	-5.22	118.21	120.30
38	A2	4888	C	C6-N1-C2	-5.22	118.21	120.30
41	A3	1057	C	O4'-C1'-N1	5.22	112.38	108.20
38	A2	3833	U	N3-C2-O2	-5.22	118.54	122.20
41	A3	853	C	C6-N1-C2	-5.22	118.21	120.30
38	A2	294	G	N3-C4-N9	5.22	129.13	126.00
38	A2	4115	G	C6-C5-N7	5.22	133.53	130.40
41	A3	548	C	C6-N1-C2	-5.22	118.21	120.30
38	A2	1368	G	OP2-P-O3'	5.21	116.67	105.20
38	A2	1847	C	C5-C6-N1	5.21	123.61	121.00
38	A2	4087	G	N3-C2-N2	-5.21	116.25	119.90
5	E1	99	MET	CG-SD-CE	-5.21	91.87	100.20
38	A2	1807	C	C5-C6-N1	5.21	123.60	121.00
38	A2	5029	C	N3-C2-O2	-5.21	118.25	121.90
39	B2	51	G	N1-C6-O6	-5.21	116.78	119.90
38	A2	1379	U	O4'-C1'-N1	5.21	112.37	108.20
38	A2	1602	U	N1-C2-O2	5.21	126.44	122.80
38	A2	3887	U	N3-C2-O2	-5.21	118.56	122.20
38	A2	2011	C	C2-N1-C1'	5.20	124.53	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A2	4336	C	N1-C2-O2	5.20	122.02	118.90
38	A2	1809	C	C2-N1-C1'	5.20	124.52	118.80
38	A2	4300	C	N3-C2-O2	-5.20	118.26	121.90
38	A2	2863	C	C6-N1-C2	-5.19	118.22	120.30
38	A2	4415	C	C6-N1-C2	-5.19	118.22	120.30
38	A2	4924	C	C2-N1-C1'	5.19	124.51	118.80
38	A2	976	C	C6-N1-C2	-5.19	118.22	120.30
38	A2	3877	C	C6-N1-C2	-5.19	118.22	120.30
38	A2	1848	C	C5-C6-N1	5.18	123.59	121.00
38	A2	1893	C	C5-C6-N1	5.18	123.59	121.00
41	A3	630	U	C6-N1-C1'	-5.18	113.94	121.20
41	A3	824	C	N3-C2-O2	-5.18	118.27	121.90
41	A3	792	C	C6-N1-C2	-5.18	118.23	120.30
40	C2	35	C	C6-N1-C2	-5.18	118.23	120.30
38	A2	741	G	C5-C6-N1	5.18	114.09	111.50
38	A2	4963	G	C4-N9-C1'	5.18	133.23	126.50
38	A2	1477	C	C2-N1-C1'	5.17	124.49	118.80
40	C2	1	C	C6-N1-C2	-5.17	118.23	120.30
38	A2	294	G	C4-N9-C1'	5.17	133.22	126.50
41	A3	494	C	N3-C2-O2	-5.17	118.28	121.90
41	A3	542	U	N1-C2-O2	5.17	126.42	122.80
38	A2	2790	A	N3-C4-N9	5.17	131.53	127.40
18	R1	89	LEU	CA-CB-CG	5.17	127.18	115.30
38	A2	2365	U	N3-C2-O2	-5.17	118.58	122.20
38	A2	1812	C	C2-N1-C1'	5.16	124.48	118.80
41	A3	1271	C	C5-C6-N1	5.16	123.58	121.00
51	K3	129	LEU	CB-CG-CD2	-5.16	102.23	111.00
36	21	61	C	C6-N1-C2	-5.16	118.24	120.30
77	l3	205	ARG	NE-CZ-NH1	5.16	122.88	120.30
38	A2	4378	G	N1-C6-O6	-5.15	116.81	119.90
41	A3	659	G	N3-C4-N9	5.15	129.09	126.00
41	A3	874	G	P-O3'-C3'	5.15	125.88	119.70
38	A2	692	C	C6-N1-C2	-5.15	118.24	120.30
38	A2	980	G	N3-C2-N2	-5.15	116.30	119.90
38	A2	1861	U	N3-C2-O2	-5.15	118.60	122.20
38	A2	4488	C	N1-C2-O2	5.15	121.99	118.90
38	A2	220	C	N1-C2-O2	5.14	121.99	118.90
41	A3	1518	C	C6-N1-C2	-5.14	118.24	120.30
41	A3	1750	C	C5-C6-N1	5.14	123.57	121.00
38	A2	4939	C	C6-N1-C2	-5.14	118.24	120.30
38	A2	1235	C	C6-N1-C2	-5.14	118.25	120.30
38	A2	4272	C	C2-N1-C1'	5.14	124.45	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A2	4405	U	C5-C6-N1	5.14	125.27	122.70
38	A2	1695	U	N1-C2-O2	5.13	126.39	122.80
38	A2	742	G	N1-C6-O6	-5.13	116.82	119.90
38	A2	1234	C	P-O3'-C3'	5.13	125.86	119.70
38	A2	125	C	P-O3'-C3'	5.13	125.85	119.70
41	A3	142	C	C2-N1-C1'	5.13	124.44	118.80
38	A2	1208	C	N3-C2-O2	-5.13	118.31	121.90
38	A2	4289	C	C6-N1-C2	-5.12	118.25	120.30
38	A2	3826	U	C2-N1-C1'	5.12	123.85	117.70
41	A3	1331	C	N1-C2-O2	5.12	121.97	118.90
41	A3	1590	C	C5-C6-N1	5.12	123.56	121.00
38	A2	2697	G	C4-C5-N7	5.12	112.85	110.80
38	A2	2863	C	N1-C2-O2	5.12	121.97	118.90
38	A2	4745	C	C5-C6-N1	5.12	123.56	121.00
41	A3	1154	U	C2-N1-C1'	5.12	123.84	117.70
41	A3	1865	C	N3-C2-O2	-5.12	118.32	121.90
38	A2	1993	C	N1-C2-O2	5.12	121.97	118.90
41	A3	183	G	C6-N1-C2	-5.11	122.03	125.10
76	k3	201	LEU	C-N-CA	5.11	134.48	121.70
41	A3	756	C	C5-C6-N1	5.11	123.55	121.00
41	A3	1535	U	N3-C2-O2	-5.11	118.63	122.20
38	A2	680	C	C6-N1-C2	-5.10	118.26	120.30
38	A2	926	G	C4-N9-C1'	5.10	133.13	126.50
41	A3	129	C	N1-C2-O2	-5.10	115.84	118.90
36	21	32	C	C6-N1-C2	-5.10	118.26	120.30
38	A2	4291	G	C4-N9-C1'	5.10	133.13	126.50
38	A2	1483	C	C2-N1-C1'	5.10	124.41	118.80
38	A2	2036	C	C6-N1-C2	-5.10	118.26	120.30
38	A2	1177	U	N1-C2-O2	5.10	126.37	122.80
38	A2	1644	C	C5-C6-N1	5.10	123.55	121.00
38	A2	4488	C	N3-C2-O2	-5.10	118.33	121.90
41	A3	465	A	OP2-P-O3'	5.10	116.41	105.20
41	A3	1303	C	C6-N1-C2	-5.10	118.26	120.30
31	e1	24	TYR	CB-CG-CD2	5.09	124.06	121.00
38	A2	3919	C	C6-N1-C2	-5.09	118.26	120.30
40	C2	123	U	N3-C2-O2	-5.09	118.64	122.20
41	A3	973	C	N3-C2-O2	-5.09	118.34	121.90
38	A2	3969	G	N1-C6-O6	5.09	122.95	119.90
38	A2	1079	C	C6-N1-C2	-5.09	118.27	120.30
41	A3	1750	C	C2-N1-C1'	5.09	124.40	118.80
38	A2	1247	C	N1-C2-O2	5.08	121.95	118.90
38	A2	1772	C	C6-N1-C2	-5.08	118.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A2	2556	A	O4'-C1'-N9	5.08	112.27	108.20
66	Z3	44	LEU	CA-CB-CG	5.08	126.99	115.30
38	A2	2670	C	N1-C2-O2	5.08	121.95	118.90
41	A3	142	C	N3-C2-O2	-5.08	118.34	121.90
41	A3	402	C	C5-C6-N1	5.08	123.54	121.00
38	A2	4940	C	C6-N1-C1'	-5.08	114.71	120.80
41	A3	695	C	C6-N1-C2	-5.08	118.27	120.30
38	A2	4884	C	C2-N1-C1'	5.07	124.38	118.80
41	A3	656	G	N9-C4-C5	-5.07	103.37	105.40
38	A2	275	C	P-O3'-C3'	5.07	125.78	119.70
38	A2	1612	G	N9-C4-C5	-5.07	103.37	105.40
41	A3	407	G	N3-C4-N9	5.07	129.04	126.00
41	A3	1556	A	N3-C4-C5	-5.07	123.25	126.80
38	A2	1632	A	C4-N9-C1'	5.07	135.42	126.30
38	A2	3716	U	N3-C2-O2	-5.07	118.65	122.20
38	A2	3883	G	C2'-C3'-O3'	5.07	121.81	113.70
38	A2	2048	U	N3-C2-O2	-5.06	118.66	122.20
58	R3	93	VAL	CA-CB-CG2	-5.06	103.31	110.90
38	A2	4185	C	N3-C2-O2	-5.06	118.36	121.90
38	A2	4931	G	O4'-C1'-N9	5.06	112.25	108.20
41	A3	130	G	N3-C4-N9	5.06	129.04	126.00
38	A2	4108	G	N3-C2-N2	-5.06	116.36	119.90
38	A2	2853	A	C4-N9-C1'	5.06	135.40	126.30
41	A3	340	C	N1-C2-O2	5.05	121.93	118.90
5	E1	106	LEU	CA-CB-CG	5.05	126.92	115.30
12	L1	77	LYS	CD-CE-NZ	5.05	123.32	111.70
38	A2	1731	C	C6-N1-C2	-5.05	118.28	120.30
84	s3	64	ARG	CB-CG-CD	5.05	124.73	111.60
38	A2	1502	G	N3-C2-N2	-5.05	116.37	119.90
38	A2	1502	G	N3-C4-C5	5.05	131.12	128.60
38	A2	4547	C	N1-C2-O2	5.05	121.93	118.90
38	A2	2505	A	P-O3'-C3'	5.04	125.75	119.70
38	A2	3965	G	N9-C4-C5	-5.04	103.38	105.40
41	A3	1556	A	N3-C4-N9	5.04	131.44	127.40
52	L3	2	LEU	CA-CB-CG	5.04	126.90	115.30
38	A2	4589	C	C6-N1-C2	-5.04	118.28	120.30
38	A2	1325	C	C6-N1-C2	-5.04	118.28	120.30
38	A2	2839	A	N7-C8-N9	-5.04	111.28	113.80
41	A3	1852	C	C5-C6-N1	5.04	123.52	121.00
38	A2	1440	U	P-O3'-C3'	5.04	125.74	119.70
41	A3	627	U	OP2-P-O3'	5.03	116.28	105.20
41	A3	1240	A	O5'-P-OP1	-5.03	101.17	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	T3	39	ARG	NE-CZ-NH1	5.03	122.81	120.30
38	A2	4072	C	C6-N1-C2	-5.03	118.29	120.30
38	A2	978	G	N1-C2-N3	5.03	126.92	123.90
38	A2	2037	C	C6-N1-C2	-5.03	118.29	120.30
38	A2	4468	U	C2-N1-C1'	5.03	123.73	117.70
42	B3	177	MET	CA-CB-CG	5.03	121.85	113.30
38	A2	1735	U	N3-C2-O2	-5.03	118.68	122.20
41	A3	1230	C	C5-C6-N1	5.03	123.51	121.00
38	A2	4289	C	O4'-C1'-N1	5.02	112.22	108.20
38	A2	4180	U	C2-N1-C1'	5.02	123.73	117.70
38	A2	4700	C	C6-N1-C2	-5.02	118.29	120.30
41	A3	1237	C	C5-C6-N1	5.02	123.51	121.00
39	B2	43	U	C2-N1-C1'	5.02	123.72	117.70
40	C2	127	U	C5-C6-N1	5.02	125.21	122.70
41	A3	898	U	C6-N1-C1'	-5.02	114.18	121.20
38	A2	365	U	C2-N1-C1'	5.02	123.72	117.70
38	A2	2365	U	N1-C2-O2	5.01	126.31	122.80
38	A2	2535	C	C6-N1-C2	-5.01	118.29	120.30
41	A3	18	C	C5-C6-N1	5.01	123.51	121.00
41	A3	188	C	C5-C6-N1	5.01	123.51	121.00
84	s3	111	GLU	OE1-CD-OE2	5.01	129.32	123.30
38	A2	644	C	N1-C2-O2	5.01	121.91	118.90
38	A2	3688	U	N3-C2-O2	-5.01	118.69	122.20
19	S1	69	VAL	CG1-CB-CG2	-5.01	102.88	110.90
33	l1	90	LEU	CB-CG-CD2	5.01	119.51	111.00
41	A3	1216	C	C6-N1-C2	-5.01	118.30	120.30
38	A2	967	A	C4-N9-C1'	5.01	135.31	126.30
38	A2	977	C	C5-C6-N1	5.01	123.50	121.00
41	A3	1304	U	C2-N1-C1'	5.01	123.71	117.70
35	n1	219	PHE	CB-CG-CD1	-5.00	117.30	120.80
38	A2	1410	C	N1-C2-O2	5.00	121.90	118.90
38	A2	2495	C	C5-C6-N1	5.00	123.50	121.00
41	A3	151	C	N1-C2-O2	5.00	121.90	118.90
38	A2	978	G	N3-C2-N2	5.00	123.40	119.90
38	A2	2790	A	C4-N9-C1'	5.00	135.30	126.30
41	A3	1130	G	C8-N9-C1'	-5.00	120.50	127.00

