



## Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 12:01 PM EST

PDB ID : 3J0Q  
EMDB ID : EMD-5329  
Title : Core of mammalian 80S pre-ribosome in complex with tRNAs fitted to a 10.6Å cryo-em map: rotated PRE state 2  
Authors : Budkevich, T.; Giesebrecht, J.; Altman, R.; Munro, J.; Mielke, T.; Nierhaus, K.; Blanchard, S.; Spahn, C.M.  
Deposited on : 2011-10-11  
Resolution : 10.60 Å (reported)  
Based on initial models : 3O58, 2XZM

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

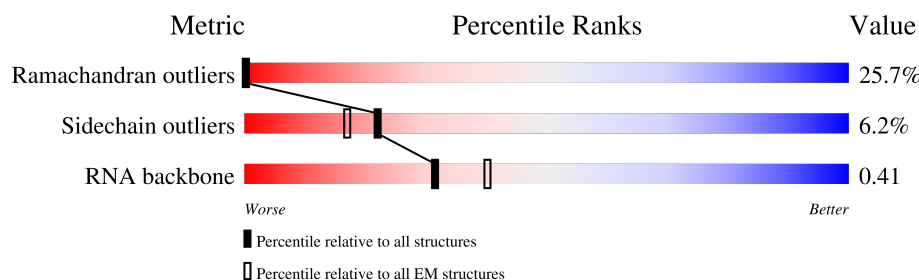
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 10.60 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.







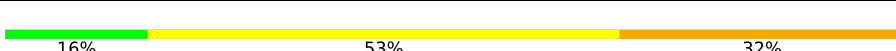
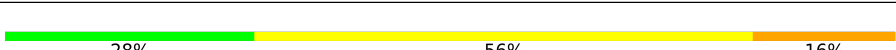
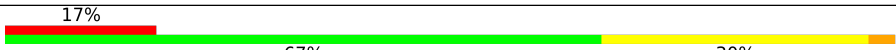
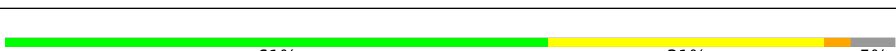
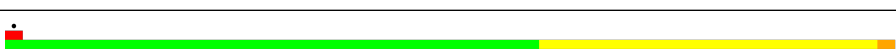
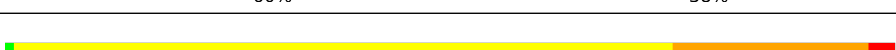

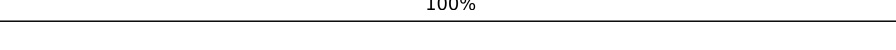
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	a	48	<div> <div>65%</div> <div>25%</div> <div>6%</div> <div>.</div> </div>
2	c	17	<div> <div>71%</div> <div>29%</div> </div>
3	d	7	<div> <div>71%</div> <div>14%</div> <div>14%</div> </div>
4	g	31	<div> <div>71%</div> <div>23%</div> <div>6%</div> </div>
5	G	13	<div> <div>85%</div> <div>15%</div> </div>
6	f	21	<div> <div>76%</div> <div>24%</div> </div>
7	h	111	<div> <div>88%</div> <div>11%</div> <div>.</div> </div>
8	S	125	<div> <div>6%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
9	L	141	
10	X	68	
11	2	112	
12	3	12	
13	9	19	
14	7	50	
15	B	213	
16	J	219	
17	k	165	
18	W	77	
18	Y	77	
19	y	3	
20	w	2	

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 18327 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 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	48	Total	C	N	O	P	0	0
			1029	459	190	332	48		

- Molecule 2 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	17	Total	C	N	O	P	0	0
			362	162	66	117	17		

- Molecule 3 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	7	Total	C	N	O	P	0	0
			155	69	33	46	7		

- Molecule 4 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	31	Total	C	N	O	P	0	0
			660	295	118	216	31		

- Molecule 5 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	13	Total	C	N	O	P	0	0
			276	123	49	91	13		

- Molecule 6 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	21	Total	C	N	O	P	0	0
			452	200	79	152	21		

- Molecule 7 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	111	Total	C	N	O	P	0	0
			2368	1060	431	766	111		

