



## Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 09:23 PM EDT

PDB ID : 5TZS  
EMDB ID : EMD-8473  
Title : Architecture of the yeast small subunit processome  
Authors : Chaker-Margot, M.; Barandun, J.; Hunziker, M.; Klinge, S.  
Deposited on : 2016-11-22  
Resolution : 5.10 Å(reported)

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

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

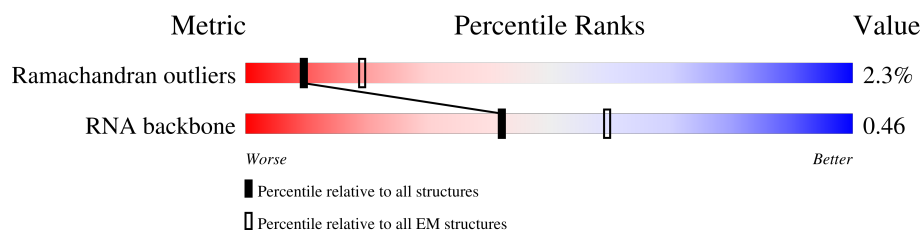
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 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 5.10 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
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	0	364	<div> <div>21%</div> <div>99%</div> </div>
2	1	1800	<div> <div>12%</div> <div>14%</div> <div>12%</div> <div>71%</div> </div>
3	2	126	<div> <div>12%</div> <div>48%</div> <div>49%</div> </div>
4	3	236	<div> <div>79%</div> <div>86%</div> <div>6%</div> <div>8%</div> </div>
5	5	261	<div> <div>48%</div> <div>86%</div> <div>7%</div> <div>8%</div> </div>
6	6	225	<div> <div>9%</div> <div>81%</div> <div>8%</div> <div>10%</div> </div>
7	7	190	<div> <div>95%</div> <div>88%</div> <div>9%</div> </div>
8	8	200	<div> <div>63%</div> <div>84%</div> <div>14%</div> </div>
9	9	197	<div> <div>21%</div> <div>86%</div> <div>8%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
10	A	39	100%
11	B	108	45% 100%
12	C	143	80% 20%
13	D	156	72% 94% 6%
14	E	130	81% 97% ..
15	F	135	21% 64% 33%
16	G	67	9% 91% 7%
17	H	544	44% 99%
18	I	176	22% 94% 6%
19	J	107	7% 98%
19	K	107	16% 95%
20	M	258	8% 99%
21	N	545	20% 99%
22	O	638	8% 98%
23	P	306	7% 100%
24	Q	710	19% 99%
25	R	717	78% 100%
26	S	250	14% 98%
27	T	781	5% 96%
28	U	284	13% 100%
29	V	263	72% 100%
30	W	104	9% 90% 10%
31	X	640	72% 100%
32	Y	641	93% 100%
33	Z	151	5% 99%

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Mol	Chain	Length	Quality of chain
34	a	312	
35	b	341	
36	c	221	
37	d	216	
38	e	126	
38	f	126	
39	g	573	
40	h	367	
41	i	511	
42	j	252	
42	k	252	
43	l	124	
44	m	156	
45	n	160	
46	o	175	
47	p	924	
48	q	372	
49	r	145	
50	s	290	
50	t	290	
50	u	290	
51	v	580	
52	y	507	
53	z	76	

## 2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 98451 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 5' external transcribed spacer.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	364	Total	C	N	O	P	0	0
			4476	1871	43	2198	364		

- Molecule 2 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	515	Total	C	N	O	P	0	0
			10978	4908	1957	3598	515		

- Molecule 3 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	126	Total	C	N	O	P	0	0
			2468	1095	388	859	126		

- Molecule 4 is a protein called rpS6\_ES6.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	3	216	Total	C	N	O	0	0
			1063	631	216	216		

- Molecule 5 is a protein called rpS4\_ES4.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	5	241	Total	C	N	O	0	0
			1185	703	241	241		

- Molecule 6 is a protein called rpS5\_US7.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	6	202	Total	C	N	O	0	0
			1000	596	202	202		

- Molecule 7 is a protein called rpS7\_eS7.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	7	186	Total	C	N	O	0	0
			923	551	186	186		

- Molecule 8 is a protein called rpS8\_eS8.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	8	173	Total	C	N	O	0	0
			849	503	173	173		

- Molecule 9 is a protein called rpS9\_uS4.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	9	185	Total	C	N	O	0	0
			915	545	185	185		

- Molecule 10 is a DNA chain called 5' domain-associated.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	A	39	Total	C	O	P	0	0
			468	195	234	39		

- Molecule 11 is a DNA chain called 3' domain-associated.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	B	108	Total	C	O	P	0	0
			1296	540	648	108		

- Molecule 12 is a protein called rpS16\_uS9.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	C	115	Total	C	N	O	0	0
			566	336	115	115		

- Molecule 13 is a protein called rpS11\_uS17.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	D	146	Total	C	N	O	0	0
			721	429	146	146		

- Molecule 14 is a protein called rpS22\_uS8.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	E	127	Total	C	N	O	0	0
			624	370	127	127		

- Molecule 15 is a protein called rpS24\_eS24.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	F	90	Total	C	N	O	0	0
			444	264	90	90		

- Molecule 16 is a protein called rpS28\_eS28.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	G	62	Total	C	N	O	0	0
			306	182	62	62		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	17	ALA	GLY	conflict	UNP Q3E7X9

- Molecule 17 is a protein called Utp4.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	H	544	Total	C	N	O	0	0
			2680	1592	544	544		

- Molecule 18 is a protein called UtpA\_CTD1.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	I	176	Total	C	N	O	0	0
			880	528	176	176		

- Molecule 19 is a protein called UtpA\_CTD2.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	J	107	Total	C	N	O	0	0
			535	321	107	107		
19	K	105	Total	C	N	O	0	0
			525	315	105	105		

- Molecule 20 is a protein called Beta-propeller 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	M	258	Total	C	N	O	0	0
			1275	759	258	258		

- Molecule 21 is a protein called Utp17.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	N	545	Total	C	N	O	0	0
			2678	1588	545	545		

- Molecule 22 is a protein called Utp1.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	O	638	Total	C	N	O	0	0
			3153	1877	638	638		

- Molecule 23 is a protein called Utp6.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	P	306	Total	C	N	O	0	0
			1530	918	306	306		

- Molecule 24 is a protein called Utp12.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Q	710	Total	C	N	O	0	0
			3503	2083	710	710		

- Molecule 25 is a protein called Utp13.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	R	717	Total	C	N	O	0	0
			3539	2105	717	717		

- Molecule 26 is a protein called Utp18.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	S	250	Total	C	N	O	0	0
			1228	728	250	250		

- Molecule 27 is a protein called Utp21.



Mol	Chain	Residues	Atoms				AltConf	Trace
27	T	749	Total	C	N	O	0	0
			3691	2193	749	749		

- Molecule 28 is a protein called Beta-propeller 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	U	284	Total	C	N	O	0	0
			1398	830	284	284		

- Molecule 29 is a protein called Enp2.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	V	263	Total	C	N	O	0	0
			1298	772	263	263		

- Molecule 30 is a protein called UtpA\_CTD4.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	W	104	Total	C	N	O	0	0
			520	312	104	104		

- Molecule 31 is a protein called Kre33.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	X	640	Total	C	N	O	0	0
			3155	1875	640	640		

- Molecule 32 is a protein called Kre33.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Y	641	Total	C	N	O	0	0
			3160	1878	641	641		

- Molecule 33 is a protein called Imp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Z	151	Total	C	N	O	0	0
			748	446	151	151		

- Molecule 34 is a protein called Nop56.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	a	312	Total	C	N	O	0	0
			1544	920	312	312		

- Molecule 35 is a protein called Nop58.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	b	341	Total	C	N	O	0	0
			1687	1005	341	341		

- Molecule 36 is a protein called Nop1.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	c	221	Total	C	N	O	0	0
			1088	646	221	221		

- Molecule 37 is a protein called Nop1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	d	216	Total	C	N	O	0	0
			1064	632	216	216		

- Molecule 38 is a protein called Snu13.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	e	122	Total	C	N	O	0	0
			606	362	122	122		
38	f	114	Total	C	N	O	0	0
			566	338	114	114		

- Molecule 39 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	g	365	Total	C	N	O	0	0
			1799	1069	365	365		

- Molecule 40 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	h	355	Total	C	N	O	0	0
			1742	1032	355	355		

- Molecule 41 is a protein called Bms1,Ribosome biogenesis protein BMS1,Bms1.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	i	475	Total	C	N	O	0	0
			2347	1398	475	474		

- Molecule 42 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	j	211	Total	C	N	O	0	0
			1047	625	211	211		
42	k	218	Total	C	N	O	0	0
			1081	645	218	218		

- Molecule 43 is a protein called Utp24.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	l	124	Total	C	N	O	0	0
			613	365	124	124		

- Molecule 44 is a protein called Imp4.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	m	156	Total	C	N	O	0	0
			775	463	156	156		

- Molecule 45 is a protein called Utp30.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	n	160	Total	C	N	O	0	0
			791	471	160	160		

- Molecule 46 is a protein called Unassigned KH domain.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	o	173	Total	C	N	O	0	0
			858	512	173	173		

- Molecule 47 is a protein called Utp20.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	p	924	Total	C	N	O	0	0
			4620	2772	924	924		

- Molecule 48 is a protein called Repeat protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	q	372	Total	C	N	O	0	0
			1860	1116	372	372		

- Molecule 49 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	r	82	Total	C	N	O	0	0
			402	238	82	82		

- Molecule 50 is a protein called Beta-propeller 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	s	290	Total	C	N	O	0	0
			1429	849	290	290		
50	t	269	Total	C	N	O	0	0
			1076	538	269	269		
50	u	274	Total	C	N	O	0	0
			1346	798	274	274		

- Molecule 51 is a protein called Repeat protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	v	577	Total	C	N	O	0	0
			2885	1731	577	577		

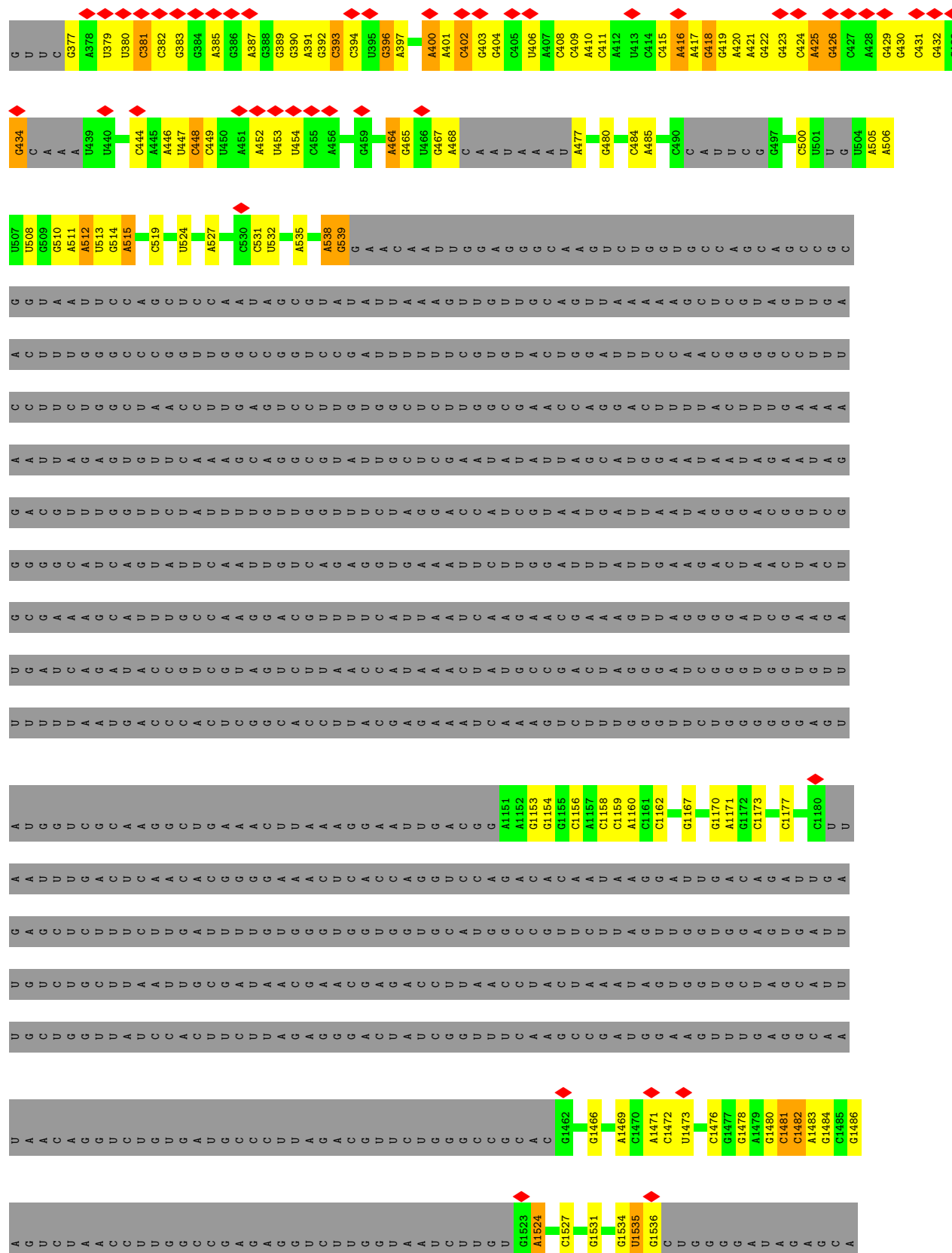
- Molecule 52 is a protein called Unassigned protein helices.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	y	507	Total	C	N	O	0	0
			2535	1521	507	507		

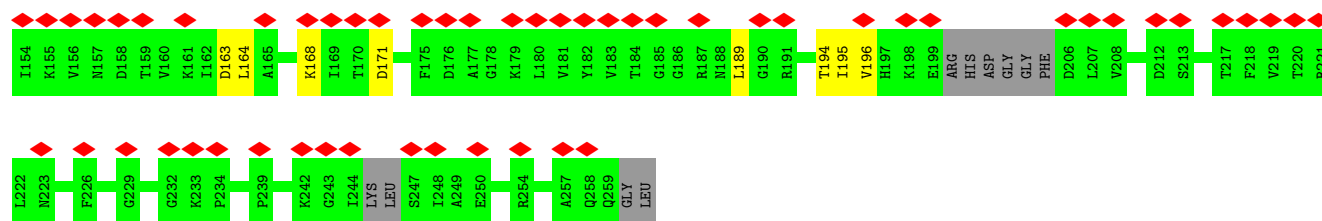
- Molecule 53 is a DNA chain called Unassigned RNA helices.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	z	76	Total	C	O	P	0	0
			912	380	456	76		

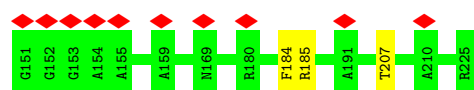
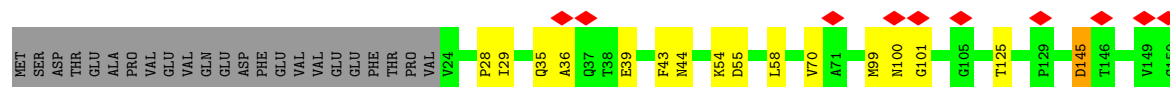
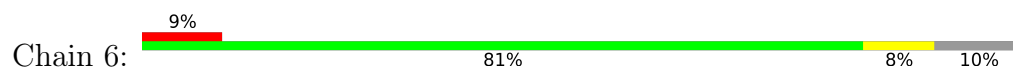




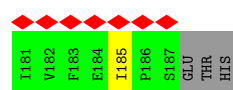
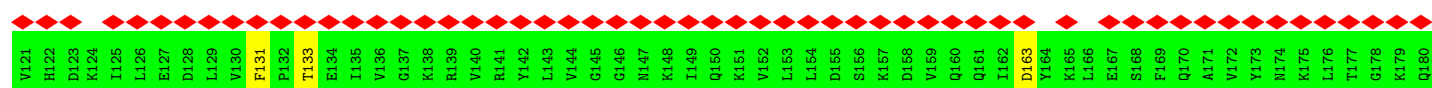
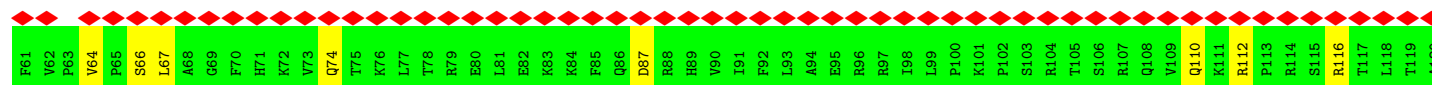
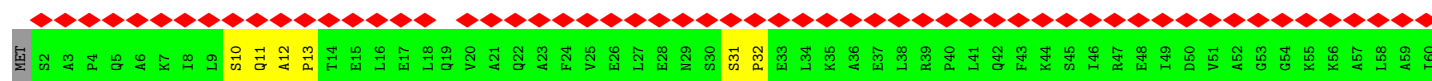
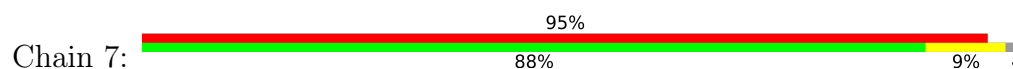




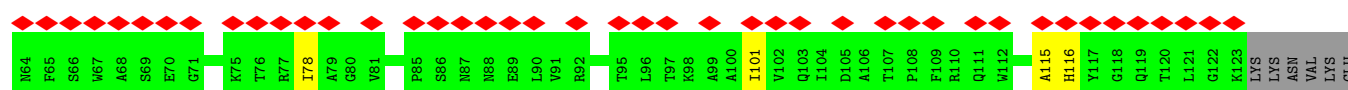
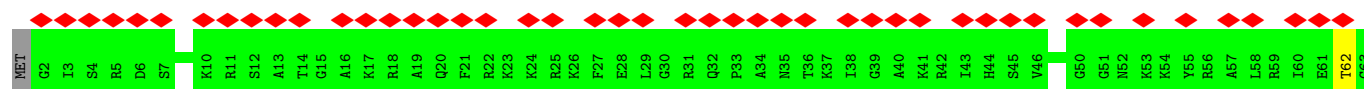
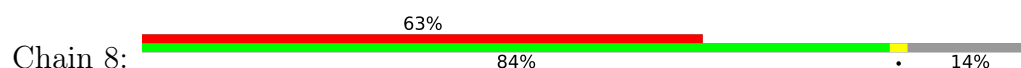
• Molecule 6: rpS5\_US7



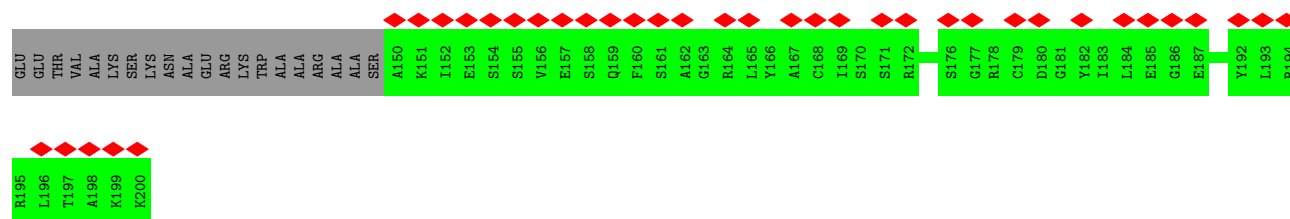
• Molecule 7: rpS7\_eS7



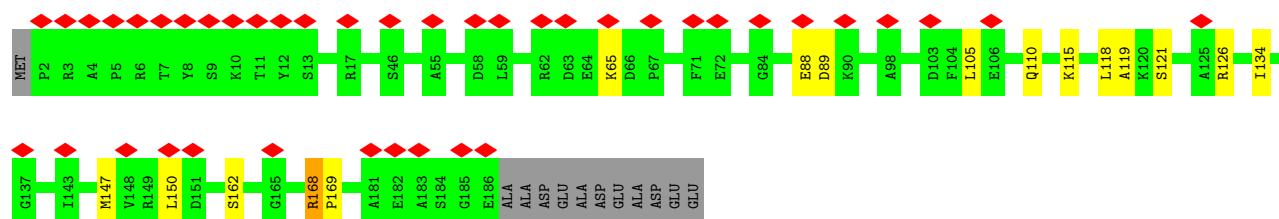
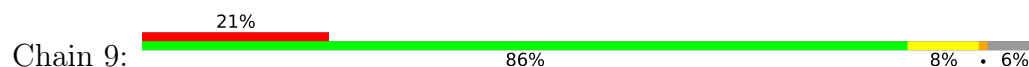
• Molecule 8: rpS8\_eS8







- Molecule 9: rpS9\_uS4

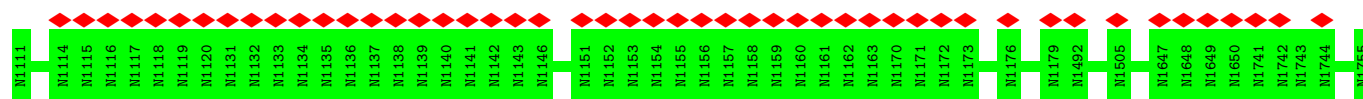


- Molecule 10: 5' domain-associated

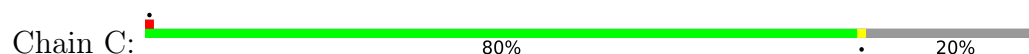


There are no outlier residues recorded for this chain.

