



## Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 01:23 am GMT

PDB ID : 6R6P  
EMDB ID : EMD-4737  
Title : Structure of XBP1u-paused ribosome nascent chain complex (rotated state)  
Authors : Shanmuganathan, V.; Cheng, J.; Berninghausen, O.; Beckmann, R.  
Deposited on : 2019-03-27  
Resolution : 3.10 Å (reported)  
Based on initial model : ?

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

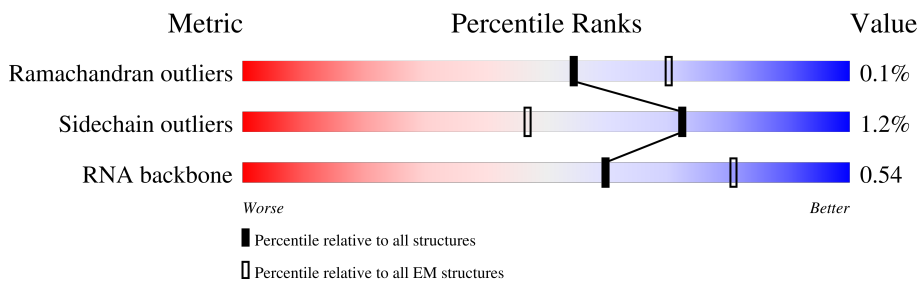
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	5	3662	
2	7	120	
3	8	156	
4	A	244	
5	B	394	
6	C	362	
7	D	292	
8	E	248	

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Mol	Chain	Length	Quality of chain
9	F	225	6% 100%
10	G	241	18% 98%
11	H	190	7% 99%
12	I	213	94%
13	J	169	11% 99%
14	L	210	15% 99%
15	M	138	6% 100%
16	N	203	100%
17	O	199	97%
18	P	153	99%
19	Q	187	100%
20	R	180	17% 98%
21	S	175	99%
22	T	159	8% 99%
23	U	99	15% 99%
24	V	131	99%
25	W	63	5% 98%
26	X	119	7% 99%
27	Y	134	7% 99%
28	Z	135	10% 98%
29	a	147	100%
30	b	75	24% 99%
31	c	94	6% 99%
32	d	107	9% 98%
33	e	128	99%

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Mol	Chain	Length	Quality of chain
34	f	109	5% 98%
35	g	114	7% 98%
36	h	122	6% 99%
37	i	102	11% 99%
38	j	86	• 98%
39	k	69	25% 99%
40	l	50	• 94% 6%
41	m	52	6% 100%
42	n	23	13% 100%
43	o	104	12% 96%
44	p	91	7% 98%
45	r	125	8% 95%
46	s	198	98% 99%
47	t	163	100% 98%
48	1	24	8% 96%
49	2	76	66% 67% 30%
50	3	75	27% 79% 20%
51	K	1698	18% 76% 22%
52	q	217	40% 100%
53	u	213	21% 99%
54	v	221	34% 99%
55	x	262	56% 99%
56	z	237	54% 99%
57	y	189	60% 97%
58	CC	206	39% 99%

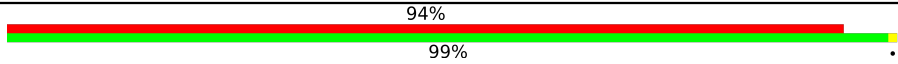

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Mol	Chain	Length	Quality of chain
59	XX	185	53% 98%
60	EE	151	27% 93% 5%
61	QQ	149	28% 99%
62	MM	136	20% 99%
63	UU	142	54% 98%
64	YY	132	70% 100%
65	HH	83	45% 99%
66	TT	129	24% 100%
67	VV	141	8% 99%
68	NN	124	63% 99%
69	ZZ	101	23% 100%
70	JJ	83	41% 99%
71	AA	55	67% 96%
72	DD	228	62% 98%
73	BB	191	44% 97%
74	SS	96	73% 99%
75	RR	117	94% 99%
76	9	120	39% 98%
77	II	144	39% 99%
78	PP	141	50% 99%
79	GG	100	71% 99%
80	OO	75	55% 100%
81	FF	62	61% 98%
82	w	55	29% 100%
83	0	68	85% 99%

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Mol	Chain	Length	Quality of chain
84	6	313	 <p>94%</p> <p>99%</p>
85	4	10	 <p>10%</p> <p>50%</p> <p>50%</p>

## 2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 218067 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	5	3662	78486	34947	14363	25515	3661	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	7	120	2558	1141	456	842	119	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	8	156	3314	1480	585	1094	155	0	0

- Molecule 4 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	244	1868	1171	382	309	6	0	0

- Molecule 5 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	394	3148	2007	591	537	13	0	0

- Molecule 6 is a protein called uL4.

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

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	292	2386	1509	437	426	14	0	0

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E	236	1898	1215	362	318	3	0	0

- Molecule 9 is a protein called uL30.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	175	ALA	THR	conflict	UNP G1SV32
F	185	GLY	ASN	conflict	UNP G1SV32
F	202	ARG	HIS	conflict	UNP G1SV32
F	233	GLU	GLY	conflict	UNP G1SV32

- Molecule 10 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	G	241	1934	1233	371	326	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	191	GLY	CYS	conflict	UNP G1STW0

- Molecule 11 is a protein called uL6.

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



- Molecule 12 is a protein called Ribosomal protein L10 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	I	204	1655	1051	319	272	13	0	0

- Molecule 13 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	J	169	1353	855	252	240	6	0	0

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	L	210	1703	1065	354	280	4	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	47	ALA	-	insertion	UNP G1TPV0
L	48	PRO	-	insertion	UNP G1TPV0
L	49	ARG	-	insertion	UNP G1TPV0
L	50	PRO	-	insertion	UNP G1TPV0
L	51	ALA	-	insertion	UNP G1TPV0
L	52	SER	-	insertion	UNP G1TPV0
L	53	GLY	-	insertion	UNP G1TPV0
L	54	PRO	-	insertion	UNP G1TPV0
L	55	LEU	-	insertion	UNP G1TPV0

- Molecule 15 is a protein called Ribosomal protein L14.

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

- Molecule 16 is a protein called Ribosomal protein L15.

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

- Molecule 17 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	199	Total	C	N	O	S	0	0
			1638	1056	321	256	5		

- Molecule 18 is a protein called uL22.

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

- Molecule 19 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	187	Total	C	N	O	S	0	0
			1506	941	311	249	5		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	6	ARG	LEU	conflict	UNP G1TX70
Q	14	ARG	TRP	conflict	UNP G1TX70
Q	23	ILE	MET	conflict	UNP G1TX70
Q	24	TYR	CYS	conflict	UNP G1TX70
Q	38	ARG	HIS	conflict	UNP G1TX70
Q	57	ASN	LYS	conflict	UNP G1TX70
Q	66	MET	VAL	conflict	UNP G1TX70
Q	74	GLY	ASP	conflict	UNP G1TX70
Q	75	ARG	PRO	conflict	UNP G1TX70
Q	77	GLY	ASN	conflict	UNP G1TX70
Q	106	SER	THR	conflict	UNP G1TX70
Q	110	ARG	HIS	conflict	UNP G1TX70
Q	117	GLY	GLU	conflict	UNP G1TX70
Q	124	ASP	HIS	conflict	UNP G1TX70
Q	134	CYS	ARG	conflict	UNP G1TX70
Q	150	ARG	GLN	conflict	UNP G1TX70
Q	172	ARG	GLY	conflict	UNP G1TX70
Q	184	ARG	TRP	conflict	UNP G1TX70

- Molecule 20 is a protein called eL19.

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

- Molecule 21 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	S	175	1454	925	284	235	10	0	0

- Molecule 22 is a protein called eL21.

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

- Molecule 23 is a protein called Ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	U	99	808	518	141	147	2	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	32	GLY	ARG	conflict	UNP G1TSG1
U	36	ALA	GLU	conflict	UNP G1TSG1
U	39	PHE	SER	conflict	UNP G1TSG1
U	54	GLY	ARG	conflict	UNP G1TSG1
U	60	VAL	ALA	conflict	UNP G1TSG1
U	97	ARG	HIS	conflict	UNP G1TSG1

- Molecule 24 is a protein called uL14.

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

- Molecule 25 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	W	63	528	337	103	85	3	0	0

- Molecule 26 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	X	119	976	624	183	168	1	0	0

- Molecule 27 is a protein called Ribosomal protein L26.

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

- Molecule 28 is a protein called 60S ribosomal protein L27.

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

- Molecule 29 is a protein called uL15.

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

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	b	75	609	378	130	98	3	0	0

- Molecule 31 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	c	94	732	465	130	131	6	0	0

- Molecule 32 is a protein called eL31.

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

- Molecule 33 is a protein called eL32.

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

- Molecule 34 is a protein called eL33.

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

- Molecule 35 is a protein called eL34.

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

- Molecule 36 is a protein called uL29.

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

- Molecule 37 is a protein called 60S ribosomal protein L36.

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

- Molecule 38 is a protein called Ribosomal protein L37.

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

- Molecule 39 is a protein called eL38.

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

- Molecule 40 is a protein called ribosomal protein eL39.

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

- Molecule 41 is a protein called eL40.

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

- Molecule 42 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	23	Total	C	N	O	S	0	0
			222	134	61	25	2		

- Molecule 43 is a protein called eL42.

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

- Molecule 44 is a protein called ribosomal protein eL43.

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

- Molecule 45 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	125	Total	C	N	O	S	0	0
			1001	621	206	168	6		

- Molecule 46 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	198	Total	C	N	O	S	0	0
			1523	969	265	280	9		

- Molecule 47 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	t	163	Total	C	N	O	S	0	0
			1238	773	230	230	5		

- Molecule 48 is a protein called X-box-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	1	24	Total	C	N	O	S	0	0
			204	137	35	30	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	255	ALA	SER	conflict	UNP P17861

- Molecule 49 is a RNA chain called A/P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	2	76	Total	C	N	O	P	0	0
			1614	722	287	530	75		

- Molecule 50 is a RNA chain called P/E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3	75	Total	C	N	O	P	0	0
			1597	714	287	522	74		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	K	1698	Total	C	N	O	P	0	0
			36248	16180	6508	11863	1697		

- Molecule 52 is a protein called uS2.

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

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

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

- Molecule 54 is a protein called uS5.

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

- Molecule 55 is a protein called 40S ribosomal protein S4.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 56 is a protein called 40S ribosomal protein S6.

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

- Molecule 57 is a protein called 40S ribosomal protein S7.

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

- Molecule 58 is a protein called 40S ribosomal protein S8.

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

There is a discrepancy between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
CC	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 59 is a protein called Ribosomal protein S9 (Predicted).

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

- Molecule 60 is a protein called Ribosomal protein S11.

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

- Molecule 61 is a protein called ribosomal protein uS15.

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

- Molecule 62 is a protein called uS11.

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

- Molecule 63 is a protein called Ribosomal protein S16.

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

- Molecule 64 is a protein called eS17.

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

- Molecule 65 is a protein called eS21.

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

- Molecule 66 is a protein called Ribosomal protein S15a.

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

- Molecule 67 is a protein called Ribosomal protein S23.

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

- Molecule 68 is a protein called eS24.

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

- Molecule 69 is a protein called eS26.

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

- Molecule 70 is a protein called 40S ribosomal protein S27.

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

- Molecule 71 is a protein called 40S ribosomal protein S30.

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

- Molecule 72 is a protein called Ribosomal protein S3.

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

- Molecule 73 is a protein called Ribosomal protein S5.

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

- Molecule 74 is a protein called eS10.

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

- Molecule 75 is a protein called 40S ribosomal protein S12.

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

- Molecule 76 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	9	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 77 is a protein called uS13.

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

- Molecule 78 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	PP	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
PP	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 79 is a protein called uS10.

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

- Molecule 80 is a protein called ribosomal protein eS25.

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

- Molecule 81 is a protein called Ribosomal protein S28.

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

- Molecule 82 is a protein called S29.

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

- Molecule 83 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
83	0	68	555	351	103	94	7	0	0

- Molecule 84 is a protein called ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	6	313	2436	1535	424	465	12	0	0

- Molecule 85 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			P
85	4	10	211	95	37	69	10	0	0

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

Mol	Chain	Residues	Atoms		AltConf
86	5	148	Total	Mg	0
			148	148	
86	7	4	Total	Mg	0
			4	4	
86	8	1	Total	Mg	0
			1	1	
86	I	1	Total	Mg	0
			1	1	
86	P	1	Total	Mg	0
			1	1	
86	Q	1	Total	Mg	0
			1	1	
86	V	1	Total	Mg	0
			1	1	
86	e	1	Total	Mg	0
			1	1	
86	g	1	Total	Mg	0
			1	1	

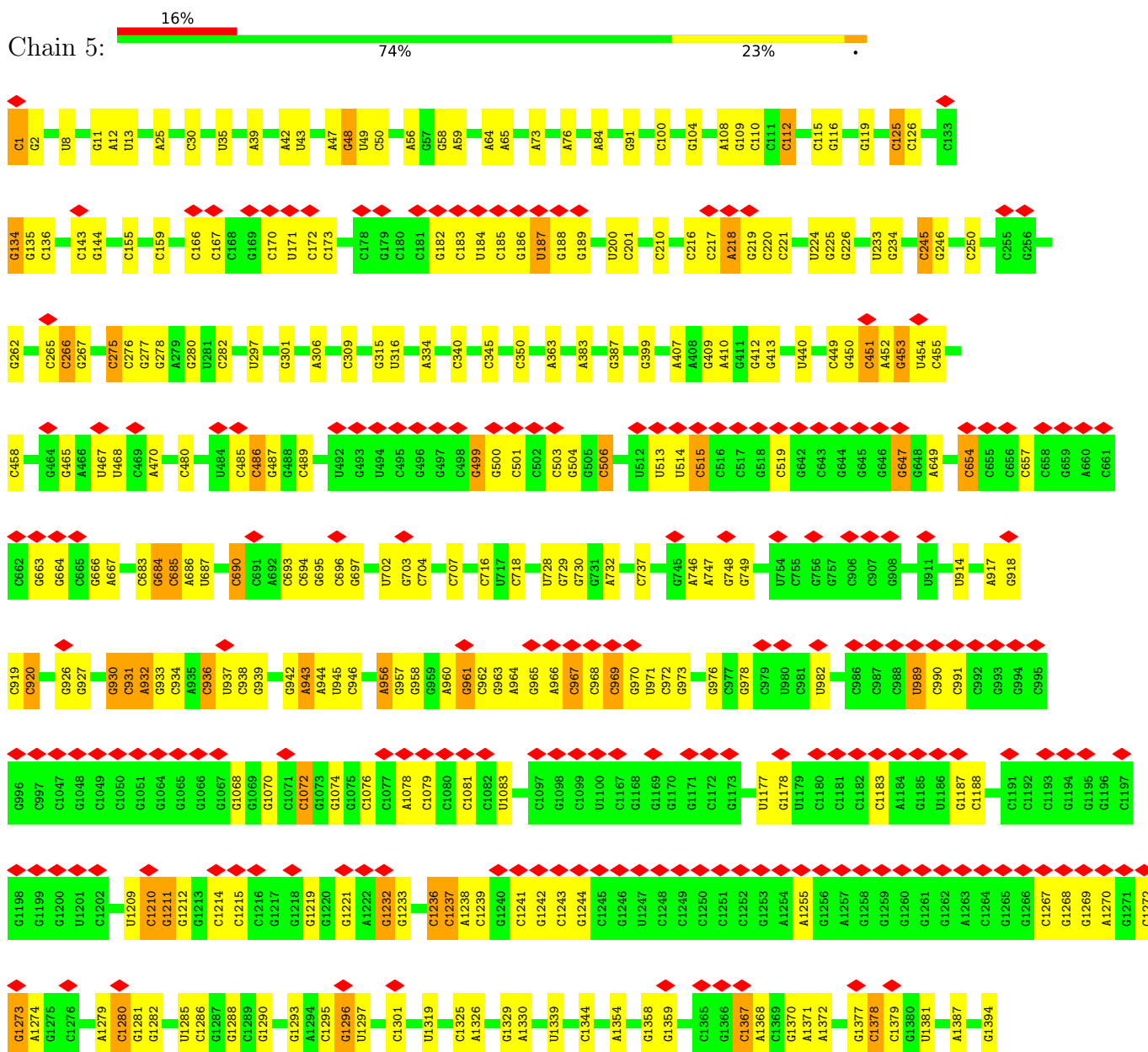
- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
87	g	1	Total	Zn	0
			1	1	
87	j	1	Total	Zn	0
			1	1	
87	m	1	Total	Zn	0
			1	1	
87	o	1	Total	Zn	0
			1	1	
87	p	1	Total	Zn	0
			1	1	

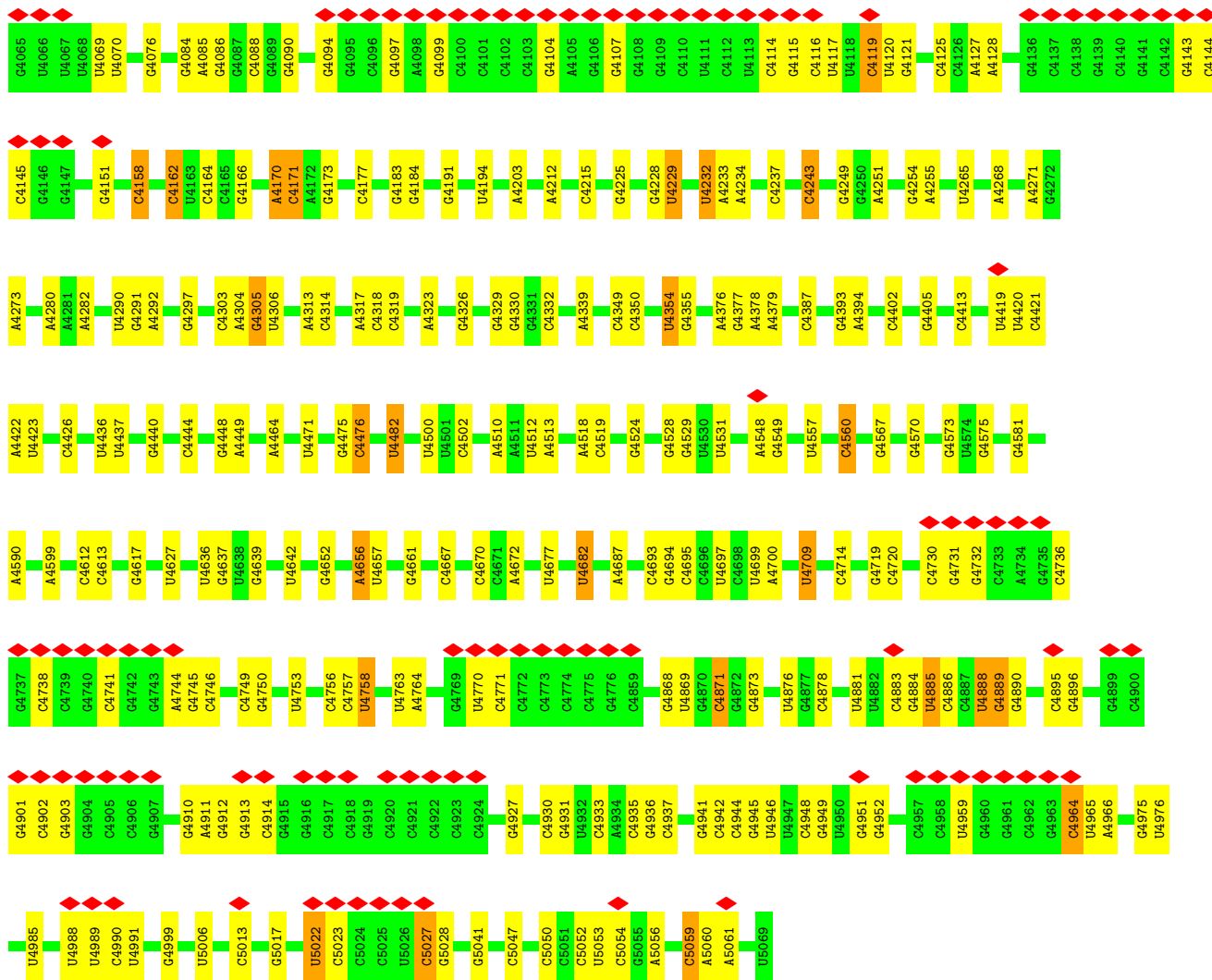
### 3 Residue-property plots

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

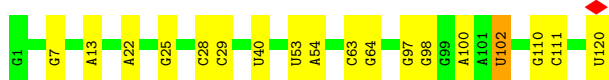
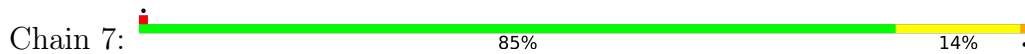
- Molecule 1: 28S ribosomal RNA







• Molecule 2: 5S ribosomal RNA



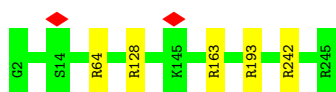
• Molecule 3: 5.8S ribosomal RNA



• Molecule 4: uL2



Chain A:  98%



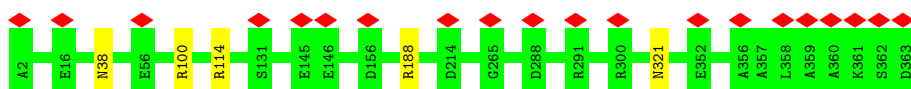
• Molecule 5: uL3

Chain B:  98%



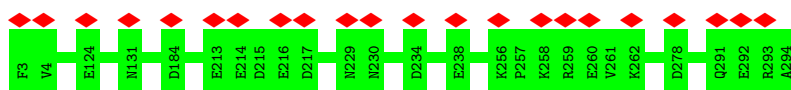
• Molecule 6: uL4

Chain C:  6% 99%

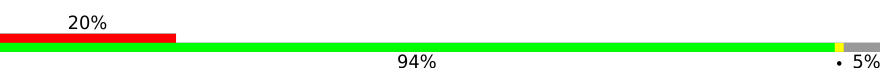


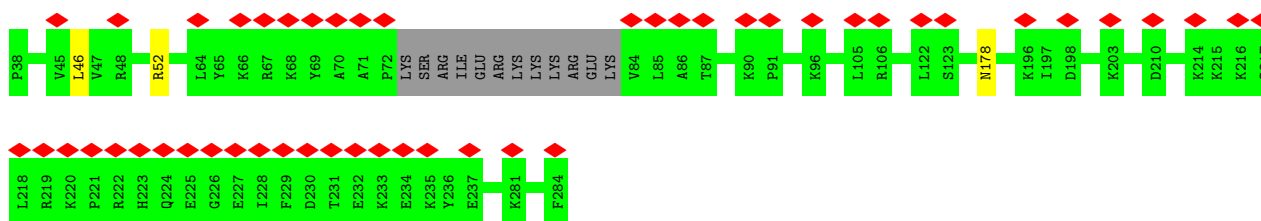
• Molecule 7: 60S ribosomal protein L5

Chain D:  8% 100%



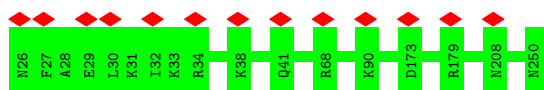
• Molecule 8: 60S ribosomal protein L6

Chain E:  20% 94% 5%



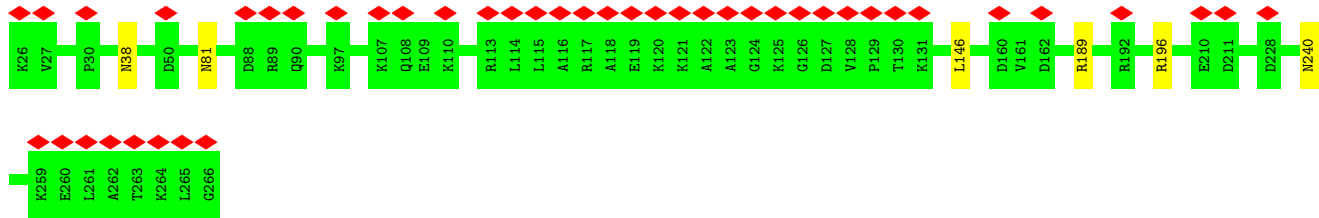
• Molecule 9: uL30

Chain F:  6% 100%

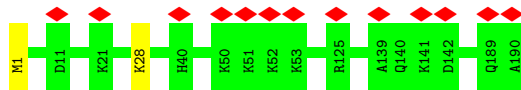


• Molecule 10: eL8

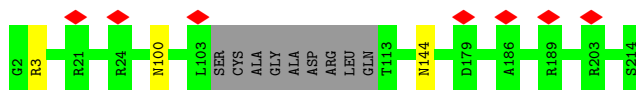
Chain G:  18% 98%



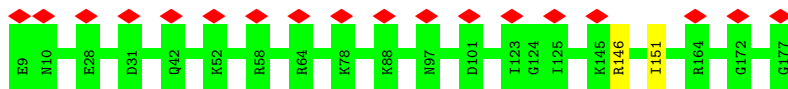
- Molecule 11: uL6



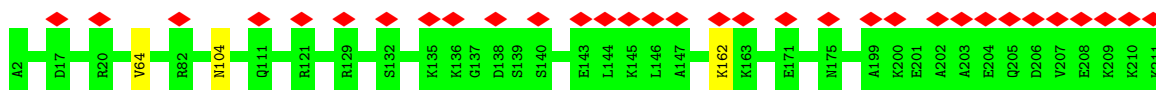
- Molecule 12: Ribosomal protein L10 (Predicted)