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A1	108	ARG	Sidechain

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Mol	Chain	Res	Type	Group
42	B3	42	LYS	Peptide
44	D3	121	ARG	Sidechain
44	D3	268	GLU	Sidechain
12	L1	74	TYR	Sidechain
52	L3	3	MET	Mainchain
52	L3	44	HIS	Peptide
14	N1	6	ARG	Sidechain
17	Q1	95	ASP	Peptide
19	S1	106	TYR	Peptide
61	U3	101	ARG	Sidechain
65	Y3	61	GLN	Peptide
76	k3	258	HIS	Peptide
33	l1	27	LYS	Peptide
33	l1	28	PHE	Peptide
77	l3	100	ARG	Sidechain
77	l3	323	ARG	Sidechain
77	l3	339	THR	Peptide
82	q3	35	ARG	Sidechain
84	s3	64	ARG	Sidechain
85	t3	129	ARG	Sidechain
85	t3	42	ARG	Sidechain
85	t3	63	THR	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	
1	A1	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
2	B1	197/199 (99%)	191 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C1	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
4	D1	185/187 (99%)	177 (96%)	8 (4%)	0	100	100
5	E1	178/180 (99%)	174 (98%)	4 (2%)	0	100	100
6	F1	174/176 (99%)	164 (94%)	10 (6%)	0	100	100
7	G1	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
8	H1	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
9	I1	137/139 (99%)	134 (98%)	3 (2%)	0	100	100
10	J1	102/106 (96%)	101 (99%)	1 (1%)	0	100	100
11	K1	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
12	L1	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
13	M1	133/135 (98%)	127 (96%)	6 (4%)	0	100	100
14	N1	145/147 (99%)	136 (94%)	9 (6%)	0	100	100
15	O1	100/116 (86%)	98 (98%)	2 (2%)	0	100	100
16	P1	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
17	Q1	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
18	R1	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
19	S1	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
20	T1	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
21	U1	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
22	V1	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
23	W1	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
24	X1	67/69 (97%)	63 (94%)	4 (6%)	0	100	100
25	Y1	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
26	Z1	50/52 (96%)	50 (100%)	0	0	100	100
27	a1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
28	b1	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
29	c1	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
30	d1	122/124 (98%)	119 (98%)	3 (2%)	0	100	100
31	e1	194/196 (99%)	176 (91%)	18 (9%)	0	100	100
32	f1	151/153 (99%)	134 (89%)	17 (11%)	0	100	100
33	l1	204/206 (99%)	173 (85%)	30 (15%)	1 (0%)	29	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	n1	234/236 (99%)	229 (98%)	5 (2%)	0	100	100
37	11	3/5 (60%)	1 (33%)	2 (67%)	0	100	100
42	B3	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
43	C3	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
44	D3	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
45	E3	226/228 (99%)	216 (96%)	10 (4%)	0	100	100
46	F3	260/262 (99%)	249 (96%)	11 (4%)	0	100	100
47	G3	181/191 (95%)	173 (96%)	8 (4%)	0	100	100
48	H3	235/237 (99%)	226 (96%)	9 (4%)	0	100	100
49	I3	181/189 (96%)	174 (96%)	7 (4%)	0	100	100
50	J3	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
51	K3	183/185 (99%)	180 (98%)	3 (2%)	0	100	100
52	L3	94/96 (98%)	83 (88%)	9 (10%)	2 (2%)	7	30
53	M3	139/151 (92%)	129 (93%)	10 (7%)	0	100	100
54	N3	115/117 (98%)	102 (89%)	13 (11%)	0	100	100
55	O3	147/149 (99%)	144 (98%)	3 (2%)	0	100	100
56	P3	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
57	Q3	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	54
58	R3	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
59	S3	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
60	T3	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
61	U3	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
62	V3	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
63	W3	81/83 (98%)	81 (100%)	0	0	100	100
64	X3	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
65	Y3	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	22	57
66	Z3	122/124 (98%)	119 (98%)	3 (2%)	0	100	100
67	a3	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
68	b3	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
69	c3	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
70	d3	60/62 (97%)	58 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	e3	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
72	f3	55/57 (96%)	53 (96%)	2 (4%)	0	100	100
73	g3	66/68 (97%)	59 (89%)	7 (11%)	0	100	100
74	h3	311/313 (99%)	287 (92%)	24 (8%)	0	100	100
75	j3	246/248 (99%)	233 (95%)	13 (5%)	0	100	100
76	k3	392/394 (100%)	373 (95%)	19 (5%)	0	100	100
77	l3	360/362 (99%)	345 (96%)	15 (4%)	0	100	100
78	m3	291/293 (99%)	282 (97%)	9 (3%)	0	100	100
79	n3	208/251 (83%)	199 (96%)	9 (4%)	0	100	100
80	o3	223/225 (99%)	215 (96%)	8 (4%)	0	100	100
81	p3	229/240 (95%)	221 (96%)	8 (4%)	0	100	100
82	q3	188/190 (99%)	179 (95%)	9 (5%)	0	100	100
83	r3	201/213 (94%)	195 (97%)	6 (3%)	0	100	100
84	s3	168/170 (99%)	168 (100%)	0	0	100	100
85	t3	208/210 (99%)	197 (95%)	10 (5%)	1 (0%)	29	64
86	u3	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
All	All	11979/12239 (98%)	11459 (96%)	514 (4%)	6 (0%)	54	83

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	l1	57	SER
52	L3	45	VAL
52	L3	46	MET
57	Q3	18	ARG
85	t3	64	VAL
65	Y3	62	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	171/171 (100%)	171 (100%)	0	100	100
2	B1	171/171 (100%)	171 (100%)	0	100	100
3	C1	134/134 (100%)	134 (100%)	0	100	100
4	D1	164/164 (100%)	164 (100%)	0	100	100
5	E1	159/159 (100%)	159 (100%)	0	100	100
6	F1	157/157 (100%)	157 (100%)	0	100	100
7	G1	139/139 (100%)	138 (99%)	1 (1%)	84	93
8	H1	89/89 (100%)	89 (100%)	0	100	100
9	I1	106/106 (100%)	105 (99%)	1 (1%)	78	91
10	J1	86/86 (100%)	86 (100%)	0	100	100
11	K1	106/106 (100%)	106 (100%)	0	100	100
12	L1	124/124 (100%)	124 (100%)	0	100	100
13	M1	117/117 (100%)	117 (100%)	0	100	100
14	N1	119/119 (100%)	118 (99%)	1 (1%)	81	92
15	O1	84/95 (88%)	82 (98%)	2 (2%)	49	76
16	P1	84/84 (100%)	84 (100%)	0	100	100
17	Q1	98/98 (100%)	98 (100%)	0	100	100
18	R1	114/114 (100%)	114 (100%)	0	100	100
19	S1	88/88 (100%)	88 (100%)	0	100	100
20	T1	98/98 (100%)	97 (99%)	1 (1%)	76	90
21	U1	109/109 (100%)	109 (100%)	0	100	100
22	V1	86/86 (100%)	86 (100%)	0	100	100
23	W1	73/73 (100%)	73 (100%)	0	100	100
24	X1	64/64 (100%)	64 (100%)	0	100	100
25	Y1	47/47 (100%)	47 (100%)	0	100	100
26	Z1	48/48 (100%)	47 (98%)	1 (2%)	53	79
27	a1	24/24 (100%)	24 (100%)	0	100	100
28	b1	92/92 (100%)	92 (100%)	0	100	100
29	c1	74/74 (100%)	73 (99%)	1 (1%)	67	86
30	d1	108/108 (100%)	108 (100%)	0	100	100
31	e1	164/164 (100%)	163 (99%)	1 (1%)	86	94
32	f1	126/126 (100%)	124 (98%)	2 (2%)	62	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
33	l1	186/186 (100%)	183 (98%)	3 (2%)	62 84
35	n1	213/219 (97%)	213 (100%)	0	100 100
37	11	4/4 (100%)	4 (100%)	0	100 100
42	B3	180/181 (99%)	180 (100%)	0	100 100
43	C3	194/194 (100%)	194 (100%)	0	100 100
44	D3	187/187 (100%)	186 (100%)	1 (0%)	88 94
45	E3	190/190 (100%)	189 (100%)	1 (0%)	88 94
46	F3	224/224 (100%)	224 (100%)	0	100 100
47	G3	158/161 (98%)	157 (99%)	1 (1%)	86 94
48	H3	207/207 (100%)	206 (100%)	1 (0%)	88 94
49	I3	165/169 (98%)	165 (100%)	0	100 100
50	J3	178/178 (100%)	178 (100%)	0	100 100
51	K3	161/161 (100%)	161 (100%)	0	100 100
52	L3	87/87 (100%)	87 (100%)	0	100 100
53	M3	130/136 (96%)	129 (99%)	1 (1%)	81 92
54	N3	99/99 (100%)	99 (100%)	0	100 100
55	O3	130/130 (100%)	130 (100%)	0	100 100
56	P3	106/106 (100%)	106 (100%)	0	100 100
57	Q3	115/115 (100%)	115 (100%)	0	100 100
58	R3	117/117 (100%)	117 (100%)	0	100 100
59	S3	119/119 (100%)	119 (100%)	0	100 100
60	T3	125/125 (100%)	124 (99%)	1 (1%)	81 92
61	U3	111/111 (100%)	111 (100%)	0	100 100
62	V3	92/92 (100%)	92 (100%)	0	100 100
63	W3	67/67 (100%)	67 (100%)	0	100 100
64	X3	112/112 (100%)	112 (100%)	0	100 100
65	Y3	113/113 (100%)	111 (98%)	2 (2%)	59 82
66	Z3	107/107 (100%)	106 (99%)	1 (1%)	78 91
67	a3	66/66 (100%)	66 (100%)	0	100 100
68	b3	88/88 (100%)	88 (100%)	0	100 100
69	c3	75/75 (100%)	75 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	d3	55/55 (100%)	55 (100%)	0	100	100
71	e3	48/48 (100%)	48 (100%)	0	100	100
72	f3	47/47 (100%)	47 (100%)	0	100	100
73	g3	61/61 (100%)	60 (98%)	1 (2%)	62	84
74	h3	272/272 (100%)	270 (99%)	2 (1%)	84	93
75	j3	190/190 (100%)	188 (99%)	2 (1%)	73	89
76	k3	342/342 (100%)	340 (99%)	2 (1%)	86	94
77	l3	302/302 (100%)	300 (99%)	2 (1%)	84	93
78	m3	247/247 (100%)	247 (100%)	0	100	100
79	n3	190/223 (85%)	190 (100%)	0	100	100
80	o3	196/196 (100%)	196 (100%)	0	100	100
81	p3	200/205 (98%)	200 (100%)	0	100	100
82	q3	169/169 (100%)	169 (100%)	0	100	100
83	r3	175/180 (97%)	174 (99%)	1 (1%)	86	94
84	s3	143/143 (100%)	143 (100%)	0	100	100
85	t3	175/175 (100%)	175 (100%)	0	100	100
86	u3	117/117 (100%)	117 (100%)	0	100	100
All	All	10458/10532 (99%)	10425 (100%)	33 (0%)	92	96

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G1	146	LYS
9	I1	48	ARG
14	N1	93	ASN
15	O1	91	ARG
15	O1	117	ARG
20	T1	54	ARG
26	Z1	80	ARG
29	c1	7	LYS
31	e1	112	ARG
32	f1	57	ARG
32	f1	123	ARG
33	l1	15	ARG
33	l1	25	ARG
33	l1	39	LYS