- Molecule 11: 3' domain-associated



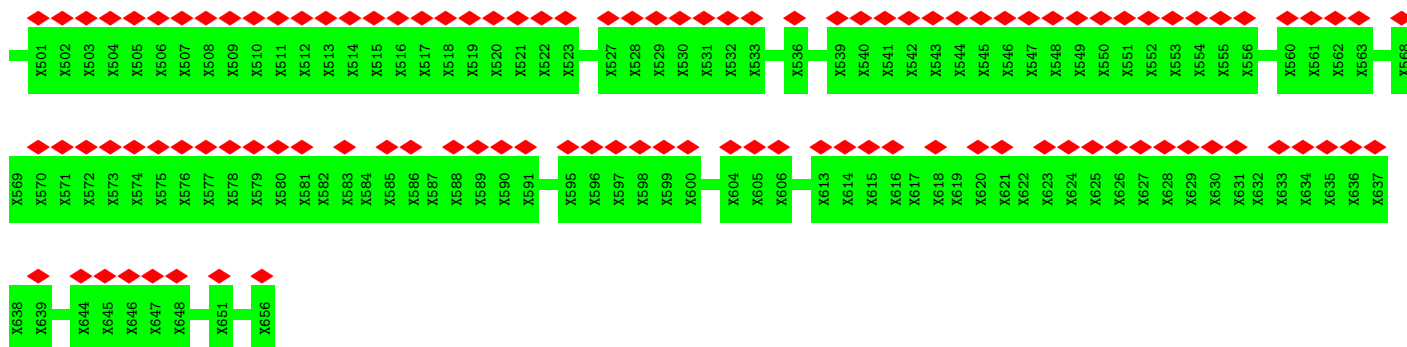
- Molecule 12: rpS16\_uS9



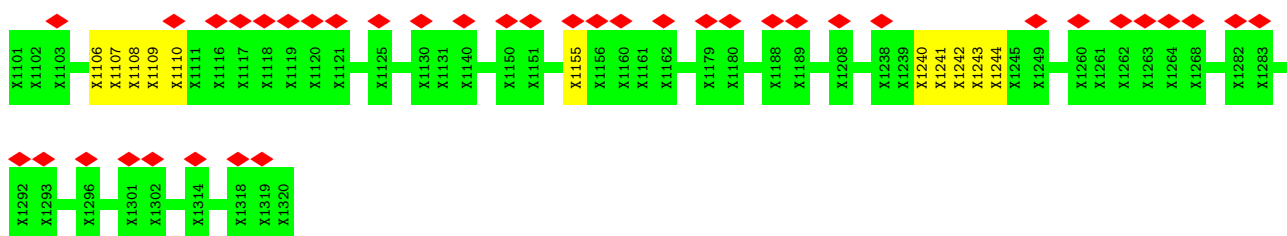
- Molecule 13: rpS11\_uS17



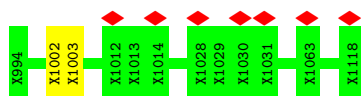




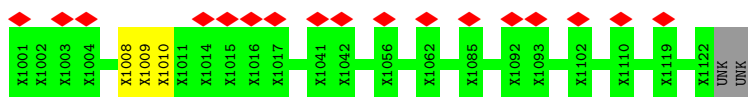
• Molecule 18: UtpA\_CTD1



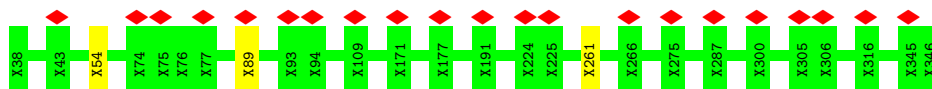
• Molecule 19: UtpA\_CTD2



• Molecule 19: UtpA\_CTD2

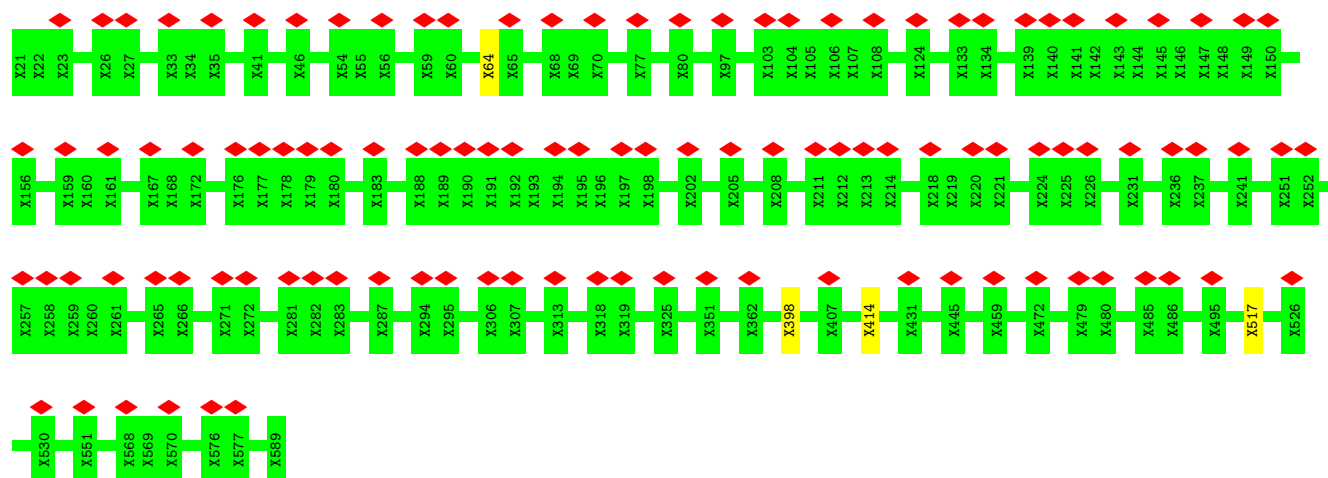


• Molecule 20: Beta-propeller 2

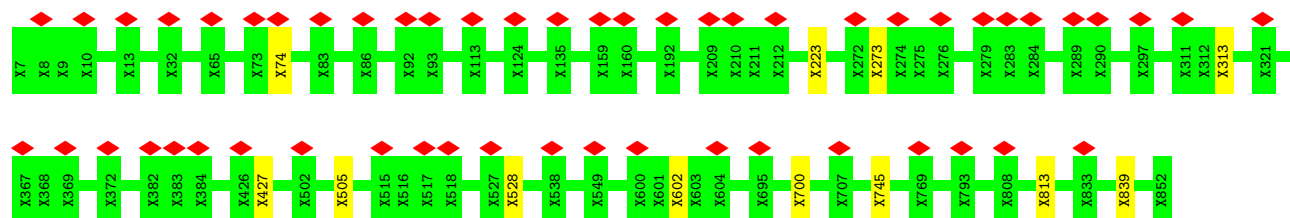


• Molecule 21: Utp17

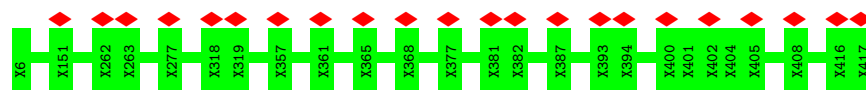




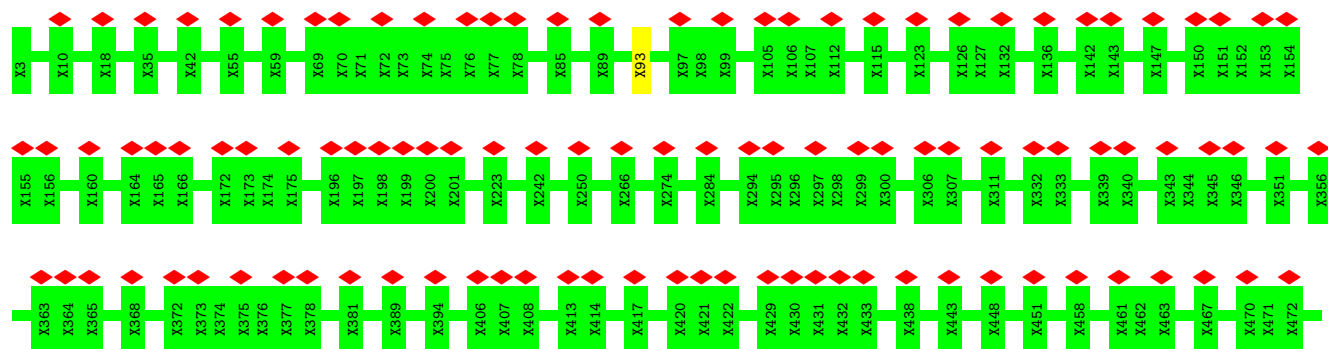
• Molecule 22: Utp1

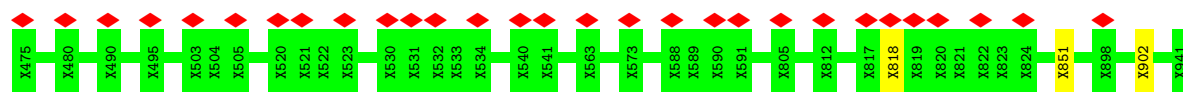


• Molecule 23: Utp6

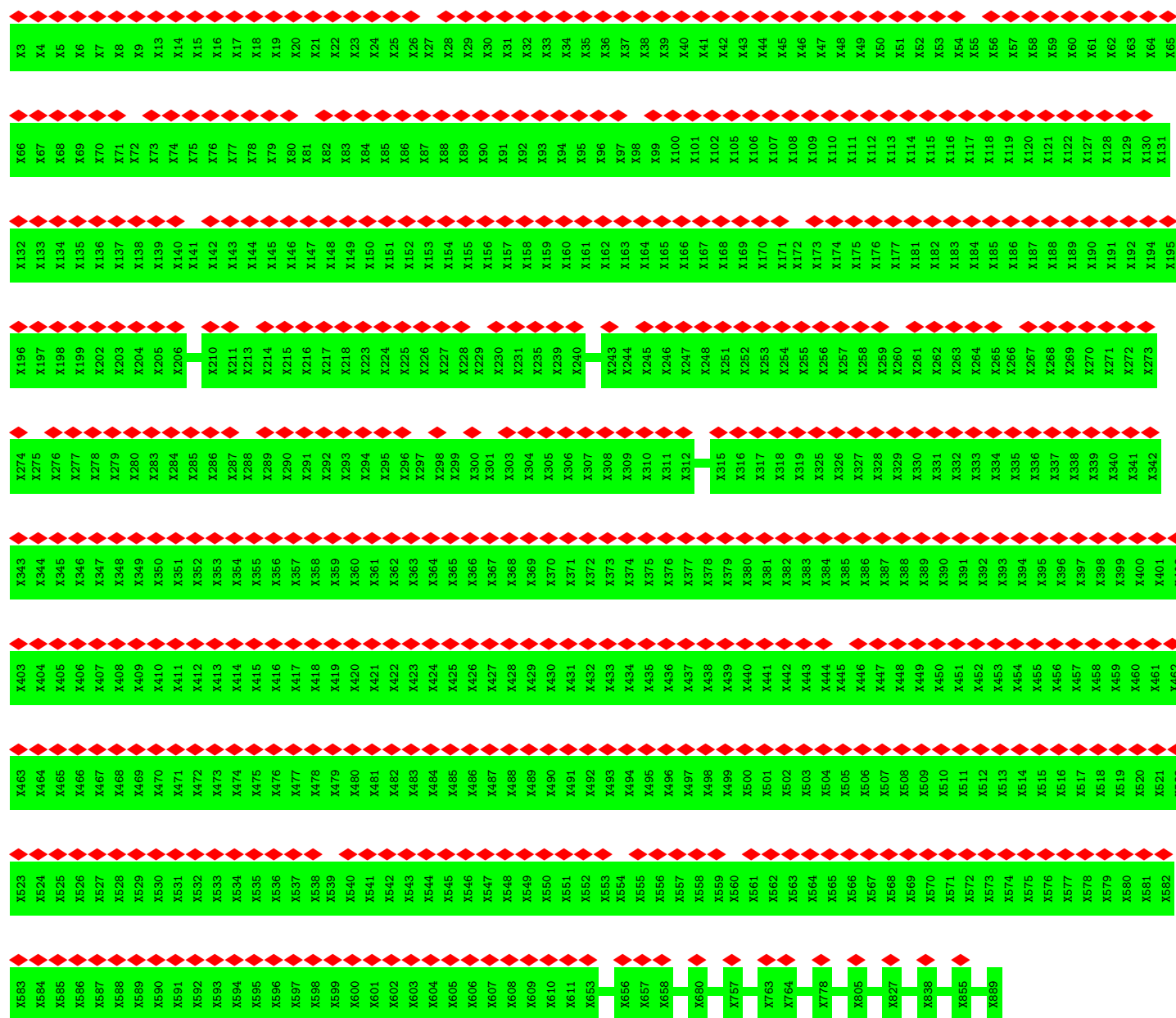
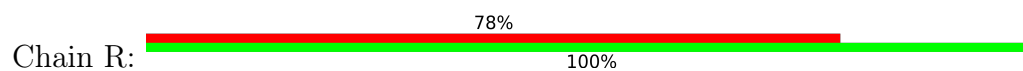


• Molecule 24: Utp12

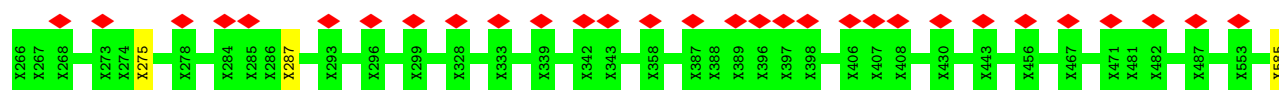


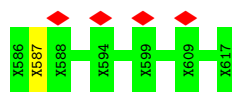


• Molecule 25: Utp13

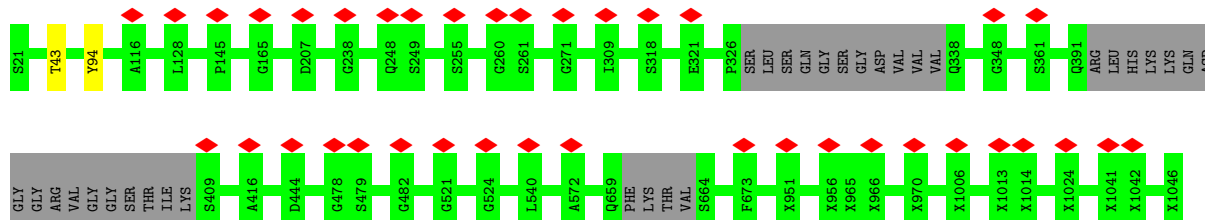


• Molecule 26: Utp18

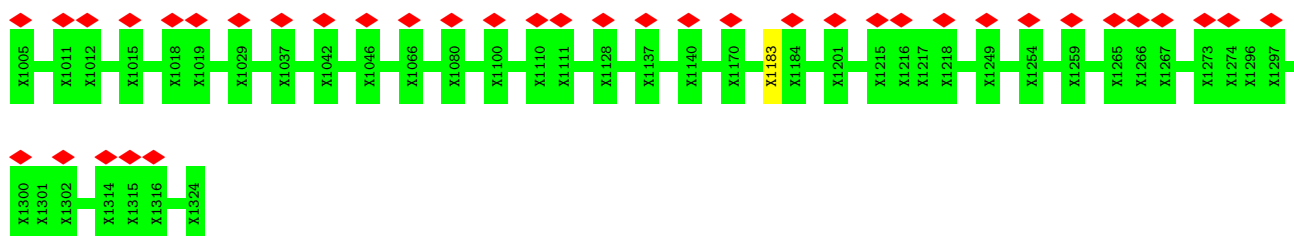




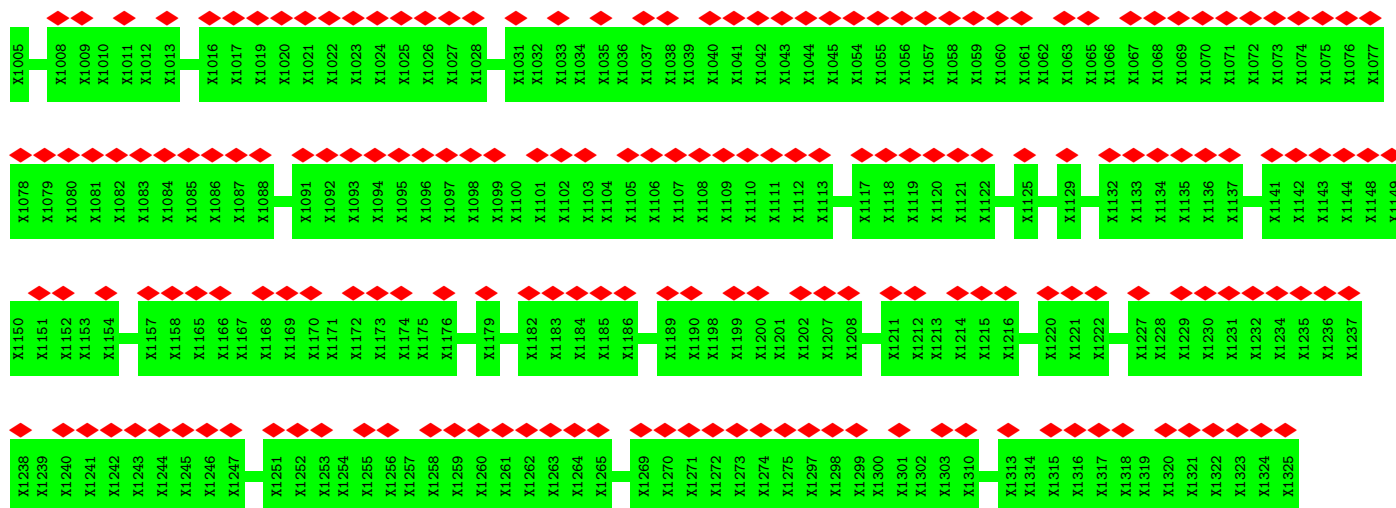
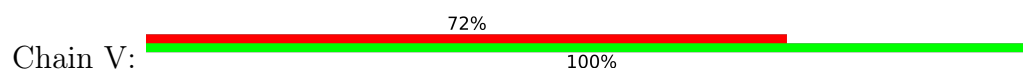
• Molecule 27: Utp21



• Molecule 28: Beta-propeller 5

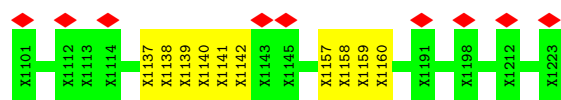


• Molecule 29: Enp2

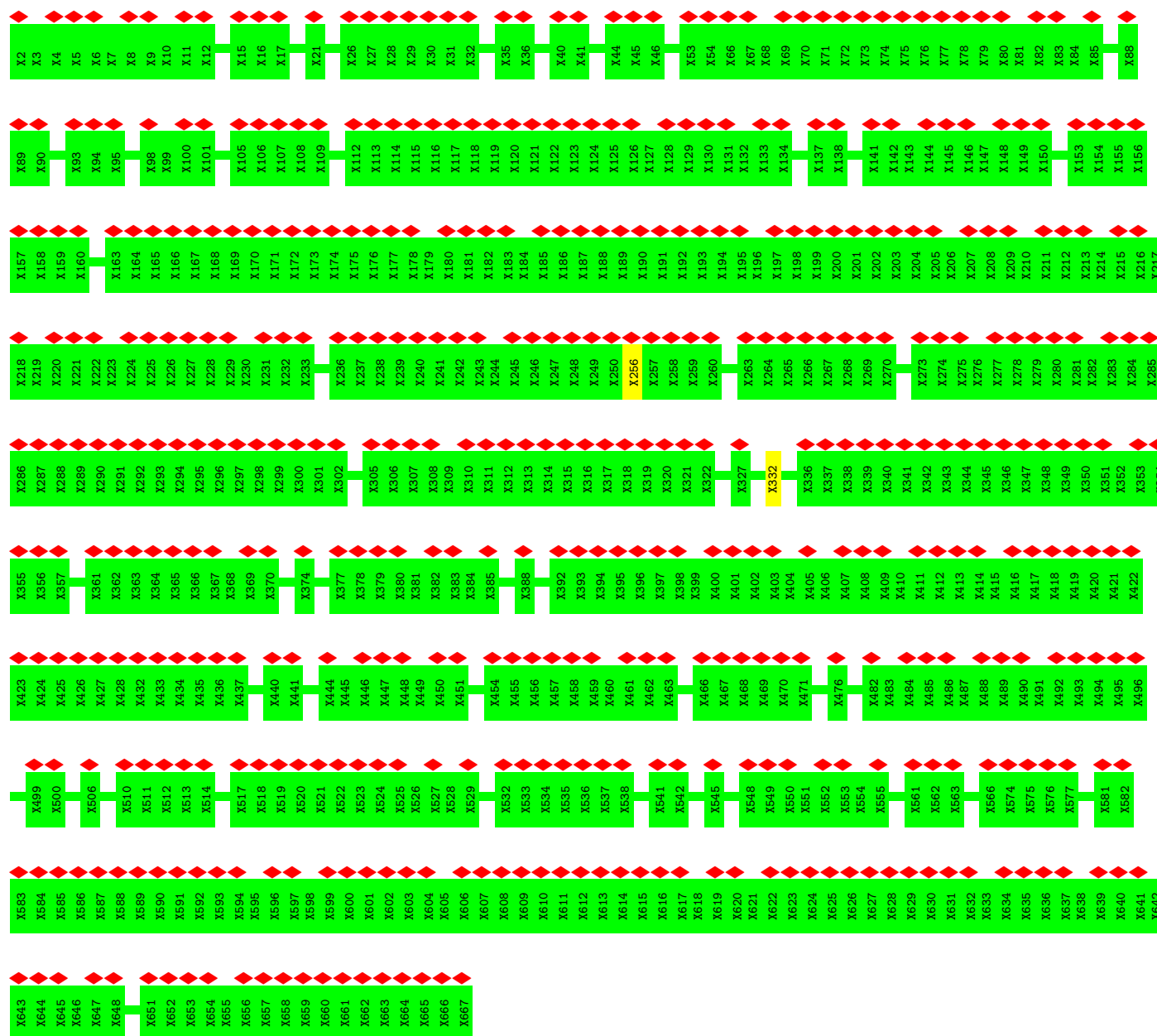
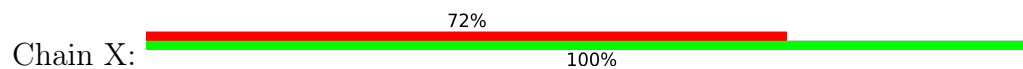