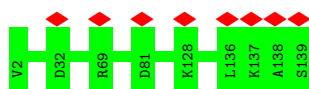
- Molecule 13: uL5



- Molecule 14: 60S ribosomal protein L13



- Molecule 15: Ribosomal protein L14



- Molecule 16: Ribosomal protein L15





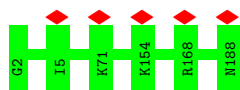
- Molecule 17: uL13



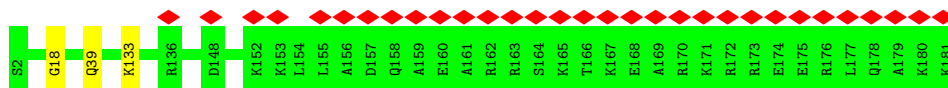
- Molecule 18: uL22



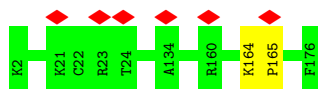
- Molecule 19: eL18



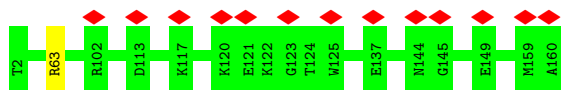
- Molecule 20: eL19



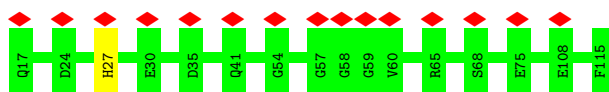
- Molecule 21: eL20



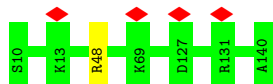
- Molecule 22: eL21



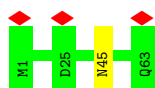
- Molecule 23: Ribosomal protein L22



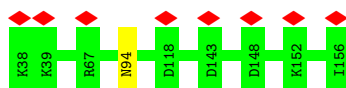
- Molecule 24: uL14



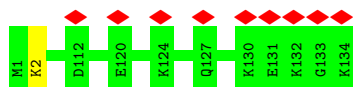
- Molecule 25: Ribosomal protein L24



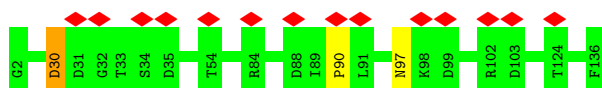
- Molecule 26: uL23



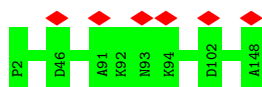
- Molecule 27: Ribosomal protein L26



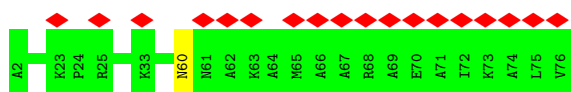
- Molecule 28: 60S ribosomal protein L27



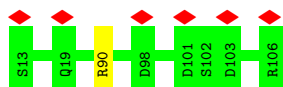
- Molecule 29: uL15



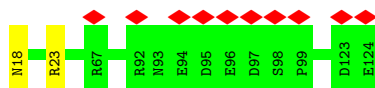
- Molecule 30: 60S ribosomal protein L29



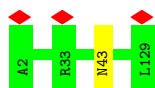
- Molecule 31: eL30



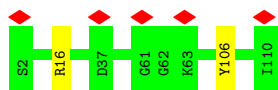
- Molecule 32: eL31



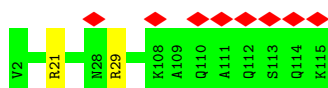
- Molecule 33: eL32



- Molecule 34: eL33

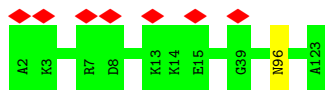


- Molecule 35: eL34

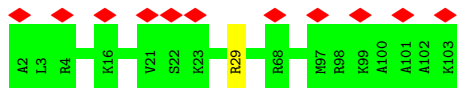


- Molecule 36: uL29





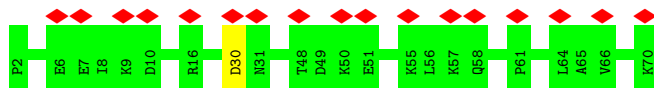
- Molecule 37: 60S ribosomal protein L36



- Molecule 38: Ribosomal protein L37



- Molecule 39: eL38



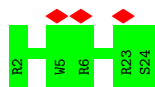
- Molecule 40: ribosomal protein eL39



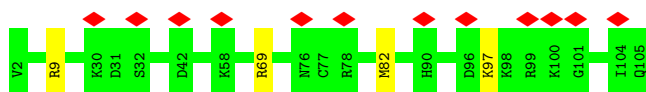
- Molecule 41: eL40



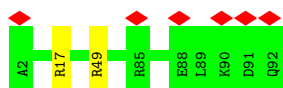
- Molecule 42: 60s ribosomal protein l41



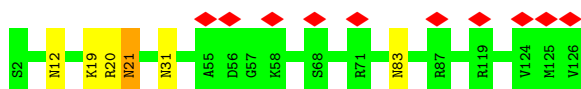
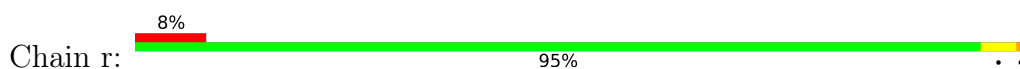
- Molecule 43: eL42



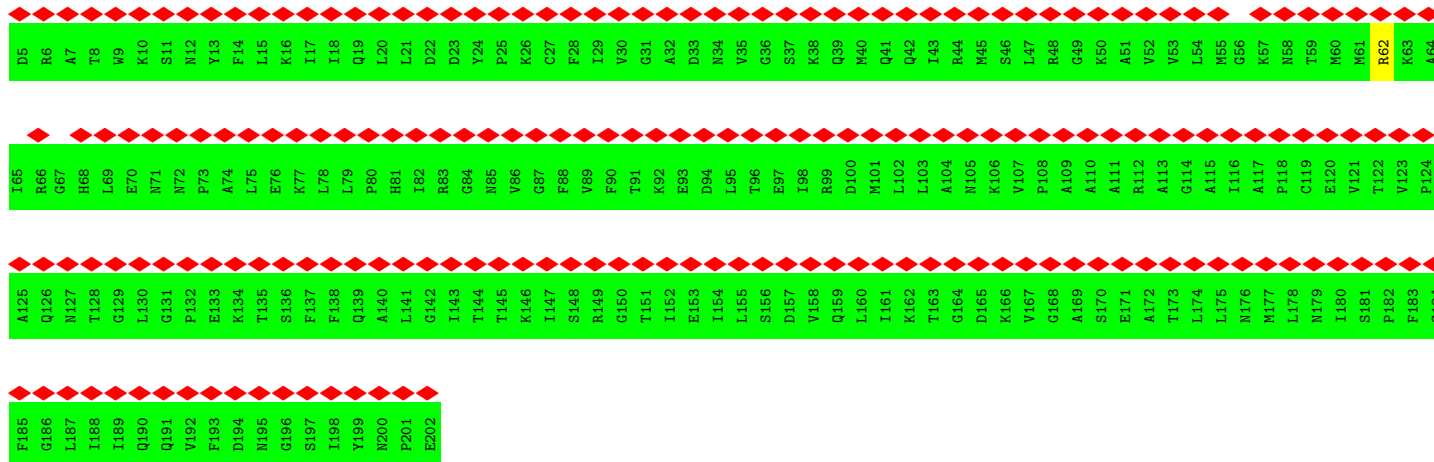
- Molecule 44: ribosomal protein eL43



- Molecule 45: eL28

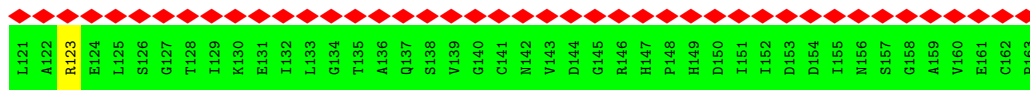


- Molecule 46: 60S acidic ribosomal protein P0

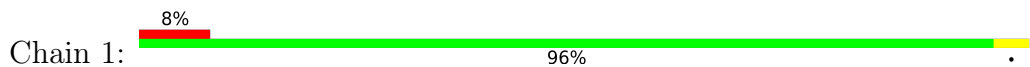


- Molecule 47: Ribosomal protein L12

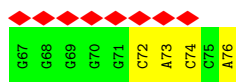
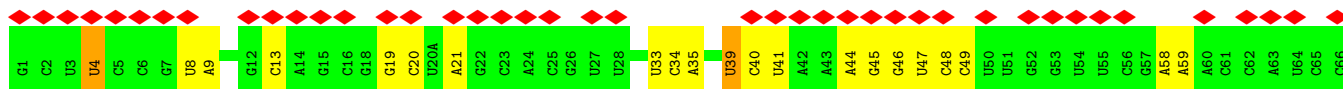




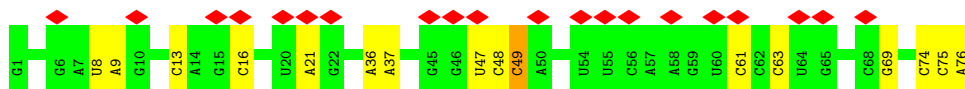
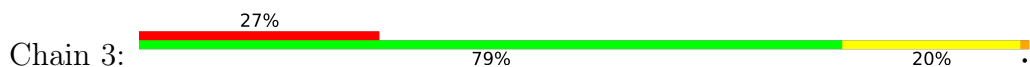
• Molecule 48: X-box-binding protein 1



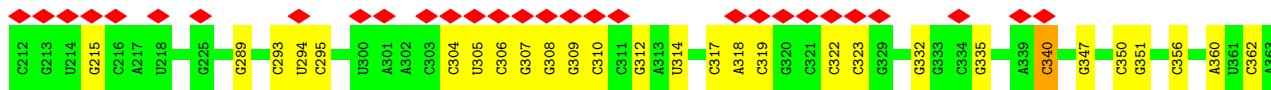
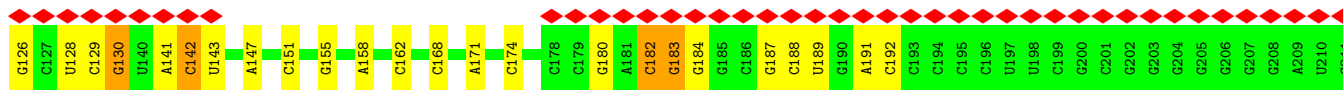
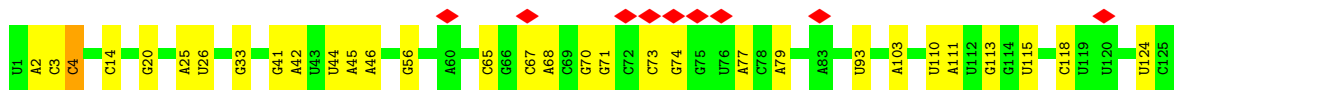
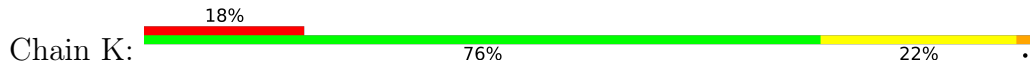
• Molecule 49: A/P-tRNA



• Molecule 50: P/E-tRNA

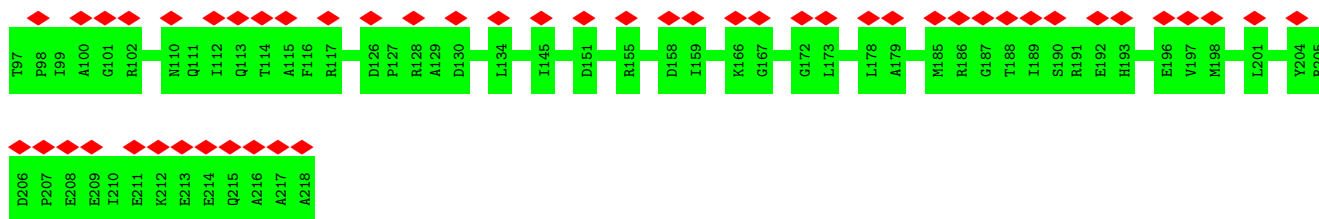


• Molecule 51: 18S rRNA

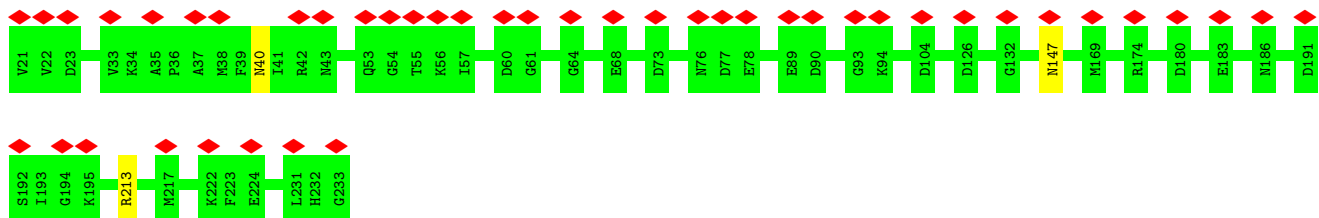




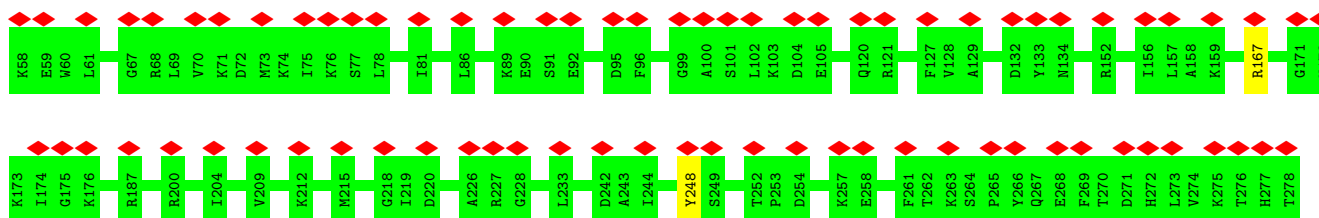




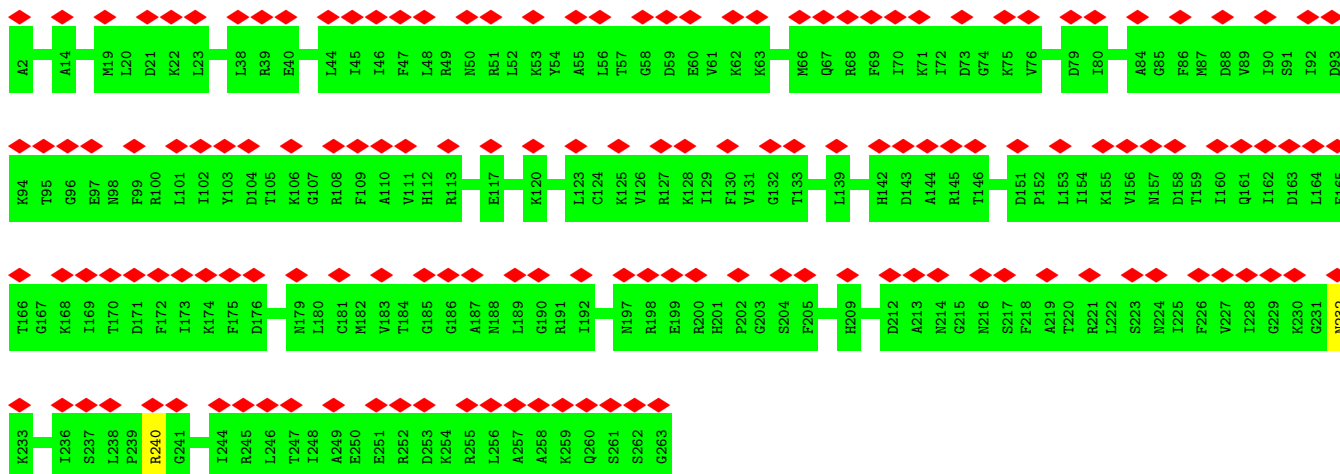
- Molecule 53: 40S ribosomal protein S3a



- Molecule 54: uS5



- Molecule 55: 40S ribosomal protein S4



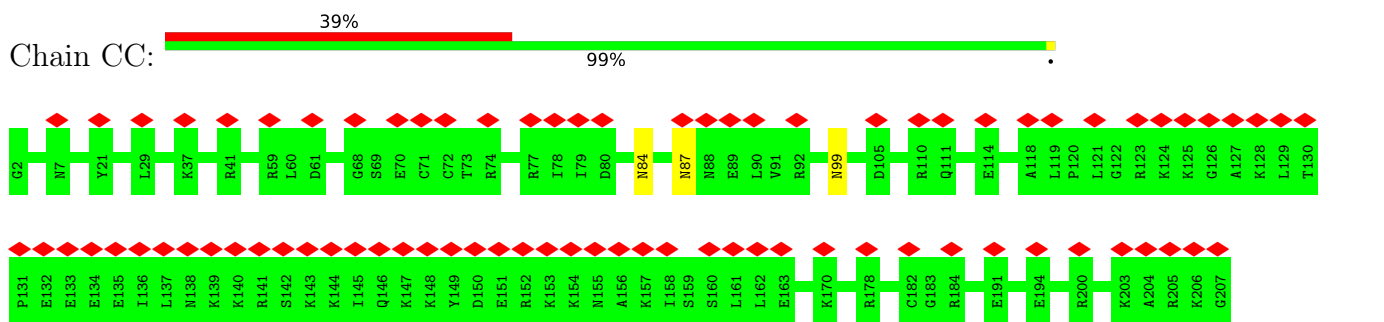
- Molecule 56: 40S ribosomal protein S6



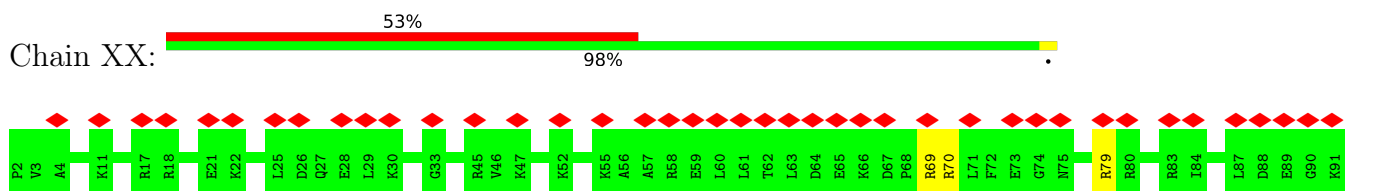
• Molecule 57: 40S ribosomal protein S7

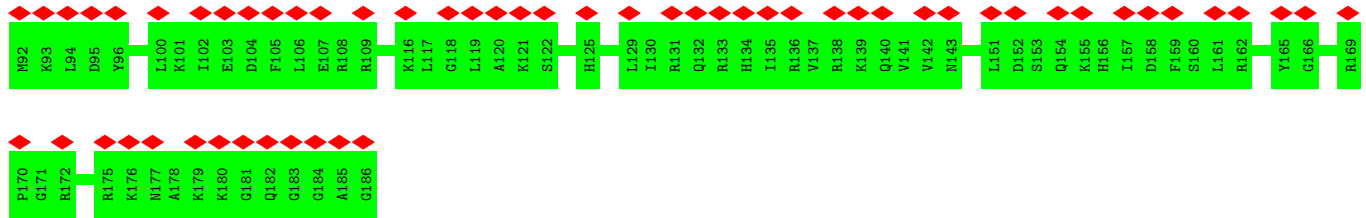


• Molecule 58: 40S ribosomal protein S8



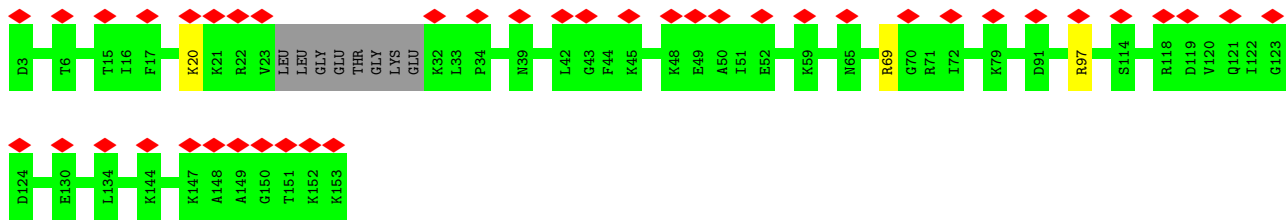
• Molecule 59: Ribosomal protein S9 (Predicted)