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Mol	Chain	Res	Type
44	D3	167	ARG
45	E3	76	ARG
47	G3	122	ARG
48	H3	98	ARG
53	M3	69	ARG
60	T3	23	ARG
65	Y3	8	ARG
65	Y3	110	HIS
66	Z3	101	LYS
73	g3	138	ARG
74	h3	57	ARG
74	h3	60	ARG
75	j3	30	ARG
75	j3	163	ARG
76	k3	154	LYS
76	k3	378	ARG
77	l3	100	ARG
77	l3	188	ARG
83	r3	24	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	B1	96	GLN
9	I1	101	ASN
18	R1	124	ASN
33	l1	171	HIS
45	E3	101	GLN
48	H3	65	GLN
49	I3	76	GLN
51	K3	154	GLN
60	T3	73	ASN
74	h3	296	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	m1	2/3 (66%)	0	0
36	21	75/76 (98%)	21 (28%)	0
38	A2	3554/5051 (70%)	731 (20%)	58 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
39	B2	118/119 (99%)	11 (9%)	0
40	C2	149/156 (95%)	28 (18%)	1 (0%)
41	A3	1678/1697 (98%)	350 (20%)	15 (0%)
All	All	5576/7102 (78%)	1141 (20%)	74 (1%)

All (1141) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
36	21	9	G
36	21	10	G
36	21	14	A
36	21	16	U
36	21	17	G
36	21	18	G
36	21	19	U
36	21	20	U
36	21	21	A
36	21	42	A
36	21	46	G
36	21	47	A
36	21	48	C
36	21	49	A
36	21	56	C
36	21	58	C
36	21	59	G
36	21	62	G
36	21	63	G
36	21	67	U
36	21	76	A
38	A2	11	G
38	A2	17	A
38	A2	25	A
38	A2	39	A
38	A2	42	A
38	A2	56	A
38	A2	58	G
38	A2	59	A
38	A2	64	A
38	A2	65	A
38	A2	66	A
38	A2	73	A
38	A2	74	G

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Mol	Chain	Res	Type
38	A2	76	A
38	A2	84	A
38	A2	91	G
38	A2	108	A
38	A2	109	G
38	A2	110	C
38	A2	117	C
38	A2	118	C
38	A2	119	G
38	A2	120	A
38	A2	126	C
38	A2	134	G
38	A2	135	G
38	A2	136	C
38	A2	142	G
38	A2	146	G
38	A2	159	C
38	A2	160	G
38	A2	170	C
38	A2	172	C
38	A2	173	C
38	A2	197	A
38	A2	200	U
38	A2	201	C
38	A2	209	U
38	A2	210	C
38	A2	216	C
38	A2	217	C
38	A2	218	A
38	A2	219	G
38	A2	224	U
38	A2	233	U
38	A2	234	G
38	A2	246	G
38	A2	256	G
38	A2	265	C
38	A2	266	C
38	A2	267	G
38	A2	268	G
38	A2	276	C
38	A2	280	G
38	A2	297	U

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Mol	Chain	Res	Type
38	A2	306	A
38	A2	309	C
38	A2	315	G
38	A2	316	U
38	A2	334	A
38	A2	340	C
38	A2	345	C
38	A2	360	A
38	A2	362	A
38	A2	363	A
38	A2	386	A
38	A2	387	G
38	A2	401	G
38	A2	407	A
38	A2	412	G
38	A2	413	G
38	A2	431	G
38	A2	432	U
38	A2	440	U
38	A2	446	C
38	A2	449	C
38	A2	450	G
38	A2	452	A
38	A2	453	G
38	A2	454	U
38	A2	463	A
38	A2	464	G
38	A2	467	U
38	A2	468	U
38	A2	472	C
38	A2	484	G
38	A2	485	U
38	A2	486	C
38	A2	487	C
38	A2	493	U
38	A2	498	G
38	A2	499	C
38	A2	500	G
38	A2	506	G
38	A2	659	C
38	A2	660	G
38	A2	667	G

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Mol	Chain	Res	Type
38	A2	668	A
38	A2	673	C
38	A2	686	C
38	A2	698	G
38	A2	705	C
38	A2	706	G
38	A2	709	G
38	A2	720	C
38	A2	730	G
38	A2	732	G
38	A2	744	G
38	A2	748	A
38	A2	749	A
38	A2	751	G
38	A2	881	G
38	A2	912	U
38	A2	915	A
38	A2	916	G
38	A2	924	C
38	A2	925	C
38	A2	926	G
38	A2	929	A
38	A2	931	C
38	A2	932	A
38	A2	933	G
38	A2	934	C
38	A2	939	C
38	A2	940	G
38	A2	942	C
38	A2	944	A
38	A2	946	U
38	A2	947	C
38	A2	957	A
38	A2	960	G
38	A2	961	A
38	A2	962	G
38	A2	967	A
38	A2	968	C
38	A2	970	C
38	A2	975	G
38	A2	981	C
38	A2	985	C

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Mol	Chain	Res	Type
38	A2	1070	C
38	A2	1071	G
38	A2	1077	C
38	A2	1078	C
38	A2	1080	C
38	A2	1095	C
38	A2	1177	U
38	A2	1178	C
38	A2	1193	G
38	A2	1196	G
38	A2	1208	C
38	A2	1209	G
38	A2	1210	G
38	A2	1212	C
38	A2	1213	C
38	A2	1214	C
38	A2	1232	G
38	A2	1233	G
38	A2	1234	C
38	A2	1235	C
38	A2	1237	C
38	A2	1247	C
38	A2	1271	G
38	A2	1273	G
38	A2	1282	G
38	A2	1285	G
38	A2	1290	C
38	A2	1291	G
38	A2	1294	G
38	A2	1299	C
38	A2	1300	U
38	A2	1301	A
38	A2	1324	A
38	A2	1335	A
38	A2	1352	A
38	A2	1356	G
38	A2	1357	G
38	A2	1368	G
38	A2	1369	A
38	A2	1375	G
38	A2	1376	C
38	A2	1378	G

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Mol	Chain	Res	Type
38	A2	1379	U
38	A2	1385	A
38	A2	1392	G
38	A2	1395	A
38	A2	1396	A
38	A2	1398	G
38	A2	1407	G
38	A2	1410	C
38	A2	1415	G
38	A2	1420	A
38	A2	1436	C
38	A2	1437	C
38	A2	1438	U
38	A2	1441	C
38	A2	1445	U
38	A2	1446	C
38	A2	1456	C
38	A2	1457	G
38	A2	1476	C
38	A2	1477	C
38	A2	1478	C
38	A2	1482	G
38	A2	1483	C
38	A2	1484	G
38	A2	1493	G
38	A2	1497	A
38	A2	1498	G
38	A2	1502	G
38	A2	1514	U
38	A2	1515	A
38	A2	1523	A
38	A2	1534	A
38	A2	1543	G
38	A2	1547	A
38	A2	1566	C
38	A2	1578	U
38	A2	1588	U
38	A2	1591	U
38	A2	1596	U
38	A2	1602	U
38	A2	1612	G
38	A2	1613	A

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Mol	Chain	Res	Type
38	A2	1624	G
38	A2	1625	G
38	A2	1631	A
38	A2	1633	G
38	A2	1634	A
38	A2	1638	A
38	A2	1640	C
38	A2	1641	G
38	A2	1642	A
38	A2	1654	G
38	A2	1661	C
38	A2	1670	G
38	A2	1676	C
38	A2	1691	G
38	A2	1694	C
38	A2	1696	C
38	A2	1724	G
38	A2	1731	C
38	A2	1734	G
38	A2	1735	U
38	A2	1741	G
38	A2	1742	A
38	A2	1750	G
38	A2	1756	U
38	A2	1760	G
38	A2	1764	G
38	A2	1768	C
38	A2	1772	C
38	A2	1773	U
38	A2	1775	A
38	A2	1776	A
38	A2	1781	U
38	A2	1787	A
38	A2	1803	G
38	A2	1804	A
38	A2	1806	G
38	A2	1815	G
38	A2	1819	G
38	A2	1821	G
38	A2	1828	C
38	A2	1835	G
38	A2	1836	G

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Mol	Chain	Res	Type
38	A2	1837	A
38	A2	1842	G
38	A2	1843	A
38	A2	1855	G
38	A2	1869	G
38	A2	1882	U
38	A2	1892	A
38	A2	1893	C
38	A2	1897	A
38	A2	1898	C
38	A2	1907	A
38	A2	1910	G
38	A2	1912	G
38	A2	1918	U
38	A2	1920	C
38	A2	1921	C
38	A2	1922	G
38	A2	1931	C
38	A2	1932	A
38	A2	1935	C
38	A2	1940	G
38	A2	1947	U
38	A2	1951	G
38	A2	1961	G
38	A2	1962	A
38	A2	1967	A
38	A2	1972	G
38	A2	1974	U
38	A2	1976	G
38	A2	1977	C
38	A2	1978	C
38	A2	1980	U
38	A2	1984	A
38	A2	1985	G
38	A2	1986	U
38	A2	1987	C
38	A2	1991	A
38	A2	1997	U
38	A2	1998	A
38	A2	2001	G
38	A2	2002	A
38	A2	2004	U

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Mol	Chain	Res	Type
38	A2	2007	G
38	A2	2008	U
38	A2	2011	C
38	A2	2021	G
38	A2	2024	G
38	A2	2025	A
38	A2	2026	A
38	A2	2046	G
38	A2	2047	A
38	A2	2048	U
38	A2	2052	G
38	A2	2055	G
38	A2	2056	G
38	A2	2069	A
38	A2	2070	U
38	A2	2071	A
38	A2	2084	U
38	A2	2089	G
38	A2	2090	U
38	A2	2092	G
38	A2	2093	G
38	A2	2094	C
38	A2	2096	G
38	A2	2097	A
38	A2	2098	G
38	A2	2100	G
38	A2	2102	G
38	A2	2104	A
38	A2	2105	A
38	A2	2106	G
38	A2	2107	A
38	A2	2108	G
38	A2	2262	G
38	A2	2263	C
38	A2	2264	G
38	A2	2266	A
38	A2	2270	U
38	A2	2271	A
38	A2	2272	C
38	A2	2277	C
38	A2	2292	C
38	A2	2303	A

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Mol	Chain	Res	Type
38	A2	2304	G
38	A2	2309	G
38	A2	2316	A
38	A2	2319	G
38	A2	2334	G
38	A2	2335	A
38	A2	2336	G
38	A2	2351	G
38	A2	2354	C
38	A2	2363	A
38	A2	2372	U
38	A2	2398	A
38	A2	2405	G
38	A2	2413	C
38	A2	2420	A
38	A2	2425	C
38	A2	2428	U
38	A2	2436	G
38	A2	2437	G
38	A2	2444	C
38	A2	2453	G
38	A2	2456	A
38	A2	2470	U
38	A2	2474	G
38	A2	2478	G
38	A2	2491	C
38	A2	2492	C
38	A2	2493	U
38	A2	2494	C
38	A2	2495	C
38	A2	2496	G
38	A2	2506	G
38	A2	2507	C
38	A2	2508	C
38	A2	2509	G
38	A2	2516	A
38	A2	2517	G
38	A2	2523	C
38	A2	2532	A
38	A2	2533	U
38	A2	2540	A
38	A2	2547	G

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Mol	Chain	Res	Type
38	A2	2549	G
38	A2	2550	G
38	A2	2557	U
38	A2	2567	G
38	A2	2569	G
38	A2	2586	C
38	A2	2589	G
38	A2	2590	A
38	A2	2592	C
38	A2	2614	A
38	A2	2630	C
38	A2	2643	G
38	A2	2650	A
38	A2	2652	G
38	A2	2656	C
38	A2	2665	G
38	A2	2672	C
38	A2	2673	C
38	A2	2679	A
38	A2	2689	G
38	A2	2690	U
38	A2	2697	G
38	A2	2698	A
38	A2	2699	A
38	A2	2708	G
38	A2	2711	U
38	A2	2712	C
38	A2	2713	C
38	A2	2714	G
38	A2	2717	G
38	A2	2724	G
38	A2	2726	U
38	A2	2729	G
38	A2	2738	G
38	A2	2743	U
38	A2	2746	A
38	A2	2747	A
38	A2	2757	G
38	A2	2763	G
38	A2	2766	U
38	A2	2767	A
38	A2	2770	U

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Mol	Chain	Res	Type
38	A2	2772	U
38	A2	2785	U
38	A2	2790	A
38	A2	2791	U
38	A2	2793	U
38	A2	2801	A
38	A2	2809	A
38	A2	2810	A
38	A2	2817	C
38	A2	2818	A
38	A2	2829	U
38	A2	2830	G
38	A2	2831	U
38	A2	2845	G
38	A2	2851	G
38	A2	2858	G
38	A2	2866	G
38	A2	2879	G
38	A2	2887	G
38	A2	3593	C
38	A2	3597	C
38	A2	3599	A
38	A2	3600	C
38	A2	3610	G
38	A2	3611	U
38	A2	3613	C
38	A2	3620	G
38	A2	3621	G
38	A2	3625	A
38	A2	3630	A
38	A2	3631	C
38	A2	3639	U
38	A2	3643	A
38	A2	3657	A
38	A2	3658	A
38	A2	3665	C
38	A2	3668	C
38	A2	3675	U
38	A2	3691	C
38	A2	3707	A
38	A2	3708	U
38	A2	3709	G