• Molecule 30: UtpA\_CTD4

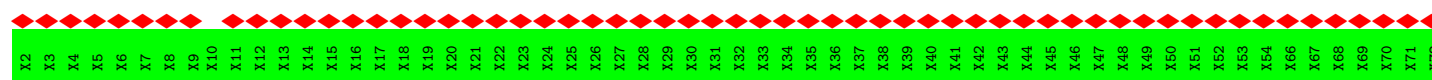


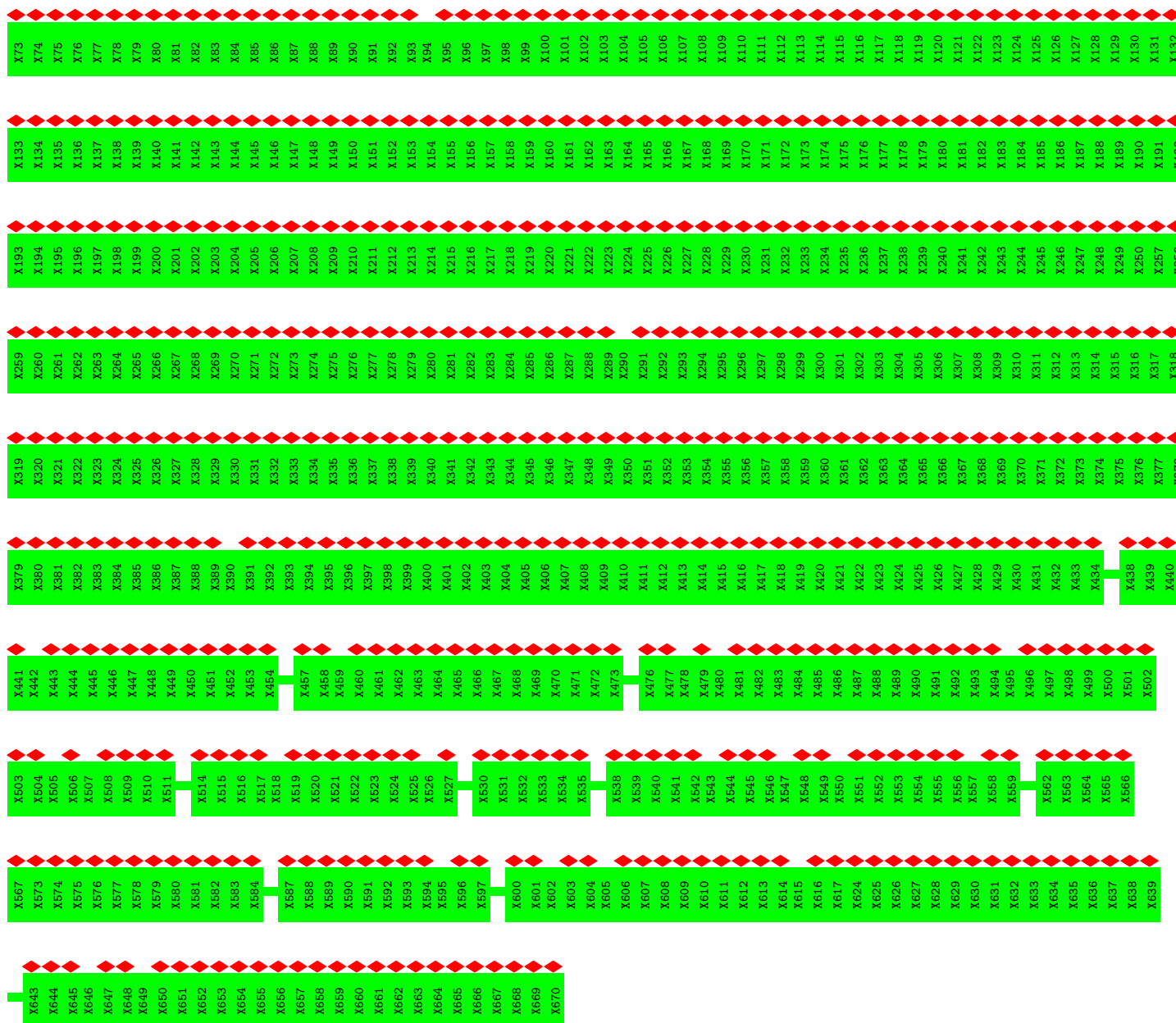


• Molecule 31: Kre33

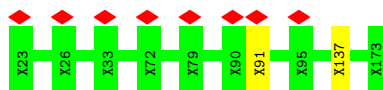


• Molecule 32: Kre33





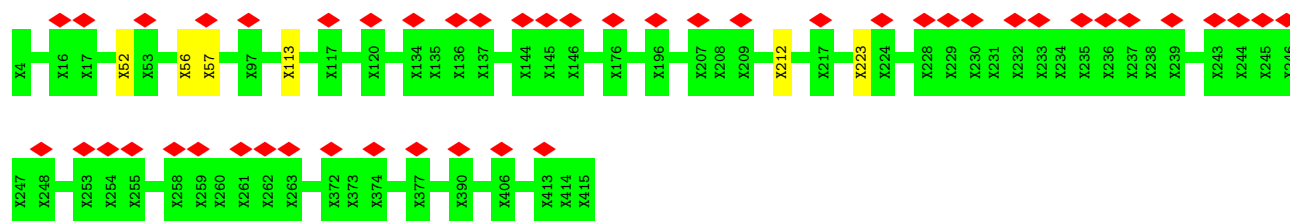
- Molecule 33: Imp3



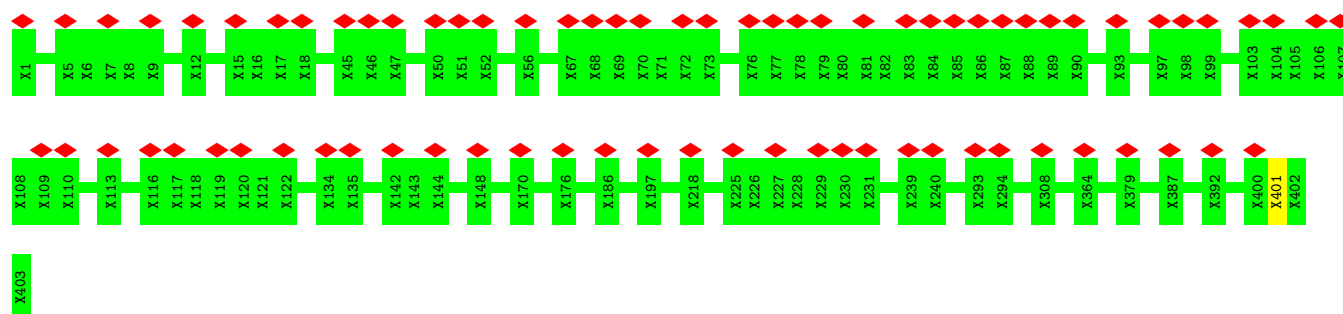
- Molecule 34: Nop56



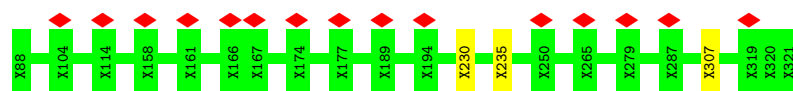




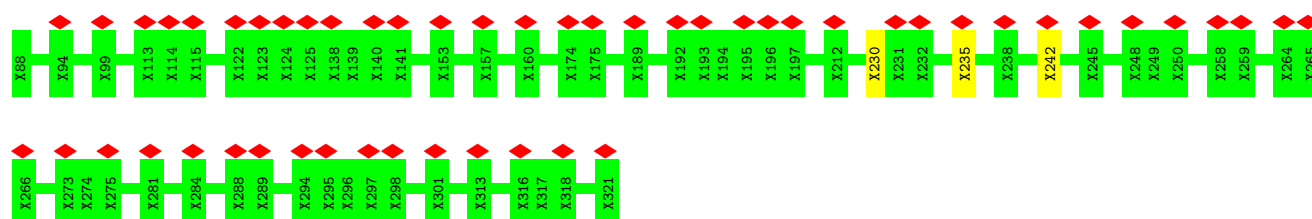
• Molecule 35: Nop58



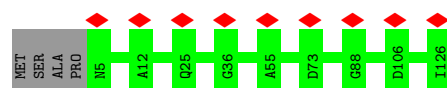
• Molecule 36: Nop1



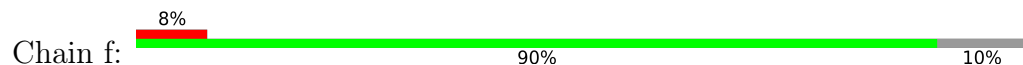
• Molecule 37: Nop1

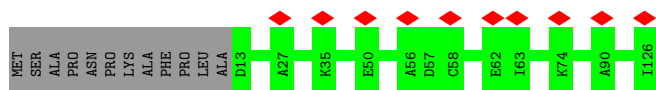


• Molecule 38: Snu13

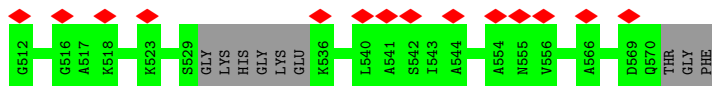
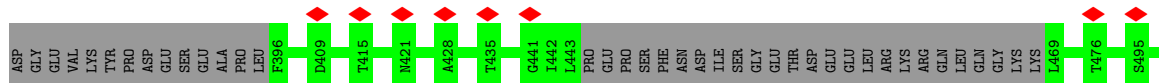
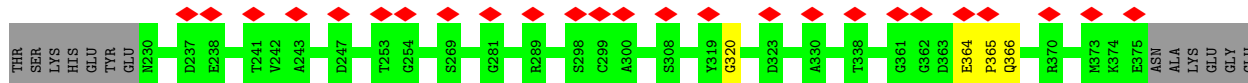
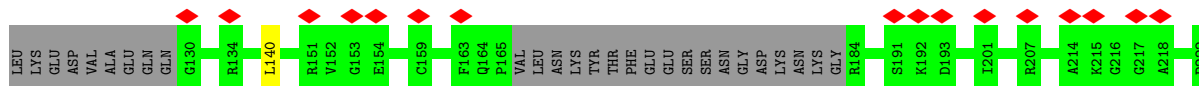
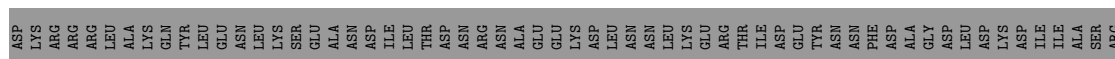


• Molecule 38: Snu13

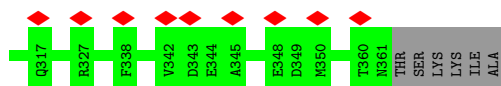
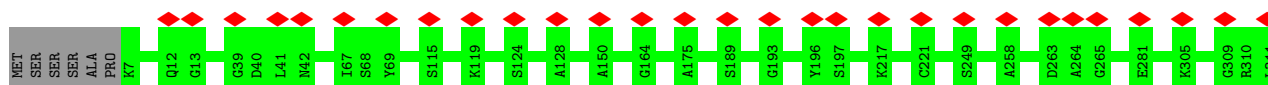




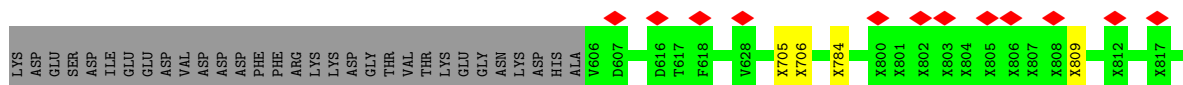
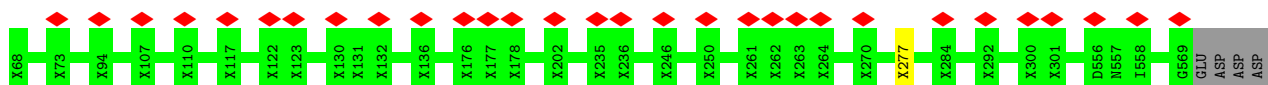
• Molecule 39: Ribosomal RNA-processing protein 9

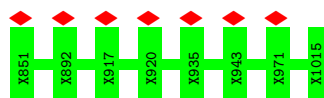


• Molecule 40: RNA 3'-terminal phosphate cyclase-like protein

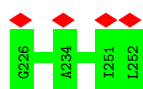
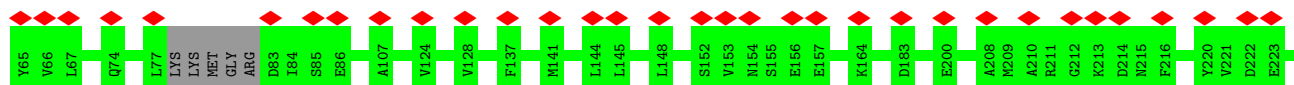
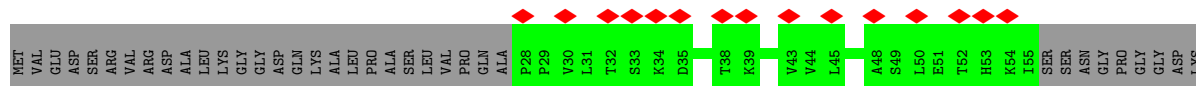
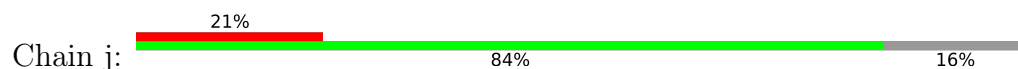


• Molecule 41: Bms1, Ribosome biogenesis protein BMS1, Bms1

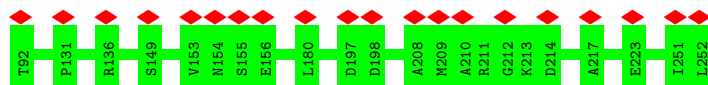
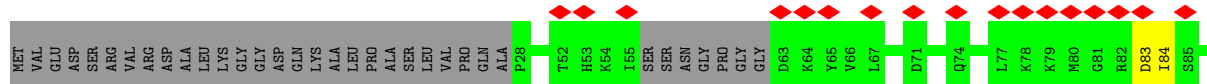
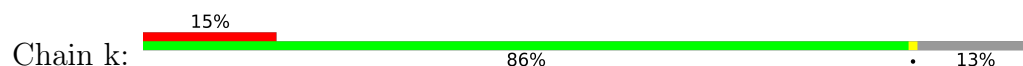




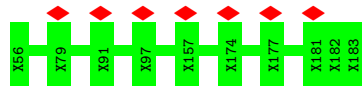
- Molecule 42: Ribosomal RNA small subunit methyltransferase NEP1



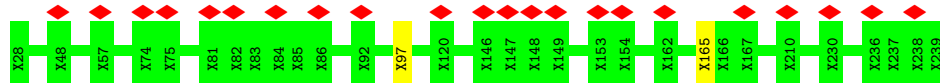
- Molecule 42: Ribosomal RNA small subunit methyltransferase NEP1



- Molecule 43: Utp24



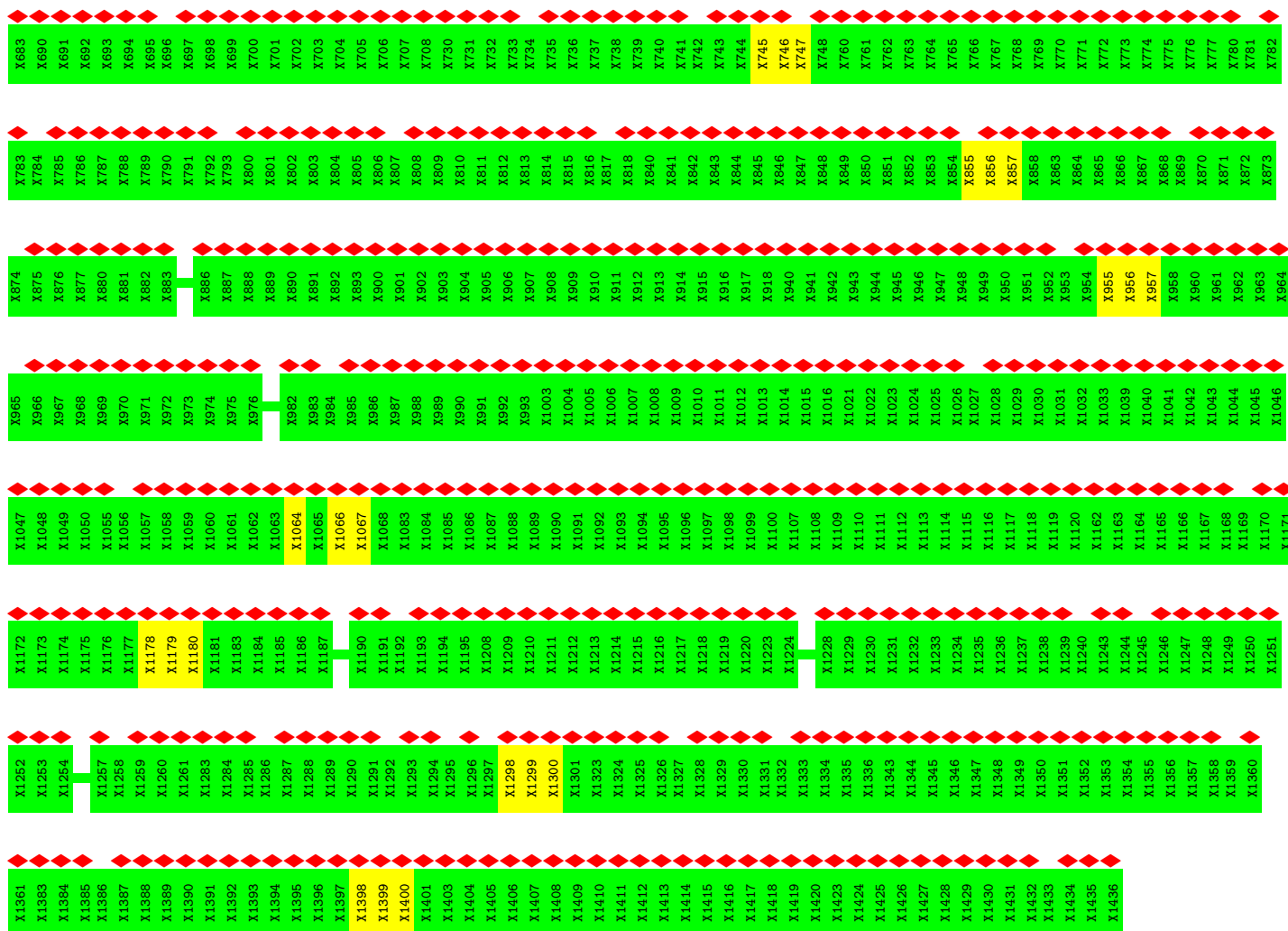
- Molecule 44: Imp4



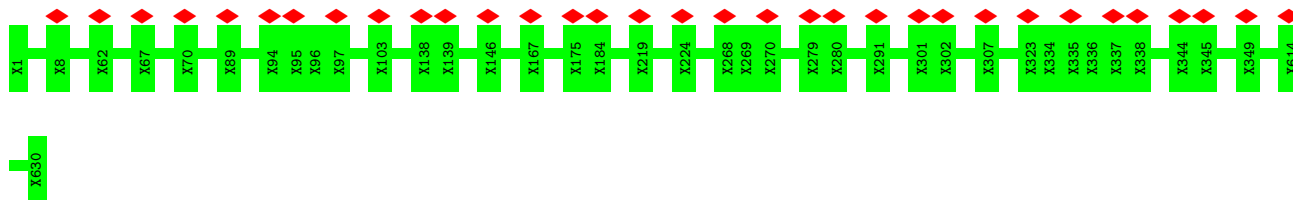
- Molecule 45: Utp30



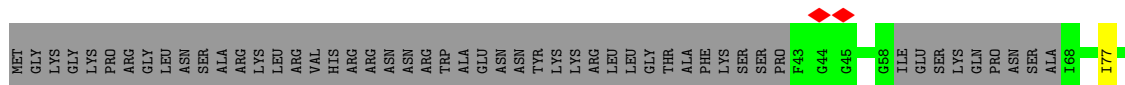




• Molecule 48: Repeat protein 2

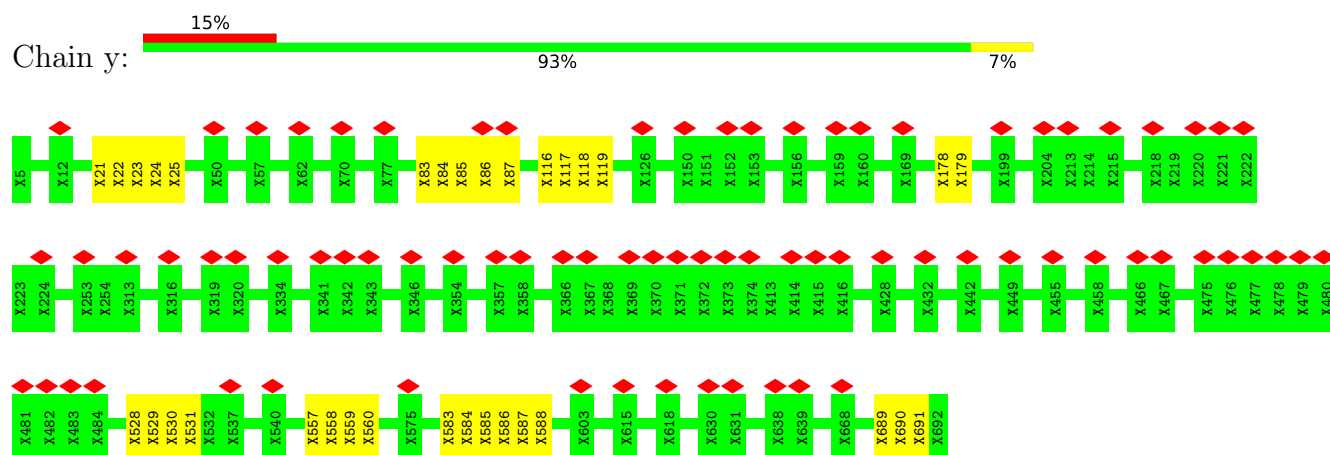


• Molecule 49: 40S ribosomal protein S23-A

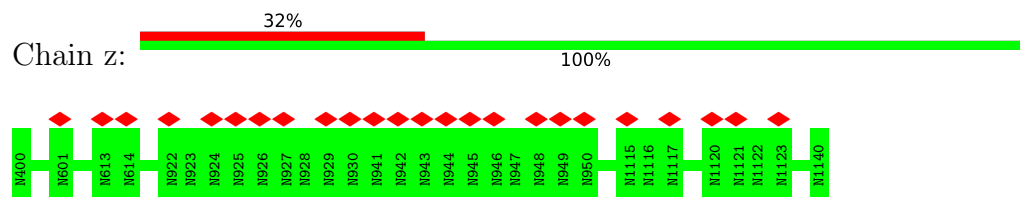




## • Molecule 52: Unassigned protein helices



## • Molecule 53: Unassigned RNA helices



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	33813	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.56	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	503.50003, 503.50003, 503.50003	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.325, 1.325, 1.325	Depositor



## 5 Model quality

### 5.1 Standard geometry

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	0	1.11	0/268	1.42	5/417 (1.2%)
2	1	1.25	39/12260 (0.3%)	1.71	368/19055 (1.9%)
3	2	1.66	26/2443 (1.1%)	1.69	73/3787 (1.9%)
4	3	0.57	0/1061	0.81	1/1472 (0.1%)
5	5	0.63	0/1182	0.92	0/1638
6	6	0.70	2/998 (0.2%)	1.22	7/1388 (0.5%)
7	7	0.51	0/922	0.85	0/1285
8	8	0.65	0/847	0.93	0/1173
9	9	0.56	0/914	0.82	0/1272
12	C	0.50	0/565	0.77	0/784
13	D	0.30	0/720	0.62	0/1001
14	E	0.34	0/623	0.63	0/864
15	F	0.38	0/443	0.73	0/615
16	G	0.46	0/305	0.80	0/423
27	T	0.51	0/3055	0.69	0/4243
38	e	0.25	0/605	0.56	0/843
38	f	0.26	0/565	0.57	0/787
39	g	0.41	0/1793	0.64	2/2485 (0.1%)
40	h	0.40	0/1741	0.59	0/2416
41	i	0.32	0/265	0.50	0/367
42	j	0.36	0/1044	0.62	0/1452
42	k	0.39	0/1079	0.57	0/1502
49	r	0.37	0/399	0.58	0/549
All	All	0.95	67/34097 (0.2%)	1.28	456/49818 (0.9%)