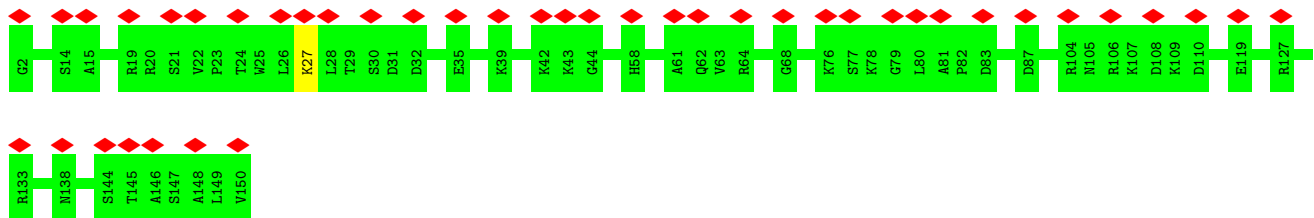
- Molecule 60: Ribosomal protein S11

Chain EE: 27% 93% 5%



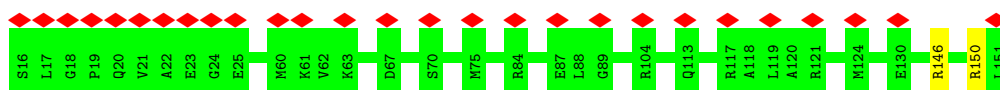
- Molecule 61: ribosomal protein uS15

Chain QQ: 28% 99%



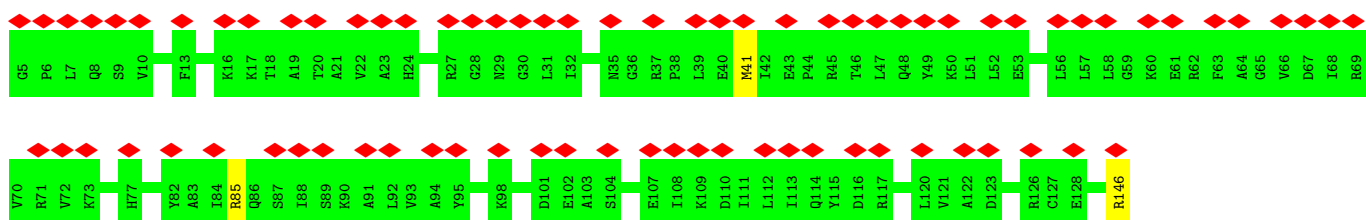
- Molecule 62: uS11

Chain MM: 20% 99%

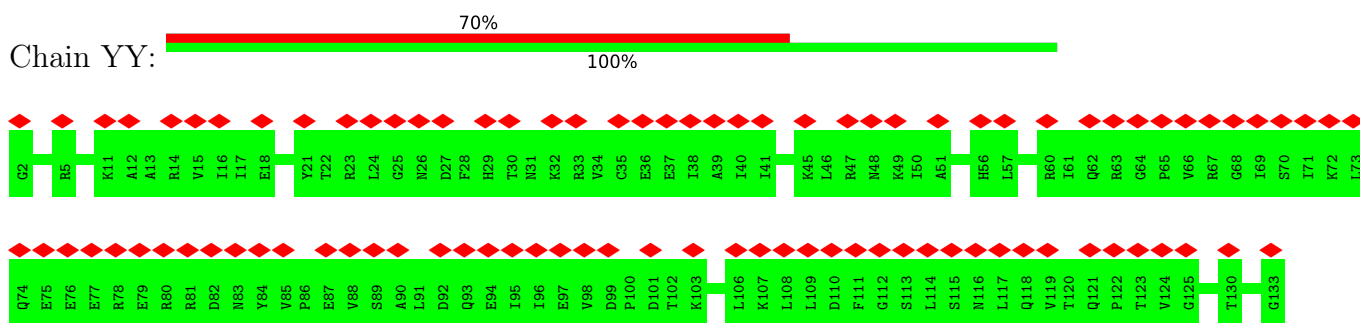


- Molecule 63: Ribosomal protein S16

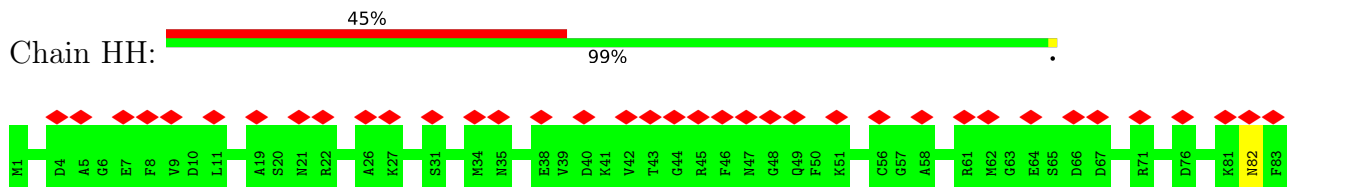
Chain UU: 54% 98%



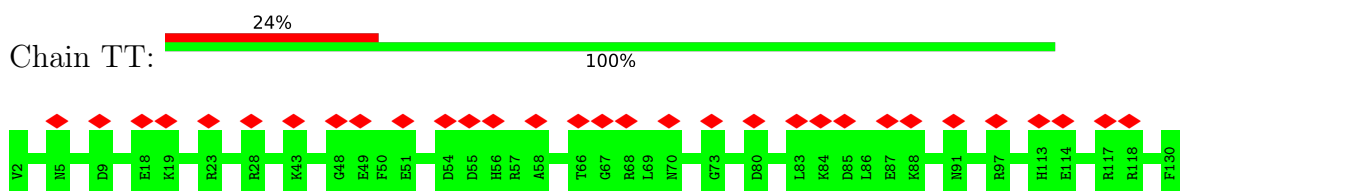
- Molecule 64: eS17



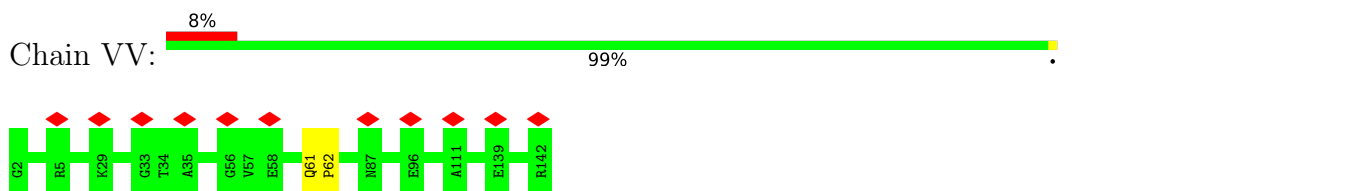
• Molecule 65: eS21



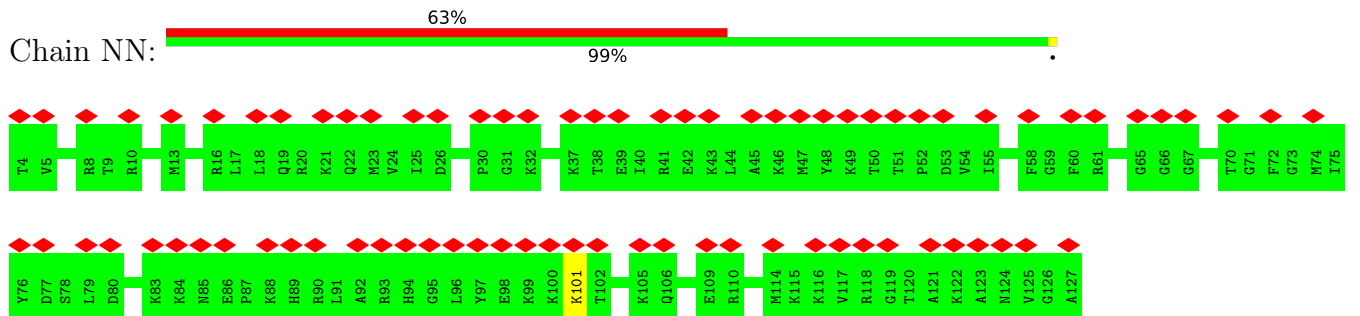
• Molecule 66: Ribosomal protein S15a



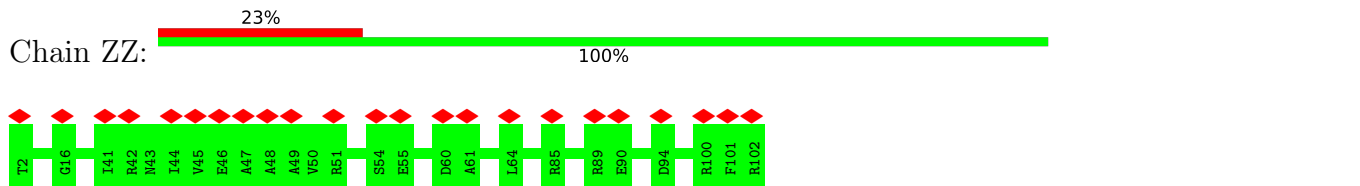
• Molecule 67: Ribosomal protein S23



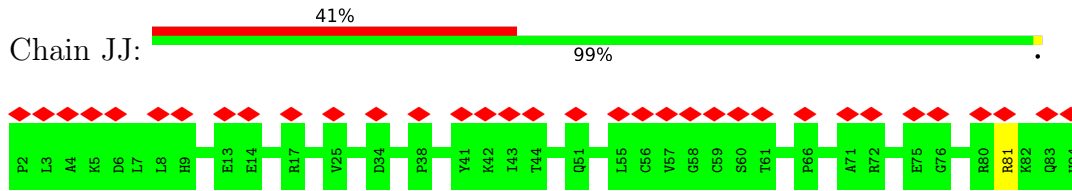
• Molecule 68: eS24



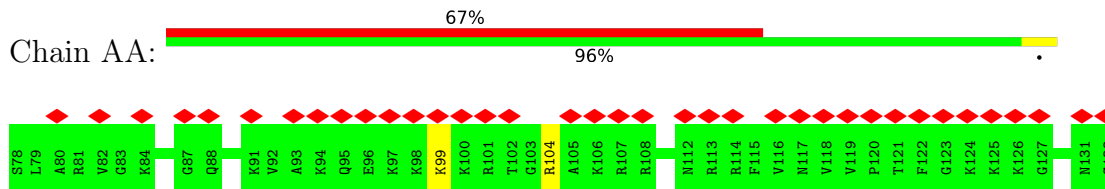
• Molecule 69: eS26



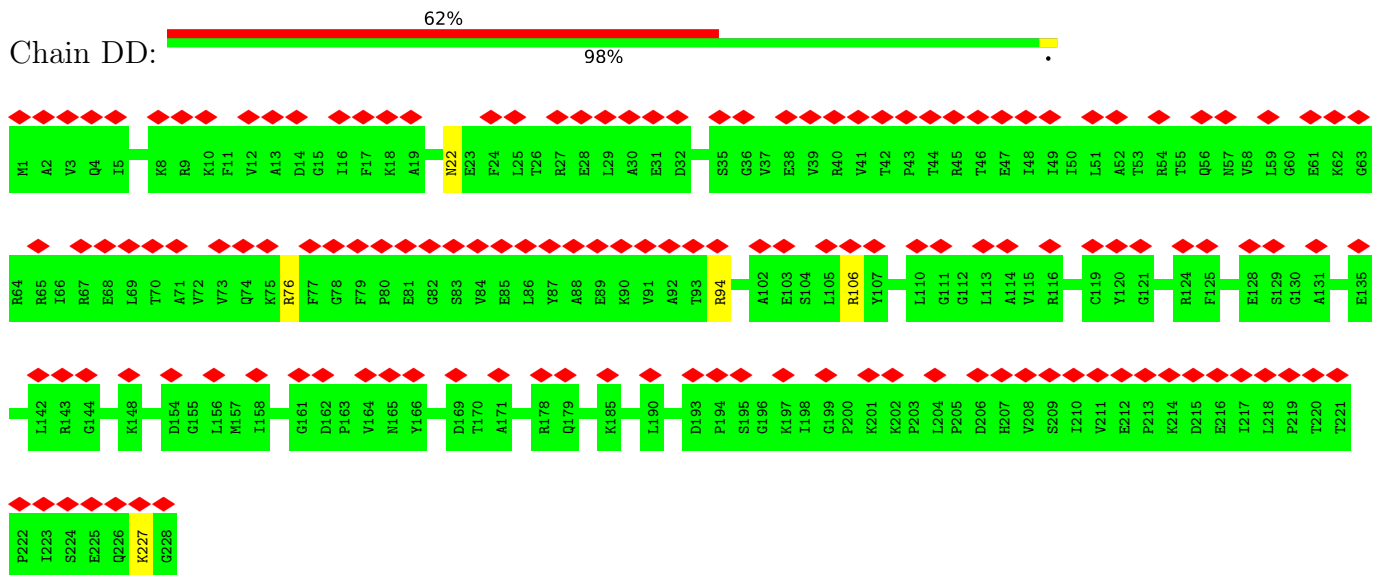
- Molecule 70: 40S ribosomal protein S27



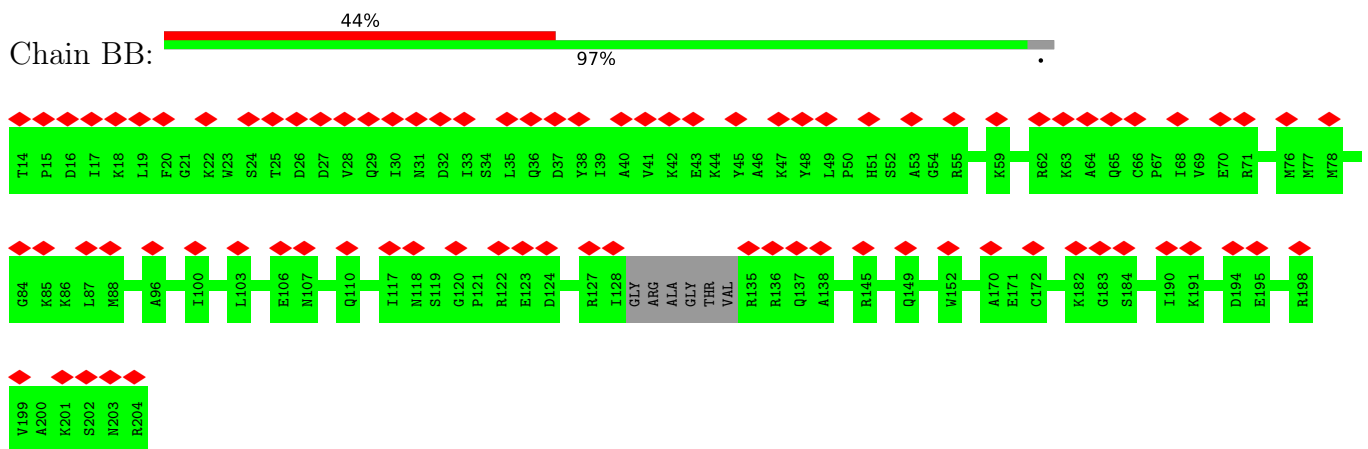
- Molecule 71: 40S ribosomal protein S30



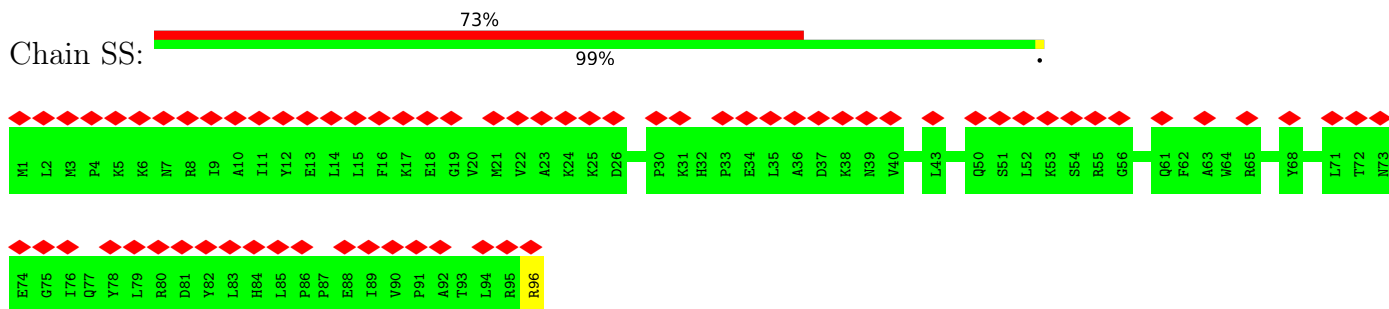
- Molecule 72: Ribosomal protein S3



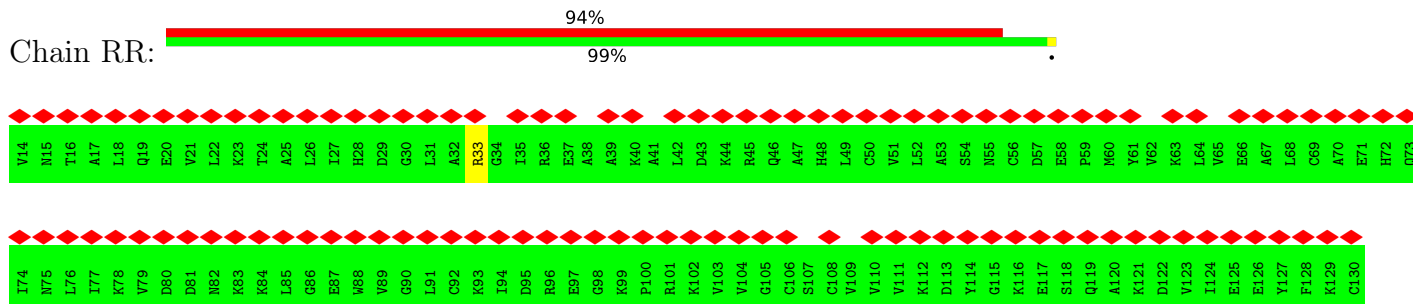
- Molecule 73: Ribosomal protein S5



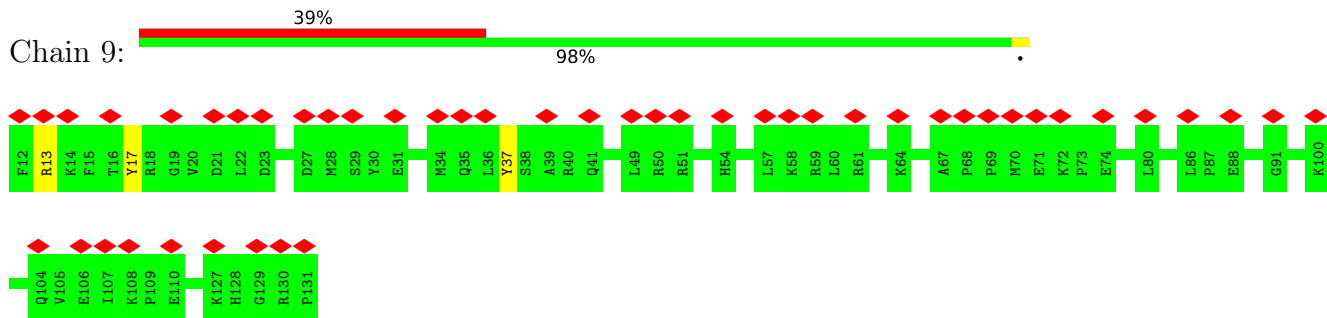
- Molecule 74: eS10



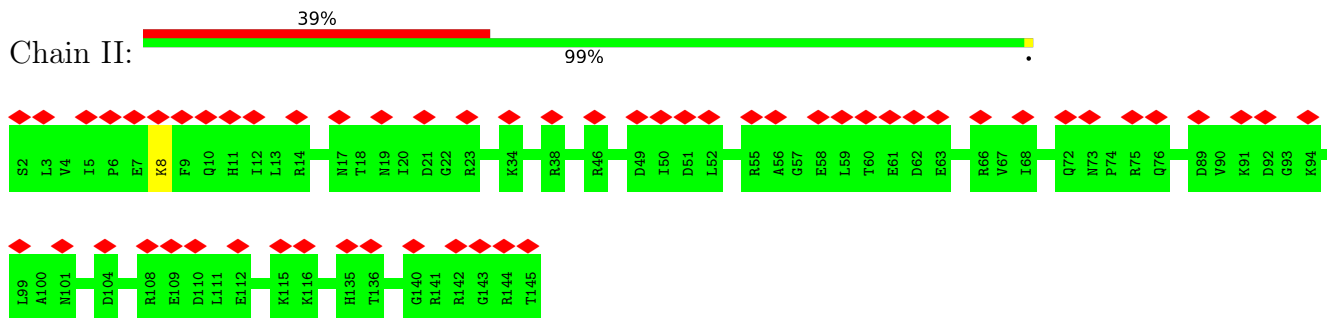
• Molecule 75: 40S ribosomal protein S12



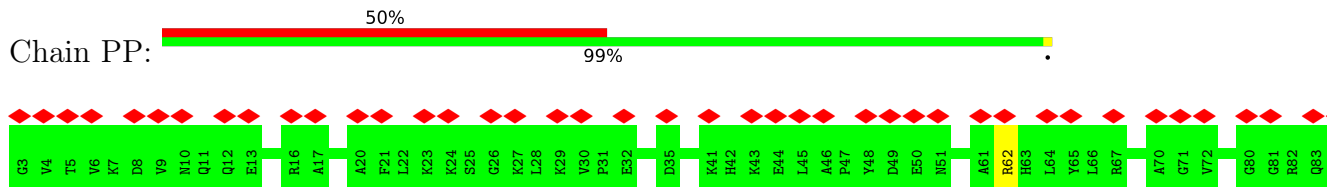
• Molecule 76: uS14

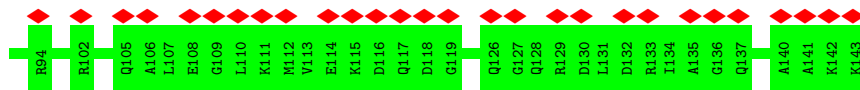


• Molecule 77: uS13

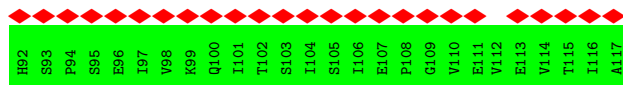
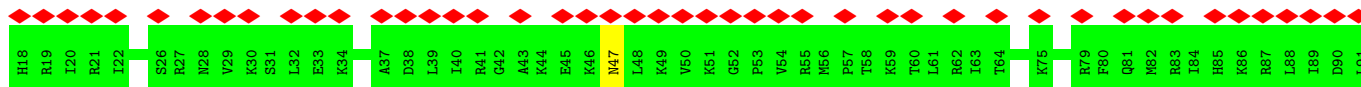
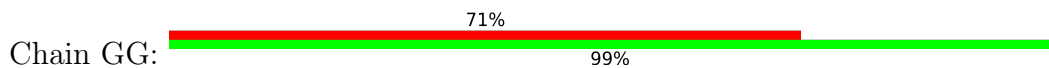


• Molecule 78: eS19

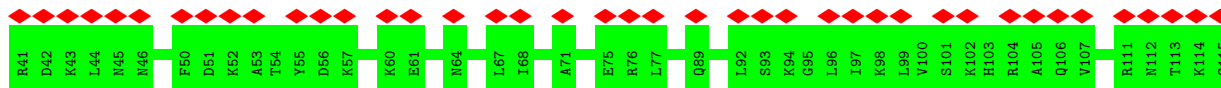




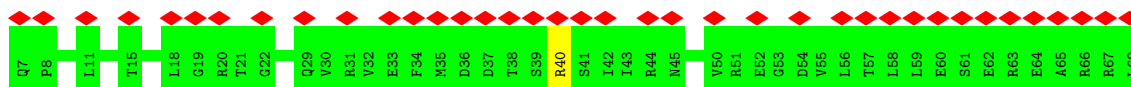
- Molecule 79: uS10



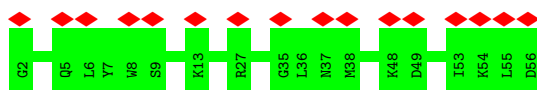
- Molecule 80: ribosomal protein eS25



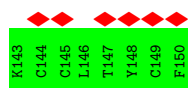
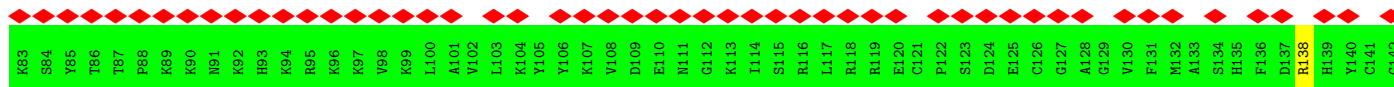
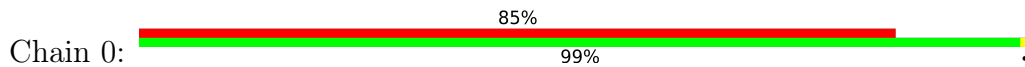
- Molecule 81: Ribosomal protein S28



- Molecule 82: S29

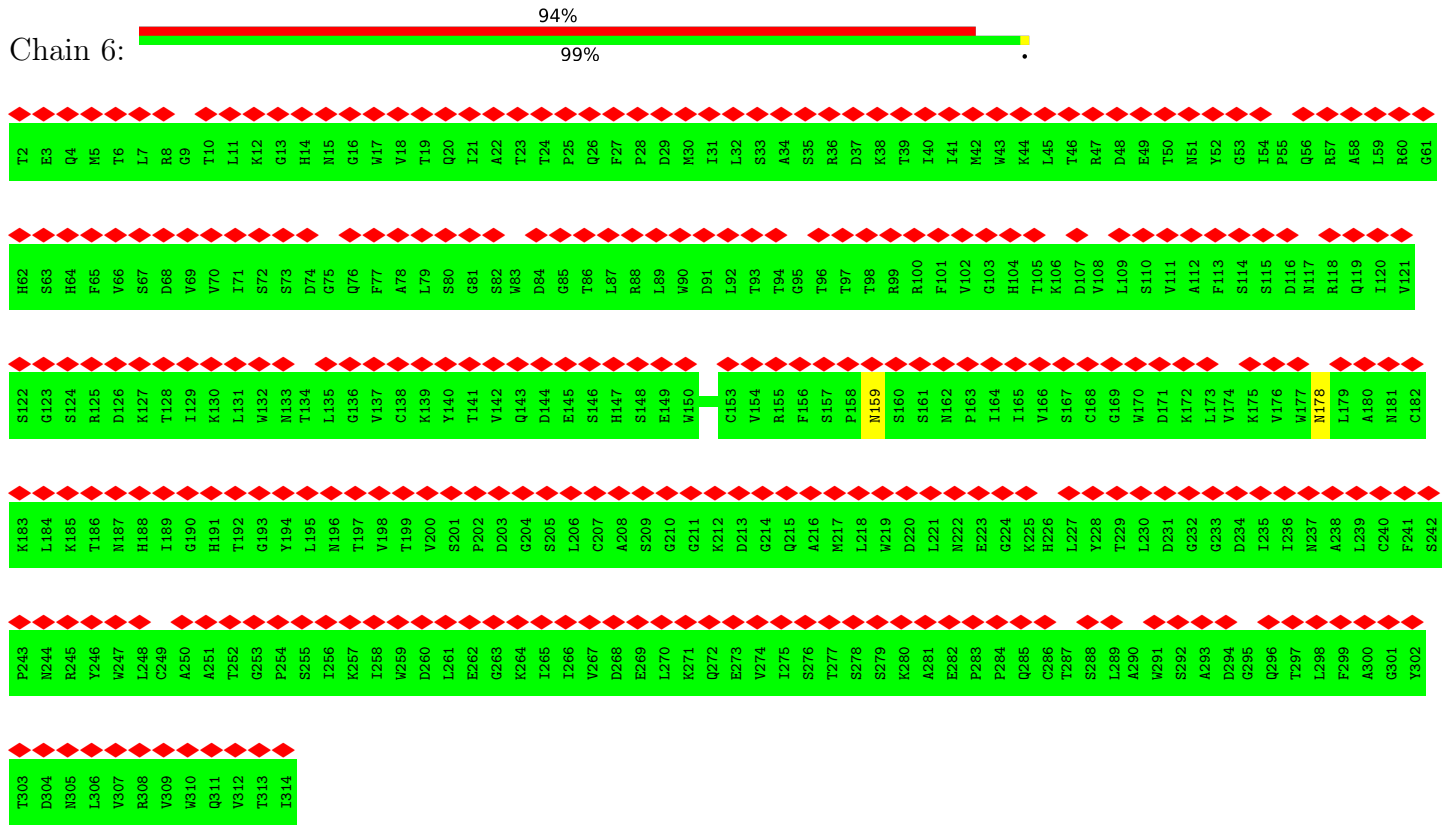


- Molecule 83: eS31



- Molecule 84: ribosomal protein RACK1





• Molecule 85: mRNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	94923	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.741	Depositor
Minimum map value	-0.435	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.08	Depositor
Map size ( $\text{\AA}$ )	429.264, 429.264, 429.264	wwPDB
Map dimensions	396, 396, 396	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.084, 1.084, 1.084	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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	5	0.31	1/87794 (0.0%)	1.05	383/136953 (0.3%)
2	7	0.28	0/2858	0.99	6/4455 (0.1%)
3	8	0.32	0/3701	1.06	10/5766 (0.2%)
4	A	0.29	0/1906	0.55	0/2556
5	B	0.27	0/3216	0.55	2/4311 (0.0%)
6	C	0.26	0/2937	0.51	0/3946
7	D	0.26	0/2432	0.50	0/3257
8	E	0.26	0/1936	0.61	1/2600 (0.0%)
9	F	0.28	0/1905	0.51	0/2539
10	G	0.27	0/1967	0.55	1/2647 (0.0%)
11	H	0.27	0/1535	0.54	0/2063
12	I	0.27	0/1693	0.49	0/2260
13	J	0.27	0/1376	0.56	0/1841
14	L	0.27	0/1734	0.53	0/2317
15	M	0.27	0/1158	0.52	0/1547
16	N	0.27	0/1746	0.51	0/2338
17	O	0.28	0/1671	0.51	0/2234
18	P	0.33	0/1268	0.53	1/1700 (0.1%)
19	Q	0.25	0/1530	0.53	0/2041
20	R	0.27	0/1524	0.54	0/2013
21	S	0.27	0/1493	0.51	0/2002
22	T	0.27	0/1326	0.49	0/1770
23	U	0.27	0/822	0.53	0/1103
24	V	0.28	0/993	0.56	0/1332
25	W	0.27	0/541	0.50	0/720
26	X	0.25	0/993	0.51	0/1334
27	Y	0.26	0/1132	0.50	0/1504
28	Z	0.28	0/1130	0.55	1/1507 (0.1%)
29	a	0.29	0/1191	0.51	0/1590
30	b	0.25	0/619	0.46	0/818
31	c	0.28	0/742	0.51	0/996
32	d	0.28	0/903	0.51	0/1216