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Mol	Chain	Res	Type
38	A2	3724	U
38	A2	3735	G
38	A2	3740	U
38	A2	3741	A
38	A2	3742	A
38	A2	3743	A
38	A2	3748	G
38	A2	3755	A
38	A2	3768	U
38	A2	3769	A
38	A2	3771	G
38	A2	3772	G
38	A2	3779	A
38	A2	3781	U
38	A2	3783	C
38	A2	3797	U
38	A2	3805	C
38	A2	3806	G
38	A2	3807	C
38	A2	3809	U
38	A2	3812	A
38	A2	3814	G
38	A2	3833	U
38	A2	3834	G
38	A2	3835	U
38	A2	3838	C
38	A2	3871	A
38	A2	3872	A
38	A2	3873	C
38	A2	3874	G
38	A2	3884	G
38	A2	3892	G
38	A2	3896	A
38	A2	3900	A
38	A2	3901	A
38	A2	3902	G
38	A2	3903	A
38	A2	3910	U
38	A2	3933	G
38	A2	3934	G
38	A2	3946	G
38	A2	3953	G

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Mol	Chain	Res	Type
38	A2	3954	U
38	A2	3955	A
38	A2	3958	A
38	A2	3959	U
38	A2	3960	A
38	A2	3962	G
38	A2	3963	U
38	A2	3964	G
38	A2	3965	G
38	A2	3966	G
38	A2	3967	A
38	A2	3969	G
38	A2	3970	C
38	A2	4031	C
38	A2	4032	C
38	A2	4033	G
38	A2	4035	C
38	A2	4037	G
38	A2	4042	A
38	A2	4043	U
38	A2	4049	U
38	A2	4050	A
38	A2	4051	C
38	A2	4060	U
38	A2	4067	A
38	A2	4070	G
38	A2	4071	A
38	A2	4078	G
38	A2	4080	G
38	A2	4082	C
38	A2	4090	C
38	A2	4091	G
38	A2	4109	C
38	A2	4111	U
38	A2	4112	C
38	A2	4113	U
38	A2	4115	G
38	A2	4120	A
38	A2	4144	C
38	A2	4148	C
38	A2	4149	U
38	A2	4156	A

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Mol	Chain	Res	Type
38	A2	4157	C
38	A2	4169	G
38	A2	4177	G
38	A2	4189	A
38	A2	4192	C
38	A2	4198	A
38	A2	4211	G
38	A2	4214	G
38	A2	4215	U
38	A2	4218	U
38	A2	4219	A
38	A2	4228	U
38	A2	4235	G
38	A2	4236	G
38	A2	4237	A
38	A2	4240	G
38	A2	4241	A
38	A2	4252	G
38	A2	4254	A
38	A2	4257	A
38	A2	4259	A
38	A2	4267	A
38	A2	4268	A
38	A2	4277	G
38	A2	4278	A
38	A2	4282	U
38	A2	4283	G
38	A2	4290	A
38	A2	4291	G
38	A2	4292	U
38	A2	4294	C
38	A2	4299	A
38	A2	4300	C
38	A2	4312	G
38	A2	4315	G
38	A2	4316	G
38	A2	4318	C
38	A2	4324	G
38	A2	4334	A
38	A2	4335	C
38	A2	4340	U
38	A2	4341	G

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Mol	Chain	Res	Type
38	A2	4359	G
38	A2	4362	A
38	A2	4363	G
38	A2	4364	A
38	A2	4366	A
38	A2	4373	C
38	A2	4377	G
38	A2	4380	A
38	A2	4381	U
38	A2	4398	C
38	A2	4405	U
38	A2	4408	A
38	A2	4412	C
38	A2	4419	G
38	A2	4426	G
38	A2	4434	G
38	A2	4435	A
38	A2	4441	G
38	A2	4450	A
38	A2	4461	G
38	A2	4474	A
38	A2	4481	G
38	A2	4486	U
38	A2	4498	U
38	A2	4499	A
38	A2	4501	G
38	A2	4504	A
38	A2	4505	C
38	A2	4508	G
38	A2	4510	G
38	A2	4517	U
38	A2	4534	A
38	A2	4546	C
38	A2	4556	G
38	A2	4559	G
38	A2	4561	G
38	A2	4567	G
38	A2	4570	A
38	A2	4576	A
38	A2	4612	A
38	A2	4613	U
38	A2	4621	A

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Mol	Chain	Res	Type
38	A2	4622	U
38	A2	4623	G
38	A2	4625	G
38	A2	4638	G
38	A2	4643	U
38	A2	4644	G
38	A2	4656	C
38	A2	4658	A
38	A2	4663	U
38	A2	4673	A
38	A2	4680	G
38	A2	4686	A
38	A2	4694	A
38	A2	4695	U
38	A2	4705	G
38	A2	4706	C
38	A2	4707	G
38	A2	4736	G
38	A2	4737	G
38	A2	4740	G
38	A2	4743	C
38	A2	4745	C
38	A2	4747	G
38	A2	4750	A
38	A2	4751	G
38	A2	4757	C
38	A2	4758	C
38	A2	4759	C
38	A2	4762	G
38	A2	4849	G
38	A2	4852	G
38	A2	4853	C
38	A2	4855	G
38	A2	4857	G
38	A2	4858	A
38	A2	4859	G
38	A2	4864	U
38	A2	4865	C
38	A2	4867	U
38	A2	4869	C
38	A2	4877	C
38	A2	4878	G

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Mol	Chain	Res	Type
38	A2	4889	G
38	A2	4894	G
38	A2	4896	G
38	A2	4901	G
38	A2	4903	C
38	A2	4904	C
38	A2	4908	C
38	A2	4916	A
38	A2	4919	C
38	A2	4920	A
38	A2	4921	C
38	A2	4925	A
38	A2	4926	C
38	A2	4929	U
38	A2	4930	C
38	A2	4931	G
38	A2	4932	U
38	A2	4933	G
38	A2	4937	A
38	A2	4938	A
38	A2	4939	C
38	A2	4940	C
38	A2	4942	G
38	A2	4945	G
38	A2	4948	A
38	A2	4949	A
38	A2	4958	U
38	A2	4967	U
38	A2	4970	U
38	A2	4971	U
38	A2	4972	C
38	A2	4975	G
38	A2	4981	G
38	A2	4996	A
38	A2	4998	A
38	A2	4999	G
38	A2	5013	G
38	A2	5023	G
38	A2	5024	A
38	A2	5029	C
38	A2	5032	C
38	A2	5035	U

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Mol	Chain	Res	Type
38	A2	5036	C
38	A2	5037	G
38	A2	5043	A
38	A2	5044	G
39	B2	7	G
39	B2	25	G
39	B2	42	A
39	B2	53	U
39	B2	54	A
39	B2	63	C
39	B2	64	G
39	B2	97	G
39	B2	100	A
39	B2	102	U
39	B2	110	G
40	C2	2	G
40	C2	3	A
40	C2	34	U
40	C2	35	C
40	C2	39	G
40	C2	59	A
40	C2	60	G
40	C2	62	A
40	C2	63	U
40	C2	75	G
40	C2	87	G
40	C2	94	G
40	C2	103	A
40	C2	105	C
40	C2	109	C
40	C2	110	U
40	C2	111	U
40	C2	114	G
40	C2	121	G
40	C2	123	U
40	C2	124	U
40	C2	125	C
40	C2	126	C
40	C2	127	U
40	C2	128	C
40	C2	147	G
40	C2	151	G

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Mol	Chain	Res	Type
40	C2	153	C
41	A3	3	C
41	A3	14	C
41	A3	17	C
41	A3	25	A
41	A3	33	G
41	A3	42	A
41	A3	44	U
41	A3	45	A
41	A3	46	A
41	A3	56	G
41	A3	58	C
41	A3	67	C
41	A3	68	A
41	A3	72	C
41	A3	73	C
41	A3	74	G
41	A3	75	G
41	A3	77	A
41	A3	79	A
41	A3	99	A
41	A3	103	A
41	A3	110	U
41	A3	111	A
41	A3	113	G
41	A3	114	G
41	A3	115	U
41	A3	116	U
41	A3	124	U
41	A3	126	G
41	A3	130	G
41	A3	143	U
41	A3	146	G
41	A3	147	A
41	A3	155	G
41	A3	157	U
41	A3	162	C
41	A3	168	C
41	A3	171	A
41	A3	173	A
41	A3	180	G
41	A3	182	C

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Mol	Chain	Res	Type
41	A3	183	G
41	A3	184	G
41	A3	186	C
41	A3	188	C
41	A3	191	A
41	A3	192	C
41	A3	202	G
41	A3	206	G
41	A3	294	U
41	A3	302	A
41	A3	307	G
41	A3	308	G
41	A3	309	G
41	A3	312	G
41	A3	319	C
41	A3	320	G
41	A3	347	G
41	A3	351	G
41	A3	356	C
41	A3	362	C
41	A3	364	A
41	A3	368	U
41	A3	369	C
41	A3	370	G
41	A3	381	C
41	A3	383	G
41	A3	385	G
41	A3	386	C
41	A3	396	U
41	A3	398	A
41	A3	400	C
41	A3	407	G
41	A3	408	A
41	A3	409	C
41	A3	418	A
41	A3	420	G
41	A3	428	U
41	A3	438	G
41	A3	441	C
41	A3	447	A
41	A3	448	A
41	A3	450	C

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Mol	Chain	Res	Type
41	A3	455	A
41	A3	464	A
41	A3	465	A
41	A3	466	G
41	A3	471	G
41	A3	472	C
41	A3	473	A
41	A3	474	G
41	A3	476	A
41	A3	482	G
41	A3	483	C
41	A3	487	U
41	A3	492	C
41	A3	496	C
41	A3	516	A
41	A3	517	C
41	A3	531	A
41	A3	532	C
41	A3	533	A
41	A3	547	G
41	A3	548	C
41	A3	549	C
41	A3	550	C
41	A3	551	U
41	A3	554	A
41	A3	555	A
41	A3	556	U
41	A3	559	G
41	A3	561	A
41	A3	562	U
41	A3	568	C
41	A3	573	U
41	A3	576	A
41	A3	583	A
41	A3	587	A
41	A3	588	G
41	A3	589	G
41	A3	590	A
41	A3	591	U
41	A3	593	C
41	A3	603	C
41	A3	604	A

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Mol	Chain	Res	Type
41	A3	606	G
41	A3	608	C
41	A3	614	C
41	A3	617	G
41	A3	621	C
41	A3	627	U
41	A3	628	A
41	A3	629	A
41	A3	631	U
41	A3	643	A
41	A3	644	G
41	A3	655	A
41	A3	659	G
41	A3	660	C
41	A3	664	A
41	A3	668	A
41	A3	669	A
41	A3	670	A
41	A3	671	A
41	A3	672	A
41	A3	673	G
41	A3	678	U
41	A3	683	G
41	A3	689	U
41	A3	734	C
41	A3	752	G
41	A3	753	C
41	A3	754	G
41	A3	808	A
41	A3	811	A
41	A3	821	G
41	A3	822	U
41	A3	827	A
41	A3	830	A
41	A3	844	U
41	A3	845	G
41	A3	847	A
41	A3	859	G
41	A3	870	A
41	A3	871	U
41	A3	872	A
41	A3	874	G

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Mol	Chain	Res	Type
41	A3	875	A
41	A3	878	G
41	A3	879	C
41	A3	888	U
41	A3	889	U
41	A3	890	U
41	A3	893	U
41	A3	896	U
41	A3	898	U
41	A3	901	G
41	A3	909	G
41	A3	913	A
41	A3	914	U
41	A3	920	A
41	A3	933	G
41	A3	934	G
41	A3	943	U
41	A3	955	A
41	A3	963	A
41	A3	971	G
41	A3	984	C
41	A3	985	G
41	A3	990	A
41	A3	992	A
41	A3	999	G
41	A3	1002	U
41	A3	1017	U
41	A3	1023	A
41	A3	1050	A
41	A3	1060	A
41	A3	1062	A
41	A3	1078	C
41	A3	1080	A
41	A3	1083	A
41	A3	1085	C
41	A3	1089	G
41	A3	1107	G
41	A3	1115	U
41	A3	1116	C
41	A3	1117	C
41	A3	1118	C
41	A3	1121	G

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Mol	Chain	Res	Type
41	A3	1123	C
41	A3	1133	A
41	A3	1138	C
41	A3	1148	A
41	A3	1150	A
41	A3	1153	C
41	A3	1154	U
41	A3	1155	U
41	A3	1168	G
41	A3	1195	A
41	A3	1203	G
41	A3	1207	G
41	A3	1208	A
41	A3	1212	G
41	A3	1215	C
41	A3	1221	G
41	A3	1224	G
41	A3	1240	A
41	A3	1242	U
41	A3	1248	U
41	A3	1251	A
41	A3	1253	A
41	A3	1256	G
41	A3	1257	G
41	A3	1259	A
41	A3	1274	G
41	A3	1275	G
41	A3	1282	A
41	A3	1284	A
41	A3	1285	G
41	A3	1286	G
41	A3	1292	C
41	A3	1298	G
41	A3	1299	A
41	A3	1300	U
41	A3	1301	A
41	A3	1302	G
41	A3	1303	C
41	A3	1308	U
41	A3	1309	C
41	A3	1311	C
41	A3	1313	A