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
3	2	0	1
6	6	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	9	0	3
12	C	0	1
15	F	0	2
16	G	0	1
17	H	0	4
18	I	0	11
19	J	0	2
19	K	0	3
20	M	0	3
21	N	0	4
22	O	0	12
24	Q	0	4
26	S	0	4
27	T	0	2
28	U	0	1
30	W	0	10
31	X	0	2
33	Z	0	2
34	a	0	6
35	b	0	1
36	c	0	3
37	d	0	3
39	g	0	2
41	i	0	5
44	m	0	2
47	p	0	38
50	s	0	9
50	t	0	11
50	u	0	1
51	v	0	13
52	y	0	33
All	All	0	202

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	308	U	O3'-P	-63.84	0.84	1.61
2	1	1615	C	O3'-P	-41.94	1.10	1.61
6	6	145	ASP	C-N	-12.45	1.05	1.34
2	1	337	G	C2-N2	10.63	1.45	1.34
3	2	118	A	C1'-N9	-10.57	1.32	1.46
6	6	207	THR	C-N	-9.46	1.12	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	163	G	N9-C4	-9.23	1.30	1.38
2	1	337	G	C8-N7	-8.96	1.25	1.30
2	1	337	G	N1-C2	8.18	1.44	1.37
2	1	337	G	C2-N3	8.08	1.39	1.32
2	1	65	A	N9-C4	-7.83	1.33	1.37
2	1	163	G	N3-C4	-7.69	1.30	1.35
2	1	1535	U	C2-N3	-7.44	1.32	1.37
2	1	100	A	P-OP2	-7.00	1.37	1.49
2	1	397	A	N9-C4	-7.00	1.33	1.37
3	2	99	U	C1'-N1	6.97	1.59	1.48
3	2	312	U	C1'-N1	6.96	1.59	1.48
3	2	304	U	C1'-N1	6.93	1.59	1.48
3	2	102	U	C1'-N1	6.93	1.59	1.48
3	2	100	U	C1'-N1	6.91	1.59	1.48
3	2	308	U	C1'-N1	6.91	1.59	1.48
3	2	203	U	C1'-N1	6.89	1.59	1.48
2	1	163	G	C5-C6	-6.73	1.35	1.42
3	2	80	U	C1'-N1	6.65	1.58	1.48
2	1	337	G	N7-C5	-6.57	1.35	1.39
2	1	101	U	P-OP2	-6.52	1.37	1.49
3	2	201	C	C1'-N1	6.42	1.58	1.48
3	2	261	U	C1'-N1	6.40	1.58	1.48
2	1	53	G	C6-N1	-6.40	1.35	1.39
3	2	314	C	C1'-N1	6.39	1.58	1.48
3	2	250	C	C1'-N1	6.38	1.58	1.48
3	2	264	C	C1'-N1	6.34	1.58	1.48
3	2	265	C	C1'-N1	6.34	1.58	1.48
3	2	200	C	C1'-N1	6.31	1.58	1.48
2	1	400	A	N9-C4	6.28	1.41	1.37
2	1	351	C	N1-C6	-6.27	1.33	1.37
3	2	106	C	C1'-N1	6.25	1.58	1.48
3	2	104	C	C1'-N1	6.25	1.58	1.48
3	2	105	C	C1'-N1	6.24	1.58	1.48
3	2	266	C	C1'-N1	6.24	1.58	1.48
2	1	538	A	N9-C4	6.08	1.41	1.37
3	2	111	G	C1'-N9	-5.89	1.38	1.46
2	1	392	G	N1-C2	-5.87	1.33	1.37
2	1	418	G	N7-C5	-5.66	1.35	1.39
2	1	331	A	N9-C4	-5.61	1.34	1.37
2	1	357	G	N9-C8	-5.56	1.33	1.37
2	1	1478	G	N7-C5	-5.54	1.35	1.39
2	1	341	A	N3-C4	-5.53	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	423	G	C6-N1	-5.49	1.35	1.39
2	1	314	C	C2-O2	-5.45	1.19	1.24
2	1	314	C	N3-C4	-5.44	1.30	1.33
2	1	392	G	C5-C4	-5.41	1.34	1.38
2	1	377	G	N1-C2	-5.39	1.33	1.37
2	1	317	C	N1-C6	-5.37	1.33	1.37
2	1	352	A	N9-C4	-5.33	1.34	1.37
2	1	539	G	C5-C4	5.23	1.42	1.38
2	1	55	A	C5-C4	-5.20	1.35	1.38
2	1	119	A	N9-C4	-5.17	1.34	1.37
2	1	337	G	C5-C6	-5.16	1.37	1.42
2	1	434	G	C6-N1	-5.14	1.35	1.39
3	2	78	G	C1'-N9	-5.13	1.39	1.46
3	2	95	A	C1'-N9	-5.06	1.39	1.46
3	2	253	G	C1'-N9	-5.04	1.39	1.46
2	1	453	U	N3-C4	-5.02	1.33	1.38
3	2	79	G	C1'-N9	-5.01	1.39	1.46
2	1	158	U	C3'-O3'	5.01	1.49	1.42
2	1	335	U	N1-C2	-5.01	1.34	1.38

All (456) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	1615	C	OP2-P-O3'	-30.61	37.85	105.20
6	6	145	ASP	O-C-N	-22.20	87.17	122.70
3	2	118	A	O4'-C1'-N9	-21.15	91.28	108.20
2	1	1615	C	OP1-P-O3'	17.13	142.90	105.20
2	1	1615	C	O3'-P-O5'	-16.35	72.93	104.00
2	1	337	G	C6-C5-N7	-15.77	120.94	130.40
3	2	118	A	N9-C1'-C2'	14.97	133.46	114.00
6	6	207	THR	O-C-N	14.91	146.55	122.70
2	1	163	G	C5-N7-C8	-14.86	96.87	104.30
2	1	337	G	C8-N9-C1'	-14.35	108.34	127.00
2	1	163	G	N3-C4-N9	-14.07	117.56	126.00
2	1	163	G	N3-C4-C5	14.00	135.60	128.60
2	1	163	G	C2-N3-C4	-13.50	105.15	111.90
2	1	337	G	C4-N9-C1'	13.37	143.88	126.50
2	1	308	C	C5-C6-N1	-13.33	114.33	121.00
3	2	308	U	P-O3'-C3'	12.84	135.11	119.70
2	1	453	U	N3-C2-O2	-12.75	113.28	122.20
2	1	308	C	C2-N3-C4	-12.49	113.66	119.90
2	1	65	A	C2-N3-C4	-12.37	104.42	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	6	145	ASP	C-N-CA	12.32	152.50	121.70
2	1	337	G	N9-C4-C5	-12.24	100.50	105.40
2	1	144	U	N3-C2-O2	-12.12	113.71	122.20
3	2	308	U	O3'-P-O5'	-11.97	81.26	104.00
6	6	207	THR	CA-C-N	-11.83	91.17	117.20
2	1	1615	C	P-O3'-C3'	-11.50	105.90	119.70
2	1	163	G	C4-C5-N7	11.46	115.38	110.80
2	1	337	G	N1-C6-O6	11.16	126.60	119.90
2	1	453	U	C5-C4-O4	10.88	132.43	125.90
2	1	163	G	N7-C8-N9	10.53	118.36	113.10
2	1	337	G	C4-C5-N7	10.46	114.99	110.80
2	1	308	C	C2-N1-C1'	-10.41	107.34	118.80
2	1	1572	G	C5-C6-O6	-10.14	122.52	128.60
2	1	314	C	C6-N1-C2	-9.87	116.35	120.30
6	6	145	ASP	CA-C-N	9.80	138.77	117.20
2	1	448	C	C6-N1-C2	-9.78	116.39	120.30
2	1	99	C	C2-N3-C4	-9.74	115.03	119.90
2	1	163	G	C8-N9-C4	-9.69	102.53	106.40
2	1	1481	C	C6-N1-C2	-9.66	116.43	120.30
2	1	1614	A	C5-N7-C8	-9.62	99.09	103.90
2	1	415	C	C6-N1-C2	9.38	124.05	120.30
6	6	207	THR	C-N-CA	-9.15	98.83	121.70
2	1	163	G	N1-C6-O6	9.08	125.35	119.90
2	1	1572	G	N1-C6-O6	9.03	125.32	119.90
2	1	321	C	N3-C2-O2	-9.02	115.59	121.90
2	1	163	G	N3-C2-N2	-8.80	113.74	119.90
2	1	539	G	N7-C8-N9	8.76	117.48	113.10
2	1	352	A	C8-N9-C4	8.75	109.30	105.80
2	1	337	G	C4-C5-C6	8.74	124.04	118.80
2	1	512	A	N1-C6-N6	8.65	123.79	118.60
2	1	314	C	N3-C2-O2	-8.60	115.88	121.90
2	1	1614	A	N1-C6-N6	8.56	123.73	118.60
2	1	144	U	C2-N1-C1'	8.53	127.94	117.70
2	1	453	U	C2-N1-C1'	8.52	127.92	117.70
2	1	1614	A	C4-C5-N7	8.45	114.92	110.70
2	1	272	U	N3-C2-O2	-8.44	116.30	122.20
3	2	118	A	C4-N9-C1'	-8.39	111.19	126.30
2	1	114	C	N1-C2-O2	8.37	123.92	118.90
2	1	1535	U	N1-C2-O2	8.36	128.65	122.80
2	1	359	A	C4-C5-C6	-8.29	112.85	117.00
2	1	102	U	N1-C2-O2	-8.24	117.03	122.80
2	1	342	C	C5-C6-N1	-8.06	116.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	1620	C	C6-N1-C2	-8.03	117.09	120.30
2	1	400	A	N1-C6-N6	7.99	123.39	118.60
2	1	100	A	C8-N9-C4	7.94	108.97	105.80
2	1	421	A	C8-N9-C4	7.89	108.96	105.80
2	1	364	G	C5-C6-O6	-7.88	123.88	128.60
2	1	418	G	C8-N9-C4	-7.86	103.26	106.40
2	1	306	U	C5-C6-N1	-7.84	118.78	122.70
2	1	1535	U	N3-C2-O2	-7.83	116.72	122.20
2	1	418	G	C6-C5-N7	-7.83	125.70	130.40
2	1	453	U	N3-C4-O4	-7.80	113.94	119.40
2	1	65	A	N1-C6-N6	7.79	123.28	118.60
2	1	1473	U	N3-C2-O2	-7.79	116.75	122.20
2	1	397	A	C2-N3-C4	-7.74	106.73	110.60
2	1	65	A	N3-C4-C5	7.68	132.18	126.80
2	1	337	G	N3-C4-N9	7.67	130.60	126.00
2	1	359	A	N1-C2-N3	-7.62	125.49	129.30
2	1	163	G	C5-C6-O6	-7.59	124.04	128.60
2	1	418	G	C4-N9-C1'	7.56	136.33	126.50
2	1	1478	G	C4-N9-C1'	7.53	136.29	126.50
2	1	453	U	N1-C2-O2	7.53	128.07	122.80
2	1	308	C	C6-N1-C1'	7.52	129.82	120.80
2	1	308	C	N1-C2-N3	7.50	124.45	119.20
2	1	144	U	C6-N1-C2	-7.50	116.50	121.00
2	1	308	C	N3-C4-N4	-7.50	112.75	118.00
2	1	539	G	C8-N9-C4	-7.48	103.41	106.40
2	1	359	A	C6-N1-C2	7.41	123.05	118.60
2	1	60	U	N1-C2-O2	7.41	127.99	122.80
2	1	160	C	N1-C2-O2	7.41	123.34	118.90
2	1	392	G	N1-C6-O6	-7.38	115.47	119.90
2	1	308	C	C4-C5-C6	7.34	121.07	117.40
2	1	321	C	N1-C2-O2	7.33	123.30	118.90
2	1	337	G	N3-C2-N2	7.30	125.01	119.90
2	1	421	A	N1-C6-N6	7.27	122.97	118.60
2	1	410	A	N1-C6-N6	-7.27	114.24	118.60
3	2	315	A	OP2-P-O3'	7.25	121.16	105.20
3	2	100	U	OP2-P-O3'	7.25	121.14	105.20
3	2	103	A	OP2-P-O3'	7.24	121.13	105.20
3	2	202	G	OP2-P-O3'	7.24	121.12	105.20
3	2	249	G	OP2-P-O3'	7.23	121.11	105.20
3	2	310	G	OP2-P-O3'	7.23	121.11	105.20
2	1	339	C	N1-C2-O2	-7.22	114.56	118.90
3	2	266	C	OP2-P-O3'	7.22	121.09	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	309	G	OP2-P-O3'	7.22	121.10	105.20
3	2	99	U	OP2-P-O3'	7.22	121.09	105.20
2	1	93	A	N1-C6-N6	7.22	122.93	118.60
3	2	104	C	OP2-P-O3'	7.22	121.08	105.20
3	2	201	C	OP2-P-O3'	7.22	121.08	105.20
3	2	305	G	OP2-P-O3'	7.21	121.07	105.20
2	1	421	A	N9-C4-C5	-7.21	102.92	105.80
3	2	102	U	OP2-P-O3'	7.21	121.06	105.20
3	2	200	C	OP2-P-O3'	7.21	121.06	105.20
3	2	264	C	OP2-P-O3'	7.21	121.05	105.20
2	1	56	U	C5-C6-N1	-7.20	119.10	122.70
3	2	263	A	OP2-P-O3'	7.20	121.05	105.20
3	2	105	C	OP2-P-O3'	7.20	121.05	105.20
2	1	310	C	N1-C2-O2	-7.20	114.58	118.90
3	2	307	G	OP2-P-O3'	7.20	121.03	105.20
3	2	312	U	OP2-P-O3'	7.20	121.03	105.20
3	2	265	C	OP2-P-O3'	7.20	121.03	105.20
3	2	313	A	OP2-P-O3'	7.19	121.03	105.20
3	2	304	U	OP2-P-O3'	7.18	121.00	105.20
3	2	306	G	OP2-P-O3'	7.18	121.00	105.20
3	2	316	A	OP2-P-O3'	7.18	121.00	105.20
3	2	101	G	OP2-P-O3'	7.18	120.99	105.20
3	2	311	G	OP2-P-O3'	7.18	120.99	105.20
3	2	320	G	N3-C4-C5	7.17	132.19	128.60
2	1	1572	G	C4-C5-N7	7.17	113.67	110.80
3	2	314	C	OP2-P-O3'	7.16	120.96	105.20
2	1	53	G	N1-C6-O6	-7.16	115.60	119.90
2	1	95	G	C8-N9-C4	-7.15	103.54	106.40
2	1	512	A	C5-C6-N6	-7.12	118.00	123.70
2	1	114	C	N3-C2-O2	-7.09	116.94	121.90
2	1	310	C	C4-C5-C6	7.09	120.94	117.40
2	1	354	C	N3-C4-C5	7.09	124.73	121.90
2	1	387	A	N1-C6-N6	-7.07	114.36	118.60
2	1	385	A	C5-N7-C8	7.04	107.42	103.90
2	1	65	A	N9-C4-C5	-7.03	102.99	105.80
2	1	424	C	C6-N1-C2	7.02	123.11	120.30
2	1	351	C	C2-N1-C1'	7.01	126.51	118.80
2	1	144	U	N1-C2-O2	7.00	127.70	122.80
2	1	408	C	C6-N1-C2	-6.99	117.50	120.30
3	2	308	U	OP1-P-O3'	6.99	120.58	105.20
2	1	411	C	C4-C5-C6	6.99	120.89	117.40
2	1	297	U	C2-N1-C1'	6.98	126.08	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	430	G	C5-C6-O6	-6.89	124.47	128.60
2	1	337	G	N1-C2-N3	-6.89	119.77	123.90
2	1	87	C	C4-C5-C6	6.88	120.84	117.40
1	0	281	G	N1-C2-N2	-6.86	110.02	116.20
2	1	1478	G	C6-C5-N7	-6.86	126.29	130.40
2	1	1606	C	C6-N1-C2	6.85	123.04	120.30
2	1	297	U	N3-C4-O4	6.85	124.19	119.40
2	1	1472	C	N3-C4-N4	-6.85	113.21	118.00
3	2	249	G	O3'-P-O5'	-6.84	91.01	104.00
2	1	1170	G	N3-C4-N9	6.82	130.09	126.00
1	0	290	G	N1-C2-N2	-6.82	110.06	116.20
2	1	418	G	N7-C8-N9	6.81	116.51	113.10
3	2	310	G	O3'-P-O5'	-6.81	91.07	104.00
3	2	101	G	O3'-P-O5'	-6.81	91.07	104.00
3	2	305	G	O3'-P-O5'	-6.80	91.08	104.00
3	2	201	C	O3'-P-O5'	-6.80	91.08	104.00
2	1	342	C	C4-C5-C6	6.80	120.80	117.40
3	2	202	G	O3'-P-O5'	-6.80	91.09	104.00
3	2	309	G	O3'-P-O5'	-6.80	91.09	104.00
3	2	313	A	O3'-P-O5'	-6.79	91.09	104.00
3	2	306	G	O3'-P-O5'	-6.79	91.10	104.00
3	2	264	C	O3'-P-O5'	-6.78	91.11	104.00
3	2	105	C	O3'-P-O5'	-6.78	91.12	104.00
2	1	1614	A	N7-C8-N9	6.78	117.19	113.80
3	2	316	A	O3'-P-O5'	-6.78	91.12	104.00
3	2	99	U	O3'-P-O5'	-6.78	91.13	104.00
3	2	315	A	O3'-P-O5'	-6.77	91.13	104.00
3	2	102	U	O3'-P-O5'	-6.77	91.14	104.00
3	2	266	C	O3'-P-O5'	-6.77	91.14	104.00
3	2	200	C	O3'-P-O5'	-6.77	91.14	104.00
3	2	100	U	O3'-P-O5'	-6.76	91.15	104.00
3	2	307	G	O3'-P-O5'	-6.76	91.15	104.00
3	2	103	A	O3'-P-O5'	-6.76	91.15	104.00
3	2	312	U	O3'-P-O5'	-6.76	91.16	104.00
3	2	314	C	O3'-P-O5'	-6.76	91.16	104.00
3	2	263	A	O3'-P-O5'	-6.75	91.17	104.00
3	2	104	C	O3'-P-O5'	-6.75	91.17	104.00
2	1	453	U	C6-N1-C2	-6.75	116.95	121.00
3	2	304	U	O3'-P-O5'	-6.75	91.18	104.00
2	1	163	G	C8-N9-C1'	6.74	135.76	127.00
3	2	265	C	O3'-P-O5'	-6.72	91.24	104.00
3	2	311	G	O3'-P-O5'	-6.72	91.24	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	539	G	C5-N7-C8	-6.70	100.95	104.30
2	1	1609	U	N3-C2-O2	6.70	126.89	122.20
2	1	119	A	C2-N3-C4	-6.70	107.25	110.60
2	1	65	A	C4-C5-N7	6.69	114.05	110.70
2	1	110	U	N3-C4-C5	6.68	118.61	114.60
2	1	467	G	N1-C6-O6	-6.68	115.89	119.90
2	1	426	G	N3-C4-C5	-6.68	125.26	128.60
2	1	351	C	N3-C4-C5	-6.67	119.23	121.90
2	1	364	G	C5-C6-N1	6.66	114.83	111.50
2	1	380	U	N3-C2-O2	-6.65	117.54	122.20
2	1	354	C	C4-C5-C6	-6.65	114.08	117.40
2	1	1619	C	C6-N1-C2	-6.61	117.66	120.30
2	1	282	C	C6-N1-C2	6.59	122.94	120.30
2	1	352	A	N7-C8-N9	-6.59	110.50	113.80
2	1	1478	G	C4-C5-C6	6.58	122.75	118.80
2	1	346	G	N1-C6-O6	-6.54	115.97	119.90
2	1	432	G	N3-C2-N2	-6.53	115.33	119.90
2	1	538	A	N1-C6-N6	-6.52	114.69	118.60
2	1	101	U	C6-N1-C2	-6.51	117.09	121.00
2	1	382	C	N3-C4-C5	6.51	124.50	121.90
2	1	448	C	C6-N1-C1'	6.49	128.59	120.80
2	1	1592	A	N1-C2-N3	6.48	132.54	129.30
2	1	402	C	C6-N1-C2	6.47	122.89	120.30
2	1	402	C	C5-C4-N4	-6.46	115.68	120.20
2	1	113	U	N1-C2-O2	-6.46	118.28	122.80
2	1	341	A	C8-N9-C4	-6.45	103.22	105.80
2	1	1473	U	C2-N1-C1'	6.44	125.43	117.70
2	1	394	C	C4-C5-C6	6.44	120.62	117.40
2	1	1627	U	C5-C4-O4	6.43	129.76	125.90
2	1	355	G	N1-C6-O6	-6.42	116.05	119.90
2	1	1484	G	N3-C4-N9	6.39	129.83	126.00
2	1	87	C	N1-C2-O2	-6.37	115.08	118.90
2	1	280	U	N3-C2-O2	-6.36	117.75	122.20
2	1	1473	U	N1-C2-N3	6.35	118.71	114.90
2	1	350	U	N3-C2-O2	-6.35	117.76	122.20
2	1	151	G	N9-C4-C5	6.34	107.94	105.40
3	2	320	G	C2-N3-C4	-6.33	108.74	111.90
2	1	101	U	N3-C2-O2	-6.32	117.77	122.20
2	1	290	G	C8-N9-C4	-6.32	103.87	106.40
1	0	290	G	N3-C2-N2	6.31	124.32	119.90
2	1	449	C	N3-C4-N4	-6.29	113.60	118.00
2	1	387	A	C2-N3-C4	6.29	113.74	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	396	G	N3-C2-N2	6.29	124.30	119.90
2	1	351	C	C4-C5-C6	6.29	120.54	117.40
2	1	400	A	C5-C6-N6	-6.29	118.67	123.70
3	2	65	C	N1-C2-O2	6.29	122.67	118.90
2	1	392	G	C5-C6-N1	6.27	114.64	111.50
2	1	65	A	C5-C6-N1	-6.27	114.56	117.70
2	1	139	C	C6-N1-C2	-6.25	117.80	120.30
2	1	453	U	N1-C2-N3	6.25	118.65	114.90
2	1	1571	C	C4-C5-C6	6.24	120.52	117.40
2	1	364	G	C8-N9-C4	6.20	108.88	106.40
2	1	382	C	C2-N3-C4	-6.20	116.80	119.90
2	1	359	A	C4-N9-C1'	-6.20	115.15	126.30
2	1	1614	A	C6-C5-N7	-6.18	127.97	132.30
2	1	84	A	N1-C6-N6	-6.17	114.90	118.60
2	1	306	U	C6-N1-C2	6.16	124.70	121.00
2	1	539	G	N3-C4-N9	-6.16	122.30	126.00
2	1	317	C	C2-N3-C4	-6.16	116.82	119.90
2	1	62	A	N1-C6-N6	6.15	122.29	118.60
2	1	364	G	C6-N1-C2	-6.13	121.42	125.10
2	1	1478	G	C8-N9-C1'	-6.13	119.03	127.00
2	1	447	U	N1-C2-N3	6.13	118.58	114.90
2	1	341	A	N9-C4-C5	6.13	108.25	105.80
2	1	152	U	C5-C4-O4	6.13	129.58	125.90
2	1	1481	C	C3'-C2'-C1'	-6.12	96.60	101.50
2	1	396	G	C4-C5-N7	6.11	113.25	110.80
2	1	1480	G	C8-N9-C4	-6.10	103.96	106.40
2	1	337	G	C5-C6-N1	-6.10	108.45	111.50
2	1	391	A	C5-N7-C8	6.10	106.95	103.90
1	0	281	G	N3-C2-N2	6.09	124.16	119.90
2	1	337	G	C5-C6-O6	-6.08	124.95	128.60
2	1	422	G	C8-N9-C4	-6.08	103.97	106.40
2	1	66	U	C5-C6-N1	-6.07	119.66	122.70
2	1	272	U	N1-C2-O2	6.06	127.04	122.80
2	1	1594	G	C8-N9-C4	6.05	108.82	106.40
2	1	87	C	C6-N1-C2	-6.05	117.88	120.30
2	1	150	U	N3-C4-O4	-6.05	115.17	119.40
2	1	429	G	C4-C5-N7	-6.04	108.38	110.80
2	1	1471	A	C8-N9-C4	-6.03	103.39	105.80
2	1	358	U	N1-C2-O2	-6.03	118.58	122.80
2	1	65	A	C5-N7-C8	-6.00	100.90	103.90
3	2	320	G	N3-C4-N9	-6.00	122.40	126.00
2	1	144	U	N1-C2-N3	5.99	118.50	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	59	C	N1-C2-O2	5.97	122.48	118.90
2	1	465	G	C8-N9-C4	5.96	108.78	106.40
2	1	1473	U	C5-C4-O4	5.96	129.48	125.90
2	1	1482	C	C6-N1-C2	5.96	122.69	120.30
2	1	1469	A	C8-N9-C4	5.95	108.18	105.80
2	1	416	A	N1-C6-N6	5.95	122.17	118.60
2	1	114	C	C2-N1-C1'	5.94	125.33	118.80
2	1	385	A	C4-C5-N7	-5.93	107.73	110.70
2	1	1572	G	C6-C5-N7	-5.93	126.84	130.40
39	g	320	GLY	N-CA-C	5.92	127.90	113.10
2	1	1594	G	N3-C4-N9	5.92	129.55	126.00
2	1	1481	C	N3-C4-C5	-5.92	119.53	121.90
2	1	1472	C	C2-N3-C4	-5.89	116.95	119.90
2	1	355	G	C5-C6-N1	5.88	114.44	111.50
2	1	355	G	C5-N7-C8	5.88	107.24	104.30
2	1	389	G	N3-C4-N9	5.87	129.53	126.00
2	1	419	G	N1-C6-O6	-5.85	116.39	119.90
2	1	339	C	C6-N1-C2	-5.81	117.97	120.30
2	1	1534	G	N3-C4-C5	-5.81	125.69	128.60
2	1	359	A	N3-C4-C5	5.81	130.87	126.80
2	1	109	G	N7-C8-N9	-5.80	110.20	113.10
2	1	298	C	C6-N1-C2	-5.79	117.98	120.30
2	1	96	G	N9-C4-C5	5.78	107.71	105.40
2	1	448	C	N1-C2-O2	-5.78	115.43	118.90
2	1	151	G	N3-C2-N2	-5.78	115.86	119.90
2	1	1473	U	C6-N1-C2	-5.78	117.53	121.00
2	1	418	G	C8-N9-C1'	-5.77	119.50	127.00
2	1	153	G	N3-C4-N9	-5.77	122.54	126.00
2	1	84	A	C5-N7-C8	5.76	106.78	103.90
3	2	83	A	N9-C4-C5	-5.76	103.50	105.80
2	1	385	A	N7-C8-N9	-5.75	110.92	113.80
2	1	129	U	N1-C2-N3	5.74	118.34	114.90
2	1	102	U	N1-C2-N3	5.73	118.34	114.90
2	1	280	U	N1-C2-O2	5.73	126.81	122.80
2	1	524	U	N3-C2-O2	-5.73	118.19	122.20
2	1	99	C	C2-N1-C1'	5.72	125.09	118.80
2	1	272	U	C2-N1-C1'	5.72	124.56	117.70
2	1	432	G	N9-C4-C5	5.71	107.69	105.40
2	1	1572	G	C5-N7-C8	-5.70	101.45	104.30
2	1	1620	C	N3-C2-O2	-5.70	117.91	121.90
2	1	96	G	C5-C6-O6	5.69	132.01	128.60
2	1	96	G	C8-N9-C4	-5.69	104.12	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	512	A	N9-C4-C5	-5.67	103.53	105.80
2	1	356	G	C5-N7-C8	5.67	107.13	104.30
2	1	158	U	P-O3'-C3'	5.65	126.48	119.70
2	1	359	A	C6-C5-N7	5.65	136.25	132.30
2	1	409	C	C5-C4-N4	-5.65	116.25	120.20
2	1	96	G	N1-C2-N3	5.64	127.29	123.90
2	1	396	G	N9-C4-C5	-5.64	103.14	105.40
2	1	411	C	N3-C2-O2	-5.63	117.96	121.90
2	1	1476	C	C6-N1-C2	-5.63	118.05	120.30
2	1	385	A	C5-C6-N6	5.63	128.20	123.70
3	2	85	G	N3-C4-N9	-5.61	122.64	126.00
2	1	66	U	C4-C5-C6	5.60	123.06	119.70
2	1	390	G	N3-C4-C5	-5.59	125.80	128.60
2	1	51	A	N1-C2-N3	5.59	132.09	129.30
2	1	99	C	C5-C4-N4	-5.58	116.29	120.20
2	1	146	U	N3-C2-O2	-5.58	118.29	122.20
2	1	1170	G	C8-N9-C1'	-5.58	119.75	127.00
1	0	287	G	N1-C2-N2	-5.57	111.19	116.20
2	1	310	C	C2-N3-C4	-5.56	117.12	119.90
2	1	72	A	N1-C6-N6	-5.56	115.27	118.60
2	1	328	A	N9-C4-C5	5.55	108.02	105.80
2	1	163	G	N1-C2-N3	5.54	127.22	123.90
2	1	272	U	P-O3'-C3'	5.54	126.34	119.70
2	1	425	A	N1-C6-N6	-5.51	115.29	118.60
2	1	1177	C	C2-N1-C1'	-5.51	112.74	118.80
2	1	403	G	N9-C4-C5	-5.51	103.20	105.40
2	1	351	C	C6-N1-C1'	-5.50	114.20	120.80
2	1	102	U	N3-C4-O4	5.49	123.24	119.40
2	1	1153	G	N3-C4-C5	5.49	131.34	128.60
2	1	538	A	C8-N9-C4	-5.49	103.61	105.80
2	1	110	U	N1-C2-O2	5.48	126.64	122.80
2	1	306	U	C5-C4-O4	-5.48	122.61	125.90
2	1	381	C	C2-N3-C4	-5.48	117.16	119.90
2	1	359	A	C8-N9-C4	5.47	107.99	105.80
2	1	356	G	N7-C8-N9	-5.47	110.37	113.10
3	2	257	A	N9-C4-C5	-5.46	103.61	105.80
2	1	336	G	C5-N7-C8	5.46	107.03	104.30
2	1	352	A	N3-C4-C5	5.46	130.62	126.80
2	1	418	G	N1-C6-O6	5.45	123.17	119.90
2	1	434	G	N1-C6-O6	-5.45	116.63	119.90
2	1	396	G	N3-C4-N9	5.44	129.27	126.00
4	3	108	VAL	CB-CA-C	-5.44	101.06	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	477	A	N9-C4-C5	-5.44	103.62	105.80
2	1	124	A	C6-N1-C2	5.43	121.86	118.60
2	1	153	G	N3-C4-C5	5.43	131.31	128.60
2	1	1573	A	C2-N3-C4	5.43	113.31	110.60
2	1	109	G	C5-N7-C8	5.42	107.01	104.30
2	1	426	G	N3-C4-N9	5.42	129.25	126.00
2	1	448	C	N1-C2-N3	5.42	122.99	119.20
2	1	328	A	N1-C6-N6	-5.41	115.36	118.60
2	1	387	A	C4-C5-N7	-5.38	108.01	110.70
2	1	146	U	N1-C2-O2	5.37	126.56	122.80
2	1	1619	C	C5-C6-N1	5.37	123.68	121.00
2	1	300	A	C8-N9-C4	5.37	107.95	105.80
2	1	411	C	C5-C6-N1	-5.35	118.33	121.00
2	1	296	U	N3-C4-C5	5.35	117.81	114.60
2	1	148	A	C8-N9-C4	-5.34	103.66	105.80
2	1	379	U	N1-C2-O2	-5.34	119.06	122.80
2	1	389	G	N3-C4-C5	-5.34	125.93	128.60
3	2	113	G	C8-N9-C4	-5.33	104.27	106.40
2	1	90	C	N3-C2-O2	-5.33	118.17	121.90
2	1	336	G	N7-C8-N9	-5.33	110.44	113.10
2	1	1609	U	N1-C2-O2	-5.33	119.07	122.80
3	2	327	G	C8-N9-C4	-5.32	104.27	106.40
2	1	254	A	C8-N9-C4	5.31	107.92	105.80
2	1	1484	G	N3-C4-C5	-5.31	125.95	128.60
2	1	95	G	N7-C8-N9	5.30	115.75	113.10
2	1	1483	A	N1-C6-N6	5.30	121.78	118.60
2	1	1615	C	N1-C2-O2	-5.30	115.72	118.90
2	1	1173	C	C6-N1-C2	-5.30	118.18	120.30
2	1	54	C	N3-C4-C5	5.30	124.02	121.90
2	1	65	A	C6-C5-N7	-5.30	128.59	132.30
2	1	308	C	C6-N1-C2	5.28	122.41	120.30
2	1	447	U	N3-C2-O2	-5.28	118.50	122.20
6	6	70	VAL	CB-CA-C	-5.28	101.38	111.40
2	1	524	U	N3-C4-O4	-5.27	115.71	119.40
2	1	305	C	N3-C4-C5	-5.27	119.79	121.90
2	1	418	G	C4-C5-C6	5.25	121.95	118.80
2	1	108	A	C6-N1-C2	-5.25	115.45	118.60
2	1	419	G	C5-C6-O6	5.25	131.75	128.60
3	2	111	G	O5'-P-OP1	-5.25	100.98	105.70
2	1	69	G	C8-N9-C4	5.24	108.50	106.40
2	1	358	U	N1-C2-N3	5.24	118.04	114.90
39	g	366	GLN	C-N-CA	5.24	134.79	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	420	A	C5-N7-C8	-5.23	101.28	103.90
2	1	1605	G	N1-C6-O6	-5.23	116.76	119.90
2	1	418	G	C5-N7-C8	-5.22	101.69	104.30
2	1	153	G	C2-N3-C4	-5.22	109.29	111.90
2	1	449	C	C5-C6-N1	-5.22	118.39	121.00
2	1	385	A	C5-C6-N1	-5.21	115.10	117.70
2	1	84	A	N7-C8-N9	-5.20	111.20	113.80
2	1	531	C	C6-N1-C2	-5.20	118.22	120.30
2	1	139	C	C5-C4-N4	5.20	123.84	120.20
2	1	1466	G	C5-C6-N1	-5.19	108.91	111.50
2	1	1472	C	C5-C6-N1	-5.19	118.41	121.00
2	1	106	U	N3-C4-C5	5.19	117.71	114.60
2	1	308	C	N3-C4-C5	5.19	123.97	121.90
2	1	54	C	C2-N3-C4	-5.19	117.31	119.90
2	1	539	G	C2-N3-C4	-5.18	109.31	111.90
2	1	1156	C	C6-N1-C2	5.18	122.37	120.30
2	1	402	C	N3-C4-C5	5.17	123.97	121.90
2	1	452	A	C8-N9-C4	5.17	107.87	105.80
2	1	342	C	C2-N3-C4	-5.17	117.32	119.90
2	1	295	A	C8-N9-C4	5.17	107.87	105.80
2	1	1171	A	N1-C6-N6	-5.16	115.50	118.60
2	1	163	G	C6-C5-N7	-5.15	127.31	130.40
3	2	118	A	C8-N9-C1'	5.15	136.97	127.70
2	1	1527	C	C2-N1-C1'	-5.15	113.14	118.80
2	1	1573	A	C5-C6-N1	5.14	120.27	117.70
2	1	310	C	C5-C6-N1	-5.14	118.43	121.00
2	1	393	C	N3-C4-C5	5.14	123.95	121.90
2	1	103	A	C5-N7-C8	-5.14	101.33	103.90
2	1	87	C	N1-C2-N3	5.12	122.79	119.20
2	1	1524	A	N3-C4-C5	5.12	130.39	126.80
2	1	85	A	C8-N9-C4	-5.12	103.75	105.80
2	1	464	A	C2-N3-C4	-5.11	108.04	110.60
2	1	431	C	N3-C2-O2	-5.11	118.32	121.90
2	1	93	A	N9-C4-C5	-5.11	103.76	105.80
3	2	81	U	N3-C2-O2	5.11	125.78	122.20
2	1	110	U	N3-C2-O2	-5.10	118.63	122.20
2	1	406	U	C6-N1-C2	5.10	124.06	121.00
2	1	430	G	C6-N1-C2	-5.10	122.04	125.10
2	1	251	A	C2-N3-C4	-5.09	108.05	110.60
2	1	1170	G	C4-N9-C1'	5.09	133.12	126.50
2	1	359	A	C8-N9-C1'	5.09	136.87	127.70
2	1	101	U	C5-C4-O4	5.08	128.95	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	403	G	C8-N9-C1'	-5.08	120.40	127.00
2	1	102	U	C2-N3-C4	-5.07	123.96	127.00
2	1	118	U	C2-N3-C4	-5.07	123.96	127.00
2	1	383	G	C8-N9-C4	-5.06	104.38	106.40
2	1	432	G	C8-N9-C4	-5.06	104.38	106.40
2	1	514	G	N3-C2-N2	5.05	123.44	119.90
3	2	80	U	C2-N1-C1'	5.05	123.76	117.70
2	1	128	U	C5-C6-N1	-5.04	120.18	122.70
2	1	363	G	C5-C6-O6	-5.03	125.58	128.60
2	1	403	G	N3-C4-N9	5.03	129.02	126.00
2	1	416	A	N7-C8-N9	5.02	116.31	113.80
2	1	101	U	N3-C4-O4	-5.01	115.89	119.40
2	1	357	G	N3-C2-N2	-5.01	116.39	119.90
2	1	96	G	C2-N3-C4	-5.01	109.40	111.90
2	1	1481	C	N3-C2-O2	-5.00	118.40	121.90
2	1	381	C	N1-C2-N3	5.00	122.70	119.20
2	1	515	A	C5-C6-N1	5.00	120.20	117.70