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	e	0.27	0/1071	0.49	0/1429
34	f	0.27	0/895	0.58	0/1198
35	g	0.26	0/916	0.55	0/1220
36	h	0.26	0/1021	0.51	0/1348
37	i	0.26	0/841	0.52	0/1112
38	j	0.26	0/720	0.51	0/952
39	k	0.30	0/575	0.70	1/761 (0.1%)
40	l	0.26	0/454	0.47	0/599
41	m	0.28	0/435	0.54	0/575
42	n	0.25	0/223	0.45	0/284
43	o	0.27	0/864	0.59	0/1140
44	p	0.26	0/718	0.54	0/953
45	r	0.29	0/1017	0.67	1/1364 (0.1%)
46	s	0.27	0/1547	0.52	0/2088
47	t	0.32	0/1257	0.65	0/1697
48	1	0.50	0/216	0.56	0/298
49	2	0.28	0/1802	0.95	6/2804 (0.2%)
50	3	0.27	0/1783	1.00	3/2773 (0.1%)
51	K	0.29	1/40530 (0.0%)	1.04	165/63160 (0.3%)
52	q	0.26	0/1747	0.50	0/2374
53	u	0.25	0/1756	0.53	0/2350
54	v	0.27	0/1753	0.51	0/2369
55	x	0.25	0/2118	0.51	0/2849
56	z	0.25	0/1946	0.48	0/2590
57	y	0.26	0/1510	0.52	1/2022 (0.0%)
58	CC	0.25	0/1715	0.49	0/2287
59	XX	0.25	0/1550	0.50	0/2069
60	EE	0.26	0/1195	0.50	0/1597
61	QQ	0.25	0/1226	0.46	0/1649
62	MM	0.26	0/1029	0.51	0/1380
63	UU	0.26	0/1146	0.50	0/1534
64	YY	0.24	0/1082	0.46	0/1452
65	HH	0.27	0/643	0.52	0/860
66	TT	0.27	0/1051	0.51	0/1406
67	VV	0.26	0/1116	0.53	0/1490
68	NN	0.26	0/1028	0.48	0/1366
69	ZZ	0.26	0/828	0.49	0/1109
70	JJ	0.25	0/665	0.48	0/891
71	AA	0.26	0/447	0.46	0/587
72	DD	0.27	0/1796	0.54	0/2417
73	BB	0.26	0/1492	0.49	0/2005
74	SS	0.27	0/834	0.55	0/1125
75	RR	0.26	0/918	0.56	0/1233

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	9	0.26	0/1017	0.50	0/1358
77	II	0.27	0/1208	0.53	0/1618
78	PP	0.26	0/1115	0.50	0/1493
79	GG	0.25	0/805	0.50	0/1081
80	OO	0.24	0/604	0.51	0/810
81	FF	0.24	0/490	0.48	0/656
82	w	0.26	0/470	0.46	0/623
83	0	0.25	0/567	0.48	0/753
84	6	0.25	0/2493	0.53	0/3394
85	4	0.45	0/235	1.14	1/363 (0.3%)
All	All	0.29	2/234252 (0.0%)	0.89	583/344191 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	B	0	2
20	R	0	1
21	S	0	1
23	U	0	1
34	f	0	1
67	VV	0	2
76	9	0	2
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	967	C	N3-C4	-5.24	1.30	1.33
51	K	1520	G	N9-C4	5.10	1.42	1.38

All (583) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	961	G	N1-C6-O6	-19.59	108.15	119.90
1	5	967	C	N3-C4-N4	-19.03	104.68	118.00
1	5	967	C	C5-C4-N4	16.73	131.91	120.20
1	5	961	G	C5-C6-O6	13.97	136.98	128.60
1	5	931	C	N1-C2-O2	13.86	127.22	118.90
1	5	931	C	C2-N1-C1'	13.23	133.35	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1072	C	N1-C2-O2	12.14	126.19	118.90
1	5	1072	C	C2-N1-C1'	11.32	131.25	118.80
1	5	931	C	N3-C2-O2	-10.89	114.27	121.90
51	K	1520	G	N3-C4-C5	-10.11	123.55	128.60
1	5	4420	U	C2-N1-C1'	10.01	129.72	117.70
1	5	4420	U	N1-C2-O2	10.01	129.80	122.80
51	K	1123	C	N1-C2-O2	9.79	124.77	118.90
1	5	100	C	C2-N1-C1'	9.70	129.47	118.80
51	K	853	C	C2-N1-C1'	9.36	129.09	118.80
51	K	1139	C	N1-C2-O2	9.35	124.51	118.90
1	5	1072	C	N3-C2-O2	-9.25	115.42	121.90
51	K	1261	C	N1-C2-O2	9.16	124.40	118.90
1	5	931	C	C6-N1-C1'	-9.12	109.85	120.80
1	5	4420	U	N3-C2-O2	-9.11	115.82	122.20
51	K	1520	G	C2-N3-C4	9.10	116.45	111.90
51	K	1078	C	N1-C2-O2	8.95	124.27	118.90
1	5	449	C	N1-C2-O2	8.90	124.24	118.90
1	5	4749	C	C2-N1-C1'	8.89	128.58	118.80
1	5	4749	C	N1-C2-O2	8.87	124.22	118.90
51	K	1078	C	C2-N1-C1'	8.85	128.54	118.80
51	K	1123	C	N3-C2-O2	-8.82	115.73	121.90
1	5	4413	C	C2-N1-C1'	8.77	128.45	118.80
1	5	931	C	C6-N1-C2	-8.77	116.79	120.30
51	K	853	C	N1-C2-O2	8.72	124.13	118.90
1	5	100	C	N1-C2-O2	8.54	124.03	118.90
51	K	1453	C	N1-C2-O2	8.44	123.96	118.90
51	K	1453	C	C2-N1-C1'	8.38	128.02	118.80
1	5	4119	C	N1-C2-O2	8.36	123.92	118.90
51	K	174	C	N3-C2-O2	-8.21	116.15	121.90
39	k	30	ASP	CB-CG-OD1	8.19	125.67	118.30
1	5	1381	U	C2-N1-C1'	8.13	127.45	117.70
1	5	1639	U	C2-N1-C1'	8.12	127.45	117.70
1	5	4119	C	C2-N1-C1'	8.11	127.72	118.80
1	5	1822	U	N1-C2-O2	8.04	128.43	122.80
1	5	972	C	N1-C2-O2	8.02	123.71	118.90
51	K	1261	C	C2-N1-C1'	8.00	127.60	118.80
1	5	1072	C	C6-N1-C1'	-7.98	111.22	120.80
1	5	4413	C	N1-C2-O2	7.98	123.69	118.90
51	K	1520	G	N3-C4-N9	7.96	130.78	126.00
51	K	1139	C	C2-N1-C1'	7.93	127.52	118.80
1	5	3594	C	N1-C2-O2	7.87	123.62	118.90
1	5	4413	C	N3-C2-O2	-7.86	116.39	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	449	C	C2-N1-C1'	7.85	127.44	118.80
1	5	1822	U	N3-C2-O2	-7.84	116.71	122.20
51	K	1139	C	N3-C2-O2	-7.84	116.41	121.90
51	K	1364	U	N1-C2-O2	7.82	128.27	122.80
51	K	1271	C	N1-C2-O2	7.77	123.56	118.90
1	5	499	G	C4-N9-C1'	7.76	136.59	126.50
1	5	453	G	C4-N9-C1'	7.73	136.55	126.50
1	5	3636	C	N3-C2-O2	-7.73	116.49	121.90
1	5	2023	C	N1-C2-O2	7.71	123.52	118.90
1	5	453	G	N3-C4-C5	-7.63	124.78	128.60
1	5	1236	C	N3-C2-O2	-7.63	116.56	121.90
3	8	128	C	N1-C2-O2	7.62	123.47	118.90
1	5	499	G	N3-C4-N9	7.60	130.56	126.00
51	K	1078	C	C6-N1-C2	-7.58	117.27	120.30
51	K	1261	C	N3-C2-O2	-7.56	116.61	121.90
51	K	1364	U	C2-N1-C1'	7.54	126.75	117.70
1	5	2499	C	N1-C2-O2	7.53	123.42	118.90
1	5	453	G	N3-C4-N9	7.53	130.52	126.00
1	5	687	U	N1-C2-O2	7.52	128.06	122.80
1	5	1639	U	N1-C2-O2	7.50	128.05	122.80
1	5	100	C	N3-C2-O2	-7.47	116.67	121.90
1	5	2015	U	C2'-C3'-O3'	7.46	125.91	109.50
51	K	1298	G	C4-N9-C1'	7.44	136.17	126.50
1	5	931	C	C5-C6-N1	7.38	124.69	121.00
51	K	1078	C	N3-C2-O2	-7.32	116.78	121.90
1	5	4305	G	C4-N9-C1'	7.31	136.00	126.50
51	K	578	C	N1-C2-O2	7.30	123.28	118.90
51	K	1298	G	N3-C4-N9	7.29	130.37	126.00
1	5	2097	U	C2-N1-C1'	7.27	126.42	117.70
1	5	1381	U	N1-C2-O2	7.26	127.88	122.80
1	5	961	G	N9-C4-C5	-7.25	102.50	105.40
51	K	183	G	C4-N9-C1'	7.25	135.92	126.50
1	5	1237	C	N1-C2-O2	7.25	123.25	118.90
51	K	1261	C	C6-N1-C2	-7.25	117.40	120.30
1	5	2097	U	N1-C2-O2	7.23	127.86	122.80
51	K	1303	C	N1-C2-O2	7.22	123.23	118.90
1	5	2819	U	N3-C2-O2	-7.21	117.15	122.20
1	5	2256	C	P-O3'-C3'	7.17	128.31	119.70
51	K	1298	G	N3-C4-C5	-7.17	125.01	128.60
1	5	2499	C	N3-C2-O2	-7.14	116.90	121.90
1	5	956	A	P-O3'-C3'	7.13	128.25	119.70
51	K	1364	U	N3-C2-O2	-7.10	117.23	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2046	G	P-O3'-C3'	7.09	128.21	119.70
1	5	1612	G	N3-C4-N9	7.08	130.25	126.00
1	5	2107	C	P-O3'-C3'	7.08	128.20	119.70
1	5	5027	C	P-O3'-C3'	7.08	128.19	119.70
51	K	1303	C	C2-N1-C1'	7.07	126.57	118.80
1	5	1772	C	N3-C2-O2	-7.06	116.96	121.90
51	K	293	C	N1-C2-O2	7.04	123.13	118.90
1	5	1076	C	C2-N1-C1'	7.03	126.54	118.80
51	K	1139	C	C6-N1-C2	-7.03	117.49	120.30
1	5	1072	C	C6-N1-C2	-7.02	117.49	120.30
1	5	4889	G	P-O3'-C3'	7.01	128.12	119.70
51	K	130	G	C4-N9-C1'	7.01	135.62	126.50
1	5	4749	C	N3-C2-O2	-7.00	117.00	121.90
1	5	687	U	N3-C2-O2	-6.98	117.32	122.20
1	5	1822	U	C2-N1-C1'	6.98	126.07	117.70
1	5	4413	C	O4'-C1'-N1	6.97	113.78	108.20
1	5	1772	C	N1-C2-O2	6.96	123.08	118.90
1	5	2695	A	P-O3'-C3'	6.96	128.05	119.70
51	K	1520	G	C4-N9-C1'	6.95	135.54	126.50
51	K	853	C	N3-C2-O2	-6.95	117.03	121.90
1	5	1639	U	N3-C2-O2	-6.92	117.36	122.20
1	5	449	C	N3-C2-O2	-6.89	117.07	121.90
51	K	130	G	N3-C4-N9	6.88	130.13	126.00
51	K	1624	U	C2-N1-C1'	6.88	125.95	117.70
1	5	1612	G	N3-C4-C5	-6.87	125.17	128.60
1	5	4757	C	C2-N1-C1'	6.86	126.34	118.80
1	5	4413	C	C6-N1-C2	-6.85	117.56	120.30
1	5	1481	C	N1-C2-O2	6.84	123.00	118.90
1	5	499	G	N3-C4-C5	-6.84	125.18	128.60
51	K	688	U	P-O3'-C3'	6.83	127.89	119.70
51	K	1274	G	C4-N9-C1'	6.82	135.36	126.50
1	5	4871	C	C2-N1-C1'	6.79	126.27	118.80
1	5	3636	C	N1-C2-O2	6.79	122.97	118.90
51	K	1624	U	N3-C2-O2	-6.78	117.45	122.20
51	K	1057	C	C2-N1-C1'	6.77	126.25	118.80
1	5	2257	C	P-O3'-C3'	6.76	127.82	119.70
51	K	1298	G	C8-N9-C1'	-6.76	118.21	127.00
1	5	499	G	C8-N9-C1'	-6.76	118.21	127.00
1	5	2528	G	C4-N9-C1'	6.76	135.28	126.50
1	5	1236	C	N1-C2-O2	6.74	122.95	118.90
1	5	972	C	N3-C2-O2	-6.74	117.19	121.90
1	5	4709	U	C2-N1-C1'	6.71	125.75	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4757	C	N1-C2-O2	6.71	122.92	118.90
1	5	4871	C	N1-C2-O2	6.69	122.92	118.90
1	5	3594	C	N3-C2-O2	-6.69	117.22	121.90
51	K	1453	C	N3-C2-O2	-6.68	117.22	121.90
1	5	3594	C	C6-N1-C2	-6.68	117.63	120.30
1	5	2528	G	N3-C4-N9	6.67	130.00	126.00
1	5	1612	G	C4-N9-C1'	6.67	135.17	126.50
49	2	4	U	N1-C2-O2	6.67	127.47	122.80
1	5	685	C	N1-C2-O2	6.66	122.89	118.90
1	5	4423	U	C2-N1-C1'	6.66	125.69	117.70
1	5	956	A	OP2-P-O3'	6.65	119.84	105.20
1	5	4714	C	N1-C2-O2	6.65	122.89	118.90
1	5	48	G	P-O3'-C3'	6.63	127.65	119.70
1	5	100	C	C6-N1-C1'	-6.61	112.86	120.80
51	K	1123	C	C2-N1-C1'	6.59	126.04	118.80
51	K	853	C	C6-N1-C1'	-6.58	112.90	120.80
1	5	1686	C	N1-C2-O2	6.58	122.85	118.90
1	5	100	C	C6-N1-C2	-6.58	117.67	120.30
1	5	2097	U	N3-C2-O2	-6.57	117.60	122.20
51	K	130	G	N3-C4-C5	-6.57	125.32	128.60
51	K	183	G	N3-C4-C5	-6.56	125.32	128.60
1	5	3741	C	N3-C2-O2	-6.55	117.32	121.90
1	5	4888	U	P-O3'-C3'	6.54	127.55	119.70
5	B	309	LEU	CA-CB-CG	6.53	130.32	115.30
51	K	1852	C	N1-C2-O2	6.52	122.81	118.90
1	5	4502	C	N1-C2-O2	6.52	122.81	118.90
1	5	2820	C	N1-C2-O2	6.52	122.81	118.90
51	K	1123	C	C6-N1-C2	-6.51	117.69	120.30
1	5	4171	C	N1-C2-O2	6.51	122.81	118.90
1	5	4305	G	N3-C4-N9	6.50	129.90	126.00
51	K	1689	C	C2-N1-C1'	6.50	125.95	118.80
1	5	50	C	N1-C2-O2	6.49	122.79	118.90
1	5	961	G	N3-C4-N9	6.49	129.90	126.00
1	5	2465	C	N1-C2-O2	6.49	122.79	118.90
1	5	1792	U	C2-N1-C1'	6.49	125.48	117.70
1	5	1481	C	C2-N1-C1'	6.48	125.93	118.80
1	5	4420	U	C6-N1-C1'	-6.48	112.13	121.20
1	5	4736	C	N1-C2-O2	6.47	122.78	118.90
1	5	1686	C	N3-C2-O2	-6.46	117.38	121.90
1	5	2011	C	N1-C2-O2	6.46	122.78	118.90
1	5	453	G	C8-N9-C1'	-6.46	118.61	127.00
1	5	4119	C	N3-C2-O2	-6.46	117.38	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	K	752	G	P-O3'-C3'	6.45	127.44	119.70
51	K	1274	G	N3-C4-N9	6.45	129.87	126.00
51	K	1274	G	N3-C4-C5	-6.44	125.38	128.60
1	5	4758	U	C2-N1-C1'	6.44	125.43	117.70
51	K	340	C	N1-C2-O2	6.43	122.76	118.90
1	5	489	C	N1-C2-O2	6.41	122.75	118.90
1	5	2023	C	C2-N1-C1'	6.41	125.85	118.80
51	K	1624	U	N1-C2-O2	6.40	127.28	122.80
1	5	1731	C	C2-N1-C1'	6.39	125.83	118.80
1	5	2819	U	N1-C2-O2	6.38	127.27	122.80
1	5	4305	G	N3-C4-C5	-6.37	125.41	128.60
1	5	1072	C	C5-C6-N1	6.37	124.18	121.00
1	5	2661	U	P-O3'-C3'	6.35	127.32	119.70
1	5	4946	U	N1-C2-O2	6.35	127.24	122.80
1	5	4229	U	N3-C2-O2	-6.35	117.76	122.20
51	K	183	G	N3-C4-N9	6.35	129.81	126.00
1	5	969	C	O4'-C1'-N1	6.33	113.27	108.20
51	K	356	C	C2-N1-C1'	6.33	125.77	118.80
1	5	4232	U	P-O3'-C3'	6.32	127.29	119.70
51	K	1689	C	N1-C2-O2	6.32	122.69	118.90
51	K	4	C	C2-N1-C1'	6.32	125.75	118.80
1	5	1812	C	C2-N1-C1'	6.32	125.75	118.80
1	5	2116	C	P-O3'-C3'	6.30	127.26	119.70
1	5	2528	G	N3-C4-C5	-6.30	125.45	128.60
1	5	1632	A	C2-N3-C4	6.29	113.74	110.60
1	5	4758	U	N1-C2-O2	6.27	127.19	122.80
1	5	1378	C	C6-N1-C2	-6.27	117.79	120.30
1	5	4237	C	C2-N1-C1'	6.27	125.69	118.80
1	5	1237	C	N3-C2-O2	-6.26	117.52	121.90
1	5	3594	C	C2-N1-C1'	6.26	125.69	118.80
1	5	4158	C	N3-C2-O2	-6.24	117.53	121.90
1	5	112	C	C2-N1-C1'	6.24	125.66	118.80
1	5	2465	C	N3-C2-O2	-6.22	117.55	121.90
1	5	1847	C	C2-N1-C1'	6.21	125.64	118.80
1	5	4749	C	C6-N1-C1'	-6.19	113.37	120.80
51	K	1271	C	N3-C2-O2	-6.19	117.57	121.90
51	K	1637	A	P-O3'-C3'	6.19	127.13	119.70
51	K	1057	C	N1-C2-O2	6.18	122.61	118.90
3	8	128	C	N3-C2-O2	-6.18	117.58	121.90
1	5	961	G	C4-C5-N7	6.17	113.27	110.80
51	K	1520	G	C8-N9-C4	-6.17	103.93	106.40
1	5	1210	C	C2-N1-C1'	6.17	125.59	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2023	C	N3-C2-O2	-6.17	117.58	121.90
49	2	49	C	N1-C2-O2	6.15	122.59	118.90
51	K	118	C	N1-C2-O2	6.13	122.58	118.90
1	5	4305	G	C8-N9-C1'	-6.13	119.04	127.00
51	K	531	A	P-O3'-C3'	6.12	127.04	119.70
1	5	4881	U	C2-N1-C1'	6.11	125.03	117.70
49	2	4	U	N3-C2-O2	-6.09	117.94	122.20
51	K	1078	C	C5-C6-N1	6.09	124.04	121.00
1	5	989	U	N1-C2-O2	6.08	127.05	122.80
51	K	1271	C	C2-N1-C1'	6.07	125.48	118.80
51	K	151	C	N1-C2-O2	6.07	122.54	118.90
1	5	1807	C	C2-N1-C1'	6.07	125.48	118.80
1	5	3636	C	C6-N1-C2	-6.07	117.87	120.30
1	5	685	C	C2-N1-C1'	6.05	125.45	118.80
1	5	687	U	C2-N1-C1'	6.05	124.96	117.70
1	5	1210	C	N1-C2-O2	6.05	122.53	118.90
51	K	293	C	C2-N1-C1'	6.05	125.45	118.80
1	5	1692	C	C2-N1-C1'	6.04	125.44	118.80
1	5	1381	U	N3-C2-O2	-6.03	117.98	122.20
51	K	578	C	N3-C2-O2	-6.03	117.68	121.90
1	5	1485	C	C2-N1-C1'	6.02	125.42	118.80
51	K	1118	C	C2-N1-C1'	6.01	125.41	118.80
2	7	29	C	C2-N1-C1'	6.00	125.40	118.80
18	P	91	LEU	CA-CB-CG	6.00	129.10	115.30
51	K	14	C	C2-N1-C1'	6.00	125.40	118.80
51	K	183	G	C8-N9-C1'	-5.99	119.21	127.00
51	K	1423	C	N1-C2-O2	5.99	122.49	118.90
1	5	2867	C	C2-N1-C1'	5.98	125.38	118.80
1	5	1273	G	C4-N9-C1'	5.98	134.27	126.50
51	K	130	G	C8-N9-C1'	-5.97	119.24	127.00
1	5	972	C	C6-N1-C2	-5.97	117.91	120.30
1	5	684	G	P-O3'-C3'	5.96	126.86	119.70
51	K	1389	C	N1-C2-O2	5.96	122.48	118.90
51	K	624	C	C6-N1-C2	-5.95	117.92	120.30
1	5	1081	C	C2-N1-C1'	5.94	125.33	118.80
1	5	2266	C	P-O3'-C3'	5.94	126.83	119.70
1	5	4177	C	C2-N1-C1'	5.94	125.33	118.80
51	K	824	C	N1-C2-O2	5.94	122.46	118.90
51	K	659	G	C4-N9-C1'	5.94	134.22	126.50
1	5	3741	C	N1-C2-O2	5.93	122.46	118.90
1	5	4215	C	N1-C2-O2	5.93	122.46	118.90
51	K	174	C	N1-C2-O2	5.92	122.45	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1485	C	N1-C2-O2	5.92	122.45	118.90
3	8	153	C	C2-N1-C1'	5.92	125.31	118.80
1	5	3778	U	N1-C2-O2	5.91	126.94	122.80
1	5	4476	C	C2-N1-C1'	5.91	125.31	118.80
1	5	4423	U	N3-C2-O2	-5.91	118.06	122.20
1	5	4656	A	P-O3'-C3'	5.91	126.79	119.70
1	5	4736	C	N3-C2-O2	-5.89	117.78	121.90
1	5	2093	A	P-O3'-C3'	5.89	126.77	119.70
1	5	4354	U	P-O3'-C3'	5.89	126.77	119.70
51	K	1358	U	N3-C2-O2	-5.89	118.08	122.20
51	K	1518	C	C2-N1-C1'	5.89	125.28	118.80
1	5	4423	U	N1-C2-O2	5.89	126.92	122.80
51	K	356	C	N1-C2-O2	5.88	122.43	118.90
1	5	930	G	P-O3'-C3'	5.88	126.75	119.70
1	5	4413	C	C6-N1-C1'	-5.88	113.75	120.80
1	5	4229	U	N1-C2-O2	5.87	126.91	122.80
51	K	1117	C	N1-C2-O2	5.87	122.42	118.90
1	5	4420	U	C5-C6-N1	5.86	125.63	122.70
3	8	124	U	P-O3'-C3'	5.86	126.73	119.70
1	5	2274	C	C2-N1-C1'	5.85	125.23	118.80
51	K	815	U	N3-C2-O2	-5.85	118.11	122.20
1	5	1835	G	P-O3'-C3'	5.84	126.71	119.70
51	K	1303	C	N3-C2-O2	-5.84	117.81	121.90
1	5	1671	U	N3-C2-O2	-5.84	118.11	122.20
1	5	3876	A	P-O3'-C3'	5.84	126.71	119.70
1	5	3739	C	N1-C2-O2	5.83	122.40	118.90
1	5	2117	G	C4-N9-C1'	5.83	134.08	126.50
1	5	2528	G	C8-N9-C1'	-5.83	119.42	127.00
1	5	4749	C	C6-N1-C2	-5.82	117.97	120.30
1	5	506	C	C2-N1-C1'	5.82	125.20	118.80
1	5	134	G	P-O3'-C3'	5.82	126.68	119.70
1	5	4952	G	N3-C4-C5	-5.81	125.69	128.60
51	K	1660	C	C2-N1-C1'	5.81	125.19	118.80
1	5	920	C	C2-N1-C1'	5.81	125.19	118.80
1	5	4758	U	N3-C2-O2	-5.81	118.14	122.20
1	5	115	C	C2-N1-C1'	5.79	125.16	118.80
1	5	4402	C	N1-C2-O2	5.79	122.37	118.90
1	5	2123	C	P-O3'-C3'	5.78	126.64	119.70
1	5	449	C	C6-N1-C2	-5.78	117.99	120.30
51	K	579	C	N1-C2-O2	5.78	122.37	118.90
51	K	1271	C	C6-N1-C2	-5.77	117.99	120.30
1	5	155	C	N3-C2-O2	-5.76	117.86	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4964	C	N1-C2-O2	5.76	122.36	118.90
1	5	1381	U	C6-N1-C1'	-5.76	113.14	121.20
1	5	4303	C	C2-N1-C1'	5.76	125.14	118.80
1	5	245	C	P-O3'-C3'	5.76	126.61	119.70
1	5	1273	G	N3-C4-C5	-5.76	125.72	128.60
1	5	1074	G	N3-C4-N9	5.75	129.45	126.00
51	K	1453	C	C6-N1-C2	-5.75	118.00	120.30
51	K	1709	G	C4-N9-C1'	5.75	133.97	126.50
1	5	1804	A	P-O3'-C3'	5.75	126.60	119.70
1	5	458	C	N1-C2-O2	5.75	122.35	118.90
51	K	1261	C	C5-C6-N1	5.74	123.87	121.00
51	K	853	C	C6-N1-C2	-5.73	118.01	120.30
1	5	1428	U	N1-C2-O2	5.72	126.81	122.80
1	5	1273	G	N3-C4-N9	5.72	129.43	126.00
1	5	1792	U	N3-C2-O2	-5.72	118.19	122.20
1	5	4682	U	N1-C2-O2	5.72	126.80	122.80
49	2	4	U	C2-N1-C1'	5.72	124.56	117.70
1	5	1367	C	C2-N1-C1'	5.71	125.08	118.80
51	K	465	A	P-O3'-C3'	5.71	126.55	119.70
51	K	1358	U	N1-C2-O2	5.71	126.80	122.80
1	5	1792	U	N1-C2-O2	5.70	126.79	122.80
51	K	1274	G	C8-N9-C1'	-5.70	119.59	127.00
2	7	28	C	N1-C2-O2	5.70	122.32	118.90
1	5	451	C	P-O3'-C3'	5.69	126.53	119.70
51	K	614	C	P-O3'-C3'	5.69	126.53	119.70
1	5	4881	U	N1-C2-O2	5.69	126.78	122.80
1	5	1848	C	N1-C2-O2	5.69	122.31	118.90
57	y	36	LEU	CA-CB-CG	5.69	128.38	115.30
1	5	690	C	N1-C2-O2	5.68	122.31	118.90
1	5	943	A	P-O3'-C3'	5.68	126.52	119.70
1	5	4170	A	P-O3'-C3'	5.68	126.52	119.70
51	K	1453	C	C6-N1-C1'	-5.68	113.98	120.80
1	5	967	C	N1-C2-O2	5.67	122.30	118.90
1	5	1612	G	C8-N9-C1'	-5.67	119.63	127.00
1	5	1671	U	N1-C2-O2	5.67	126.77	122.80
1	5	4946	U	N3-C2-O2	-5.66	118.24	122.20
51	K	182	C	P-O3'-C3'	5.66	126.49	119.70
1	5	1429	C	N1-C2-O2	5.66	122.30	118.90
1	5	4612	C	N1-C2-O2	5.66	122.29	118.90
1	5	4482	U	N3-C2-O2	-5.65	118.25	122.20
51	K	531	A	OP1-P-O3'	5.65	117.63	105.20
51	K	4	C	N1-C2-O2	5.65	122.29	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	4682	U	N3-C2-O2	-5.64	118.25	122.20
1	5	4119	C	C6-N1-C1'	-5.64	114.03	120.80
1	5	4952	G	N3-C4-N9	5.63	129.38	126.00
1	5	1076	C	N1-C2-O2	5.62	122.28	118.90
51	K	1289	U	N1-C2-O2	5.62	126.74	122.80
51	K	870	A	P-O3'-C3'	5.61	126.43	119.70
1	5	4682	U	C2-N1-C1'	5.61	124.43	117.70
51	K	1742	C	C2-N1-C1'	5.61	124.97	118.80
1	5	4714	C	N3-C2-O2	-5.60	117.98	121.90
1	5	1232	G	P-O3'-C3'	5.60	126.42	119.70
1	5	690	C	C2-N1-C1'	5.60	124.96	118.80
51	K	1057	C	N3-C2-O2	-5.59	117.99	121.90
1	5	218	A	P-O3'-C3'	5.59	126.41	119.70
1	5	2083	C	P-O3'-C3'	5.58	126.40	119.70
1	5	1079	C	N1-C2-O2	5.58	122.25	118.90
51	K	1022	U	C2-N1-C1'	5.58	124.40	117.70
51	K	1116	C	N1-C2-O2	5.58	122.25	118.90
51	K	1078	C	C6-N1-C1'	-5.57	114.12	120.80
1	5	2820	C	N3-C2-O2	-5.56	118.01	121.90
1	5	972	C	C2-N1-C1'	5.55	124.90	118.80
1	5	1598	C	N1-C2-O2	5.54	122.23	118.90
1	5	4964	C	N3-C2-O2	-5.54	118.02	121.90
1	5	2410	C	C2-N1-C1'	5.53	124.89	118.80
1	5	2560	C	C2-N1-C1'	5.53	124.88	118.80
1	5	3657	U	N3-C2-O2	-5.53	118.33	122.20
51	K	1826	G	N3-C4-N9	5.53	129.32	126.00
1	5	1378	C	C5-C6-N1	5.52	123.76	121.00
1	5	2023	C	C6-N1-C2	-5.52	118.09	120.30
51	K	1551	U	C2-N1-C1'	5.52	124.33	117.70
51	K	1826	G	C4-N9-C1'	5.52	133.68	126.50
1	5	221	C	C2-N1-C1'	5.50	124.86	118.80
1	5	453	G	C2-N3-C4	5.50	114.65	111.90
1	5	1893	C	C2-N1-C1'	5.50	124.86	118.80
51	K	1073	U	N3-C2-O2	-5.50	118.35	122.20
1	5	4237	C	C6-N1-C2	-5.50	118.10	120.30
51	K	151	C	C2-N1-C1'	5.49	124.84	118.80
1	5	2704	C	N1-C2-O2	5.47	122.19	118.90
1	5	1359	G	C4-N9-C1'	5.46	133.60	126.50
1	5	1929	A	C4-N9-C1'	5.45	136.12	126.30
1	5	4952	G	C4-N9-C1'	5.45	133.59	126.50
1	5	2787	A	C2-N3-C4	5.45	113.33	110.60
1	5	1359	G	N7-C8-N9	5.45	115.82	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2085	G	C4-N9-C1'	5.45	133.58	126.50
1	5	155	C	N1-C2-O2	5.44	122.17	118.90
1	5	685	C	N3-C2-O2	-5.44	118.09	121.90
50	3	49	C	N1-C2-O2	5.44	122.16	118.90
1	5	961	G	C8-N9-C1'	-5.43	119.93	127.00
51	K	151	C	C6-N1-C2	-5.43	118.13	120.30
1	5	4757	C	N3-C2-O2	-5.43	118.10	121.90
51	K	427	U	C2-N1-C1'	5.43	124.21	117.70
1	5	4560	C	N1-C2-O2	5.42	122.16	118.90
1	5	4627	U	N1-C2-O2	5.42	126.60	122.80
1	5	4749	C	O4'-C1'-N1	5.42	112.54	108.20
1	5	4171	C	N3-C2-O2	-5.42	118.11	121.90
1	5	100	C	O4'-C1'-N1	5.41	112.53	108.20
51	K	1709	G	N3-C4-N9	5.41	129.24	126.00
1	5	989	U	N3-C2-O2	-5.41	118.42	122.20
1	5	1458	C	N1-C2-O2	5.41	122.14	118.90
1	5	2117	G	N3-C4-C5	-5.41	125.90	128.60
1	5	2117	G	N3-C4-N9	5.41	129.24	126.00
1	5	2083	C	OP2-P-O3'	5.40	117.08	105.20
1	5	4482	U	N1-C2-O2	5.40	126.58	122.80
85	4	44	C	N1-C2-O2	5.40	122.14	118.90
1	5	4243	C	C6-N1-C2	-5.40	118.14	120.30
51	K	1298	G	O4'-C1'-N9	-5.39	103.89	108.20
1	5	2256	C	N1-C2-O2	5.39	122.14	118.90
1	5	1339	U	N1-C2-O2	5.39	126.57	122.80
1	5	2454	U	N3-C2-O2	-5.38	118.43	122.20
5	B	214	ASP	CB-CG-OD1	5.38	123.14	118.30
2	7	28	C	N3-C2-O2	-5.38	118.14	121.90
3	8	128	C	C2-N1-C1'	5.38	124.71	118.80
1	5	3772	U	C2-N1-C1'	5.37	124.15	117.70
51	K	168	C	N1-C2-O2	5.37	122.12	118.90
51	K	1118	C	N1-C2-O2	5.37	122.12	118.90
1	5	1656	U	N1-C2-O2	5.36	126.55	122.80
1	5	2470	C	N1-C2-O2	5.36	122.12	118.90
1	5	4171	C	C6-N1-C2	-5.36	118.16	120.30
1	5	1929	A	C2-N3-C4	5.36	113.28	110.60
1	5	1	C	P-O3'-C3'	5.35	126.12	119.70
1	5	3778	U	N3-C2-O2	-5.35	118.45	122.20
1	5	5022	U	P-O3'-C3'	5.35	126.12	119.70
51	K	1314	U	C2-N1-C1'	5.35	124.12	117.70
1	5	2072	C	C6-N1-C2	-5.35	118.16	120.30
1	5	4881	U	N3-C2-O2	-5.34	118.46	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2257	C	OP1-P-O3'	5.34	116.95	105.20
1	5	245	C	N1-C2-O2	5.34	122.10	118.90
1	5	4502	C	N3-C2-O2	-5.34	118.16	121.90
51	K	624	C	C5-C6-N1	5.33	123.67	121.00
1	5	449	C	C6-N1-C1'	-5.33	114.40	120.80
1	5	48	G	OP2-P-O3'	5.33	116.92	105.20
1	5	1367	C	N1-C2-O2	5.33	122.10	118.90
51	K	1395	C	P-O3'-C3'	5.33	126.09	119.70
1	5	4177	C	C6-N1-C2	-5.32	118.17	120.30
2	7	29	C	N1-C2-O2	5.32	122.09	118.90
1	5	1848	C	C2-N1-C1'	5.32	124.65	118.80
1	5	961	G	N1-C2-N3	-5.32	120.71	123.90
51	K	630	U	C2-N1-C1'	5.31	124.07	117.70
1	5	4171	C	C2-N1-C1'	5.31	124.64	118.80
1	5	1915	C	N1-C2-O2	5.31	122.08	118.90
51	K	537	C	C2-N1-C1'	5.30	124.63	118.80
51	K	1057	C	C6-N1-C2	-5.30	118.18	120.30
1	5	647	G	C4-N9-C1'	5.30	133.39	126.50
51	K	14	C	C6-N1-C2	-5.30	118.18	120.30
51	K	823	U	C2-N1-C1'	5.30	124.06	117.70
51	K	532	C	P-O3'-C3'	5.30	126.06	119.70
1	5	2661	U	OP1-P-O3'	5.29	116.85	105.20
1	5	1639	U	C6-N1-C1'	-5.29	113.79	121.20
1	5	2904	U	C2-N1-C1'	5.29	124.05	117.70
1	5	2726	G	C4-N9-C1'	5.29	133.38	126.50
1	5	489	C	N3-C2-O2	-5.29	118.20	121.90
1	5	3622	C	N1-C2-O2	5.29	122.07	118.90
1	5	2704	C	C2-N1-C1'	5.29	124.61	118.80
51	K	1073	U	N1-C2-O2	5.28	126.49	122.80
1	5	1853	G	C4-N9-C1'	5.27	133.35	126.50
51	K	1139	C	C5-C6-N1	5.27	123.64	121.00
1	5	458	C	C2-N1-C1'	5.27	124.59	118.80
51	K	340	C	N3-C2-O2	-5.27	118.21	121.90
51	K	369	C	N1-C2-O2	5.26	122.06	118.90
1	5	961	G	C5-C6-N1	5.26	114.13	111.50
1	5	1686	C	C6-N1-C2	-5.26	118.20	120.30
1	5	30	C	C2-N1-C1'	5.25	124.58	118.80
1	5	2499	C	C6-N1-C2	-5.25	118.20	120.30
51	K	983	A	N3-C4-N9	5.25	131.60	127.40
1	5	654	C	C6-N1-C2	-5.25	118.20	120.30
1	5	3778	U	C2-N1-C1'	5.25	124.00	117.70
1	5	4162	C	N1-C2-O2	5.25	122.05	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1241	C	OP1-P-O3'	5.24	116.74	105.20
1	5	3772	U	N3-C2-O2	-5.24	118.53	122.20
51	K	1061	U	P-O3'-C3'	5.24	125.98	119.70
1	5	3772	U	N1-C2-O2	5.23	126.46	122.80
1	5	50	C	N3-C2-O2	-5.23	118.24	121.90
1	5	3673	C	N1-C2-O2	5.23	122.04	118.90
1	5	266	C	O5'-P-OP2	-5.23	101.00	105.70
1	5	1211	G	P-O3'-C3'	5.22	125.97	119.70
1	5	1807	C	N1-C2-O2	5.22	122.03	118.90
1	5	4871	C	C6-N1-C1'	-5.22	114.53	120.80
51	K	815	U	N1-C2-O2	5.22	126.45	122.80
1	5	1214	C	N1-C2-O2	5.22	122.03	118.90
51	K	142	C	N1-C2-O2	5.22	122.03	118.90
1	5	3670	C	N1-C2-O2	5.21	122.03	118.90
51	K	1518	C	N1-C2-O2	5.21	122.03	118.90
51	K	1798	C	C6-N1-C2	-5.21	118.21	120.30
1	5	1339	U	N3-C2-O2	-5.21	118.55	122.20
51	K	1364	U	C5-C6-N1	5.21	125.31	122.70
51	K	659	G	C8-N9-C1'	-5.21	120.23	127.00
1	5	2011	C	N3-C2-O2	-5.21	118.25	121.90
8	E	46	LEU	CA-CB-CG	5.21	127.28	115.30
1	5	932	A	C4-N9-C1'	5.20	135.66	126.30
1	5	3926	C	C2-N1-C1'	5.20	124.52	118.80
1	5	2362	U	N3-C2-O2	-5.20	118.56	122.20
1	5	1859	C	N1-C2-O2	5.19	122.02	118.90
1	5	2860	C	N1-C2-O2	5.19	122.02	118.90
51	K	1397	U	N3-C2-O2	-5.19	118.56	122.20
3	8	54	C	N1-C2-O2	5.19	122.01	118.90
1	5	1325	C	N1-C2-O2	5.18	122.01	118.90
1	5	2096	G	C4-N9-C1'	5.18	133.24	126.50
1	5	1633	G	P-O3'-C3'	5.18	125.92	119.70
51	K	1389	C	N3-C2-O2	-5.18	118.27	121.90
1	5	2089	G	N3-C4-N9	5.18	129.11	126.00
28	Z	30	ASP	CB-CG-OD1	5.17	122.96	118.30
1	5	486	C	P-O3'-C3'	5.17	125.91	119.70
1	5	1428	U	N3-C2-O2	-5.17	118.58	122.20
51	K	183	G	C2-N3-C4	5.17	114.49	111.90
51	K	1289	U	N3-C2-O2	-5.17	118.58	122.20
51	K	1624	U	O4'-C1'-N1	5.17	112.34	108.20
1	5	3882	C	C2-N1-C1'	5.17	124.49	118.80
1	5	2502	G	P-O3'-C3'	5.17	125.90	119.70
1	5	4942	C	C2-N1-C1'	5.17	124.48	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	657	C	N3-C2-O2	-5.16	118.29	121.90
1	5	2096	G	N3-C4-C5	-5.16	126.02	128.60
45	r	20	ARG	CA-CB-CG	5.16	124.75	113.40
50	3	8	U	C2-N1-C1'	5.16	123.89	117.70
1	5	1241	C	P-O3'-C3'	5.16	125.89	119.70
51	K	1331	C	N1-C2-O2	5.16	121.99	118.90
1	5	690	C	C6-N1-C2	-5.15	118.24	120.30
51	K	293	C	N3-C2-O2	-5.15	118.29	121.90
51	K	687	C	N1-C2-O2	5.15	121.99	118.90
1	5	125	C	P-O3'-C3'	5.15	125.88	119.70
51	K	1709	G	N3-C4-C5	-5.14	126.03	128.60
3	8	135	C	C2-N1-C1'	5.14	124.45	118.80
1	5	218	A	OP1-P-O3'	5.13	116.50	105.20
2	7	28	C	C6-N1-C2	-5.13	118.25	120.30
51	K	914	U	C2-N1-C1'	5.13	123.86	117.70
51	K	93	U	N1-C2-O2	5.13	126.39	122.80
1	5	4119	C	C6-N1-C2	-5.13	118.25	120.30
51	K	1397	U	N1-C2-O2	5.13	126.39	122.80
1	5	515	C	C5-C6-N1	5.12	123.56	121.00
1	5	1848	C	C6-N1-C2	-5.12	118.25	120.30
3	8	2	G	C4-N9-C1'	5.11	133.15	126.50
3	8	64	U	N3-C2-O2	-5.11	118.62	122.20
1	5	250	C	C2-N1-C1'	5.11	124.42	118.80
1	5	2532	C	C2-N1-C1'	5.11	124.42	118.80
1	5	2572	C	C2-N1-C1'	5.11	124.42	118.80
1	5	3594	C	C5-C6-N1	5.10	123.55	121.00
51	K	295	C	C2-N1-C1'	5.10	124.41	118.80
1	5	1816	C	C5-C6-N1	5.10	123.55	121.00
1	5	2362	U	N1-C2-O2	5.09	126.37	122.80
1	5	2856	C	N1-C2-O2	5.09	121.96	118.90
1	5	2502	G	OP1-P-O3'	5.09	116.40	105.20
1	5	275	C	P-O3'-C3'	5.09	125.81	119.70
51	K	1595	U	N1-C2-O2	5.09	126.36	122.80
1	5	1296	G	P-O3'-C3'	5.09	125.80	119.70
1	5	1731	C	C5-C6-N1	5.09	123.54	121.00
1	5	4237	C	C5-C6-N1	5.09	123.54	121.00
1	5	489	C	C2-N1-C1'	5.08	124.39	118.80
51	K	442	C	C5-C6-N1	5.08	123.54	121.00
51	K	1389	C	C2-N1-C1'	5.08	124.39	118.80
1	5	5027	C	N1-C2-O2	5.07	121.94	118.90
50	3	74	C	C2-N1-C1'	5.07	124.38	118.80
3	8	55	U	N3-C2-O2	-5.07	118.65	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1694	C	C6-N1-C2	-5.07	118.27	120.30
1	5	515	C	C2-N1-C1'	5.06	124.37	118.80
1	5	4627	U	N3-C2-O2	-5.06	118.66	122.20
1	5	187	U	P-O3'-C3'	5.06	125.77	119.70
1	5	2410	C	C6-N1-C2	-5.06	118.28	120.30
49	2	33	U	C2-N1-C1'	5.06	123.77	117.70
51	K	887	U	C2-N1-C1'	5.06	123.77	117.70
1	5	2274	C	C6-N1-C2	-5.06	118.28	120.30
1	5	647	G	N3-C4-N9	5.05	129.03	126.00
1	5	919	C	C2-N1-C1'	5.05	124.36	118.80
1	5	1656	U	N3-C2-O2	-5.05	118.67	122.20
1	5	5059	C	P-O3'-C3'	5.04	125.75	119.70
1	5	1280	C	C6-N1-C2	-5.04	118.28	120.30
1	5	4613	C	N1-C2-O2	5.04	121.92	118.90
1	5	506	C	C5-C6-N1	5.04	123.52	121.00
51	K	578	C	C6-N1-C2	-5.03	118.29	120.30
1	5	4885	U	P-O3'-C3'	5.02	125.72	119.70
1	5	1295	C	C2-N1-C1'	5.02	124.32	118.80
51	K	1798	C	C5-C6-N1	5.02	123.51	121.00
49	2	39	U	P-O3'-C3'	5.02	125.72	119.70
51	K	1067	C	C2-N1-C1'	5.02	124.32	118.80
1	5	936	C	N1-C2-O2	5.01	121.91	118.90
1	5	2008	U	C2-N1-C1'	5.01	123.72	117.70
10	G	146	LEU	CA-CB-CG	5.01	126.83	115.30
2	7	102	U	N1-C2-O2	5.01	126.31	122.80
51	K	1185	C	N1-C2-O2	5.01	121.91	118.90
51	K	1649	U	N1-C2-O2	5.01	126.31	122.80
1	5	2410	C	C5-C6-N1	5.01	123.50	121.00
1	5	282	C	N1-C2-O2	5.01	121.90	118.90
51	K	1271	C	C5-C6-N1	5.01	123.50	121.00
1	5	4194	U	C2-N1-C1'	5.00	123.71	117.70