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Mol	Chain	Res	Type
41	A3	1318	G
41	A3	1333	U
41	A3	1341	C
41	A3	1342	U
41	A3	1348	G
41	A3	1354	G
41	A3	1363	C
41	A3	1371	U
41	A3	1372	U
41	A3	1378	A
41	A3	1382	A
41	A3	1395	C
41	A3	1396	A
41	A3	1397	U
41	A3	1401	A
41	A3	1402	A
41	A3	1404	U
41	A3	1424	G
41	A3	1428	G
41	A3	1429	G
41	A3	1442	U
41	A3	1449	G
41	A3	1452	A
41	A3	1454	A
41	A3	1462	U
41	A3	1463	U
41	A3	1466	G
41	A3	1473	G
41	A3	1476	A
41	A3	1480	A
41	A3	1487	A
41	A3	1489	A
41	A3	1490	G
41	A3	1498	A
41	A3	1509	U
41	A3	1519	U
41	A3	1520	G
41	A3	1521	C
41	A3	1522	A
41	A3	1531	A
41	A3	1533	A
41	A3	1544	C

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Mol	Chain	Res	Type
41	A3	1548	G
41	A3	1552	G
41	A3	1553	C
41	A3	1554	C
41	A3	1555	U
41	A3	1556	A
41	A3	1560	U
41	A3	1570	G
41	A3	1574	C
41	A3	1580	A
41	A3	1585	U
41	A3	1587	G
41	A3	1588	A
41	A3	1597	C
41	A3	1601	A
41	A3	1606	G
41	A3	1621	U
41	A3	1623	A
41	A3	1629	C
41	A3	1637	A
41	A3	1638	G
41	A3	1648	G
41	A3	1654	G
41	A3	1661	A
41	A3	1665	G
41	A3	1671	G
41	A3	1683	C
41	A3	1698	C
41	A3	1699	A
41	A3	1701	C
41	A3	1721	U
41	A3	1722	G
41	A3	1726	G
41	A3	1730	U
41	A3	1744	G
41	A3	1753	C
41	A3	1777	G
41	A3	1783	C
41	A3	1784	G
41	A3	1785	C
41	A3	1787	G
41	A3	1805	G

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Mol	Chain	Res	Type
41	A3	1823	A
41	A3	1825	A
41	A3	1826	G
41	A3	1829	G
41	A3	1831	A
41	A3	1836	G
41	A3	1838	U
41	A3	1849	G
41	A3	1851	A
41	A3	1861	G
41	A3	1862	G
41	A3	1863	A
41	A3	1864	U
41	A3	1865	C
41	A3	1869	A

All (74) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
38	A2	125	C
38	A2	134	G
38	A2	217	C
38	A2	245	C
38	A2	265	C
38	A2	267	G
38	A2	275	C
38	A2	385	A
38	A2	406	C
38	A2	449	C
38	A2	486	C
38	A2	505	G
38	A2	930	G
38	A2	960	G
38	A2	1070	C
38	A2	1209	G
38	A2	1234	C
38	A2	1236	A
38	A2	1289	G
38	A2	1368	G
38	A2	1440	U
38	A2	1445	U
38	A2	1455	G

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Mol	Chain	Res	Type
38	A2	1477	C
38	A2	1633	G
38	A2	1818	G
38	A2	1979	A
38	A2	1983	A
38	A2	2046	G
38	A2	2068	C
38	A2	2089	G
38	A2	2269	C
38	A2	2505	A
38	A2	2642	U
38	A2	2698	A
38	A2	3598	G
38	A2	3620	G
38	A2	3667	G
38	A2	3705	G
38	A2	3871	A
38	A2	3883	G
38	A2	3899	G
38	A2	3954	U
38	A2	3969	G
38	A2	4030	G
38	A2	4059	G
38	A2	4112	C
38	A2	4218	U
38	A2	4340	U
38	A2	4364	A
38	A2	4381	U
38	A2	4434	G
38	A2	4685	U
38	A2	4705	G
38	A2	4866	G
38	A2	4907	U
38	A2	4918	G
38	A2	4929	U
40	C2	124	U
41	A3	24	C
41	A3	110	U
41	A3	465	A
41	A3	532	C
41	A3	553	U
41	A3	561	A

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Mol	Chain	Res	Type
41	A3	627	U
41	A3	688	U
41	A3	752	G
41	A3	870	A
41	A3	874	G
41	A3	1061	U
41	A3	1137	U
41	A3	1395	C
41	A3	1637	A

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 282 ligands modelled in this entry, 282 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
38	A2	27
41	A3	18
10	J1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J1	63:GLN	C	79:GLN	N	38.60
1	A2	1403:C	O3’	1404:G	P	20.34
1	A2	1407:G	O3’	1408:C	P	19.15
1	A2	1408:C	O3’	1409:G	P	17.91
1	A2	1404:G	O3’	1405:G	P	17.70
1	A3	697:G	O3’	729:C	P	17.34
1	A2	4131:C	O3’	4132:G	P	17.24
1	A3	834:C	O3’	841:G	P	17.04
1	A3	1761:U	O3’	1771:G	P	16.73
1	A3	130:G	O3’	141:A	P	16.21
1	A3	756:C	O3’	788:G	P	15.47
1	A3	1417:C	O3’	1423:C	P	14.74
1	A3	323:C	O3’	329:G	P	14.37
1	A2	919:C	O3’	920:C	P	13.26
1	A2	481:G	O3’	482:C	P	10.77
1	A2	920:C	O3’	921:G	P	10.22
1	A2	739:C	O3’	740:C	P	9.43
1	A2	482:C	O3’	483:G	P	8.98
1	A2	480:C	O3’	481:G	P	8.17
1	A3	745:C	O3’	749:U	P	8.08
1	A2	936:G	O3’	937:C	P	7.91
1	A2	973:G	O3’	974:C	P	7.66
1	A2	972:U	O3’	973:G	P	7.59
1	A2	1411:C	O3’	1412:G	P	7.49
1	A2	935:A	O3’	936:G	P	7.31
1	A3	225:G	O3’	287:U	P	7.10
1	A2	971:G	O3’	972:U	P	6.71
1	A3	736:C	O3’	743:U	P	6.58
1	A3	689:U	O3’	690:G	P	6.30
1	A2	922:C	O3’	923:C	P	6.29
1	A2	4058:C	O3’	4059:G	P	6.27
1	A3	322:C	O3’	323:C	P	6.10
1	A2	1956:A	O3’	1957:U	P	5.80
1	A2	738:C	O3’	739:C	P	5.73
1	A3	798:G	O3’	799:U	P	5.24
1	A2	934:C	O3’	935:A	P	5.05
1	A2	740:C	O3’	741:G	P	4.93

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A2	3943:C	O3'	3944:A	P	4.37
1	A3	304:C	O3'	305:U	P	4.25
1	A3	1432:U	O3'	1438:A	P	4.24
1	A2	1957:U	O3'	1958:A	P	4.06
1	A3	902:G	O3'	903:A	P	4.02
1	A2	5002:G	O3'	5003:C	P	3.56
1	A3	886:A	O3'	887:U	P	3.32
1	A2	170:C	O3'	171:U	P	3.25
1	A3	903:A	O3'	904:A	P	3.25

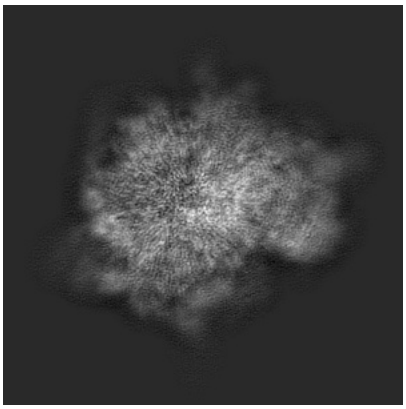
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16052. These allow visual inspection of the internal detail of the map and identification of artifacts.

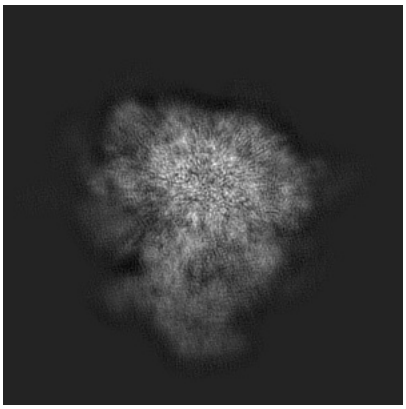
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

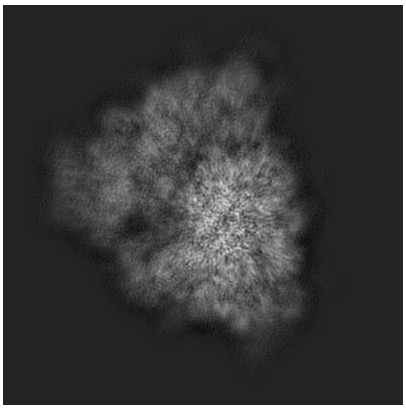
6.1.1 Primary map



X

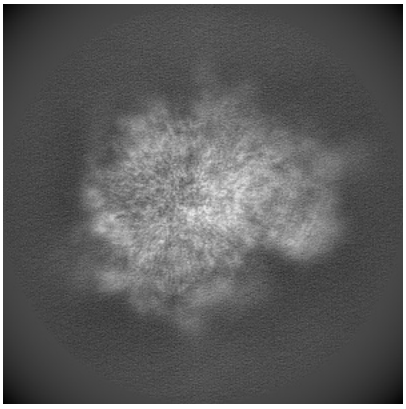


Y

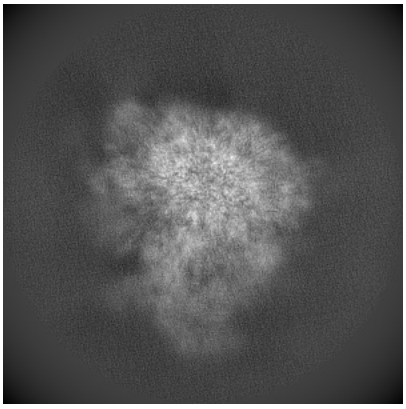


Z

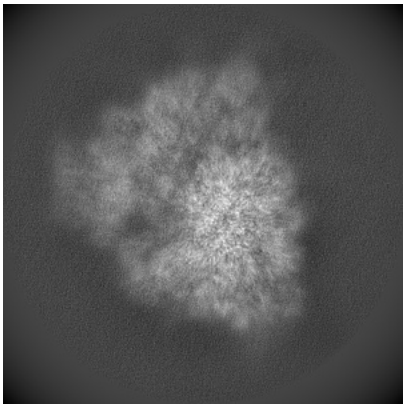
6.1.2 Raw map



X



Y

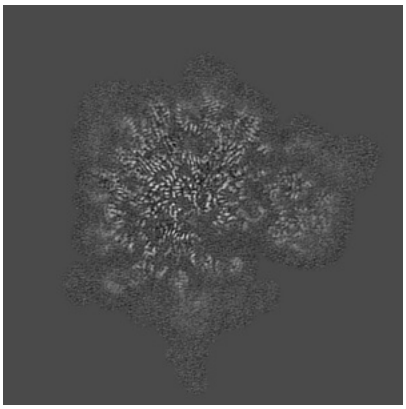


Z

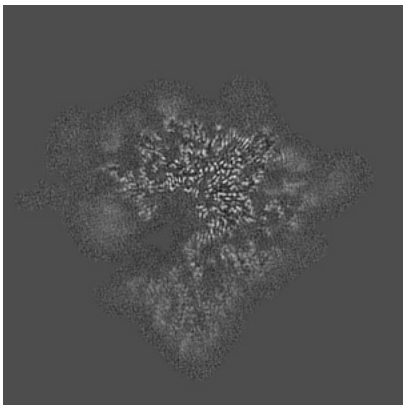
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