There are no chirality outliers.

All (202) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	118	A	Sidechain
6	6	145	ASP	Mainchain
6	6	44	ASN	Peptide
6	6	99	MET	Peptide
9	9	168	ARG	Peptide
9	9	88	GLU	Peptide
9	9	89	ASP	Peptide
12	C	40	GLU	Peptide
15	F	32	ARG	Peptide
15	F	51	GLU	Peptide
16	G	19	THR	Peptide
17	H	177	UNK	Peptide
17	H	218	UNK	Peptide
17	H	86	UNK	Peptide
17	H	94	UNK	Peptide
18	I	1106	UNK	Mainchain
18	I	1107	UNK	Mainchain
18	I	1108	UNK	Mainchain
18	I	1109	UNK	Mainchain
18	I	1110	UNK	Mainchain

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Mol	Chain	Res	Type	Group
18	I	1155	UNK	Mainchain
18	I	1240	UNK	Mainchain
18	I	1241	UNK	Mainchain
18	I	1242	UNK	Mainchain
18	I	1243	UNK	Mainchain
18	I	1244	UNK	Mainchain
19	J	1002	UNK	Mainchain
19	J	1003	UNK	Peptide
19	K	1008	UNK	Mainchain
19	K	1009	UNK	Mainchain
19	K	1010	UNK	Mainchain
20	M	261	UNK	Peptide
20	M	54	UNK	Peptide
20	M	89	UNK	Peptide
21	N	398	UNK	Peptide
21	N	414	UNK	Peptide
21	N	517	UNK	Peptide
21	N	64	UNK	Peptide
22	O	223	UNK	Peptide
22	O	273	UNK	Peptide
22	O	313	UNK	Peptide
22	O	427	UNK	Peptide
22	O	505	UNK	Peptide
22	O	528	UNK	Peptide
22	O	602	UNK	Peptide
22	O	700	UNK	Mainchain
22	O	74	UNK	Peptide
22	O	745	UNK	Peptide
22	O	813	UNK	Peptide
22	O	839	UNK	Peptide
24	Q	818	UNK	Peptide
24	Q	851	UNK	Peptide
24	Q	902	UNK	Peptide
24	Q	93	UNK	Peptide
26	S	275	UNK	Peptide
26	S	287	UNK	Peptide
26	S	585	UNK	Peptide
26	S	587	UNK	Peptide
27	T	43	THR	Peptide
27	T	94	TYR	Peptide
28	U	1183	UNK	Peptide
30	W	1137	UNK	Mainchain

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Mol	Chain	Res	Type	Group
30	W	1138	UNK	Mainchain
30	W	1139	UNK	Mainchain
30	W	1140	UNK	Mainchain
30	W	1141	UNK	Mainchain
30	W	1142	UNK	Mainchain
30	W	1157	UNK	Mainchain
30	W	1158	UNK	Mainchain
30	W	1159	UNK	Mainchain
30	W	1160	UNK	Mainchain
31	X	256	UNK	Peptide
31	X	332	UNK	Mainchain
33	Z	137	UNK	Peptide
33	Z	91	UNK	Peptide
34	a	113	UNK	Peptide
34	a	212	UNK	Peptide
34	a	223	UNK	Peptide
34	a	52	UNK	Peptide
34	a	56	UNK	Peptide
34	a	57	UNK	Peptide
35	b	401	UNK	Peptide
36	c	230	UNK	Peptide
36	c	235	UNK	Peptide
36	c	307	UNK	Peptide
37	d	230	UNK	Peptide
37	d	235	UNK	Peptide
37	d	242	UNK	Peptide
39	g	140	LEU	Peptide
39	g	364	GLU	Peptide
41	i	277	UNK	Peptide
41	i	705	UNK	Peptide
41	i	706	UNK	Peptide
41	i	784	UNK	Peptide
41	i	809	UNK	Peptide
44	m	165	UNK	Peptide
44	m	97	UNK	Peptide
47	p	1064	UNK	Mainchain
47	p	1066	UNK	Mainchain
47	p	1067	UNK	Mainchain
47	p	1178	UNK	Mainchain
47	p	1179	UNK	Mainchain
47	p	1180	UNK	Mainchain
47	p	1298	UNK	Mainchain

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Mol	Chain	Res	Type	Group
47	p	1299	UNK	Mainchain
47	p	1300	UNK	Mainchain
47	p	1398	UNK	Mainchain
47	p	1399	UNK	Mainchain
47	p	1400	UNK	Mainchain
47	p	152	UNK	Mainchain
47	p	153	UNK	Mainchain
47	p	154	UNK	Mainchain
47	p	302	UNK	Mainchain
47	p	303	UNK	Mainchain
47	p	304	UNK	Mainchain
47	p	407	UNK	Mainchain
47	p	408	UNK	Mainchain
47	p	409	UNK	Mainchain
47	p	523	UNK	Mainchain
47	p	524	UNK	Mainchain
47	p	525	UNK	Mainchain
47	p	526	UNK	Mainchain
47	p	545	UNK	Mainchain
47	p	645	UNK	Mainchain
47	p	646	UNK	Mainchain
47	p	647	UNK	Mainchain
47	p	745	UNK	Mainchain
47	p	746	UNK	Mainchain
47	p	747	UNK	Mainchain
47	p	855	UNK	Mainchain
47	p	856	UNK	Mainchain
47	p	857	UNK	Mainchain
47	p	955	UNK	Mainchain
47	p	956	UNK	Mainchain
47	p	957	UNK	Mainchain
50	s	419	UNK	Peptide
50	s	421	UNK	Peptide
50	s	462	UNK	Peptide
50	s	528	UNK	Peptide
50	s	563	UNK	Peptide
50	s	566	UNK	Peptide
50	s	581	UNK	Peptide
50	s	582	UNK	Peptide
50	s	643	UNK	Peptide
50	t	105	UNK	Peptide
50	t	141	UNK	Peptide

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Mol	Chain	Res	Type	Group
50	t	152	UNK	Peptide
50	t	164	UNK	Peptide
50	t	180	UNK	Peptide
50	t	202	UNK	Peptide
50	t	277	UNK	Peptide
50	t	288	UNK	Peptide
50	t	54	UNK	Peptide
50	t	69	UNK	Peptide
50	t	99	UNK	Peptide
50	u	188	UNK	Peptide
51	v	135	UNK	Mainchain
51	v	282	UNK	Mainchain
51	v	283	UNK	Mainchain
51	v	429	UNK	Mainchain
51	v	58	UNK	Mainchain
51	v	59	UNK	Mainchain
51	v	598	UNK	Mainchain
51	v	599	UNK	Mainchain
51	v	727	UNK	Mainchain
51	v	728	UNK	Mainchain
51	v	783	UNK	Mainchain
51	v	784	UNK	Mainchain
51	v	809	UNK	Mainchain
52	y	116	UNK	Mainchain
52	y	117	UNK	Mainchain
52	y	118	UNK	Mainchain
52	y	119	UNK	Mainchain
52	y	178	UNK	Mainchain
52	y	179	UNK	Mainchain
52	y	21	UNK	Mainchain
52	y	22	UNK	Mainchain
52	y	23	UNK	Mainchain
52	y	24	UNK	Mainchain
52	y	25	UNK	Mainchain
52	y	528	UNK	Mainchain
52	y	529	UNK	Mainchain
52	y	530	UNK	Mainchain
52	y	531	UNK	Mainchain
52	y	557	UNK	Mainchain
52	y	558	UNK	Mainchain
52	y	559	UNK	Mainchain
52	y	560	UNK	Mainchain

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Mol	Chain	Res	Type	Group
52	y	583	UNK	Mainchain
52	y	584	UNK	Mainchain
52	y	585	UNK	Mainchain
52	y	586	UNK	Mainchain
52	y	587	UNK	Mainchain
52	y	588	UNK	Mainchain
52	y	689	UNK	Mainchain
52	y	690	UNK	Mainchain
52	y	691	UNK	Mainchain
52	y	83	UNK	Mainchain
52	y	84	UNK	Mainchain
52	y	85	UNK	Mainchain
52	y	86	UNK	Mainchain
52	y	87	UNK	Mainchain