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
76	9	17	TYR	Peptide
76	9	37	TYR	Peptide
5	B	17	LEU	Peptide
5	B	258	HIS	Peptide
20	R	18	GLY	Peptide
21	S	164	LYS	Peptide

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Mol	Chain	Res	Type	Group
23	U	27	HIS	Peptide
67	VV	61	GLN	Mainchain,Peptide
34	f	106	TYR	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	
4	A	242/244 (99%)	222 (92%)	20 (8%)	0	100	100
5	B	392/394 (100%)	370 (94%)	21 (5%)	1 (0%)	41	73
6	C	360/362 (99%)	338 (94%)	22 (6%)	0	100	100
7	D	290/292 (99%)	273 (94%)	17 (6%)	0	100	100
8	E	232/248 (94%)	195 (84%)	37 (16%)	0	100	100
9	F	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
10	G	239/241 (99%)	213 (89%)	26 (11%)	0	100	100
11	H	188/190 (99%)	174 (93%)	14 (7%)	0	100	100
12	I	200/213 (94%)	192 (96%)	8 (4%)	0	100	100
13	J	167/169 (99%)	155 (93%)	12 (7%)	0	100	100
14	L	208/210 (99%)	190 (91%)	17 (8%)	1 (0%)	29	64
15	M	136/138 (99%)	128 (94%)	8 (6%)	0	100	100
16	N	201/203 (99%)	190 (94%)	11 (6%)	0	100	100
17	O	197/199 (99%)	191 (97%)	6 (3%)	0	100	100
18	P	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
19	Q	185/187 (99%)	176 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	R	178/180 (99%)	170 (96%)	8 (4%)	0	100	100
21	S	173/175 (99%)	164 (95%)	8 (5%)	1 (1%)	25	59
22	T	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
23	U	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
24	V	129/131 (98%)	120 (93%)	9 (7%)	0	100	100
25	W	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
26	X	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
27	Y	132/134 (98%)	126 (96%)	6 (4%)	0	100	100
28	Z	133/135 (98%)	122 (92%)	9 (7%)	2 (2%)	10	39
29	a	145/147 (99%)	136 (94%)	9 (6%)	0	100	100
30	b	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
31	c	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
32	d	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
33	e	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
34	f	107/109 (98%)	99 (92%)	8 (8%)	0	100	100
35	g	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
36	h	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
37	i	100/102 (98%)	92 (92%)	8 (8%)	0	100	100
38	j	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
39	k	67/69 (97%)	59 (88%)	8 (12%)	0	100	100
40	l	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
41	m	50/52 (96%)	50 (100%)	0	0	100	100
42	n	21/23 (91%)	21 (100%)	0	0	100	100
43	o	102/104 (98%)	94 (92%)	7 (7%)	1 (1%)	15	49
44	p	89/91 (98%)	84 (94%)	5 (6%)	0	100	100
45	r	123/125 (98%)	110 (89%)	11 (9%)	2 (2%)	9	37
46	s	196/198 (99%)	178 (91%)	18 (9%)	0	100	100
47	t	161/163 (99%)	124 (77%)	36 (22%)	1 (1%)	25	59
48	l	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
52	q	215/217 (99%)	204 (95%)	11 (5%)	0	100	100
53	u	211/213 (99%)	199 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	v	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
55	x	260/262 (99%)	247 (95%)	13 (5%)	0	100	100
56	z	235/237 (99%)	232 (99%)	3 (1%)	0	100	100
57	y	181/189 (96%)	172 (95%)	9 (5%)	0	100	100
58	CC	204/206 (99%)	189 (93%)	15 (7%)	0	100	100
59	XX	183/185 (99%)	178 (97%)	5 (3%)	0	100	100
60	EE	139/151 (92%)	131 (94%)	8 (6%)	0	100	100
61	QQ	147/149 (99%)	146 (99%)	1 (1%)	0	100	100
62	MM	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
63	UU	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
64	YY	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
65	HH	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
66	TT	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
67	VV	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22	57
68	NN	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
69	ZZ	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
70	JJ	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
71	AA	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
72	DD	226/228 (99%)	221 (98%)	5 (2%)	0	100	100
73	BB	181/191 (95%)	170 (94%)	11 (6%)	0	100	100
74	SS	94/96 (98%)	88 (94%)	6 (6%)	0	100	100
75	RR	115/117 (98%)	106 (92%)	9 (8%)	0	100	100
76	9	118/120 (98%)	110 (93%)	8 (7%)	0	100	100
77	II	142/144 (99%)	129 (91%)	13 (9%)	0	100	100
78	PP	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
79	GG	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
80	OO	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
81	FF	60/62 (97%)	60 (100%)	0	0	100	100
82	w	53/55 (96%)	53 (100%)	0	0	100	100
83	0	66/68 (97%)	61 (92%)	5 (8%)	0	100	100
84	6	311/313 (99%)	289 (93%)	22 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	11507/11712 (98%)	10831 (94%)	666 (6%)	10 (0%)	54	83