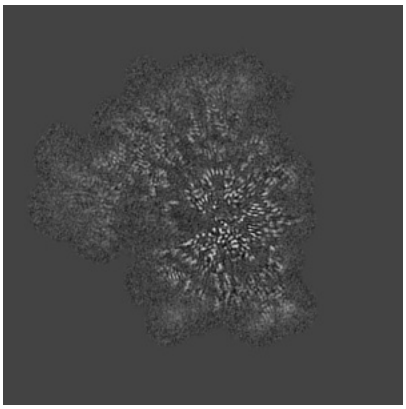
6.2.1 Primary map



X Index: 250

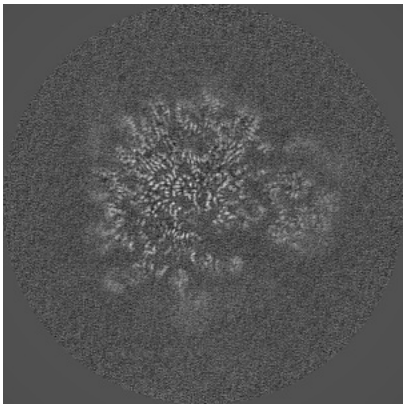


Y Index: 250

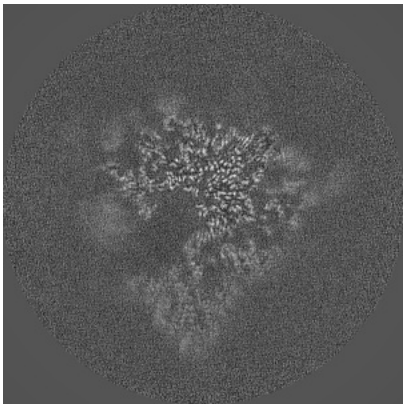


Z Index: 250

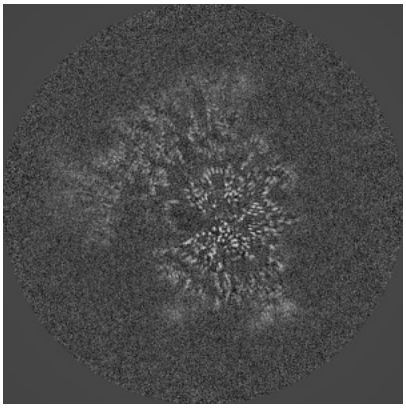
6.2.2 Raw map



X Index: 250



Y Index: 250

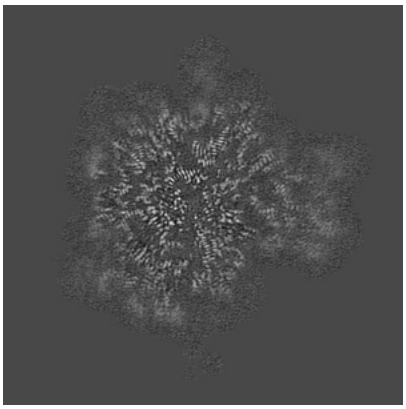


Z Index: 250

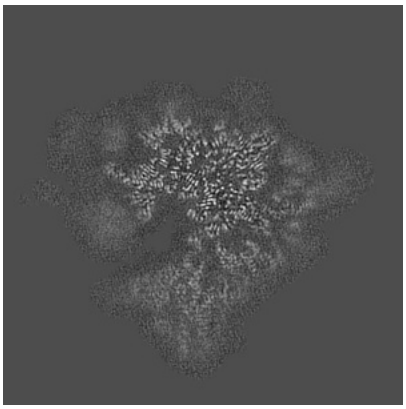
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

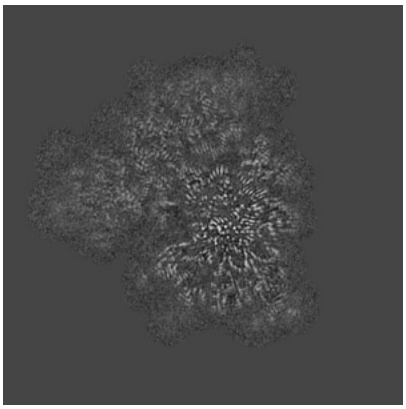
6.3.1 Primary map



X Index: 276

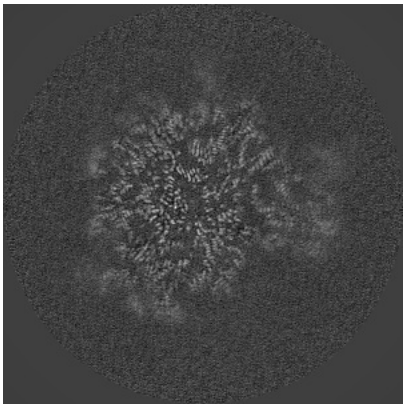


Y Index: 255

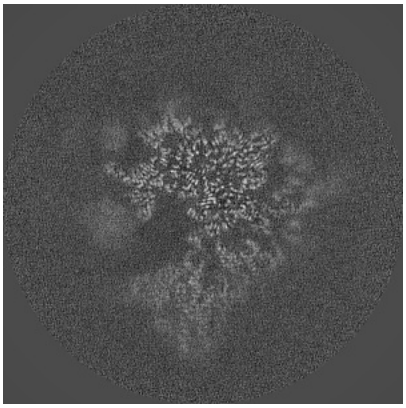


Z Index: 244

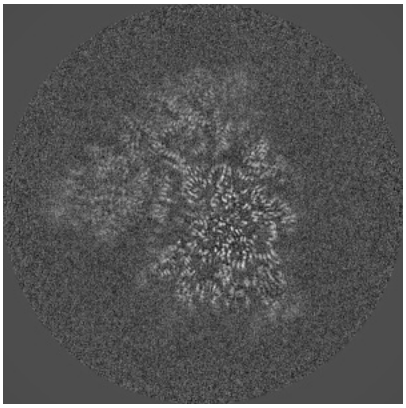
6.3.2 Raw map



X Index: 275



Y Index: 255

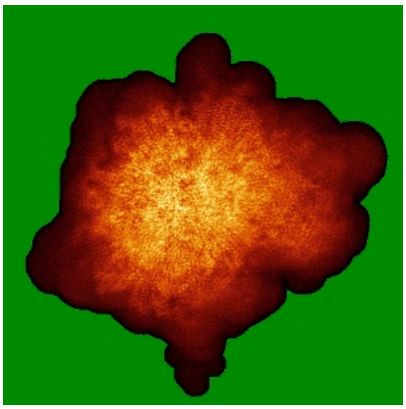


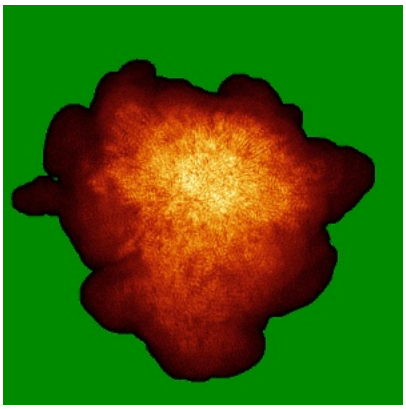
Z Index: 241

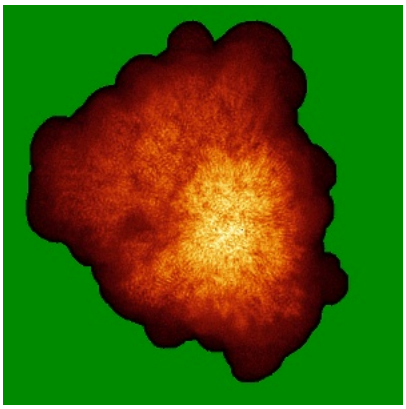
The images above show the largest variance slices of the map in three orthogonal directions.

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

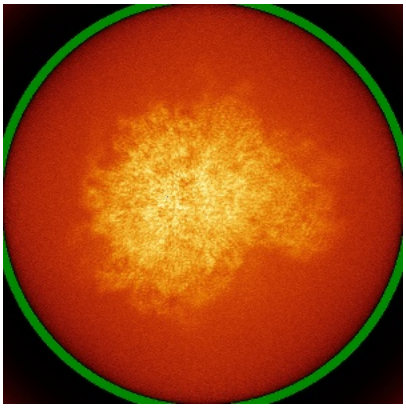
6.4.1 Primary map

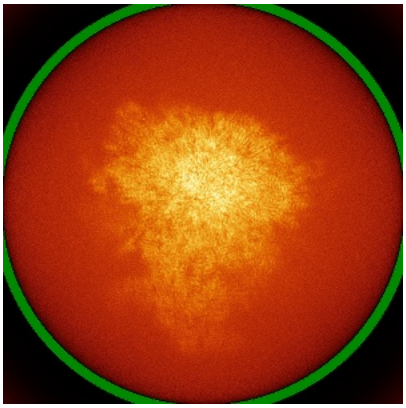

X

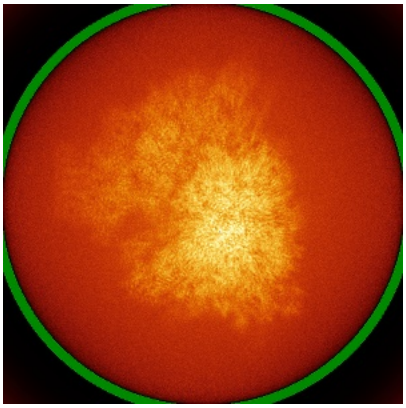

Y


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.

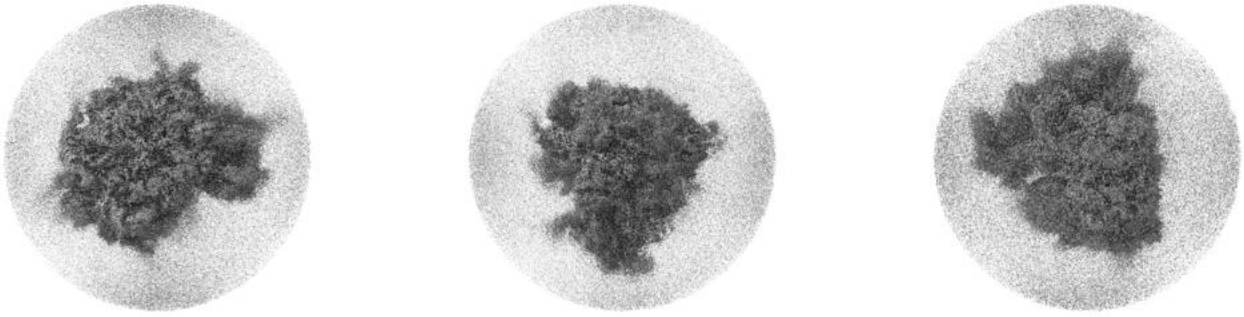
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

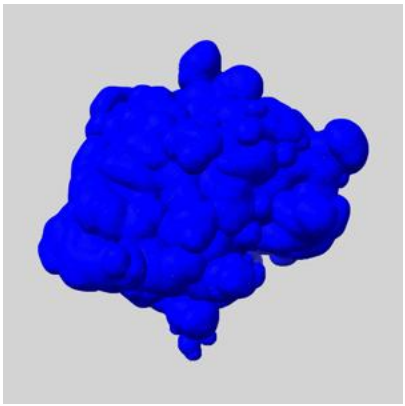
6.6 Mask visualisation (i)

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

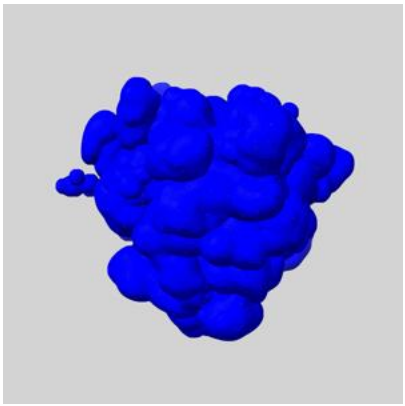
A mask typically either:

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

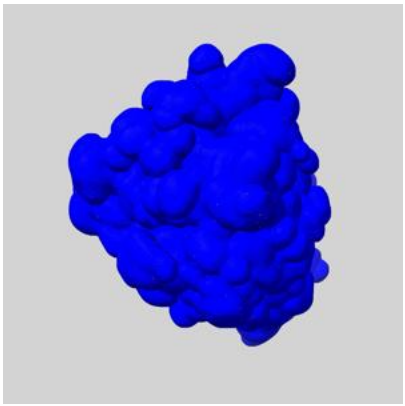
6.6.1 emd_16052_msk_1.map (i)