## 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	3	212/236 (90%)	180 (85%)	20 (9%)	12 (6%)	1	20
5	5	235/261 (90%)	199 (85%)	19 (8%)	17 (7%)	1	16
6	6	198/225 (88%)	148 (75%)	36 (18%)	14 (7%)	1	16
7	7	184/190 (97%)	143 (78%)	23 (12%)	18 (10%)	0	10
8	8	169/200 (84%)	150 (89%)	14 (8%)	5 (3%)	4	31
9	9	183/197 (93%)	152 (83%)	17 (9%)	14 (8%)	1	14
12	C	113/143 (79%)	107 (95%)	6 (5%)	0	100	100
13	D	144/156 (92%)	125 (87%)	19 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	E	125/130 (96%)	113 (90%)	11 (9%)	1 (1%)	19	60
15	F	88/135 (65%)	72 (82%)	13 (15%)	3 (3%)	3	29
16	G	60/67 (90%)	53 (88%)	7 (12%)	0	100	100
27	T	613/781 (78%)	565 (92%)	48 (8%)	0	100	100
38	e	120/126 (95%)	118 (98%)	2 (2%)	0	100	100
38	f	112/126 (89%)	110 (98%)	2 (2%)	0	100	100
39	g	353/573 (62%)	337 (96%)	15 (4%)	1 (0%)	41	76
40	h	353/367 (96%)	340 (96%)	13 (4%)	0	100	100
41	i	50/511 (10%)	48 (96%)	2 (4%)	0	100	100
42	j	205/252 (81%)	190 (93%)	15 (7%)	0	100	100
42	k	214/252 (85%)	201 (94%)	11 (5%)	2 (1%)	17	56
49	r	76/145 (52%)	66 (87%)	9 (12%)	1 (1%)	12	48
All	All	3807/5073 (75%)	3417 (90%)	302 (8%)	88 (2%)	9	36

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	3	153	VAL
4	3	173	PRO
4	3	174	LYS
5	5	24	SER
5	5	95	THR
5	5	163	ASP
5	5	164	LEU
5	5	196	VAL
6	6	28	PRO
6	6	39	GLU
6	6	54	LYS
6	6	58	LEU
6	6	125	THR
7	7	10	SER
7	7	11	GLN
7	7	31	SER
7	7	64	VAL
7	7	67	LEU
7	7	74	GLN
7	7	110	GLN
7	7	116	ARG

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Mol	Chain	Res	Type
7	7	131	PHE
7	7	163	ASP
7	7	185	ILE
8	8	116	HIS
9	9	118	LEU
9	9	121	SER
9	9	168	ARG
15	F	52	LYS
4	3	25	ARG
4	3	68	LEU
4	3	152	ASP
4	3	154	ARG
5	5	12	LEU
5	5	104	ASP
6	6	35	GLN
6	6	36	ALA
6	6	55	ASP
6	6	100	ASN
7	7	87	ASP
7	7	112	ARG
8	8	62	THR
8	8	115	ALA
9	9	105	LEU
9	9	110	GLN
9	9	134	ILE
9	9	147	MET
9	9	169	PRO
4	3	142	ARG
4	3	165	GLY
5	5	57	ASN
5	5	94	ALA
5	5	168	LYS
5	5	171	ASP
6	6	43	PHE
7	7	133	THR
8	8	101	ILE
9	9	162	SER
42	k	84	ILE
4	3	2	LYS
4	3	70	PRO
5	5	189	LEU
6	6	29	ILE

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Mol	Chain	Res	Type
6	6	101	GLY
6	6	184	PHE
6	6	185	ARG
7	7	66	SER
9	9	65	LYS
9	9	126	ARG
15	F	37	LYS
15	F	51	GLU
42	k	83	ASP
5	5	90	ILE
7	7	12	ALA
7	7	13	PRO
8	8	78	ILE
9	9	115	LYS
9	9	119	ALA
9	9	150	LEU
5	5	194	THR
4	3	69	LEU
7	7	32	PRO
14	E	6	VAL
5	5	150	PRO
5	5	195	ILE
39	g	365	PRO
49	r	77	ILE
5	5	30	ARG

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	10/364 (2%)	1 (10%)	0
2	1	496/1800 (27%)	119 (23%)	22 (4%)
3	2	95/126 (75%)	20 (21%)	3 (3%)
All	All	601/2290 (26%)	140 (23%)	25 (4%)

All (140) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	287	G
2	1	57	G
2	1	60	U
2	1	67	A
2	1	68	A
2	1	69	G
2	1	72	A
2	1	73	U
2	1	74	U
2	1	75	U
2	1	76	A
2	1	77	U
2	1	101	U
2	1	104	A
2	1	111	U
2	1	114	C
2	1	115	G
2	1	140	A
2	1	141	U
2	1	144	U
2	1	145	A
2	1	146	U
2	1	153	G
2	1	158	U
2	1	159	U
2	1	161	U
2	1	166	C
2	1	175	G
2	1	178	U
2	1	249	U
2	1	250	C
2	1	260	U
2	1	261	U
2	1	262	U
2	1	265	A
2	1	268	C
2	1	271	A
2	1	272	U
2	1	273	G
2	1	275	C
2	1	277	U
2	1	278	U
2	1	280	U

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Mol	Chain	Res	Type
2	1	281	G
2	1	283	U
2	1	287	G
2	1	299	A
2	1	301	A
2	1	308	C
2	1	314	C
2	1	316	A
2	1	319	U
2	1	320	U
2	1	321	C
2	1	322	G
2	1	323	A
2	1	325	G
2	1	337	G
2	1	338	C
2	1	341	A
2	1	352	A
2	1	359	A
2	1	360	A
2	1	361	C
2	1	381	C
2	1	393	C
2	1	396	G
2	1	400	A
2	1	401	A
2	1	402	C
2	1	404	G
2	1	416	A
2	1	418	G
2	1	425	A
2	1	426	G
2	1	434	G
2	1	444	C
2	1	446	A
2	1	448	C
2	1	454	U
2	1	464	A
2	1	468	A
2	1	480	G
2	1	484	C
2	1	485	A

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Mol	Chain	Res	Type
2	1	500	C
2	1	505	A
2	1	506	A
2	1	508	U
2	1	510	G
2	1	511	A
2	1	513	U
2	1	515	A
2	1	519	C
2	1	527	A
2	1	532	U
2	1	535	A
2	1	538	A
2	1	539	G
2	1	1154	G
2	1	1158	C
2	1	1159	C
2	1	1160	A
2	1	1162	C
2	1	1167	G
2	1	1481	C
2	1	1482	C
2	1	1486	G
2	1	1524	A
2	1	1531	G
2	1	1535	U
2	1	1536	G
2	1	1573	A
2	1	1574	G
2	1	1575	G
2	1	1582	U
2	1	1583	A
2	1	1584	G
2	1	1616	G
2	1	1621	U
3	2	63	C
3	2	64	A
3	2	72	C
3	2	87	G
3	2	88	U
3	2	95	A
3	2	96	C

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Mol	Chain	Res	Type
3	2	114	A
3	2	115	G
3	2	248	G
3	2	318	U
3	2	319	G
3	2	320	G
3	2	321	C
3	2	322	A
3	2	323	G
3	2	324	U
3	2	325	C
3	2	328	A
3	2	329	C

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	1	66	U
2	1	72	A
2	1	75	U
2	1	76	A
2	1	103	A
2	1	114	C
2	1	139	C
2	1	158	U
2	1	249	U
2	1	272	U
2	1	277	U
2	1	352	A
2	1	400	A
2	1	417	A
2	1	512	A
2	1	1481	C
2	1	1535	U
2	1	1572	G
2	1	1573	A
2	1	1574	G
2	1	1575	G
2	1	1620	C
3	2	308	U
3	2	317	A
3	2	318	U

## 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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
47	p	58
1	0	45
51	v	31
22	O	27
48	q	23
25	R	20
52	y	18
24	Q	18
41	i	16
17	H	16
23	P	15
26	S	13
21	N	11
18	I	11
29	V	11
20	M	11
45	n	10
11	B	9
3	2	8
2	1	8

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Mol	Chain	Number of breaks
53	z	7
34	a	7
44	m	7
31	X	7
32	Y	7
50	t	6
35	b	6
30	W	6
50	s	6
19	K	5
10	A	5
19	J	5
28	U	5
50	u	4
27	T	3
43	l	3
6	6	3
46	o	2
37	d	2
36	c	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	y	204:UNK	C	213:UNK	N	135.82
1	y	180:UNK	C	185:UNK	N	133.64
1	y	618:UNK	C	625:UNK	N	128.71
1	z	950:N	O3'	1110:N	P	127.24
1	y	144:UNK	C	150:UNK	N	117.41
1	y	254:UNK	C	313:UNK	N	109.65
1	y	532:UNK	C	537:UNK	N	106.19
1	y	484:UNK	C	500:UNK	N	104.64
1	B	1143:N	O3'	1146:N	P	103.51
1	y	374:UNK	C	413:UNK	N	93.23
1	z	622:N	O3'	921:N	P	93.14
1	y	640:UNK	C	650:UNK	N	88.80
1	B	1149:N	O3'	1151:N	P	88.51
1	B	1516:N	O3'	1630:N	P	81.08
1	i	636:LEU	C	704:UNK	N	79.82
1	R	611:UNK	C	653:UNK	N	75.10
1	y	589:UNK	C	600:UNK	N	73.02
1	q	446:UNK	C	600:UNK	N	71.23
1	y	26:UNK	C	30:UNK	N	67.25

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1179:N	O3'	1492:N	P	66.63
1	Q	619:UNK	C	787:UNK	N	65.68
1	O	324:N	O3'	332:N	P	64.96
1	H	346:UNK	C	348:UNK	N	61.99
1	O	75:N	O3'	90:N	P	60.05
1	v	430:UNK	C	487:UNK	N	57.90
1	H	30:UNK	C	33:UNK	N	57.25
1	i	715:UNK	C	783:UNK	N	56.46
1	y	88:UNK	C	95:UNK	N	55.59
1	N	300:UNK	C	302:UNK	N	53.57
1	z	407:N	O3'	600:N	P	52.76
1	O	479:N	O3'	495:N	P	50.20
1	y	50:UNK	C	55:UNK	N	46.05
1	Q	11:UNK	C	17:UNK	N	44.58
1	T	673:PHE	C	900:UNK	N	43.63
1	Q	326:UNK	C	332:UNK	N	43.16
1	O	712:UNK	C	734:UNK	N	41.53
1	R	319:UNK	C	325:UNK	N	40.52
1	O	131:N	O3'	133:N	P	39.12
1	R	9:UNK	C	13:UNK	N	39.08
1	y	120:UNK	C	125:UNK	N	37.71
1	O	341:UNK	C	347:UNK	N	36.50
1	O	13:UNK	C	16:UNK	N	35.25
1	i	305:UNK	C	547:TRP	N	35.22
1	p	1120:UNK	C	1162:UNK	N	34.22
1	q	377:UNK	C	386:UNK	N	32.47
1	q	404:UNK	C	416:UNK	N	30.67
1	y	561:UNK	C	563:UNK	N	30.23
1	p	1361:UNK	C	1383:UNK	N	28.83
1	a	321:UNK	C	372:UNK	N	28.39
1	T	911:UNK	C	923:UNK	N	25.95
1	O	274:N	O3'	281:G	P	24.41
1	q	104:UNK	C	116:UNK	N	23.59
1	O	234:N	O3'	241:N	P	23.56
1	O	390:N	O3'	400:N	P	23.43
1	m	126:UNK	C	137:UNK	N	23.31
1	t	224:UNK	C	239:UNK	N	23.18
1	q	277:UNK	C	279:UNK	N	23.16
1	2	106:C	O3'	111:G	P	23.13
1	q	323:UNK	C	334:UNK	N	22.82
1	i	202:UNK	C	215:UNK	N	22.64
1	I	1131:UNK	C	1140:UNK	N	21.34

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	p	1261:UNK	C	1283:UNK	N	20.44
1	n	51:UNK	C	59:UNK	N	19.56
1	v	180:UNK	C	192:UNK	N	19.55
1	i	94:UNK	C	104:UNK	N	19.54
1	0	291:G	O3'	305:N	P	19.47
1	i	227:UNK	C	235:UNK	N	19.32
1	p	1068:UNK	C	1083:UNK	N	19.31
1	q	175:UNK	C	184:UNK	N	18.71
1	p	1195:UNK	C	1208:UNK	N	18.41
1	0	189:N	O3'	201:N	P	18.36
1	B	1120:N	O3'	1131:N	P	17.97
1	0	251:N	O3'	262:N	P	17.83
1	p	349:UNK	C	361:UNK	N	17.81
1	n	77:UNK	C	82:UNK	N	17.79
1	v	24:UNK	C	32:UNK	N	17.74
1	i	923:UNK	C	930:UNK	N	17.70
1	0	521:N	O3'	525:N	P	17.57
1	H	391:UNK	C	418:UNK	N	17.45
1	0	226:N	O3'	228:N	P	17.41
1	p	958:UNK	C	960:UNK	N	17.41
1	q	153:UNK	C	165:UNK	N	17.37
1	2	267:A	O3'	304:U	P	17.36
1	B	1650:N	O3'	1741:N	P	17.36
1	z	930:N	O3'	941:N	P	17.36
1	z	1130:N	O3'	1134:N	P	17.36
1	0	359:N	O3'	361:N	P	17.35
1	X	566:UNK	C	574:UNK	N	17.31
1	2	203:U	O3'	246:A	P	17.03
1	q	80:UNK	C	89:UNK	N	16.60
1	K	1079:UNK	C	1085:UNK	N	16.58
1	v	507:UNK	C	531:UNK	N	16.54
1	p	1100:UNK	C	1107:UNK	N	16.47
1	0	97:N	O3'	100:N	P	16.40
1	0	121:N	O3'	125:N	P	16.39
1	0	309:N	O3'	321:N	P	16.39
1	0	425:N	O3'	432:N	P	16.39
1	0	564:N	O3'	570:N	P	16.39
1	B	1502:N	O3'	1505:N	P	16.39
1	0	109:N	O3'	115:N	P	16.38
1	H	72:UNK	C	79:UNK	N	16.37
1	p	748:UNK	C	760:UNK	N	16.28
1	A	594:N	O3'	604:N	P	16.21

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	18:N	O3'	60:N	P	16.20
1	A	562:N	O3'	570:N	P	16.20
1	p	199:UNK	C	206:UNK	N	16.20
1	v	284:UNK	C	290:UNK	N	16.08
1	v	703:UNK	C	708:UNK	N	15.99
1	v	157:UNK	C	164:UNK	N	15.92
1	A	575:N	O3'	580:N	P	15.86
1	P	76:UNK	C	84:UNK	N	15.83
1	O	455:N	O3'	464:N	P	15.70
1	p	858:UNK	C	863:UNK	N	15.63
1	q	291:UNK	C	297:UNK	N	15.62
1	Y	567:UNK	C	573:UNK	N	15.60
1	v	678:UNK	C	686:UNK	N	15.59
1	b	153:UNK	C	160:UNK	N	15.41
1	p	583:UNK	C	590:UNK	N	15.37
1	z	1124:N	O3'	1128:N	P	15.34
1	W	1177:UNK	C	1189:UNK	N	15.26
1	O	337:N	O3'	340:N	P	15.07
1	T	956:UNK	C	965:UNK	N	14.76
1	p	458:UNK	C	470:UNK	N	14.57
1	v	624:UNK	C	637:UNK	N	14.55
1	p	305:UNK	C	311:UNK	N	14.54
1	q	224:UNK	C	229:UNK	N	14.51
1	I	1201:UNK	C	1208:UNK	N	14.41
1	p	1336:UNK	C	1343:UNK	N	14.38
1	n	19:UNK	C	27:UNK	N	14.37
1	p	74:UNK	C	81:UNK	N	14.30
1	p	410:UNK	C	420:UNK	N	13.97
1	p	33:UNK	C	56:UNK	N	13.95
1	y	672:UNK	C	674:UNK	N	13.88
1	P	402:UNK	C	404:UNK	N	13.85
1	O	142:N	O3'	146:N	P	13.80
1	Y	617:UNK	C	624:UNK	N	13.72
1	B	1163:N	O3'	1170:N	P	13.70
1	P	341:UNK	C	346:UNK	N	13.68
1	2	118:A	O3'	200:C	P	13.59
1	m	167:UNK	C	178:UNK	N	13.59
1	p	1181:UNK	C	1183:UNK	N	13.59
1	p	1220:UNK	C	1223:UNK	N	13.50
1	p	893:UNK	C	900:UNK	N	13.42
1	v	755:UNK	C	759:UNK	N	13.42
1	n	102:UNK	C	107:UNK	N	13.38

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	361:UNK	C	363:UNK	N	13.16
1	v	600:UNK	C	606:UNK	N	13.13
1	0	448:N	O3'	450:N	P	13.08
1	p	438:UNK	C	445:UNK	N	13.02
1	I	1156:UNK	C	1160:UNK	N	12.97
1	q	349:UNK	C	358:UNK	N	12.95
1	S	361:UNK	C	375:UNK	N	12.92
1	K	1064:UNK	C	1067:UNK	N	12.84
1	0	438:N	O3'	440:N	P	12.77
1	p	527:UNK	C	530:UNK	N	12.76
1	n	187:UNK	C	196:UNK	N	12.55
1	0	368:N	O3'	372:N	P	12.51
1	I	1264:UNK	C	1268:UNK	N	12.50
1	p	487:UNK	C	492:UNK	N	12.42
1	p	244:UNK	C	256:UNK	N	12.38
1	z	614:N	O3'	615:N	P	12.35
1	p	683:UNK	C	690:UNK	N	12.24
1	v	570:UNK	C	576:UNK	N	12.24
1	N	577:UNK	C	580:UNK	N	12.23
1	v	329:UNK	C	338:UNK	N	12.08
1	I	1285:UNK	C	1292:UNK	N	12.07
1	p	94:UNK	C	106:UNK	N	12.05
1	A	585:N	O3'	590:N	P	12.02
1	p	1033:UNK	C	1039:UNK	N	12.02
1	a	139:UNK	C	144:UNK	N	12.00
1	q	48:UNK	C	51:UNK	N	11.94
1	v	211:UNK	C	219:UNK	N	11.89
1	H	204:UNK	C	210:UNK	N	11.84
1	o	192:UNK	C	194:UNK	N	11.82
1	2	88:U	O3'	93:U	P	11.74
1	q	248:UNK	C	250:UNK	N	11.74
1	p	1301:UNK	C	1323:UNK	N	11.70
1	O	51:UNK	C	59:UNK	N	11.62
1	p	993:UNK	C	1003:UNK	N	11.60
1	p	328:UNK	C	336:UNK	N	11.57
1	S	571:UNK	C	581:UNK	N	11.43
1	H	324:UNK	C	344:UNK	N	11.38
1	P	199:UNK	C	259:UNK	N	11.24
1	v	234:UNK	C	239:UNK	N	11.21
1	a	392:UNK	C	399:UNK	N	11.16
1	O	613:UNK	C	618:UNK	N	11.15
1	p	1420:UNK	C	1423:UNK	N	11.15

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	v	307:UNK	C	314:UNK	N	11.13
1	I	1172:UNK	C	1177:UNK	N	11.11
1	q	134:UNK	C	137:UNK	N	11.08
1	Q	576:UNK	C	583:UNK	N	10.99
1	q	614:UNK	C	618:UNK	N	10.98
1	p	607:UNK	C	631:UNK	N	10.94
1	v	386:UNK	C	397:UNK	N	10.85
1	p	1050:UNK	C	1055:UNK	N	10.76
1	p	378:UNK	C	391:UNK	N	10.72
1	0	528:N	O3'	531:N	P	10.70
1	s	391:UNK	C	410:UNK	N	10.67
1	a	87:UNK	C	96:UNK	N	10.66
1	i	178:UNK	C	182:UNK	N	10.64
1	n	133:UNK	C	137:UNK	N	10.57
1	0	153:N	O3'	155:N	P	10.52
1	v	548:UNK	C	553:UNK	N	10.49
1	p	504:UNK	C	512:UNK	N	10.48
1	J	1052:UNK	C	1061:UNK	N	10.37
1	v	256:UNK	C	262:UNK	N	10.34
1	V	1190:UNK	C	1198:UNK	N	10.33
1	v	655:UNK	C	659:UNK	N	10.33
1	M	287:UNK	C	298:UNK	N	10.31
1	O	621:UNK	C	686:UNK	N	10.28
1	P	285:UNK	C	295:UNK	N	10.17
1	v	84:UNK	C	92:UNK	N	10.09
1	p	567:UNK	C	570:UNK	N	10.08
1	N	546:UNK	C	551:UNK	N	9.88
1	p	179:UNK	C	186:UNK	N	9.87
1	H	445:UNK	C	451:UNK	N	9.86
1	R	764:UNK	C	768:UNK	N	9.86
1	X	54:UNK	C	66:UNK	N	9.84
1	Y	54:UNK	C	66:UNK	N	9.84
1	p	155:UNK	C	161:UNK	N	9.84
1	p	777:UNK	C	780:UNK	N	9.84
1	n	164:UNK	C	170:UNK	N	9.83
1	p	224:UNK	C	231:UNK	N	9.74
1	M	112:UNK	C	116:UNK	N	9.72
1	t	244:UNK	C	248:UNK	N	9.64
1	P	103:UNK	C	108:UNK	N	9.57
1	O	298:UNK	C	305:UNK	N	9.54
1	I	1219:UNK	C	1223:UNK	N	9.53
1	O	465:UNK	C	471:UNK	N	9.49