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	L	64	VAL
67	VV	62	PRO
43	o	97	LYS
45	r	19	LYS
45	r	21	ASN
28	Z	30	ASP
47	t	3	PRO
21	S	165	PRO
28	Z	90	PRO
5	B	259	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	
4	A	187/187 (100%)	182 (97%)	5 (3%)	44	74
5	B	336/342 (98%)	334 (99%)	2 (1%)	86	94
6	C	302/302 (100%)	297 (98%)	5 (2%)	60	83
7	D	247/247 (100%)	247 (100%)	0	100	100
8	E	208/221 (94%)	206 (99%)	2 (1%)	76	90
9	F	194/195 (100%)	194 (100%)	0	100	100
10	G	206/206 (100%)	201 (98%)	5 (2%)	49	76
11	H	169/169 (100%)	167 (99%)	2 (1%)	71	88
12	I	174/180 (97%)	171 (98%)	3 (2%)	60	83
13	J	142/142 (100%)	140 (99%)	2 (1%)	67	86
14	L	176/176 (100%)	174 (99%)	2 (1%)	73	89
15	M	117/117 (100%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	N	171/171 (100%)	170 (99%)	1 (1%)	86	94
17	O	171/171 (100%)	165 (96%)	6 (4%)	36	68
18	P	134/134 (100%)	133 (99%)	1 (1%)	84	93
19	Q	163/163 (100%)	163 (100%)	0	100	100
20	R	159/159 (100%)	157 (99%)	2 (1%)	69	87
21	S	156/156 (100%)	156 (100%)	0	100	100
22	T	139/139 (100%)	138 (99%)	1 (1%)	84	93
23	U	89/89 (100%)	89 (100%)	0	100	100
24	V	101/101 (100%)	100 (99%)	1 (1%)	76	90
25	W	55/55 (100%)	54 (98%)	1 (2%)	59	82
26	X	107/107 (100%)	106 (99%)	1 (1%)	78	91
27	Y	124/124 (100%)	123 (99%)	1 (1%)	81	92
28	Z	117/117 (100%)	116 (99%)	1 (1%)	78	91
29	a	119/119 (100%)	119 (100%)	0	100	100
30	b	62/62 (100%)	61 (98%)	1 (2%)	62	84
31	c	79/79 (100%)	78 (99%)	1 (1%)	69	87
32	d	98/98 (100%)	96 (98%)	2 (2%)	55	80
33	e	114/114 (100%)	113 (99%)	1 (1%)	78	91
34	f	88/88 (100%)	87 (99%)	1 (1%)	73	89
35	g	98/98 (100%)	96 (98%)	2 (2%)	55	80
36	h	109/109 (100%)	108 (99%)	1 (1%)	78	91
37	i	86/86 (100%)	85 (99%)	1 (1%)	71	88
38	j	73/73 (100%)	71 (97%)	2 (3%)	44	74
39	k	64/64 (100%)	64 (100%)	0	100	100
40	l	47/47 (100%)	44 (94%)	3 (6%)	17	48
41	m	48/48 (100%)	48 (100%)	0	100	100
42	n	22/22 (100%)	22 (100%)	0	100	100
43	o	92/92 (100%)	89 (97%)	3 (3%)	38	69
44	p	74/74 (100%)	72 (97%)	2 (3%)	44	74
45	r	109/109 (100%)	105 (96%)	4 (4%)	34	66
46	s	166/166 (100%)	165 (99%)	1 (1%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	t	136/136 (100%)	133 (98%)	3 (2%)	52	78
48	l	22/22 (100%)	21 (96%)	1 (4%)	27	60
52	q	180/181 (99%)	179 (99%)	1 (1%)	86	94
53	u	194/194 (100%)	191 (98%)	3 (2%)	65	85
54	v	187/187 (100%)	185 (99%)	2 (1%)	73	89
55	x	224/224 (100%)	222 (99%)	2 (1%)	78	91
56	z	207/207 (100%)	205 (99%)	2 (1%)	76	90
57	y	165/169 (98%)	165 (100%)	0	100	100
58	CC	178/178 (100%)	175 (98%)	3 (2%)	60	83
59	XX	161/161 (100%)	158 (98%)	3 (2%)	57	81
60	EE	130/136 (96%)	127 (98%)	3 (2%)	50	77
61	QQ	130/130 (100%)	129 (99%)	1 (1%)	81	92
62	MM	106/106 (100%)	104 (98%)	2 (2%)	57	81
63	UU	117/117 (100%)	114 (97%)	3 (3%)	46	74
64	YY	119/119 (100%)	119 (100%)	0	100	100
65	HH	67/67 (100%)	66 (98%)	1 (2%)	65	85
66	TT	112/112 (100%)	112 (100%)	0	100	100
67	VV	113/113 (100%)	113 (100%)	0	100	100
68	NN	107/107 (100%)	106 (99%)	1 (1%)	78	91
69	ZZ	88/88 (100%)	88 (100%)	0	100	100
70	JJ	75/75 (100%)	74 (99%)	1 (1%)	69	87
71	AA	46/46 (100%)	44 (96%)	2 (4%)	29	62
72	DD	190/190 (100%)	185 (97%)	5 (3%)	46	74
73	BB	158/161 (98%)	158 (100%)	0	100	100
74	SS	87/87 (100%)	86 (99%)	1 (1%)	73	89
75	RR	99/99 (100%)	98 (99%)	1 (1%)	76	90
76	9	109/109 (100%)	108 (99%)	1 (1%)	78	91
77	II	125/125 (100%)	124 (99%)	1 (1%)	81	92
78	PP	111/111 (100%)	110 (99%)	1 (1%)	78	91
79	GG	92/92 (100%)	91 (99%)	1 (1%)	73	89
80	OO	66/66 (100%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
81	FF	55/55 (100%)	54 (98%)	1 (2%)	59	82
82	w	48/48 (100%)	48 (100%)	0	100	100
83	0	61/61 (100%)	60 (98%)	1 (2%)	62	84
84	6	272/272 (100%)	270 (99%)	2 (1%)	84	93
All	All	10029/10069 (100%)	9911 (99%)	118 (1%)	72	88

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	64	ARG
4	A	128	ARG
4	A	163	ARG
4	A	193	ARG
4	A	242	ARG
5	B	24	ARG
5	B	62	ARG
6	C	38	ASN
6	C	100	ARG
6	C	114	ARG
6	C	188	ARG
6	C	321	ASN
8	E	52	ARG
8	E	178	ASN
10	G	38	ASN
10	G	81	ASN
10	G	189	ARG
10	G	196	ARG
10	G	240	ASN
11	H	1	MET
11	H	28	LYS
12	I	3	ARG
12	I	100	ASN
12	I	144	ASN
13	J	146	ARG
13	J	151	ILE
14	L	104	ASN
14	L	162	LYS
16	N	38	ARG
17	O	12	ARG
17	O	65	ASN
17	O	94	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	O	117	ARG
17	O	187	LYS
17	O	191	ARG
18	P	128	ARG
20	R	39	GLN
20	R	133	LYS
22	T	63	ARG
24	V	48	ARG
25	W	45	ASN
26	X	94	ASN
27	Y	2	LYS
28	Z	97	ASN
30	b	60	ASN
31	c	90	ARG
32	d	18	ASN
32	d	23	ARG
33	e	43	ASN
34	f	16	ARG
35	g	21	ARG
35	g	29	ARG
36	h	96	ASN
37	i	29	ARG
38	j	20	ARG
38	j	45	ARG
40	l	21	ARG
40	l	33	ASN
40	l	36	ARG
43	o	9	ARG
43	o	69	ARG
43	o	82	MET
44	p	17	ARG
44	p	49	ARG
45	r	12	ASN
45	r	21	ASN
45	r	31	ASN
45	r	83	ASN
46	s	62	ARG
47	t	1	MET
47	t	40	LYS
47	t	123	ARG
48	l	260	MET
52	q	50	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
53	u	40	ASN
53	u	147	ASN
53	u	213	ARG
54	v	167	ARG
54	v	248	TYR
55	x	232	ASN
55	x	240	ARG
56	z	63	MET
56	z	191	ARG
58	CC	84	ASN
58	CC	87	ASN
58	CC	99	ASN
59	XX	69	ARG
59	XX	70	ARG
59	XX	79	ARG
60	EE	20	LYS
60	EE	69	ARG
60	EE	97	ARG
61	QQ	27	LYS
62	MM	146	ARG
62	MM	150	ARG
63	UU	41	MET
63	UU	85	ARG
63	UU	146	ARG
65	HH	82	ASN
68	NN	101	LYS
70	JJ	81	ARG
71	AA	99	LYS
71	AA	104	ARG
72	DD	22	ASN
72	DD	76	ARG
72	DD	94	ARG
72	DD	106	ARG
72	DD	227	LYS
74	SS	96	ARG
75	RR	33	ARG
76	9	13	ARG
77	II	8	LYS
78	PP	62	ARG
79	GG	47	ASN
81	FF	40	ARG
83	0	138	ARG

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Mol	Chain	Res	Type
84	6	159	ASN
84	6	178	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
5	B	167	GLN
5	B	204	GLN
5	B	245	HIS
5	B	302	ASN
5	B	354	GLN
6	C	38	ASN
6	C	50	GLN
7	D	225	GLN
8	E	178	ASN
8	E	275	ASN
8	E	280	HIS
9	F	41	GLN
9	F	112	GLN
9	F	133	ASN
10	G	38	ASN
10	G	46	GLN
10	G	81	ASN
10	G	112	GLN
10	G	240	ASN
11	H	8	GLN
11	H	39	ASN
12	I	95	HIS
12	I	144	ASN
14	L	19	GLN
16	N	181	HIS
16	N	201	HIS
17	O	50	ASN
17	O	65	ASN
17	O	199	HIS
18	P	75	GLN
18	P	80	GLN
20	R	58	HIS
20	R	130	ASN
21	S	50	GLN
21	S	163	HIS
22	T	3	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
22	T	95	HIS
22	T	127	GLN
24	V	77	HIS
25	W	17	HIS
25	W	45	ASN
26	X	93	ASN
26	X	94	ASN
26	X	111	GLN
28	Z	97	ASN
29	a	14	HIS
31	c	15	ASN
31	c	51	ASN
32	d	18	ASN
32	d	30	HIS
33	e	43	ASN
33	e	52	GLN
34	f	80	ASN
34	f	99	HIS
35	g	100	GLN
35	g	112	GLN
36	h	63	GLN
36	h	96	ASN
40	l	33	ASN
44	p	92	GLN
45	r	12	ASN
45	r	21	ASN
45	r	31	ASN
45	r	83	ASN
46	s	191	GLN
48	l	253	GLN
52	q	50	ASN
52	q	111	GLN
52	q	141	ASN
53	u	101	HIS
53	u	124	HIS
53	u	147	ASN
53	u	157	GLN
54	v	113	GLN
54	v	272	HIS
55	x	36	HIS
55	x	67	GLN
55	x	232	ASN

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Mol	Chain	Res	Type
56	z	81	HIS
56	z	202	ASN
57	y	186	ASN
58	CC	84	ASN
58	CC	87	ASN
58	CC	88	ASN
58	CC	99	ASN
58	CC	138	ASN
58	CC	165	GLN
60	EE	83	GLN
62	MM	94	HIS
63	UU	11	GLN
63	UU	35	ASN
63	UU	80	GLN
63	UU	97	GLN
64	YY	62	GLN
65	HH	47	ASN
65	HH	82	ASN
66	TT	113	HIS
68	NN	15	ASN
68	NN	63	HIS
71	AA	117	ASN
72	DD	22	ASN
73	BB	114	ASN
74	SS	44	HIS
75	RR	48	HIS
75	RR	82	ASN
76	9	41	GLN
79	GG	47	ASN
81	FF	29	GLN
84	6	159	ASN
84	6	178	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3649/3662 (99%)	841 (23%)	72 (1%)
2	7	119/120 (99%)	16 (13%)	0
3	8	155/156 (99%)	40 (25%)	1 (0%)
49	2	74/76 (97%)	23 (31%)	1 (1%)
50	3	72/75 (96%)	13 (18%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	K	1686/1698 (99%)	352 (20%)	22 (1%)
85	4	9/10 (90%)	4 (44%)	0
All	All	5764/5797 (99%)	1289 (22%)	97 (1%)

All (1289) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	2	G
1	5	8	U
1	5	11	G
1	5	12	A
1	5	13	U
1	5	25	A
1	5	35	U
1	5	39	A
1	5	42	A
1	5	43	U
1	5	47	A
1	5	48	G
1	5	49	U
1	5	56	A
1	5	58	G
1	5	59	A
1	5	64	A
1	5	65	A
1	5	73	A
1	5	76	A
1	5	84	A
1	5	91	G
1	5	104	G
1	5	108	A
1	5	109	G
1	5	110	C
1	5	112	C
1	5	116	G
1	5	119	G
1	5	126	C
1	5	134	G
1	5	135	G
1	5	136	C
1	5	143	C
1	5	144	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	159	C
1	5	166	C
1	5	167	C
1	5	171	U
1	5	172	C
1	5	173	C
1	5	182	G
1	5	183	C
1	5	184	U
1	5	185	C
1	5	186	G
1	5	187	U
1	5	188	G
1	5	189	G
1	5	200	U
1	5	201	C
1	5	210	C
1	5	216	C
1	5	217	C
1	5	218	A
1	5	219	G
1	5	220	C
1	5	224	U
1	5	225	G
1	5	226	G
1	5	233	U
1	5	234	G
1	5	246	G
1	5	262	G
1	5	265	C
1	5	266	C
1	5	267	G
1	5	276	C
1	5	277	G
1	5	278	G
1	5	280	G
1	5	297	U
1	5	301	G
1	5	306	A
1	5	309	C
1	5	315	G
1	5	316	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	334	A
1	5	340	C
1	5	345	C
1	5	350	C
1	5	363	A
1	5	383	A
1	5	387	G
1	5	399	G
1	5	407	A
1	5	409	G
1	5	410	A
1	5	412	G
1	5	413	G
1	5	440	U
1	5	450	G
1	5	451	C
1	5	452	A
1	5	453	G
1	5	454	U
1	5	455	C
1	5	465	G
1	5	467	U
1	5	468	U
1	5	470	A
1	5	480	C
1	5	485	C
1	5	486	C
1	5	487	G
1	5	499	G
1	5	500	G
1	5	501	C
1	5	503	C
1	5	504	G
1	5	506	C
1	5	513	U
1	5	514	U
1	5	515	C
1	5	519	C
1	5	647	G
1	5	649	A
1	5	654	C
1	5	663	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	664	G
1	5	666	G
1	5	667	A
1	5	683	C
1	5	684	G
1	5	685	C
1	5	686	A
1	5	690	C
1	5	694	C
1	5	695	G
1	5	696	C
1	5	697	G
1	5	702	U
1	5	703	G
1	5	704	C
1	5	707	C
1	5	716	C
1	5	718	C
1	5	728	U
1	5	729	G
1	5	730	G
1	5	732	A
1	5	737	C
1	5	746	A
1	5	747	A
1	5	748	G
1	5	749	G
1	5	914	U
1	5	917	A
1	5	918	G
1	5	920	C
1	5	926	G
1	5	927	G
1	5	930	G
1	5	931	C
1	5	932	A
1	5	933	G
1	5	934	C
1	5	936	C
1	5	937	U
1	5	938	C
1	5	939	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	942	G
1	5	944	A
1	5	945	U
1	5	946	C
1	5	957	G
1	5	958	G
1	5	960	A
1	5	961	G
1	5	962	C
1	5	963	G
1	5	964	A
1	5	965	G
1	5	966	A
1	5	967	C
1	5	968	C
1	5	969	C
1	5	970	G
1	5	971	U
1	5	973	G
1	5	976	G
1	5	978	G
1	5	982	U
1	5	989	U
1	5	990	C
1	5	991	C
1	5	1068	G
1	5	1070	G
1	5	1072	C
1	5	1078	A
1	5	1083	U
1	5	1177	U
1	5	1178	G
1	5	1183	C
1	5	1187	G
1	5	1188	C
1	5	1209	U
1	5	1210	C
1	5	1211	G
1	5	1212	G
1	5	1215	C
1	5	1219	G
1	5	1221	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	1233	G
1	5	1237	C
1	5	1238	A
1	5	1239	C
1	5	1242	G
1	5	1243	C
1	5	1244	G
1	5	1255	A
1	5	1267	C
1	5	1268	G
1	5	1269	G
1	5	1270	A
1	5	1272	C
1	5	1273	G
1	5	1274	A
1	5	1279	A
1	5	1280	C
1	5	1281	G
1	5	1282	G
1	5	1285	U
1	5	1286	C
1	5	1288	G
1	5	1290	G
1	5	1293	G
1	5	1297	U
1	5	1301	C
1	5	1319	U
1	5	1326	A
1	5	1330	A
1	5	1344	C
1	5	1354	A
1	5	1358	G
1	5	1367	C
1	5	1368	A
1	5	1370	G
1	5	1371	A
1	5	1372	A
1	5	1377	G
1	5	1378	C
1	5	1379	C
1	5	1387	A
1	5	1394	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	1397	A
1	5	1399	G
1	5	1408	G
1	5	1410	U
1	5	1411	C
1	5	1419	G
1	5	1420	A
1	5	1421	G
1	5	1429	C
1	5	1437	C
1	5	1439	C
1	5	1440	U
1	5	1441	C
1	5	1445	U
1	5	1446	C
1	5	1448	G
1	5	1451	G
1	5	1456	C
1	5	1457	G
1	5	1458	C
1	5	1465	G
1	5	1475	G
1	5	1482	G
1	5	1483	C
1	5	1497	A
1	5	1498	G
1	5	1501	C
1	5	1502	G
1	5	1514	U
1	5	1516	G
1	5	1518	A
1	5	1523	A
1	5	1525	A
1	5	1534	A
1	5	1535	C
1	5	1547	A
1	5	1563	A
1	5	1564	A
1	5	1566	C
1	5	1574	G
1	5	1578	U
1	5	1591	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	1596	U
1	5	1597	G
1	5	1602	U
1	5	1607	C
1	5	1612	G
1	5	1613	A
1	5	1624	G
1	5	1625	G
1	5	1631	A
1	5	1633	G
1	5	1634	A
1	5	1638	A
1	5	1640	C
1	5	1641	G
1	5	1649	U
1	5	1650	A
1	5	1654	G
1	5	1660	U
1	5	1661	C
1	5	1676	C
1	5	1677	U
1	5	1680	G
1	5	1694	C
1	5	1698	C
1	5	1719	A
1	5	1720	C
1	5	1721	G
1	5	1724	G
1	5	1731	C
1	5	1741	G
1	5	1742	A
1	5	1754	U
1	5	1755	C
1	5	1756	U
1	5	1757	U
1	5	1759	G
1	5	1760	G
1	5	1761	G
1	5	1764	G
1	5	1765	A
1	5	1768	C
1	5	1769	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	1772	C
1	5	1775	A
1	5	1776	A
1	5	1777	C
1	5	1780	A
1	5	1781	U
1	5	1787	A
1	5	1799	G
1	5	1803	G
1	5	1804	A
1	5	1805	A
1	5	1812	C
1	5	1815	G
1	5	1819	G
1	5	1820	C
1	5	1821	G
1	5	1822	U
1	5	1828	C
1	5	1833	G
1	5	1834	U
1	5	1835	G
1	5	1836	G
1	5	1840	G
1	5	1848	C
1	5	1855	G
1	5	1869	G
1	5	1882	U
1	5	1888	A
1	5	1889	U
1	5	1890	G
1	5	1897	A
1	5	1906	U
1	5	1910	G
1	5	1916	G
1	5	1918	U
1	5	1920	C
1	5	1921	C
1	5	1922	G
1	5	1925	G
1	5	1928	C
1	5	1930	U
1	5	1931	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	1932	A
1	5	1957	U
1	5	1958	A
1	5	1959	U
1	5	1960	A
1	5	1961	G
1	5	1962	A
1	5	1964	A
1	5	1966	C
1	5	1967	A
1	5	1968	G
1	5	1969	G
1	5	1970	A
1	5	1971	C
1	5	1975	G
1	5	1976	G
1	5	1978	C
1	5	1980	U
1	5	1981	G
1	5	1985	G
1	5	1987	C
1	5	1988	G
1	5	1991	A
1	5	1993	C
1	5	1997	U
1	5	2001	G
1	5	2002	A
1	5	2003	G
1	5	2007	G
1	5	2010	A
1	5	2011	C
1	5	2016	C
1	5	2017	A
1	5	2026	A
1	5	2044	U
1	5	2047	A
1	5	2048	U
1	5	2052	G
1	5	2055	G
1	5	2056	G
1	5	2069	A
1	5	2084	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	2085	G
1	5	2089	G
1	5	2090	U
1	5	2092	G
1	5	2093	A
1	5	2094	G
1	5	2095	A
1	5	2097	U
1	5	2101	C
1	5	2105	A
1	5	2107	C
1	5	2108	G
1	5	2109	G
1	5	2110	C
1	5	2111	G
1	5	2112	G
1	5	2113	G
1	5	2114	G
1	5	2116	C
1	5	2117	G
1	5	2119	C
1	5	2120	G
1	5	2122	G
1	5	2123	C
1	5	2124	G
1	5	2126	G
1	5	2127	C
1	5	2247	C
1	5	2248	C
1	5	2250	C
1	5	2251	G
1	5	2252	G
1	5	2253	A
1	5	2254	G
1	5	2257	C
1	5	2258	C
1	5	2259	G
1	5	2260	C
1	5	2261	G
1	5	2263	A
1	5	2264	C
1	5	2265	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	2266	C
1	5	2267	U
1	5	2268	A
1	5	2279	A
1	5	2289	C
1	5	2300	A
1	5	2301	G
1	5	2306	G
1	5	2313	A
1	5	2314	G
1	5	2316	G
1	5	2322	G
1	5	2331	G
1	5	2333	G
1	5	2348	G
1	5	2350	U
1	5	2351	C
1	5	2360	A
1	5	2395	A
1	5	2396	A
1	5	2410	C
1	5	2417	A
1	5	2422	C
1	5	2425	U
1	5	2433	G
1	5	2438	A
1	5	2440	U
1	5	2441	C
1	5	2450	G
1	5	2471	G
1	5	2488	C
1	5	2489	C
1	5	2490	U
1	5	2491	C
1	5	2503	G
1	5	2504	C
1	5	2505	C
1	5	2506	G
1	5	2513	A
1	5	2514	G
1	5	2517	A
1	5	2529	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	2530	U
1	5	2537	A
1	5	2544	G
1	5	2546	G
1	5	2547	G
1	5	2549	G
1	5	2553	A
1	5	2554	U
1	5	2571	C
1	5	2572	C
1	5	2575	U
1	5	2581	A
1	5	2583	C
1	5	2587	A
1	5	2589	C
1	5	2618	G
1	5	2638	G
1	5	2661	U
1	5	2662	G
1	5	2669	C
1	5	2670	C
1	5	2681	G
1	5	2686	G
1	5	2687	U
1	5	2694	G
1	5	2695	A
1	5	2696	A
1	5	2710	C
1	5	2711	G
1	5	2712	G
1	5	2714	G
1	5	2721	G
1	5	2725	A
1	5	2726	G
1	5	2740	U
1	5	2752	G
1	5	2754	G
1	5	2761	U
1	5	2762	G
1	5	2763	U
1	5	2767	U
1	5	2768	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	2769	U
1	5	2770	C
1	5	2787	A
1	5	2788	U
1	5	2790	U
1	5	2794	C
1	5	2798	A
1	5	2806	A
1	5	2814	C
1	5	2826	U
1	5	2827	G
1	5	2828	U
1	5	2833	A
1	5	2842	G
1	5	2849	A
1	5	2855	G
1	5	2857	A
1	5	2867	C
1	5	2897	G
1	5	2898	G
1	5	2904	U
1	5	2905	C
1	5	3593	C
1	5	3595	U
1	5	3596	A
1	5	3597	G
1	5	3602	C
1	5	3605	C
1	5	3616	U
1	5	3617	G
1	5	3625	G
1	5	3626	G
1	5	3630	A
1	5	3635	A
1	5	3636	C
1	5	3648	A
1	5	3662	A
1	5	3670	C
1	5	3673	C
1	5	3692	A
1	5	3705	G
1	5	3710	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	3711	A
1	5	3729	U
1	5	3748	A
1	5	3760	A
1	5	3761	C
1	5	3772	U
1	5	3774	A
1	5	3777	G
1	5	3778	U
1	5	3784	A
1	5	3786	U
1	5	3799	A
1	5	3802	U
1	5	3810	C
1	5	3811	G
1	5	3812	C
1	5	3814	U
1	5	3817	A
1	5	3819	G
1	5	3840	U
1	5	3843	C
1	5	3860	A
1	5	3870	C
1	5	3876	A
1	5	3877	A
1	5	3878	C
1	5	3879	G
1	5	3889	G
1	5	3892	U
1	5	3897	G
1	5	3898	G
1	5	3901	A
1	5	3905	A
1	5	3906	A
1	5	3907	G
1	5	3908	A
1	5	3915	U
1	5	3926	C
1	5	3938	G
1	5	3939	G
1	5	3943	A
1	5	4069	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	4070	U
1	5	4076	G
1	5	4084	G
1	5	4085	A
1	5	4086	G
1	5	4088	C
1	5	4090	G
1	5	4094	G
1	5	4097	G
1	5	4099	G
1	5	4104	G
1	5	4107	G
1	5	4114	C
1	5	4115	G
1	5	4116	C
1	5	4117	U
1	5	4119	C
1	5	4120	U
1	5	4121	G
1	5	4125	C
1	5	4127	A
1	5	4128	A
1	5	4143	G
1	5	4144	C
1	5	4145	C
1	5	4151	G
1	5	4158	C
1	5	4162	C
1	5	4164	C
1	5	4166	G
1	5	4170	A
1	5	4171	C
1	5	4173	G
1	5	4183	G
1	5	4184	G
1	5	4191	G
1	5	4203	A
1	5	4212	A
1	5	4225	G
1	5	4228	G
1	5	4229	U
1	5	4233	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	4234	A
1	5	4243	C
1	5	4249	G
1	5	4251	A
1	5	4254	G
1	5	4255	A
1	5	4265	U
1	5	4268	A
1	5	4271	A
1	5	4273	A
1	5	4280	A
1	5	4282	A
1	5	4290	U
1	5	4291	G
1	5	4292	A
1	5	4297	G
1	5	4304	A
1	5	4305	G
1	5	4306	U
1	5	4313	A
1	5	4314	C
1	5	4317	A
1	5	4318	C
1	5	4319	C
1	5	4323	A
1	5	4326	G
1	5	4329	G
1	5	4330	G
1	5	4332	C
1	5	4339	A
1	5	4349	C
1	5	4350	C
1	5	4354	U
1	5	4355	G
1	5	4376	A
1	5	4377	G
1	5	4378	A
1	5	4379	A
1	5	4387	C
1	5	4393	G
1	5	4394	A
1	5	4405	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	4419	U
1	5	4421	C
1	5	4422	A
1	5	4426	C
1	5	4436	U
1	5	4437	U
1	5	4440	G
1	5	4444	C
1	5	4448	G
1	5	4449	A
1	5	4464	A
1	5	4471	U
1	5	4475	G
1	5	4476	C
1	5	4482	U
1	5	4500	U
1	5	4510	A
1	5	4512	U
1	5	4513	A
1	5	4518	A
1	5	4519	C
1	5	4524	G
1	5	4528	G
1	5	4529	G
1	5	4531	U
1	5	4548	A
1	5	4549	G
1	5	4557	U
1	5	4560	C
1	5	4567	G
1	5	4570	G
1	5	4573	G
1	5	4575	G
1	5	4581	G
1	5	4590	A
1	5	4599	A
1	5	4617	G
1	5	4636	U
1	5	4637	G
1	5	4639	G
1	5	4642	U
1	5	4652	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	4656	A
1	5	4657	U
1	5	4661	G
1	5	4667	C
1	5	4670	C
1	5	4672	A
1	5	4677	U
1	5	4682	U
1	5	4687	A
1	5	4693	C
1	5	4694	G
1	5	4695	C
1	5	4697	U
1	5	4700	A
1	5	4709	U
1	5	4719	G
1	5	4720	C
1	5	4730	C
1	5	4731	G
1	5	4732	G
1	5	4738	C
1	5	4741	C
1	5	4744	A
1	5	4745	G
1	5	4746	C
1	5	4750	G
1	5	4753	U
1	5	4756	C
1	5	4758	U
1	5	4763	U
1	5	4764	A
1	5	4770	U
1	5	4771	C
1	5	4868	G
1	5	4869	U
1	5	4871	C
1	5	4873	G
1	5	4876	U
1	5	4878	C
1	5	4883	C
1	5	4884	G
1	5	4886	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	4889	G
1	5	4890	G
1	5	4895	C
1	5	4896	G
1	5	4901	G
1	5	4902	C
1	5	4903	G
1	5	4910	G
1	5	4911	A
1	5	4912	G
1	5	4913	G
1	5	4914	C
1	5	4927	G
1	5	4930	C
1	5	4931	G
1	5	4933	C
1	5	4936	G
1	5	4937	C
1	5	4941	G
1	5	4944	C
1	5	4945	G
1	5	4949	G
1	5	4951	G
1	5	4959	U
1	5	4964	C
1	5	4965	U
1	5	4966	A
1	5	4975	G
1	5	4976	U
1	5	4985	U
1	5	4988	U
1	5	4989	U
1	5	4990	C
1	5	4991	U
1	5	4999	G
1	5	5006	U
1	5	5013	C
1	5	5017	G
1	5	5023	C
1	5	5027	C
1	5	5028	G
1	5	5041	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	5047	C
1	5	5050	C
1	5	5052	C
1	5	5053	U
1	5	5054	C
1	5	5056	A
1	5	5060	A
1	5	5061	A
2	7	7	G
2	7	13	A
2	7	22	A
2	7	25	G
2	7	40	U
2	7	53	U
2	7	54	A
2	7	63	C
2	7	64	G
2	7	97	G
2	7	98	G
2	7	100	A
2	7	102	U
2	7	110	G
2	7	111	C
2	7	120	U
3	8	2	G
3	8	34	U
3	8	35	C
3	8	37	A
3	8	39	G
3	8	49	G
3	8	51	U
3	8	59	A
3	8	60	G
3	8	61	A
3	8	62	A
3	8	63	U
3	8	75	G
3	8	80	A
3	8	81	C
3	8	82	A
3	8	83	C
3	8	84	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	8	85	U
3	8	86	U
3	8	87	G
3	8	90	C
3	8	94	G
3	8	99	U
3	8	103	A
3	8	105	C
3	8	107	C
3	8	109	C
3	8	110	U
3	8	111	U
3	8	114	G
3	8	123	U
3	8	124	U
3	8	125	C
3	8	126	C
3	8	127	U
3	8	128	C
3	8	147	G
3	8	150	C
3	8	153	C
49	2	4	U
49	2	8	U
49	2	9	A
49	2	13	C
49	2	19	G
49	2	20	C
49	2	21	A
49	2	34	C
49	2	35	A
49	2	39	U
49	2	40	C
49	2	41	U
49	2	44	A
49	2	45	G
49	2	46	G
49	2	47	U
49	2	48	C
49	2	58	A
49	2	59	A
49	2	72	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	2	73	A
49	2	74	C
49	2	76	A
50	3	9	A
50	3	13	C
50	3	16	C
50	3	21	A
50	3	37	A
50	3	47	U
50	3	48	C
50	3	49	C
50	3	61	C
50	3	63	C
50	3	69	G
50	3	75	C
50	3	76	A
51	K	2	A
51	K	3	C
51	K	4	C
51	K	20	G
51	K	25	A
51	K	26	U
51	K	33	G
51	K	41	G
51	K	42	A
51	K	44	U
51	K	45	A
51	K	46	A
51	K	56	G
51	K	65	C
51	K	67	C
51	K	68	A
51	K	70	G
51	K	71	G
51	K	73	C
51	K	74	G
51	K	77	A
51	K	79	A
51	K	103	A
51	K	111	A
51	K	113	G
51	K	115	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
51	K	124	U
51	K	126	G
51	K	128	U
51	K	129	C
51	K	130	G
51	K	141	A
51	K	142	C
51	K	143	U
51	K	147	A
51	K	155	G
51	K	158	A
51	K	162	C
51	K	171	A
51	K	180	G
51	K	182	C
51	K	183	G
51	K	184	G
51	K	187	G
51	K	188	C
51	K	189	U
51	K	191	A
51	K	192	C
51	K	215	G
51	K	289	G
51	K	294	U
51	K	304	C
51	K	305	U
51	K	306	C
51	K	307	G
51	K	308	G
51	K	309	G
51	K	310	C
51	K	312	G
51	K	314	U
51	K	317	C
51	K	318	A
51	K	319	C
51	K	323	C
51	K	332	G
51	K	335	G
51	K	340	C
51	K	347	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
51	K	350	C
51	K	351	G
51	K	360	A
51	K	362	C
51	K	364	A
51	K	368	U
51	K	369	C
51	K	370	G
51	K	381	C
51	K	385	G
51	K	386	C
51	K	398	A
51	K	400	C
51	K	408	A
51	K	409	C
51	K	417	C
51	K	418	A
51	K	421	G
51	K	426	A
51	K	435	A
51	K	438	G
51	K	448	A
51	K	450	C
51	K	455	A
51	K	464	A
51	K	465	A
51	K	466	G
51	K	471	G
51	K	472	C
51	K	473	A
51	K	474	G
51	K	476	A
51	K	482	G
51	K	487	U
51	K	492	C
51	K	525	A
51	K	530	U
51	K	532	C
51	K	533	A
51	K	547	G
51	K	548	C
51	K	549	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
51	K	550	C
51	K	551	U
51	K	554	A
51	K	555	A
51	K	556	U
51	K	559	G
51	K	560	A
51	K	564	A
51	K	568	C
51	K	576	A
51	K	583	A
51	K	588	G
51	K	590	A
51	K	591	U
51	K	606	G
51	K	608	C
51	K	614	C
51	K	615	C
51	K	617	G
51	K	621	C
51	K	624	C
51	K	626	A
51	K	628	A
51	K	643	A
51	K	644	G
51	K	660	C
51	K	662	G
51	K	663	C
51	K	664	A
51	K	668	A
51	K	669	A
51	K	671	A
51	K	672	A
51	K	673	G
51	K	683	G
51	K	688	U
51	K	689	U
51	K	752	G
51	K	753	C
51	K	754	G
51	K	798	G
51	K	799	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
51	K	810	A
51	K	811	A
51	K	821	G
51	K	822	U
51	K	830	A
51	K	834	C
51	K	844	U
51	K	845	G
51	K	847	A
51	K	870	A
51	K	871	U
51	K	872	A
51	K	873	G
51	K	875	A
51	K	878	G
51	K	887	U
51	K	890	U
51	K	892	U
51	K	901	G
51	K	903	A
51	K	904	A
51	K	909	G
51	K	913	A
51	K	914	U
51	K	917	U
51	K	920	A
51	K	933	G
51	K	934	G
51	K	970	G
51	K	971	G
51	K	978	G
51	K	990	A
51	K	992	A
51	K	999	G
51	K	1017	U
51	K	1023	A
51	K	1041	G
51	K	1045	U
51	K	1060	A
51	K	1061	U
51	K	1062	A
51	K	1078	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
51	K	1083	A
51	K	1085	C
51	K	1086	G
51	K	1089	G
51	K	1097	G
51	K	1100	A
51	K	1113	A
51	K	1115	U
51	K	1116	C
51	K	1117	C
51	K	1118	C
51	K	1121	G
51	K	1126	G
51	K	1131	G
51	K	1133	A
51	K	1138	C
51	K	1139	C
51	K	1149	A
51	K	1150	A
51	K	1153	C
51	K	1154	U
51	K	1155	U
51	K	1161	U
51	K	1170	A
51	K	1195	A
51	K	1208	A
51	K	1215	C
51	K	1221	G
51	K	1224	G
51	K	1242	U
51	K	1251	A
51	K	1253	A
51	K	1256	G
51	K	1257	G
51	K	1259	A
51	K	1264	C
51	K	1271	C
51	K	1274	G
51	K	1275	G
51	K	1284	A
51	K	1285	G
51	K	1286	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
51	K	1298	G
51	K	1299	A
51	K	1301	A
51	K	1302	G
51	K	1303	C
51	K	1307	U
51	K	1308	U
51	K	1310	U
51	K	1314	U
51	K	1333	U
51	K	1341	C
51	K	1342	U
51	K	1345	G
51	K	1348	G
51	K	1371	U
51	K	1372	U
51	K	1376	A
51	K	1378	A
51	K	1382	A
51	K	1394	G
51	K	1395	C
51	K	1396	A
51	K	1397	U
51	K	1401	A
51	K	1402	A
51	K	1409	A
51	K	1410	C
51	K	1412	C
51	K	1428	G
51	K	1442	U
51	K	1447	G
51	K	1449	G
51	K	1452	A
51	K	1454	A
51	K	1455	A
51	K	1462	U
51	K	1463	U
51	K	1466	G
51	K	1473	G
51	K	1476	A
51	K	1477	U
51	K	1489	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
51	K	1490	G
51	K	1494	U
51	K	1497	G
51	K	1498	A
51	K	1507	G
51	K	1509	U
51	K	1510	G
51	K	1521	C
51	K	1522	A
51	K	1533	A
51	K	1535	U
51	K	1536	G
51	K	1544	C
51	K	1548	G
51	K	1552	G
51	K	1553	C
51	K	1554	C
51	K	1555	U
51	K	1556	A
51	K	1557	C
51	K	1567	G
51	K	1570	G
51	K	1574	C
51	K	1575	G
51	K	1580	A
51	K	1585	U
51	K	1586	U
51	K	1587	G
51	K	1588	A
51	K	1598	G
51	K	1601	A
51	K	1604	G
51	K	1606	G
51	K	1621	U
51	K	1623	A
51	K	1637	A
51	K	1638	G
51	K	1646	C
51	K	1648	G
51	K	1664	A
51	K	1665	G
51	K	1680	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
51	K	1682	C
51	K	1683	C
51	K	1695	A
51	K	1699	A
51	K	1715	A
51	K	1721	U
51	K	1722	G
51	K	1725	U
51	K	1726	G
51	K	1744	G
51	K	1748	G
51	K	1753	C
51	K	1756	C
51	K	1783	C
51	K	1799	G
51	K	1814	G
51	K	1815	A
51	K	1823	A
51	K	1824	A
51	K	1825	A
51	K	1826	G
51	K	1831	A
51	K	1836	G
51	K	1838	U
51	K	1849	G
51	K	1851	A
51	K	1852	C
51	K	1861	G
51	K	1862	G
51	K	1863	A
51	K	1865	C
51	K	1869	A
85	4	45	A
85	4	46	U
85	4	49	A
85	4	50	U