X



Y

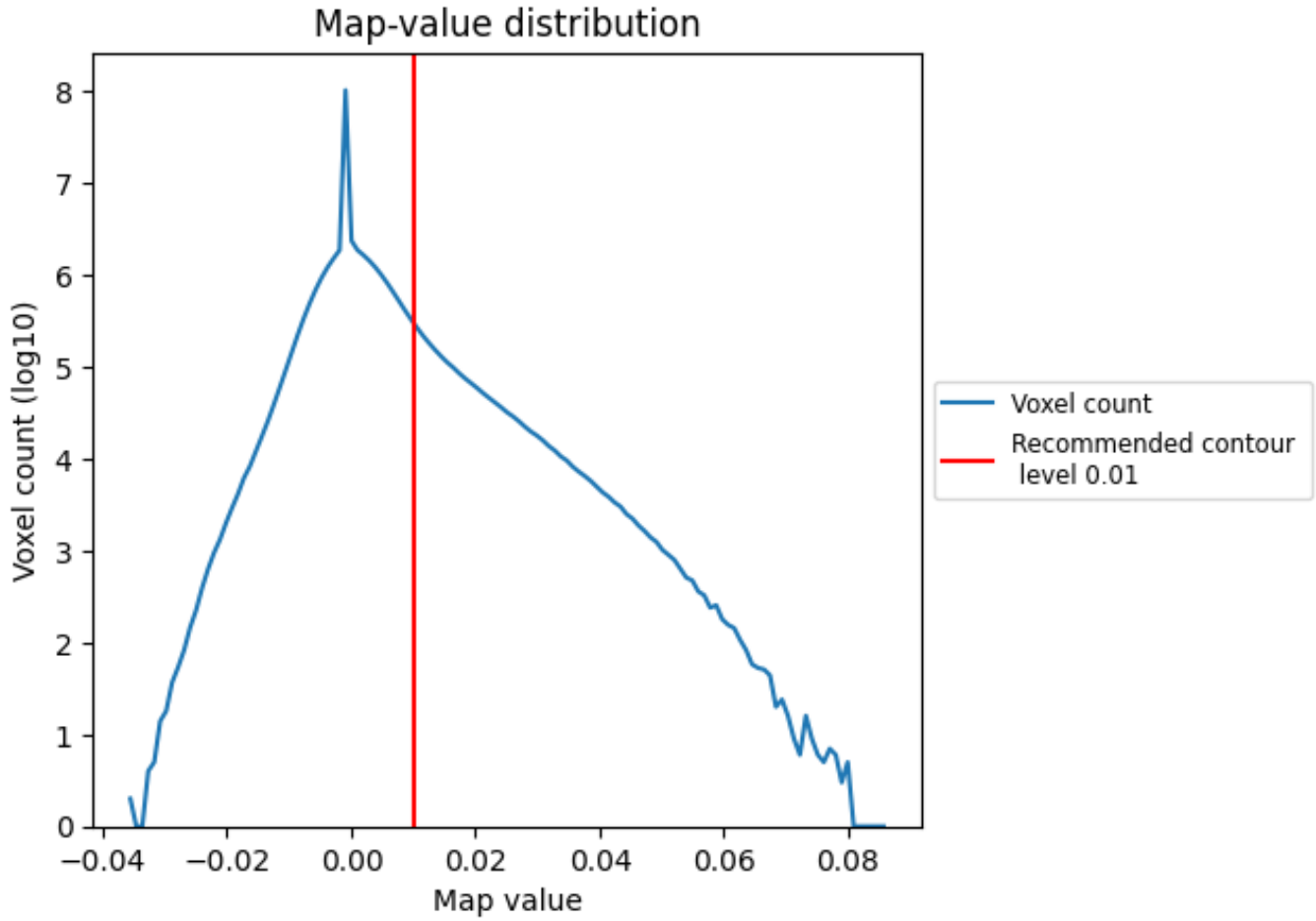


Z

7 Map analysis

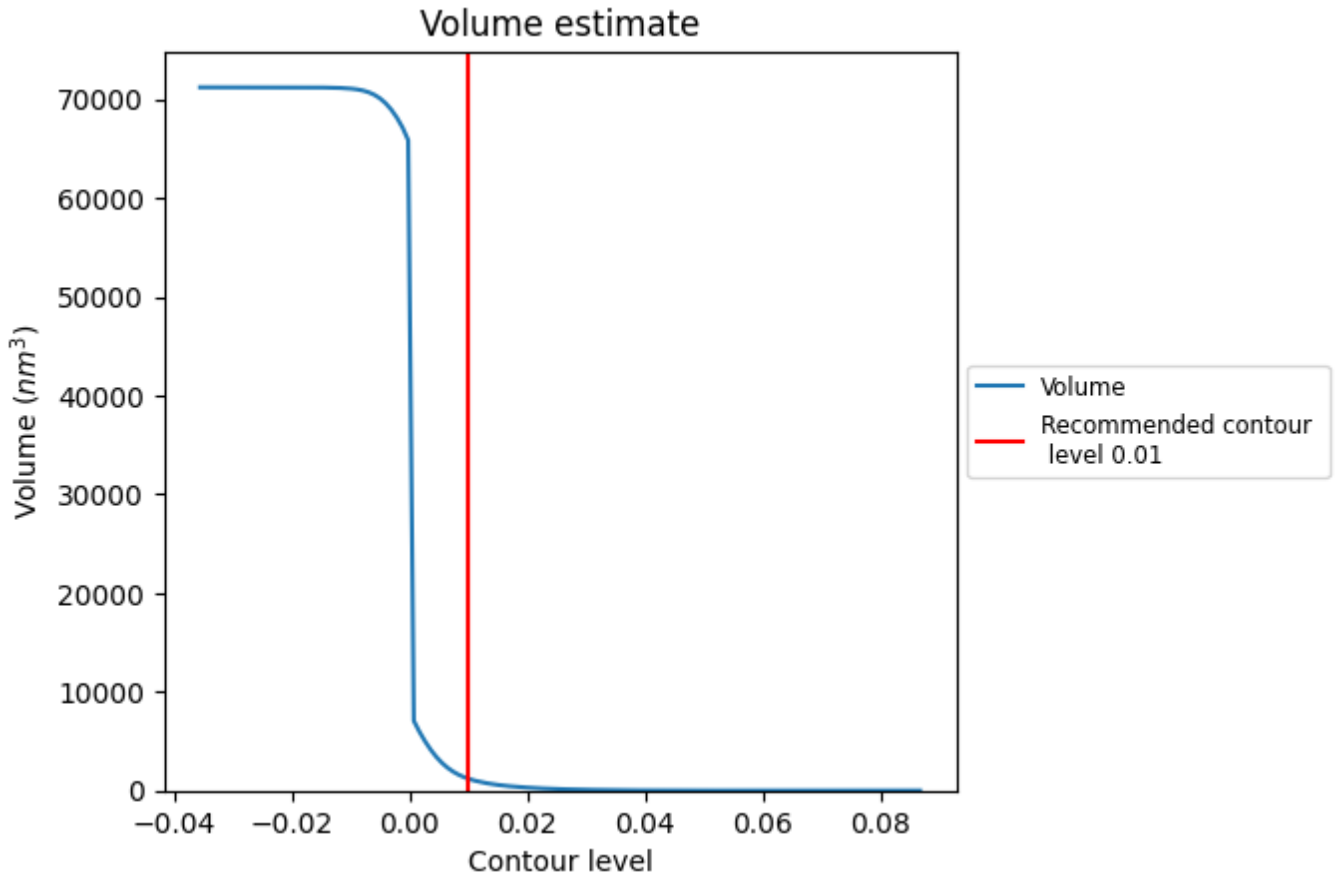
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

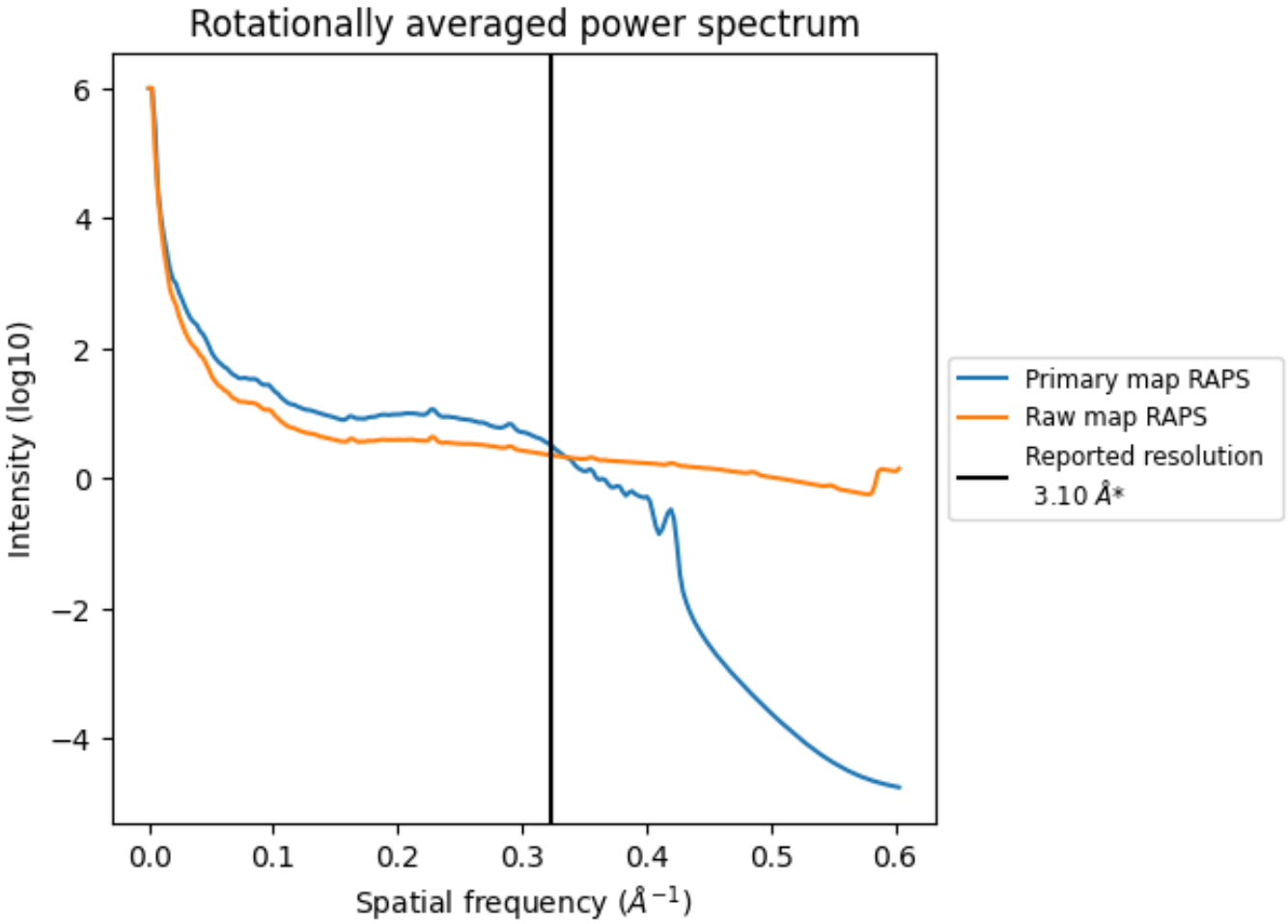
7.2 Volume estimate



The volume at the recommended contour level is 1202 nm^3; this corresponds to an approximate mass of 1086 kDa.

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

7.3 Rotationally averaged power spectrum (i)

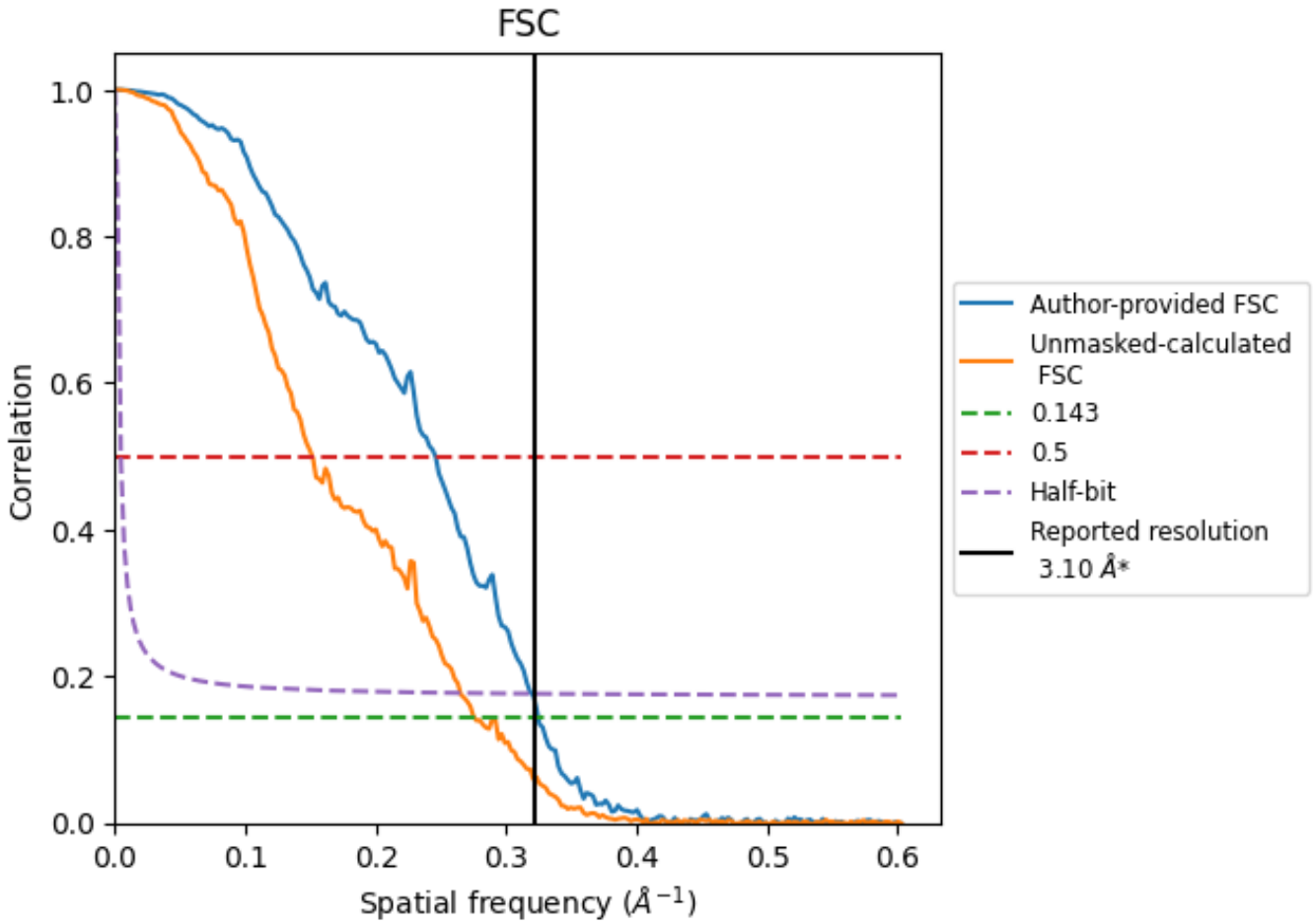


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

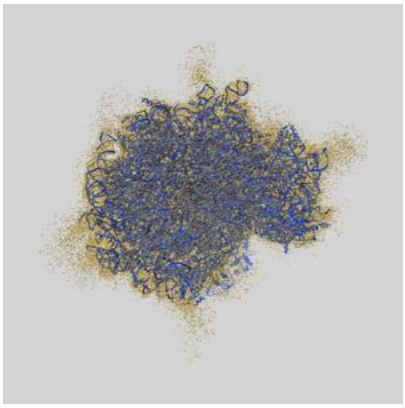
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	4.07	3.13
Unmasked-calculated*	3.62	6.61	3.77