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	261:U	O3'	263:A	P	9.46
1	M	160:UNK	C	166:UNK	N	9.46
1	q	307:UNK	C	311:UNK	N	9.42
1	a	164:UNK	C	169:UNK	N	9.35
1	I	1233:UNK	C	1236:UNK	N	9.25
1	X	428:UNK	C	432:UNK	N	9.24
1	Q	107:UNK	C	112:UNK	N	9.16
1	v	60:UNK	C	64:UNK	N	9.11
1	N	168:UNK	C	172:UNK	N	9.01
1	P	23:UNK	C	26:UNK	N	8.98
1	V	1158:UNK	C	1165:UNK	N	8.96
1	I	1245:UNK	C	1249:UNK	N	8.93
1	I	1111:UNK	C	1116:UNK	N	8.91
1	Q	127:UNK	C	132:UNK	N	8.91
1	R	680:UNK	C	751:UNK	N	8.89
1	p	648:UNK	C	650:UNK	N	8.88
1	p	1401:UNK	C	1403:UNK	N	8.83
1	J	1074:UNK	C	1081:UNK	N	8.79
1	K	1025:UNK	C	1030:UNK	N	8.75
1	W	1114:UNK	C	1118:UNK	N	8.68
1	p	708:UNK	C	730:UNK	N	8.57
1	I	1189:UNK	C	1192:UNK	N	8.55
1	R	235:UNK	C	239:UNK	N	8.54
1	v	106:UNK	C	117:UNK	N	8.54
1	P	321:UNK	C	326:UNK	N	8.49
1	p	918:UNK	C	940:UNK	N	8.48
1	v	785:UNK	C	789:UNK	N	8.48
1	W	1161:UNK	C	1164:UNK	N	8.42
1	A	552:N	O3'	555:N	P	8.32
1	p	667:UNK	C	670:UNK	N	8.32
1	H	144:UNK	C	151:UNK	N	8.28
1	0	380:N	O3'	384:N	P	8.23
1	R	122:UNK	C	127:UNK	N	8.15
1	V	1275:UNK	C	1297:UNK	N	8.04
1	i	146:UNK	C	149:UNK	N	8.03
1	R	845:UNK	C	855:UNK	N	7.97
1	W	1128:UNK	C	1131:UNK	N	7.91
1	0	405:N	O3'	407:N	P	7.88
1	M	101:UNK	C	106:UNK	N	7.80
1	U	1160:UNK	C	1165:UNK	N	7.80
1	W	1143:UNK	C	1145:UNK	N	7.80
1	p	1240:UNK	C	1243:UNK	N	7.79

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	231:UNK	C	235:UNK	N	7.72
1	Q	223:UNK	C	228:UNK	N	7.68
1	O	161:N	O3'	166:N	P	7.65
1	H	114:UNK	C	116:UNK	N	7.64
1	K	1042:UNK	C	1047:UNK	N	7.63
1	l	177:UNK	C	178:UNK	N	7.63
1	u	46:UNK	C	49:UNK	N	7.63
1	P	120:UNK	C	124:UNK	N	7.61
1	U	1274:UNK	C	1296:UNK	N	7.61
1	n	37:UNK	C	44:UNK	N	7.58
1	s	30:UNK	C	348:UNK	N	7.57
1	y	571:UNK	C	573:UNK	N	7.56
1	i	77:UNK	C	82:UNK	N	7.52
1	p	272:UNK	C	288:UNK	N	7.52
1	V	1303:UNK	C	1310:UNK	N	7.42
1	S	497:UNK	C	531:UNK	N	7.41
1	v	136:UNK	C	141:UNK	N	7.34
1	l	511:A	O3'	512:A	P	7.29
1	U	1046:UNK	C	1052:UNK	N	7.28
1	O	279:UNK	C	283:UNK	N	7.27
1	v	729:UNK	C	732:UNK	N	7.26
1	q	201:UNK	C	205:UNK	N	7.18
1	O	93:UNK	C	97:UNK	N	7.15
1	P	138:UNK	C	140:UNK	N	7.13
1	V	1063:UNK	C	1065:UNK	N	7.12
1	K	1011:UNK	C	1014:UNK	N	7.11
1	s	444:UNK	C	452:UNK	N	7.10
1	N	372:UNK	C	376:UNK	N	7.09
1	P	154:UNK	C	161:UNK	N	7.07
1	a	21:UNK	C	48:UNK	N	7.07
1	P	382:UNK	C	383:UNK	N	7.04
1	P	175:UNK	C	179:UNK	N	7.01
1	O	432:UNK	C	436:UNK	N	6.99
1	U	1244:UNK	C	1248:UNK	N	6.99
1	B	1635:N	O3'	1637:N	P	6.96
1	Q	182:UNK	C	186:UNK	N	6.91
1	n	89:UNK	C	92:UNK	N	6.90
1	O	549:N	O3'	555:N	P	6.89
1	O	259:UNK	C	261:UNK	N	6.89
1	p	1016:UNK	C	1021:UNK	N	6.80
1	q	27:UNK	C	30:UNK	N	6.78
1	R	280:UNK	C	283:UNK	N	6.77

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	t	266:UNK	C	270:UNK	N	6.75
1	v	356:UNK	C	360:UNK	N	6.74
1	Q	116:UNK	C	120:UNK	N	6.72
1	R	780:UNK	C	791:UNK	N	6.67
1	0	535:N	O3'	537:N	P	6.65
1	M	279:UNK	C	281:UNK	N	6.65
1	p	818:UNK	C	840:UNK	N	6.65
1	p	1239:UNK	C	1240:UNK	N	6.65
1	Q	21:UNK	C	27:UNK	N	6.63
1	m	186:UNK	C	198:UNK	N	6.63
1	s	488:UNK	C	493:UNK	N	6.59
1	Q	284:UNK	C	290:UNK	N	6.57
1	R	177:UNK	C	181:UNK	N	6.56
1	d	99:UNK	C	106:UNK	N	6.54
1	l	387:A	O3'	388:G	P	6.53
1	J	1038:UNK	C	1042:UNK	N	6.49
1	P	47:UNK	C	50:UNK	N	6.48
1	R	102:UNK	C	105:UNK	N	6.48
1	H	160:UNK	C	166:UNK	N	6.47
1	N	518:UNK	C	521:UNK	N	6.43
1	c	125:UNK	C	139:UNK	N	6.42
1	J	1014:UNK	C	1016:UNK	N	6.38
1	V	1202:UNK	C	1207:UNK	N	6.35
1	O	387:UNK	C	392:UNK	N	6.31
1	t	213:UNK	C	216:UNK	N	6.30
1	Y	250:UNK	C	257:UNK	N	6.29
1	O	192:UNK	C	194:UNK	N	6.28
1	l	423:G	O3'	424:C	P	6.27
1	S	378:UNK	C	384:UNK	N	6.22
1	Q	204:UNK	C	208:UNK	N	6.20
1	t	291:UNK	C	293:UNK	N	6.18
1	n	64:UNK	C	66:UNK	N	6.17
1	p	793:UNK	C	800:UNK	N	6.14
1	v	376:UNK	C	380:UNK	N	6.14
1	H	43:UNK	C	47:UNK	N	6.13
1	S	389:UNK	C	396:UNK	N	6.12
1	p	877:UNK	C	880:UNK	N	6.08
1	v	613:UNK	C	618:UNK	N	6.07
1	O	331:UNK	C	334:UNK	N	6.06
1	i	901:UNK	C	912:UNK	N	6.03
1	p	121:UNK	C	139:UNK	N	6.01
1	l	146:U	O3'	147:A	P	6.00

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	218:UNK	C	223:UNK	N	5.99
1	N	497:UNK	C	500:UNK	N	5.97
1	M	192:UNK	C	195:UNK	N	5.95
1	O	32:UNK	C	36:UNK	N	5.93
1	l	110:UNK	C	113:UNK	N	5.92
1	H	246:UNK	C	250:UNK	N	5.91
1	q	64:UNK	C	67:UNK	N	5.88
1	S	302:UNK	C	312:UNK	N	5.86
1	Q	233:UNK	C	241:UNK	N	5.83
1	N	384:UNK	C	386:UNK	N	5.76
1	N	560:UNK	C	562:UNK	N	5.72
1	Q	252:UNK	C	256:UNK	N	5.69
1	b	312:UNK	C	314:UNK	N	5.65
1	i	862:UNK	C	870:UNK	N	5.63
1	V	1045:UNK	C	1054:UNK	N	5.60
1	O	131:UNK	C	134:UNK	N	5.53
1	S	414:UNK	C	419:UNK	N	5.52
1	V	1017:UNK	C	1019:UNK	N	5.49
1	O	143:UNK	C	149:UNK	N	5.48
1	l	167:U	O3'	168:A	P	5.46
1	0	206:N	O3'	208:N	P	5.41
1	s	584:UNK	C	587:UNK	N	5.38
1	O	124:UNK	C	131:UNK	N	5.30
1	b	123:UNK	C	132:UNK	N	5.28
1	S	355:UNK	C	357:UNK	N	5.25
1	o	176:UNK	C	178:UNK	N	5.25
1	M	236:UNK	C	238:UNK	N	5.19
1	V	1232:UNK	C	1234:UNK	N	5.18
1	m	53:UNK	C	56:UNK	N	5.18
1	N	35:UNK	C	39:UNK	N	5.13
1	p	546:UNK	C	550:UNK	N	5.09
1	m	63:UNK	C	71:UNK	N	5.04
1	S	458:UNK	C	463:UNK	N	4.97
1	l	1470:C	O3'	1471:A	P	4.95
1	y	661:UNK	C	666:UNK	N	4.91
1	X	250:UNK	C	256:UNK	N	4.90
1	v	408:UNK	C	410:UNK	N	4.88
1	H	55:UNK	C	57:UNK	N	4.86
1	M	142:UNK	C	151:UNK	N	4.86
1	R	218:UNK	C	223:UNK	N	4.86
1	S	471:UNK	C	481:UNK	N	4.86
1	H	258:UNK	C	262:UNK	N	4.81

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	203:UNK	C	205:UNK	N	4.80
1	V	1144:UNK	C	1148:UNK	N	4.79
1	R	208:UNK	C	210:UNK	N	4.73
1	b	319:UNK	C	340:UNK	N	4.73
1	q	434:UNK	C	436:UNK	N	4.72
1	u	207:UNK	C	214:UNK	N	4.71
1	H	133:UNK	C	135:UNK	N	4.66
1	O	518:UNK	C	520:UNK	N	4.66
1	N	506:UNK	C	508:UNK	N	4.62
1	p	977:UNK	C	980:UNK	N	4.61
1	S	269:UNK	C	272:UNK	N	4.58
1	i	817:UNK	C	818:UNK	N	4.50
1	s	635:UNK	C	638:UNK	N	4.50
1	2	250:C	O3'	252:C	P	4.44
1	O	290:UNK	C	292:UNK	N	4.33
1	i	134:UNK	C	136:UNK	N	4.31
1	0	183:N	O3'	185:N	P	4.28
1	0	416:N	O3'	418:N	P	4.25
1	O	175:UNK	C	181:UNK	N	4.23
1	m	210:UNK	C	220:UNK	N	4.22
1	0	512:N	O3'	514:N	P	4.17
1	O	422:UNK	C	424:UNK	N	4.17
1	v	499:UNK	C	502:UNK	N	4.01
1	Q	52:UNK	C	54:UNK	N	3.94
1	R	199:UNK	C	202:UNK	N	3.93
1	R	192:UNK	C	194:UNK	N	3.82
1	b	19:UNK	C	43:UNK	N	3.73
1	O	410:UNK	C	414:UNK	N	3.71
1	R	248:UNK	C	251:UNK	N	3.67
1	a	306:UNK	C	309:UNK	N	3.67
1	M	324:UNK	C	340:UNK	N	3.65
1	X	336:UNK	C	337:UNK	N	3.64
1	Y	336:UNK	C	337:UNK	N	3.64
1	i	1006:UNK	C	1007:UNK	N	3.60
1	U	1144:UNK	C	1148:UNK	N	3.58
1	i	793:UNK	C	795:UNK	N	3.53
1	q	11:UNK	C	13:UNK	N	3.53
1	0	507:N	O3'	509:N	P	3.51
1	O	455:UNK	C	458:UNK	N	3.51
1	X	171:UNK	C	172:UNK	N	3.48
1	Y	171:UNK	C	172:UNK	N	3.48
1	O	166:UNK	C	168:UNK	N	3.44

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	381:UNK	C	383:UNK	N	3.36
1	u	283:UNK	C	285:UNK	N	3.35
1	u	149:UNK	C	152:UNK	N	3.33
1	M	177:UNK	C	179:UNK	N	3.29
1	d	125:UNK	C	138:UNK	N	3.26
1	R	211:UNK	C	213:UNK	N	3.25
1	Q	543:UNK	C	545:UNK	N	3.24
1	Q	832:UNK	C	834:UNK	N	3.20
1	S	539:UNK	C	541:UNK	N	3.18
1	O	543:N	O3'	544:N	P	3.17
1	O	562:UNK	C	583:UNK	N	3.17
1	t	127:UNK	C	133:UNK	N	3.16
1	S	560:UNK	C	565:UNK	N	3.15
1	Q	61:UNK	C	63:UNK	N	3.13
1	m	104:UNK	C	112:UNK	N	3.13
1	q	267:UNK	C	268:UNK	N	3.10
1	p	1237:UNK	C	1238:UNK	N	3.06
1	R	301:UNK	C	303:UNK	N	3.02
1	O	332:N	O3'	333:N	P	3.01
1	l	75:UNK	C	78:UNK	N	2.97
1	O	266:N	O3'	268:N	P	2.87
1	1	1169:G	O3'	1170:G	P	2.75
1	6	159:ALA	C	160:VAL	N	2.63
1	O	348:N	O3'	350:N	P	2.58
1	p	1238:UNK	C	1239:UNK	N	2.15
1	V	1016:UNK	C	1017:UNK	N	1.97
1	O	66:N	O3'	68:N	P	1.95
1	O	218:N	O3'	220:N	P	1.88
1	Y	332:UNK	C	333:UNK	N	1.79
1	O	334:N	O3'	335:N	P	1.38
1	W	1142:UNK	C	1143:UNK	N	1.19
1	6	207:THR	C	208:SER	N	1.12
1	1	1615:C	O3'	1616:G	P	1.10
1	J	1002:UNK	C	1003:UNK	N	1.09
1	6	145:ASP	C	146:THR	N	1.05
1	X	332:UNK	C	333:UNK	N	1.02
1	2	308:U	O3'	309:G	P	0.84



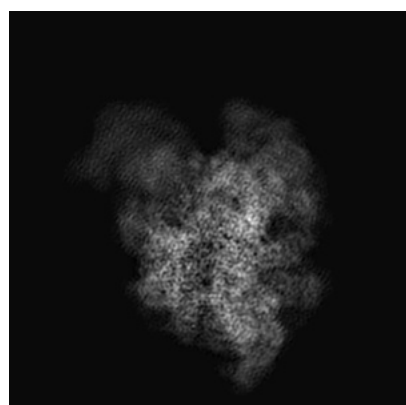
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8473. These allow visual inspection of the internal detail of the map and identification of artifacts.

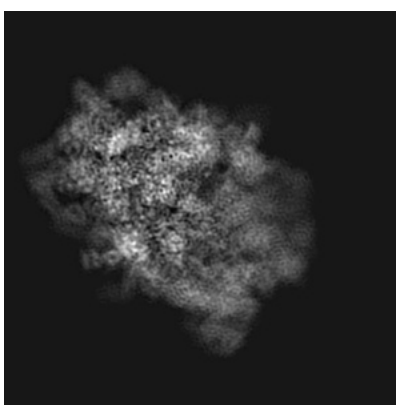
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

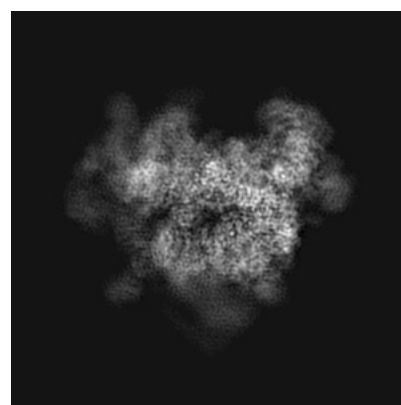
#### 6.1.1 Primary map



X



Y

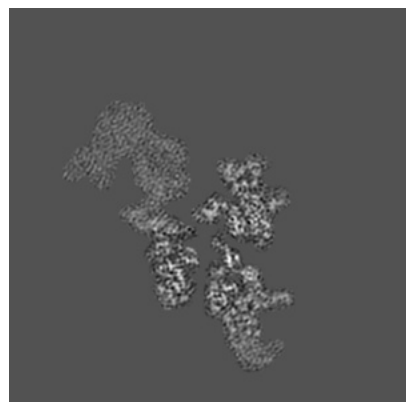


Z

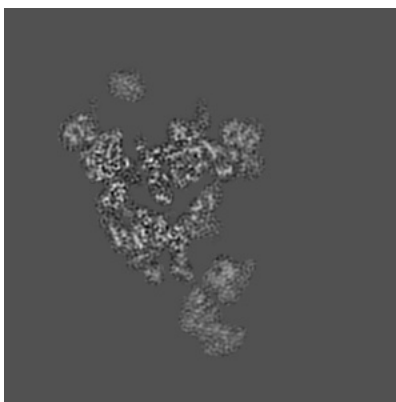
The images above show the map projected in three orthogonal directions.

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

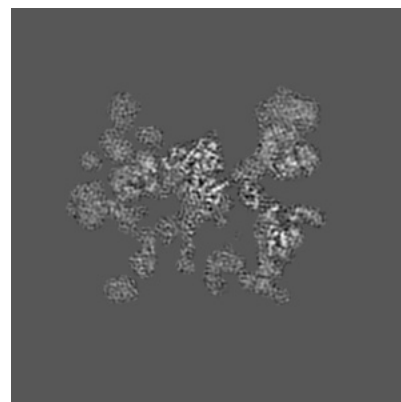
#### 6.2.1 Primary map



X Index: 190



Y Index: 190

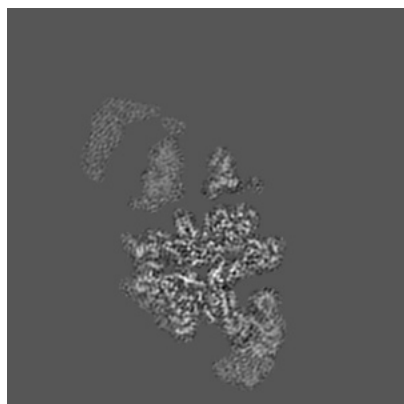


Z Index: 190

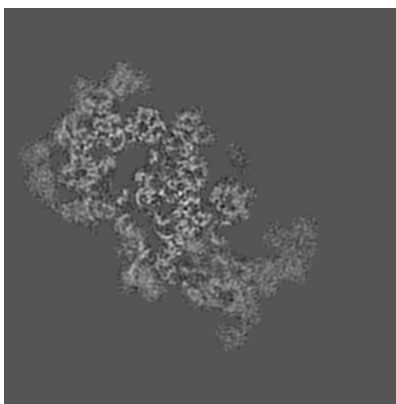
The images above show central slices of the map in three orthogonal directions.

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

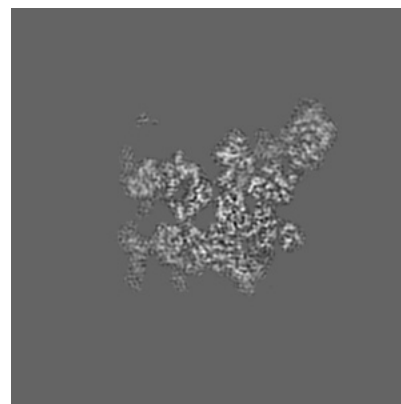
### 6.3.1 Primary map



X Index: 217



Y Index: 219



Z Index: 151

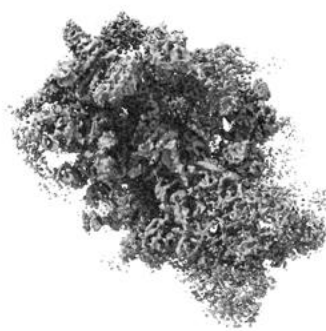
The images above show the largest variance slices of the map in three orthogonal directions.

## 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 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

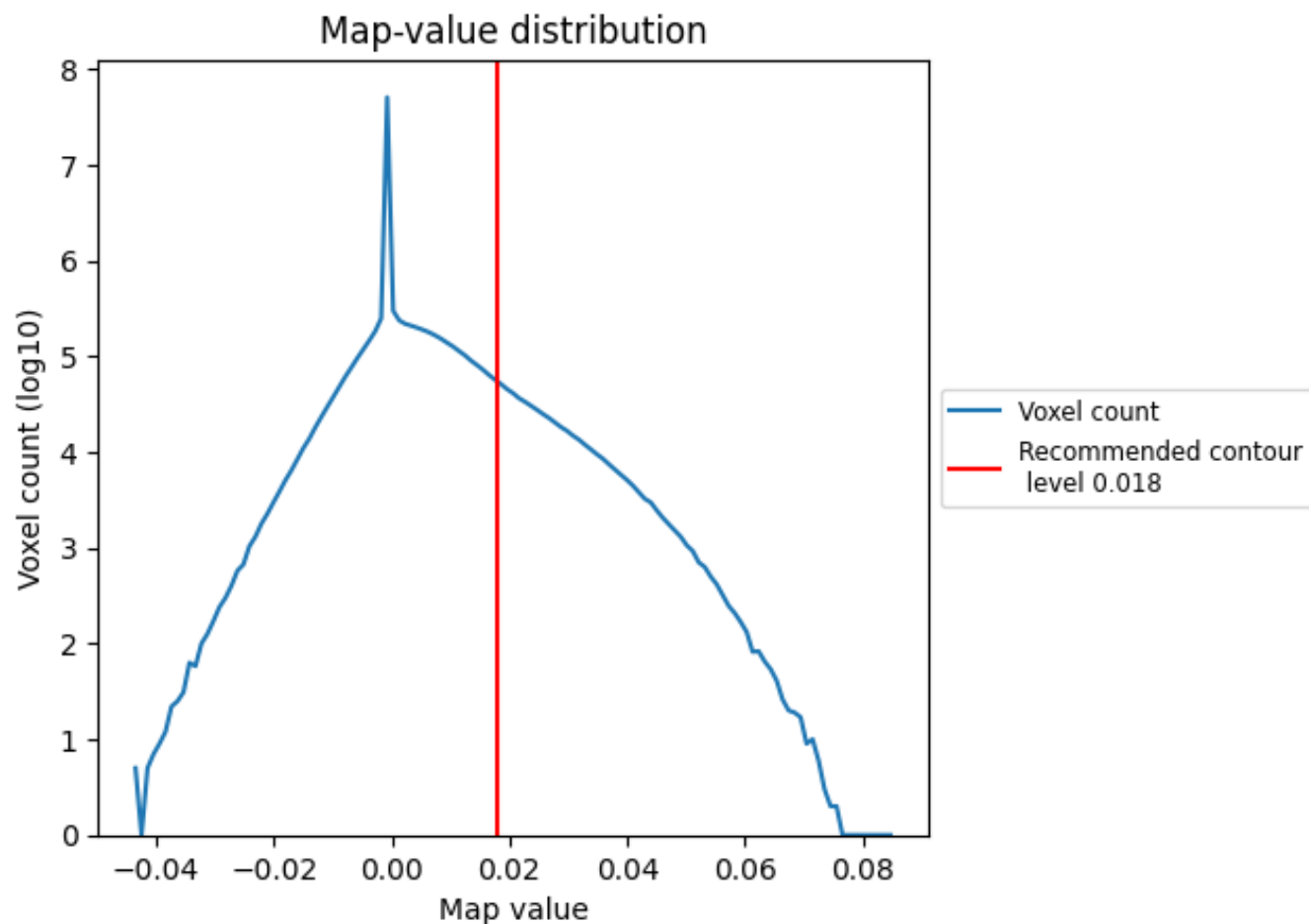
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