All (97) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	1	C
1	5	48	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	125	C
1	5	134	G
1	5	170	C
1	5	187	U
1	5	216	C
1	5	218	A
1	5	245	C
1	5	265	C
1	5	275	C
1	5	451	C
1	5	454	U
1	5	486	C
1	5	684	G
1	5	693	C
1	5	930	G
1	5	943	A
1	5	956	A
1	5	989	U
1	5	1211	G
1	5	1232	G
1	5	1236	C
1	5	1238	A
1	5	1296	G
1	5	1329	G
1	5	1407	C
1	5	1440	U
1	5	1455	G
1	5	1633	G
1	5	1804	A
1	5	1818	G
1	5	1835	G
1	5	2015	U
1	5	2017	A
1	5	2046	G
1	5	2083	C
1	5	2089	G
1	5	2093	A
1	5	2107	C
1	5	2116	C
1	5	2123	C
1	5	2256	C
1	5	2257	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	5	2260	C
1	5	2262	G
1	5	2266	C
1	5	2502	G
1	5	2661	U
1	5	2695	A
1	5	3625	G
1	5	3771	C
1	5	3876	A
1	5	4119	C
1	5	4170	A
1	5	4232	U
1	5	4354	U
1	5	4448	G
1	5	4528	G
1	5	4548	A
1	5	4656	A
1	5	4699	U
1	5	4719	G
1	5	4885	U
1	5	4888	U
1	5	4889	G
1	5	4935	C
1	5	4948	C
1	5	5022	U
1	5	5027	C
1	5	5059	C
1	5	5060	A
3	8	124	U
49	2	39	U
50	3	36	A
51	K	110	U
51	K	182	C
51	K	304	C
51	K	305	U
51	K	322	C
51	K	434	G
51	K	465	A
51	K	532	C
51	K	553	U
51	K	614	C
51	K	642	U

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Mol	Chain	Res	Type
51	K	688	U
51	K	752	G
51	K	798	G
51	K	870	A
51	K	902	G
51	K	1061	U
51	K	1137	U
51	K	1395	C
51	K	1520	G
51	K	1637	A
51	K	1664	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 164 ligands modelled in this entry, 164 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	5	12
51	K	11
50	3	2
49	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	697:G	O3'	729:C	P	18.34
1	K	756:C	O3'	788:G	P	17.89
1	K	1761:U	O3'	1771:G	P	17.79
1	5	4776:G	O3'	4859:C	P	17.38
1	5	757:G	O3'	906:C	P	17.23
1	5	2910:G	O3'	3583:U	P	17.01
1	5	519:C	O3'	642:G	P	17.00
1	K	834:C	O3'	841:G	P	16.21
1	K	323:C	O3'	329:G	P	15.96
1	K	1417:C	O3'	1423:C	P	15.13
1	5	3950:U	O3'	4065:G	P	14.95
1	5	997:C	O3'	1047:C	P	14.50
1	5	2131:C	O3'	2243:C	P	14.18
1	K	130:G	O3'	140:U	P	14.04
1	5	1051:G	O3'	1064:G	P	10.03
1	K	745:C	O3'	749:U	P	7.98
1	K	225:G	O3'	287:U	P	7.30
1	K	736:C	O3'	743:U	P	6.33
1	3	19:G	O3'	20:U	P	6.15
1	2	16:C	O3'	18:G	P	5.67
1	5	1699:A	O3'	1718:C	P	5.39
1	3	16:C	O3'	18:U	P	5.26
1	K	1432:U	O3'	1438:A	P	4.82
1	5	1840:G	O3'	1842:G	P	4.76
1	5	1100:U	O3'	1167:C	P	4.13
1	5	1222:A	O3'	1232:G	P	3.81

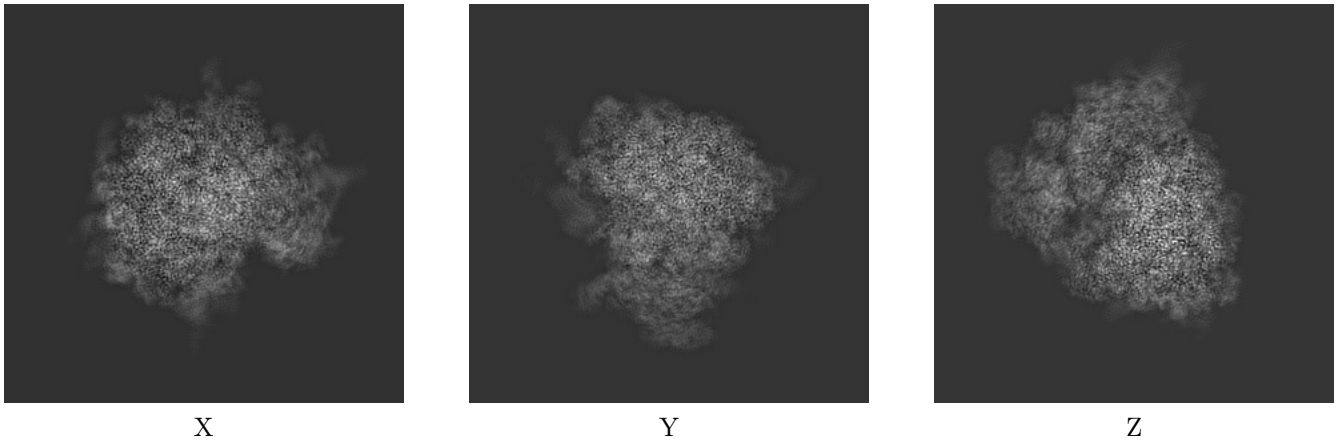
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4737. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

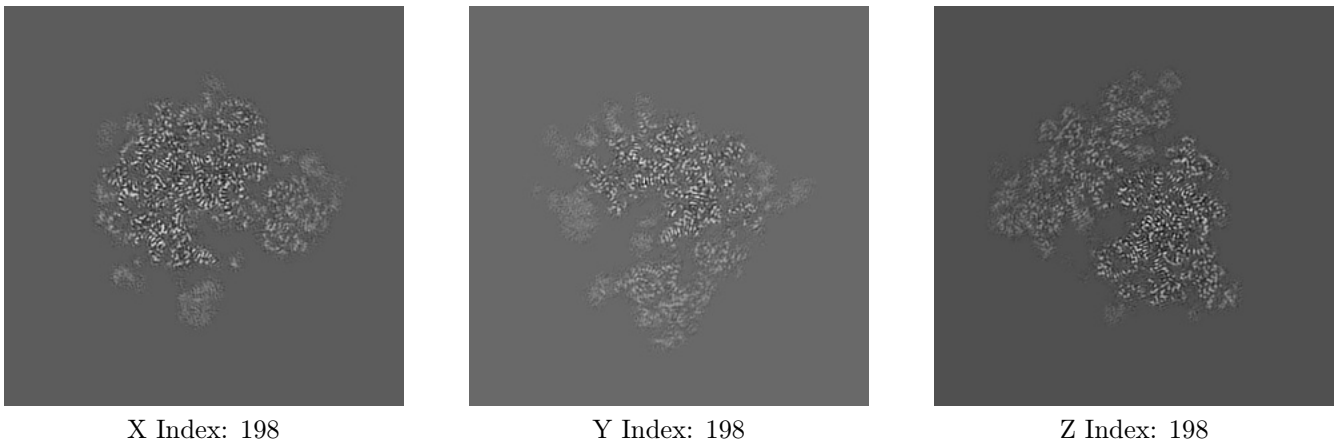
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

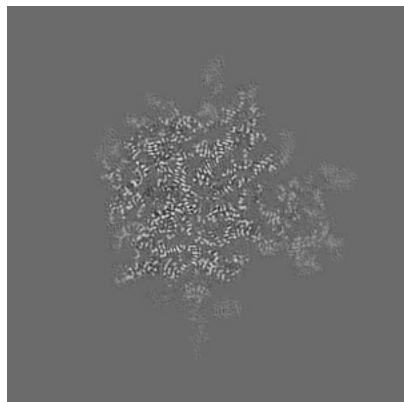
#### 6.2.1 Primary map



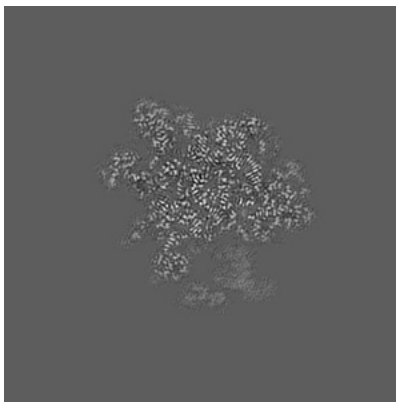
The images above show central slices of the map in three orthogonal directions.

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

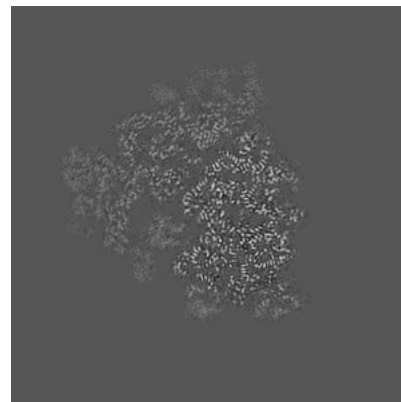
### 6.3.1 Primary map



X Index: 215



Y Index: 154

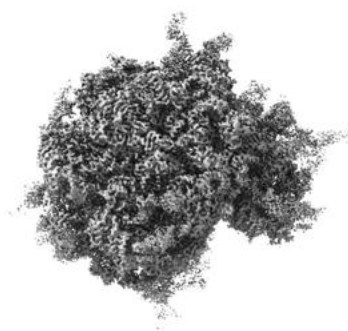


Z Index: 212

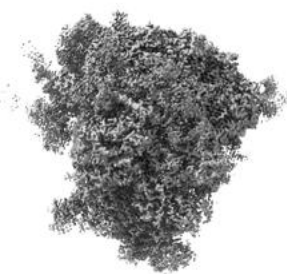
The images above show the largest variance slices of the map in three orthogonal directions.