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.62 differs from the reported value 3.1 by more than 10 %

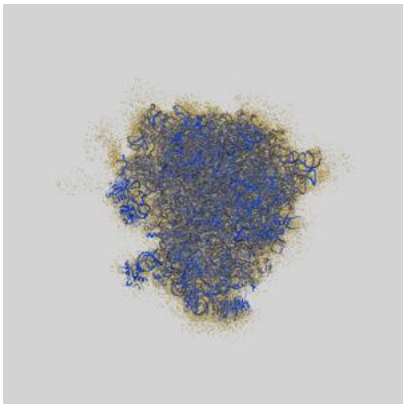
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16052 and PDB model 8BHF. Per-residue inclusion information can be found in section 3 on page 22.

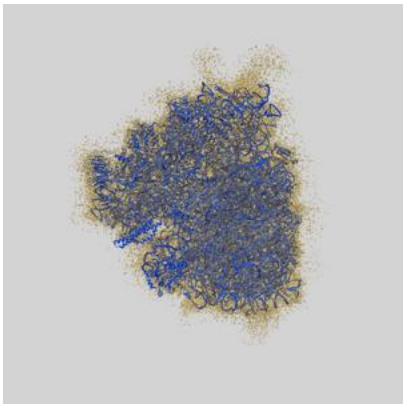
9.1 Map-model overlay



X



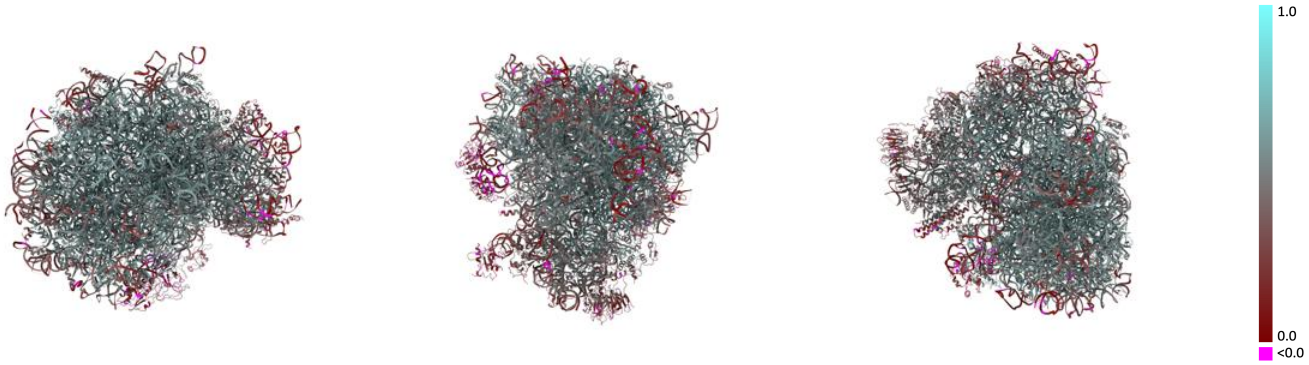
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

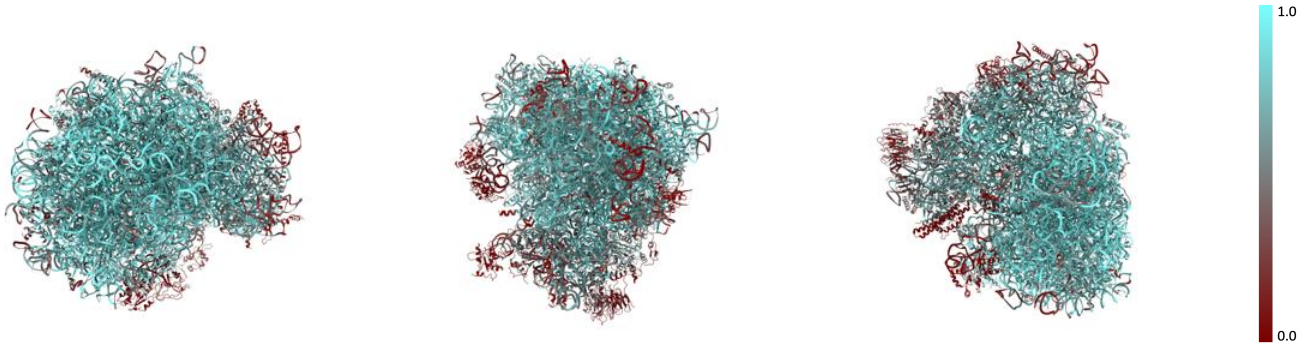
9.2 Q-score mapped to coordinate model



X Y Z

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

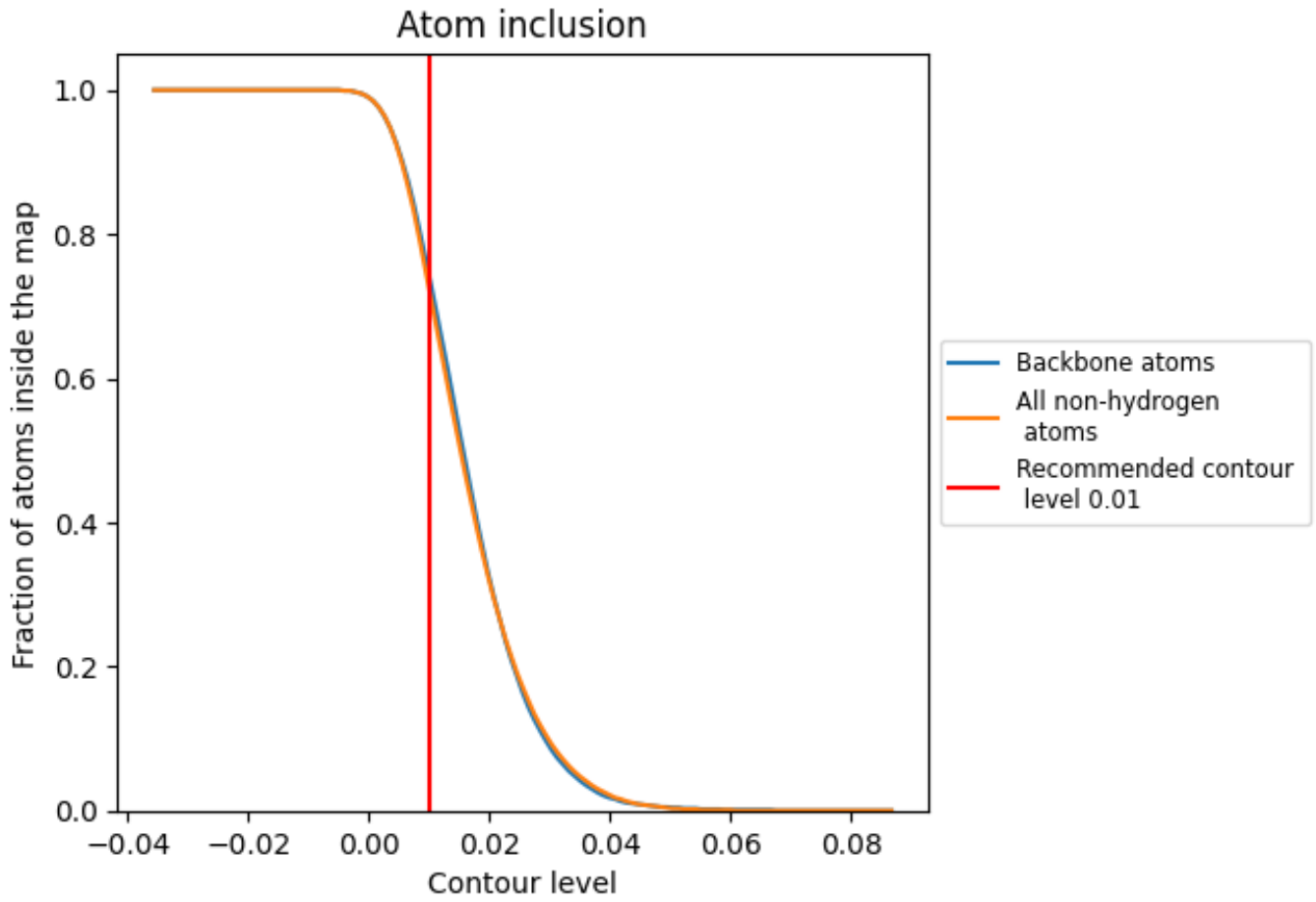
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7250	0.4920
11	0.3240	0.3870
21	0.6740	0.4480
A1	0.8670	0.5820
A2	0.8330	0.5090
A3	0.7330	0.4720
B1	0.8360	0.5710
B2	0.9380	0.5760
B3	0.5220	0.4700
C1	0.8330	0.5680
C2	0.9040	0.5530
C3	0.6090	0.4970
D1	0.8330	0.5700
D3	0.6360	0.5010
E1	0.7340	0.5220
E3	0.3540	0.3690
F1	0.8320	0.5700
F3	0.6040	0.4890
G1	0.7820	0.5450
G3	0.5350	0.4560
H1	0.6550	0.4750
H3	0.4400	0.3870
I1	0.7610	0.5480
I3	0.3260	0.3730
J1	0.5200	0.4220
J3	0.6090	0.5010
K1	0.7810	0.5430
K3	0.6350	0.4830
L1	0.8100	0.5470
L3	0.2720	0.3370
M1	0.7550	0.5370
M3	0.6720	0.5450
N1	0.8700	0.5850
N3	0.0650	0.2000
O1	0.6580	0.5030

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Chain	Atom inclusion	Q-score
O3	0.6690	0.5200
P1	0.7610	0.5420
P3	0.6680	0.5140
Q1	0.7600	0.5370
Q3	0.4030	0.3740
R1	0.8500	0.5750
R3	0.5150	0.4300
S1	0.8470	0.5750
S3	0.3960	0.3910
T1	0.7590	0.5510
T3	0.4570	0.4090
U1	0.7770	0.5460
U3	0.4880	0.4100
V1	0.7510	0.5420
V3	0.3810	0.4100
W1	0.9120	0.5920
W3	0.5390	0.4760
X1	0.6500	0.4800
X3	0.7350	0.5470
Y1	0.7960	0.5440
Y3	0.6650	0.5310
Z1	0.8100	0.5610
Z3	0.5560	0.4400
a1	0.7890	0.5860
a3	0.3960	0.4130
b1	0.7930	0.5690
b3	0.6970	0.5340
c1	0.7630	0.5470
c3	0.5380	0.4480
d1	0.8110	0.5620
d3	0.5060	0.4760
e1	0.0490	0.1620
e3	0.5320	0.4550
f1	0.0550	0.1720
f3	0.4570	0.4340
g3	0.0870	0.2050
h3	0.2280	0.2930
j3	0.8360	0.5790
k3	0.8320	0.5730
l1	0.0220	0.1540
l3	0.8320	0.5660
m1	0.8710	0.5660

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Chain	Atom inclusion	Q-score
m3	0.8030	0.5430
n1	0.1820	0.3090
n3	0.7290	0.5140
o3	0.8040	0.5550
p3	0.6620	0.4980
q3	0.7460	0.5350
r3	0.7860	0.5530
s3	0.7130	0.5150
t3	0.7640	0.5430
u3	0.7940	0.5490