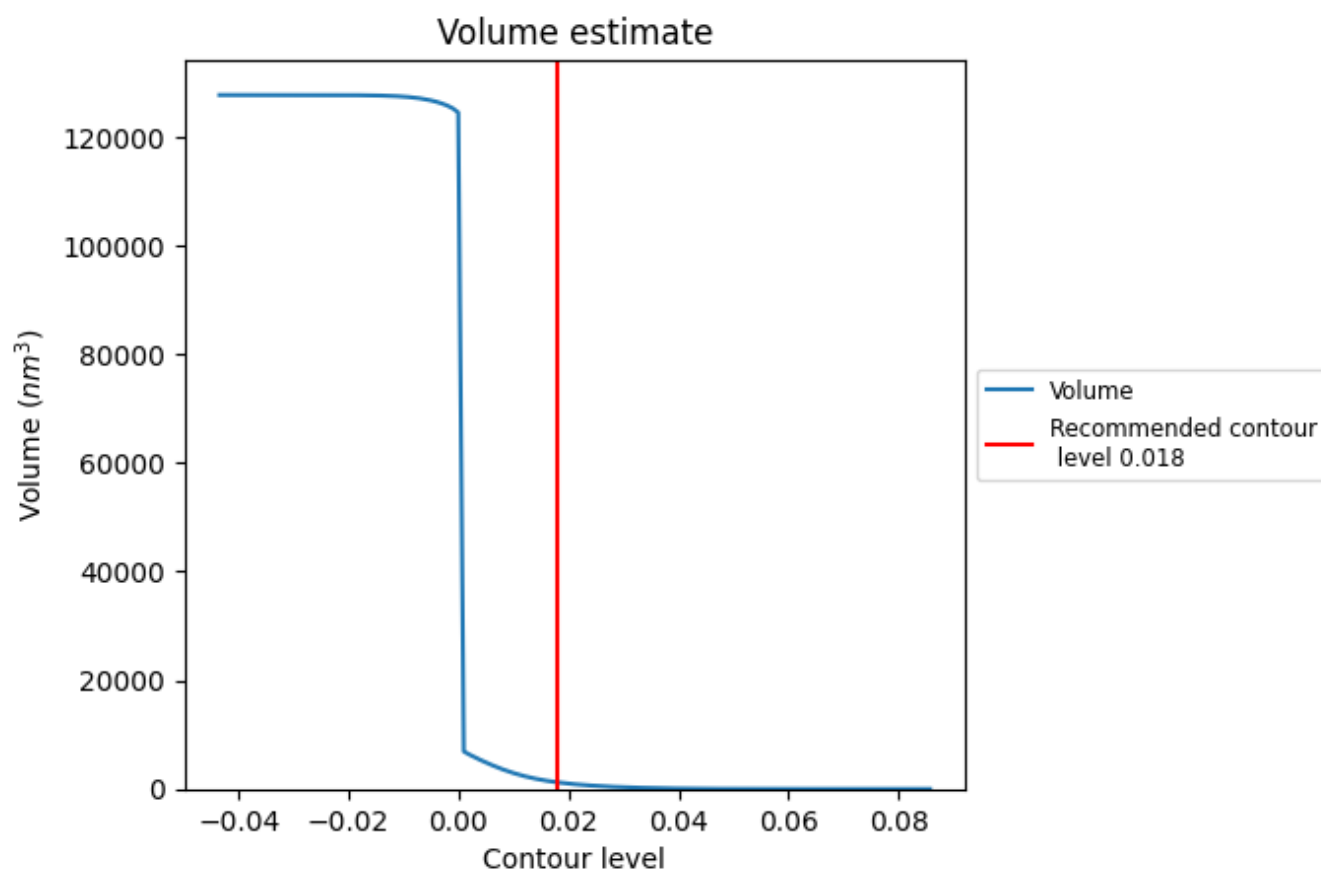
This section contains the results of statistical analysis of the map.

### 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.

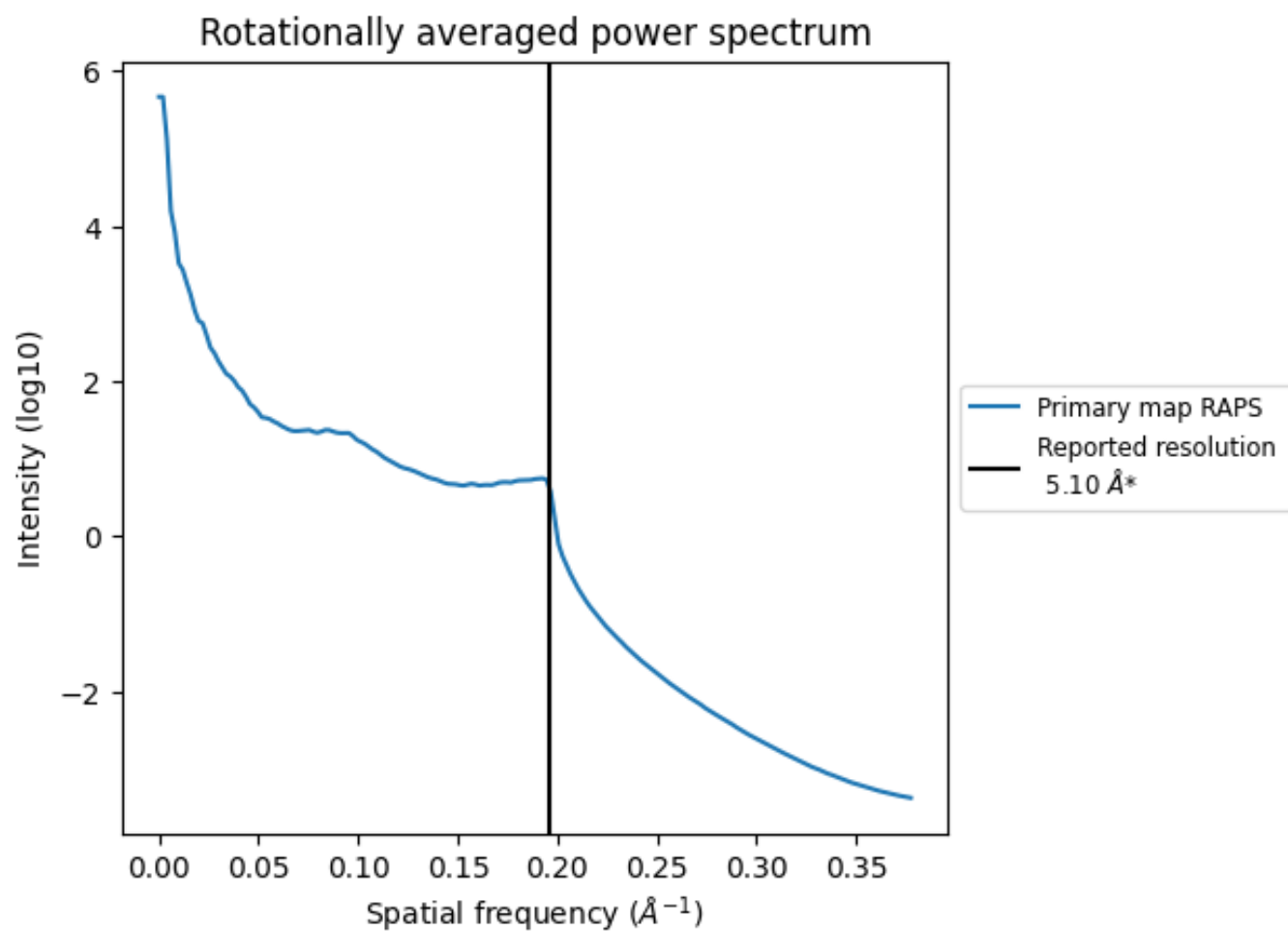
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1219 nm<sup>3</sup>; this corresponds to an approximate mass of 1101 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

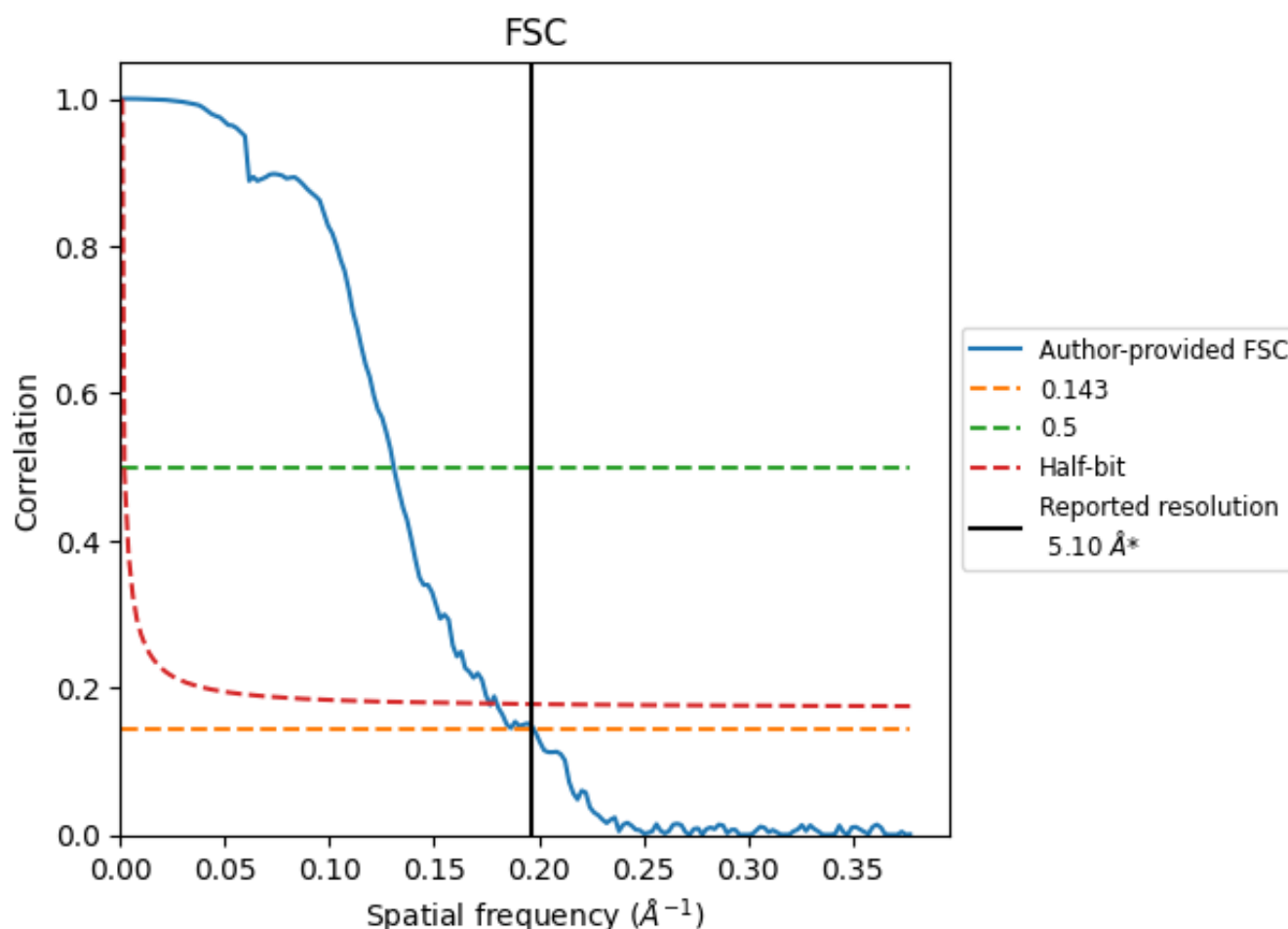


\*Reported resolution corresponds to spatial frequency of 0.196 Å<sup>-1</sup>

## 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 0.196 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	5.10	-	-
Author-provided FSC curve	5.06	7.66	5.67
Unmasked-calculated*	-	-	-

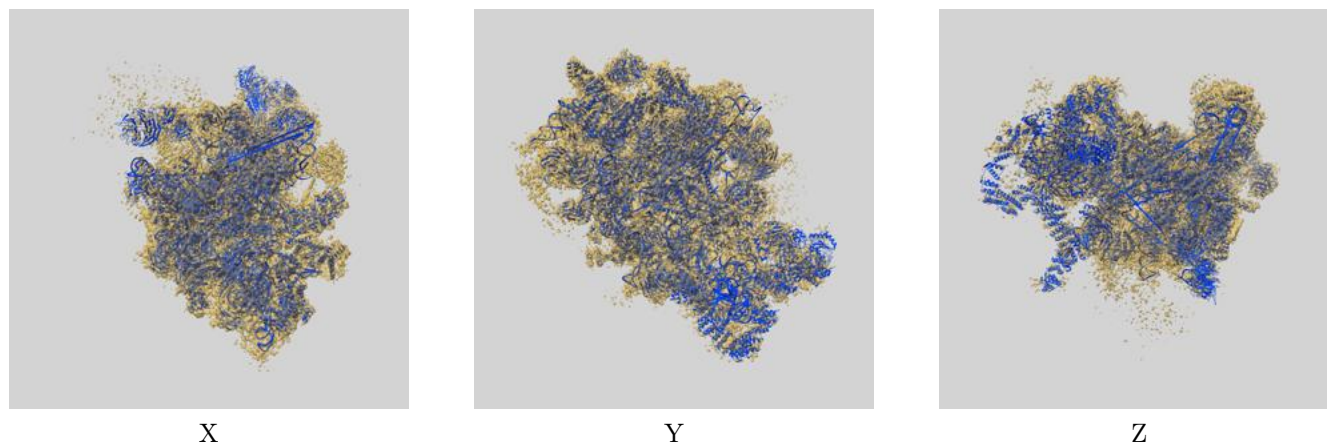
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



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

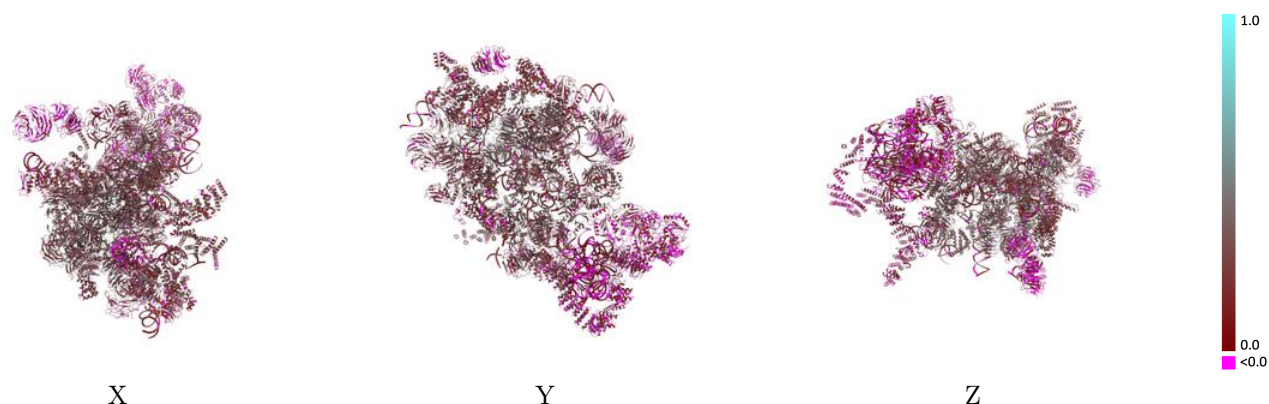
This section contains information regarding the fit between EMDB map EMD-8473 and PDB model 5TZS. Per-residue inclusion information can be found in section [3](#) on page [13](#).

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



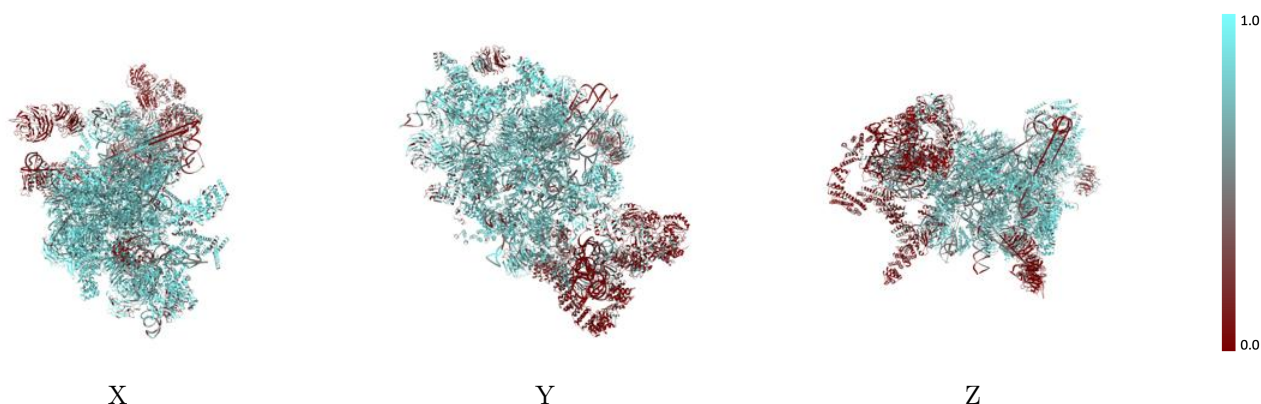
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



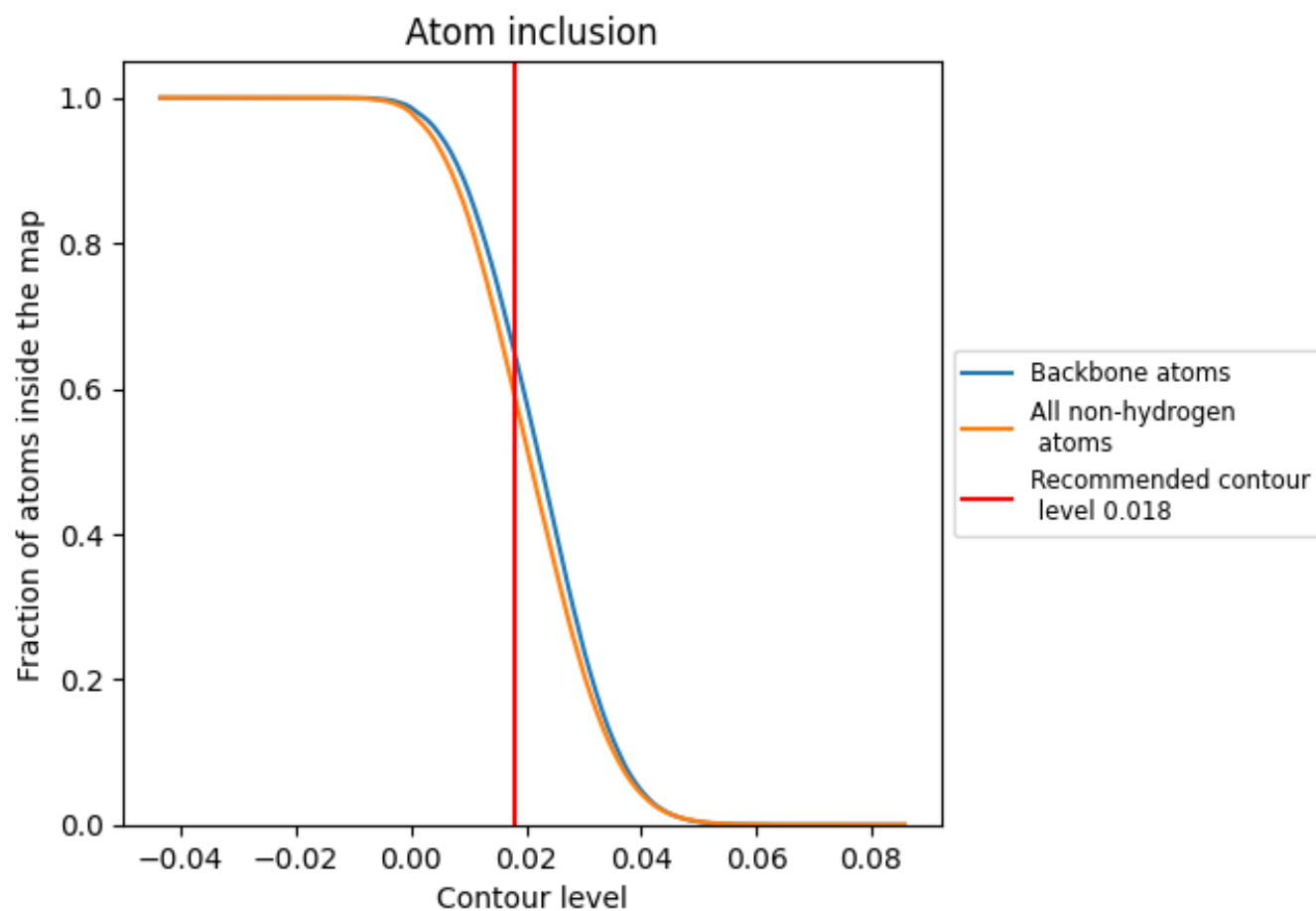
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 59% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5913	 0.2220
0	 0.6070	 0.2240
1	 0.4535	 0.1320
2	 0.7484	 0.2460
3	 0.1552	 0.0920
5	 0.4785	 0.2120
6	 0.7840	 0.3030
7	 0.0628	 0.1230
8	 0.2992	 0.1450
9	 0.6984	 0.2580
A	 0.7051	 0.2770
B	 0.4344	 0.1860
C	 0.8675	 0.3440
D	 0.2524	 0.0990
E	 0.2212	 0.2220
F	 0.6014	 0.2400
G	 0.8170	 0.3800
H	 0.5254	 0.1500
I	 0.7205	 0.2200
J	 0.8112	 0.2700
K	 0.7600	 0.2390
M	 0.8220	 0.3410
N	 0.7084	 0.2560
O	 0.8240	 0.3370
P	 0.8320	 0.2500
Q	 0.7259	 0.2480
R	 0.2292	 0.0620
S	 0.7891	 0.3220
T	 0.8464	 0.3420
U	 0.7639	 0.2990
V	 0.2935	 0.1150
W	 0.8269	 0.2800
X	 0.2849	 0.1060
Y	 0.0924	 0.0530
Z	 0.8275	 0.3300



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Chain	Atom inclusion	Q-score
a	 0.7591	 0.2500
b	 0.7178	 0.2690
c	 0.8281	 0.3400
d	 0.6758	 0.3030
e	 0.7921	 0.3070
f	 0.7827	 0.2920
g	 0.7399	 0.2740
h	 0.7830	 0.3100
i	 0.7836	 0.3150
j	 0.6714	 0.2490
k	 0.7151	 0.2920
l	 0.8548	 0.3440
m	 0.7832	 0.3260
n	 0.7661	 0.2590
o	 0.3089	 0.1520
p	 0.1710	 0.1420
q	 0.8022	 0.2450
r	 0.8010	 0.3590
s	 0.7180	 0.2400
t	 0.9126	 0.3770
u	 0.8105	 0.3320
v	 0.7584	 0.2380
y	 0.7499	 0.2570
z	 0.4704	 0.2040