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

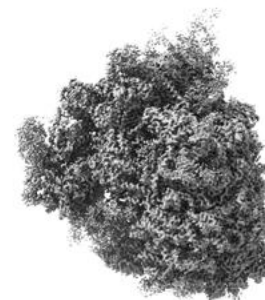
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

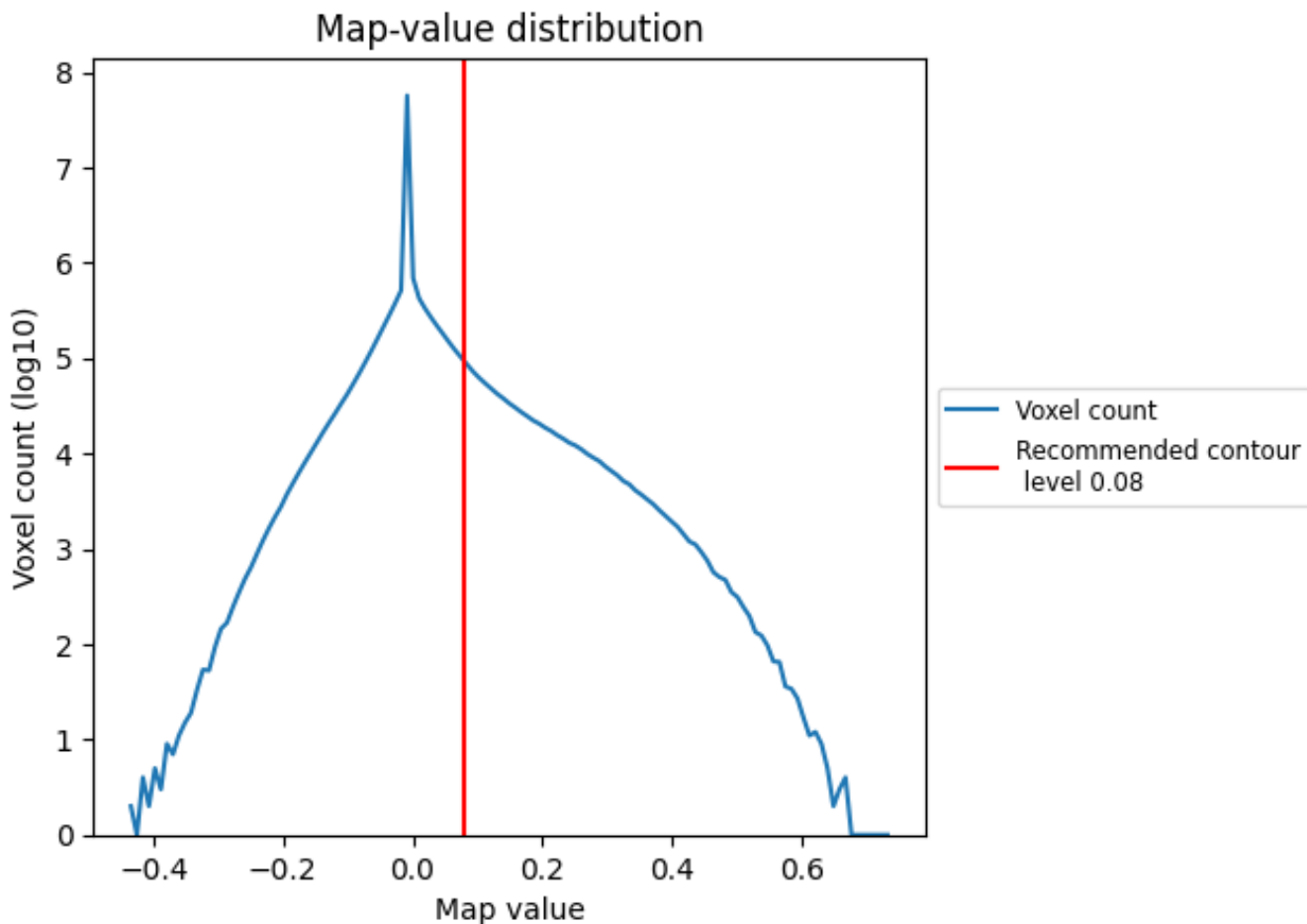
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

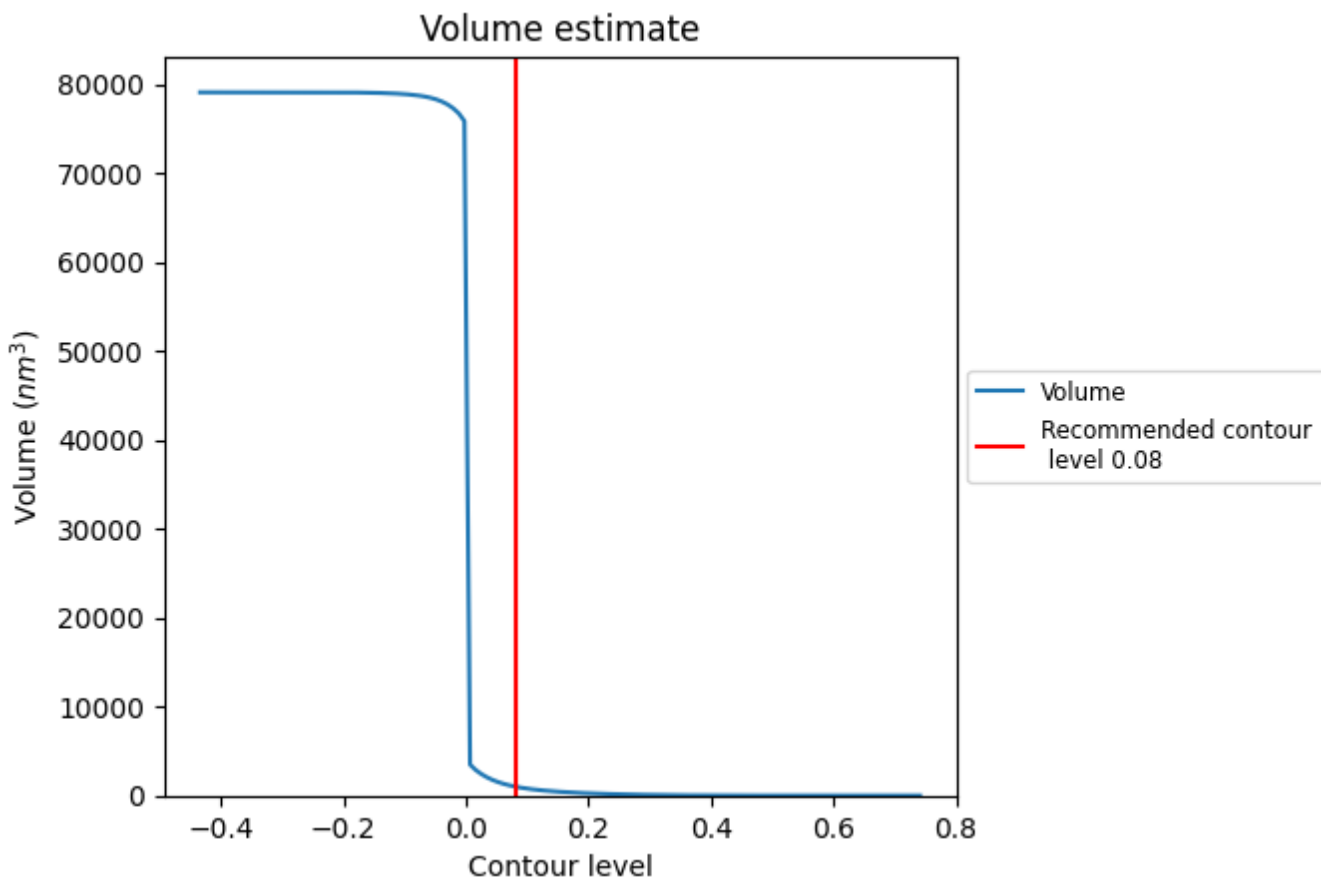
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

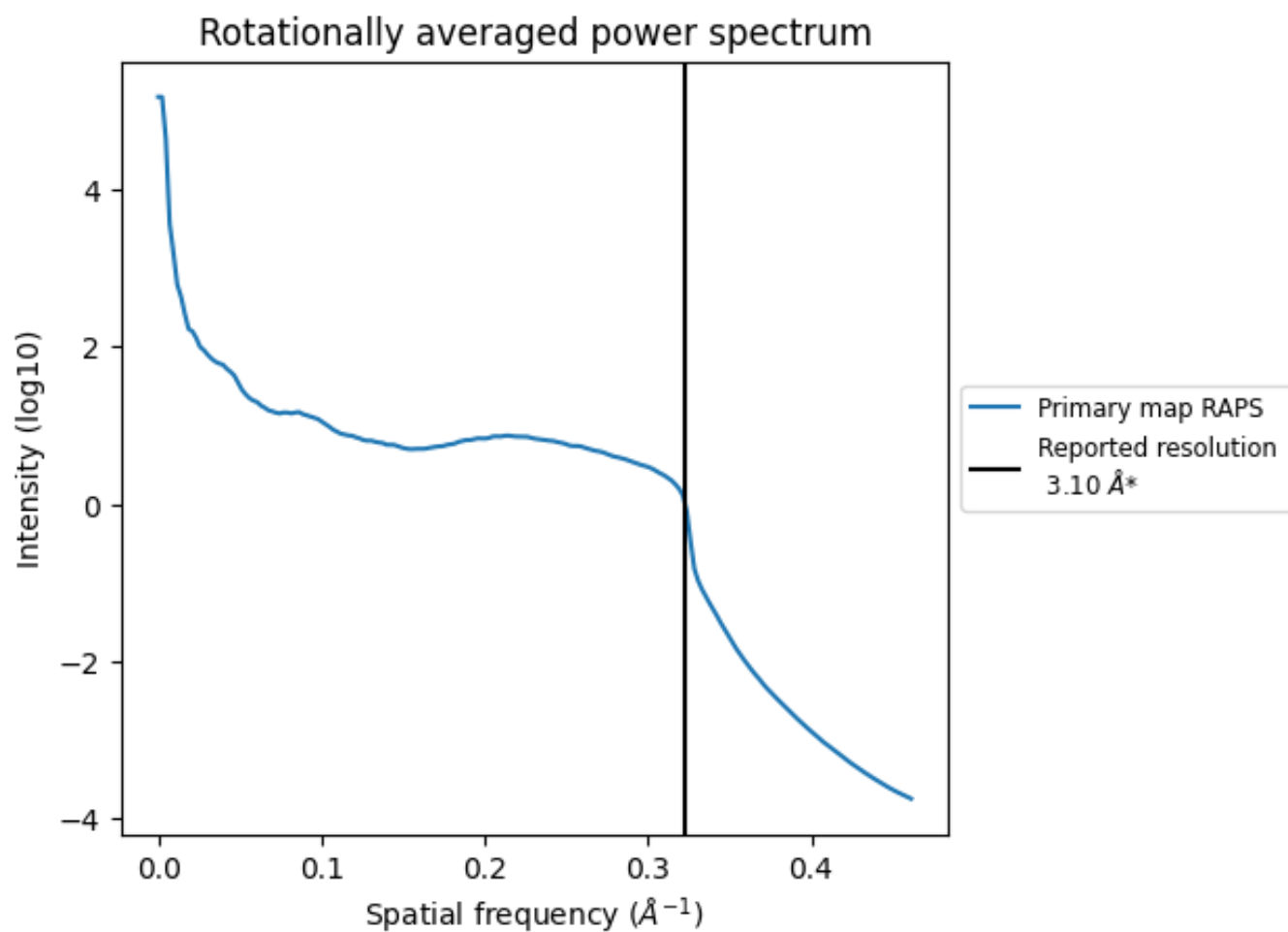


The volume at the recommended contour level is 1009 nm<sup>3</sup>; this corresponds to an approximate mass of 911 kDa.

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](#)

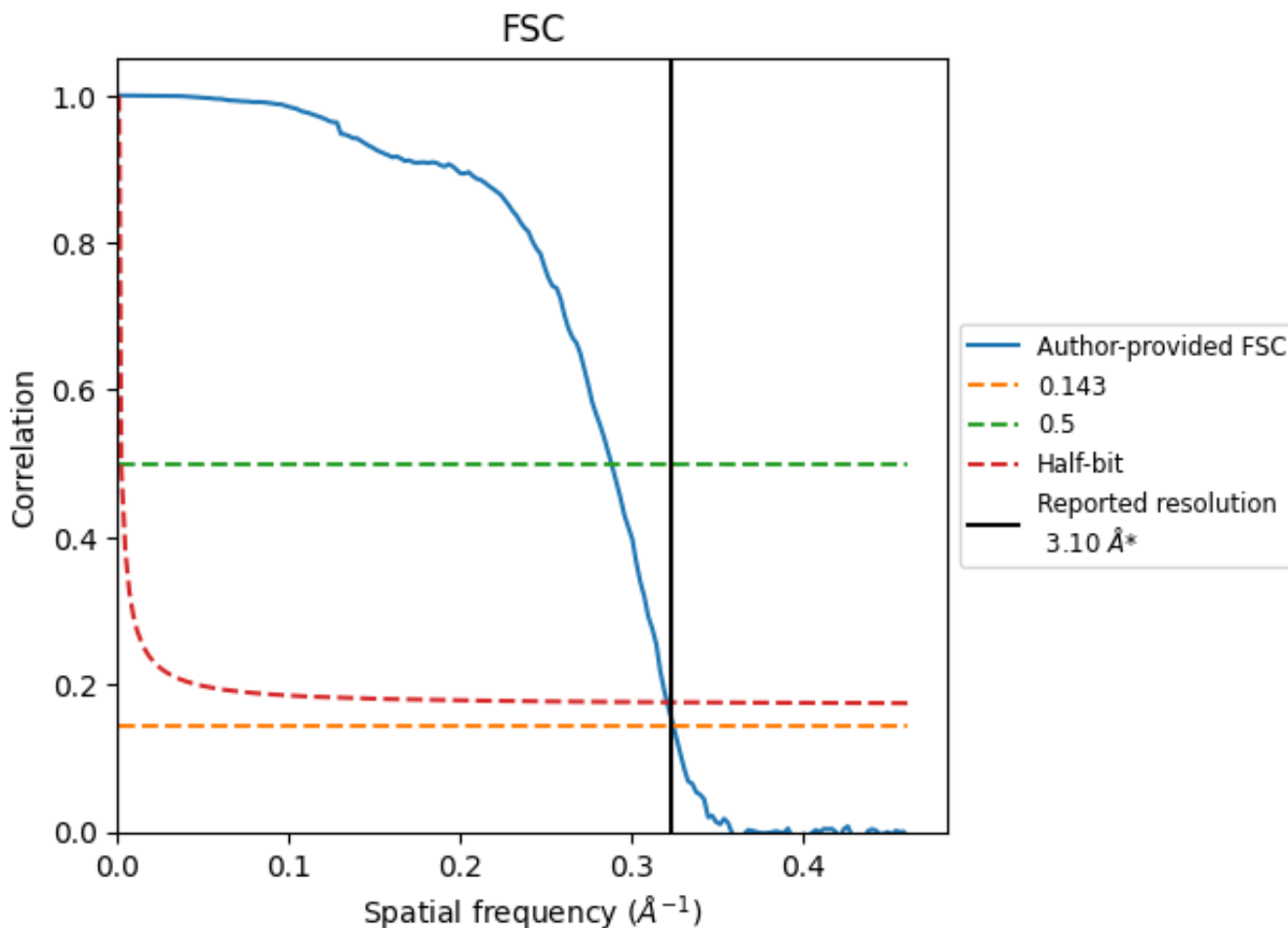


\*Reported resolution corresponds to spatial frequency of  $0.323 \text{\AA}^{-1}$

## 8 Fourier-Shell correlation [\(i\)](#)

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

### 8.1 FSC [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

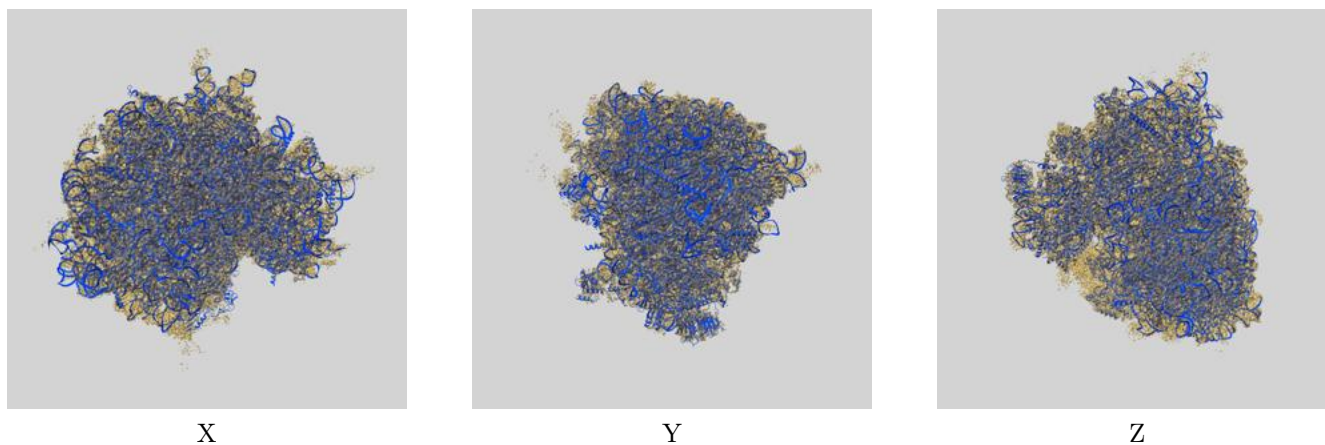
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.47	3.12
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

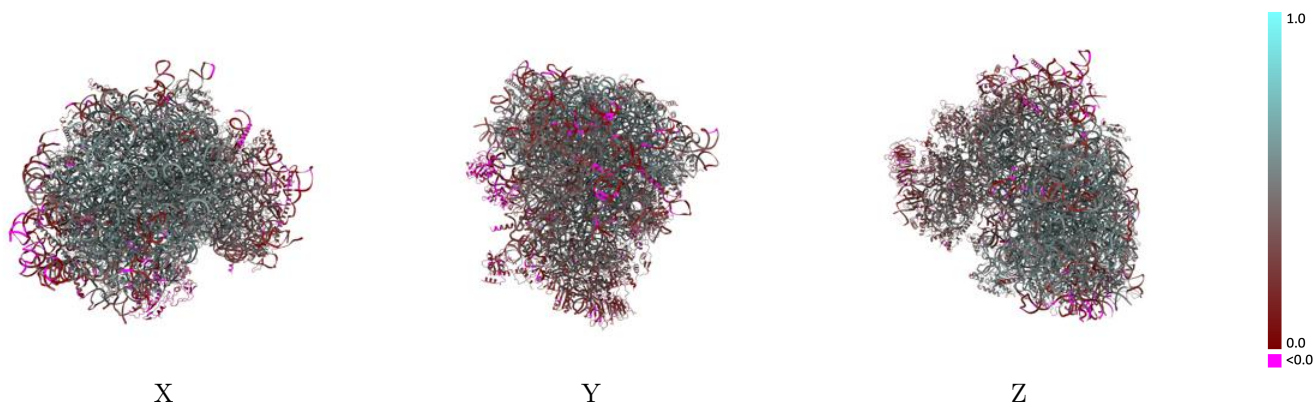
This section contains information regarding the fit between EMDB map EMD-4737 and PDB model 6R6P. Per-residue inclusion information can be found in section 3 on page 22.

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



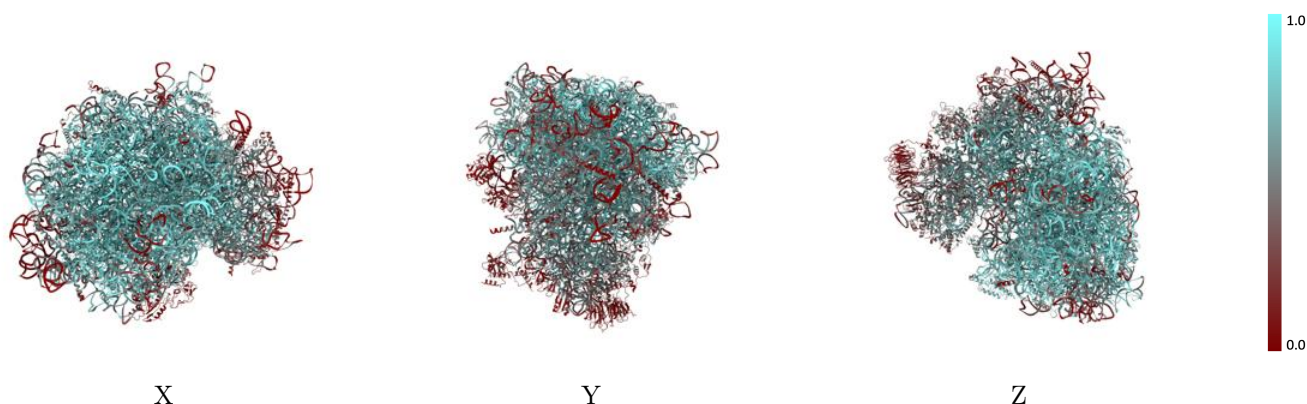
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



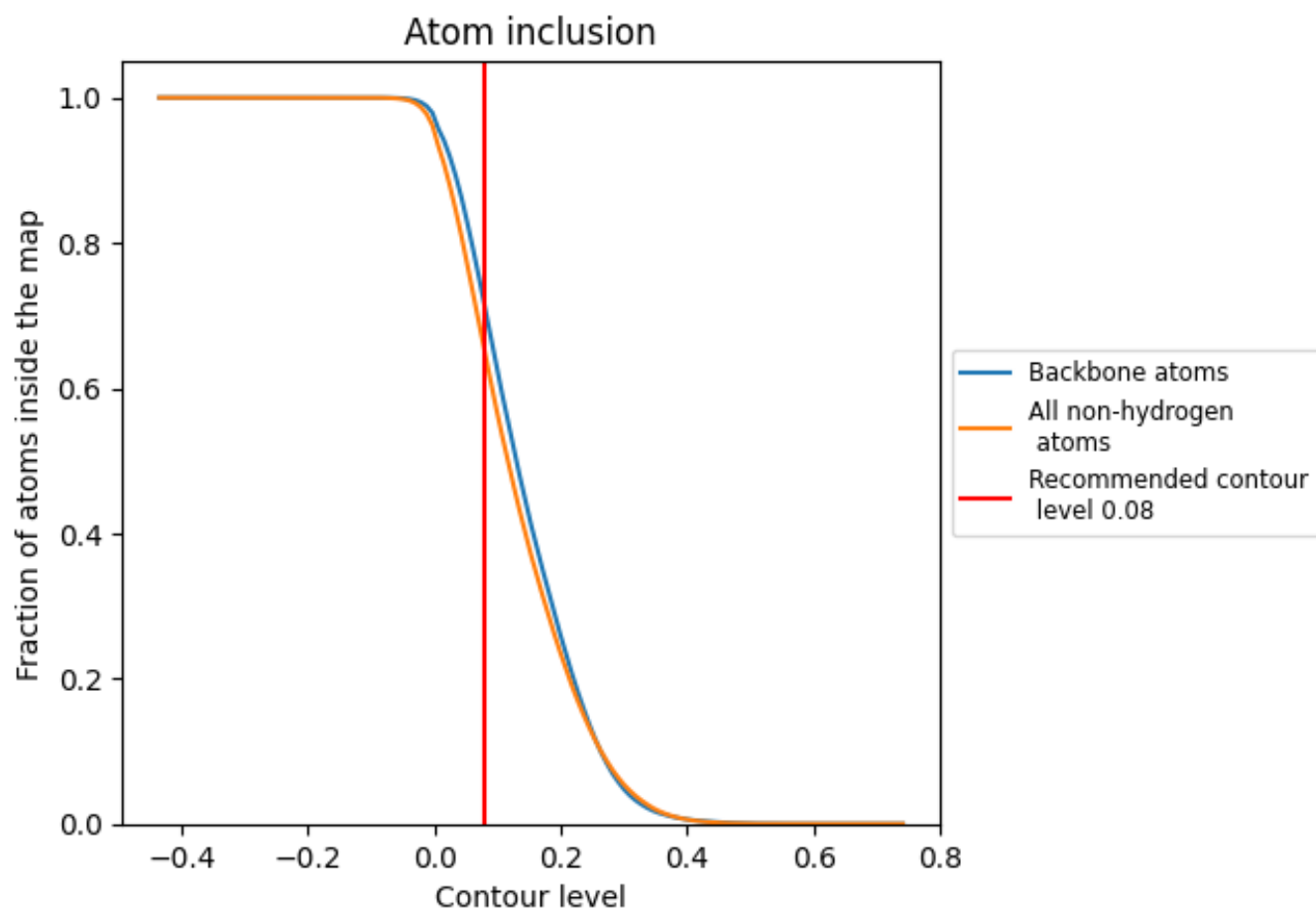
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 65% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6499	 0.4290
0	 0.1778	 0.1680
1	 0.7035	 0.5380
2	 0.3426	 0.3240
3	 0.5535	 0.3530
4	 0.7014	 0.4530
5	 0.7442	 0.4610
6	 0.1376	 0.1930
7	 0.8895	 0.5500
8	 0.7931	 0.4960
9	 0.4736	 0.3200
A	 0.7803	 0.5370
AA	 0.3169	 0.2900
B	 0.7664	 0.5170
BB	 0.4127	 0.3620
C	 0.7482	 0.5000
CC	 0.4468	 0.3500
D	 0.7174	 0.4640
DD	 0.3252	 0.2960
E	 0.6053	 0.3850
EE	 0.5465	 0.4230
F	 0.7449	 0.4970
FF	 0.3085	 0.3270
G	 0.6085	 0.4330
GG	 0.2687	 0.2660
H	 0.7118	 0.4930
HH	 0.4469	 0.3600
I	 0.7478	 0.4990
II	 0.4830	 0.3640
J	 0.6646	 0.4450
JJ	 0.4444	 0.3590
K	 0.6400	 0.4080
L	 0.6624	 0.4540
M	 0.7152	 0.4840
MM	 0.5319	 0.4100



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Chain	Atom inclusion	Q-score
N	 0.7988	 0.5320
NN	 0.3690	 0.3220
O	 0.7669	 0.5070
OO	 0.3774	 0.3290
P	 0.7804	 0.5280
PP	 0.4096	 0.3310
Q	 0.7632	 0.5060
QQ	 0.5523	 0.4270
R	 0.6155	 0.4080
RR	 0.1331	 0.1510
S	 0.7714	 0.5060
SS	 0.3076	 0.2490
T	 0.7070	 0.4840
TT	 0.5396	 0.4080
U	 0.5899	 0.4060
UU	 0.3764	 0.3380
V	 0.7495	 0.5240
VV	 0.6162	 0.4600
W	 0.7387	 0.5150
X	 0.6913	 0.4870
XX	 0.4232	 0.3350
Y	 0.7254	 0.4770
YY	 0.3247	 0.2980
Z	 0.6841	 0.4500
ZZ	 0.5455	 0.4200
a	 0.7828	 0.5220
b	 0.6088	 0.3960
c	 0.6895	 0.4770
d	 0.6989	 0.4890
e	 0.7741	 0.5300
f	 0.7803	 0.5240
g	 0.7049	 0.4910
h	 0.7181	 0.4760
i	 0.6633	 0.4640
j	 0.7786	 0.5150
k	 0.5763	 0.4060
l	 0.7376	 0.5060
m	 0.7524	 0.4900
n	 0.6318	 0.4310
o	 0.7034	 0.4880
p	 0.7054	 0.5120
q	 0.4620	 0.3600

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Chain	Atom inclusion	Q-score
r	 0.7313	 0.4760
s	 0.0300	 0.0030
t	 0.0074	 0.0090
u	 0.5462	 0.4130
v	 0.4685	 0.3530
w	 0.5147	 0.3870
x	 0.3906	 0.3360
y	 0.3559	 0.2900
z	 0.3644	 0.2960