- Molecule 8 is a protein called Ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	125	Total	C	N	O	S	0	0
			985	632	173	176	4		

- Molecule 9 is a protein called Ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	141	Total	C	N	O	S	0	0
			1097	691	221	180	5		

- Molecule 10 is a protein called Ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	68	Total	C	N	O	S	0	0
			554	350	113	90	1		

- Molecule 11 is a RNA chain called 60S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2	112	Total	C	N	O	P	0	0
			2392	1070	435	775	112		

- Molecule 12 is a RNA chain called 60S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	3	12	Total	C	N	O	P	0	0
			259	116	50	81	12		

- Molecule 13 is a RNA chain called 60S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	9	19	Total	C	N	O	P	0	0
			408	183	78	128	19		

- Molecule 14 is a RNA chain called 60S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	7	50	Total	C	N	O	P	0	0
			1054	471	173	360	50		

- Molecule 15 is a protein called Ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	B	213	Total	C	N	O		0	0
			1055	629	213	213			

- Molecule 16 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	208	Total	C	N	O		0	0
			1027	611	208	208			

- Molecule 17 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	k	165	Total	C	N	O		0	0
			810	480	165	165			

- Molecule 18 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		
18	W	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 19 is a RNA chain called mRNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	y	3	Total	C	N	O	P	0	0
			60	27	7	23	3		

- Molecule 20 is a RNA chain called mRNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	w	2	Total	C	N	O	P	0	0
			44	20	10	12	2		

### 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.

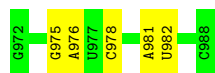
- Molecule 1: 40S ribosomal RNA fragment

Chain a: 



- Molecule 2: 40S ribosomal RNA fragment

Chain c: 



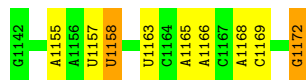
- Molecule 3: 40S ribosomal RNA fragment

Chain d: 




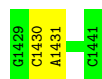
- Molecule 4: 40S ribosomal RNA fragment

Chain g: 



- Molecule 5: 40S ribosomal RNA fragment

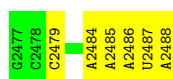
Chain G: 



- Molecule 6: 40S ribosomal RNA fragment

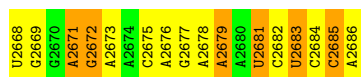
Chain 3:  50% 50%





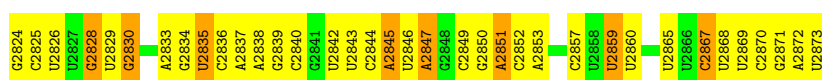
- Molecule 13: 60S ribosomal RNA fragment

Chain 9: 16% 53% 32%



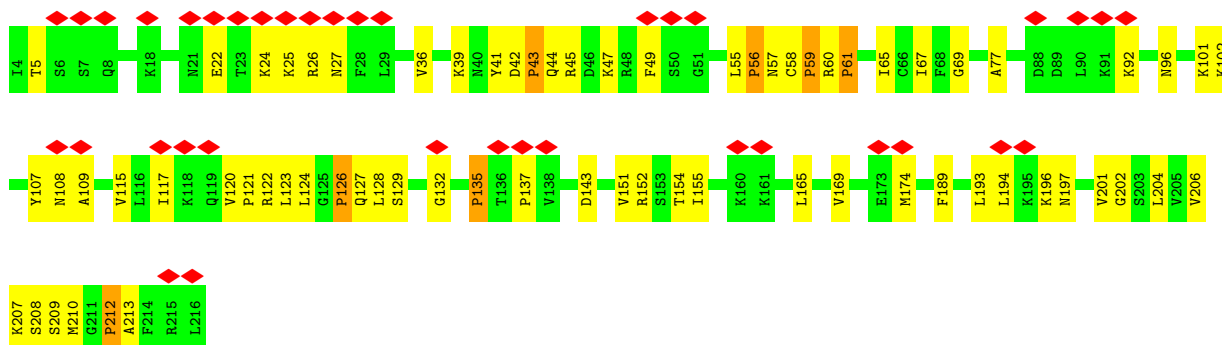
- Molecule 14: 60S ribosomal RNA fragment

Chain 7: 28% 56% 16%



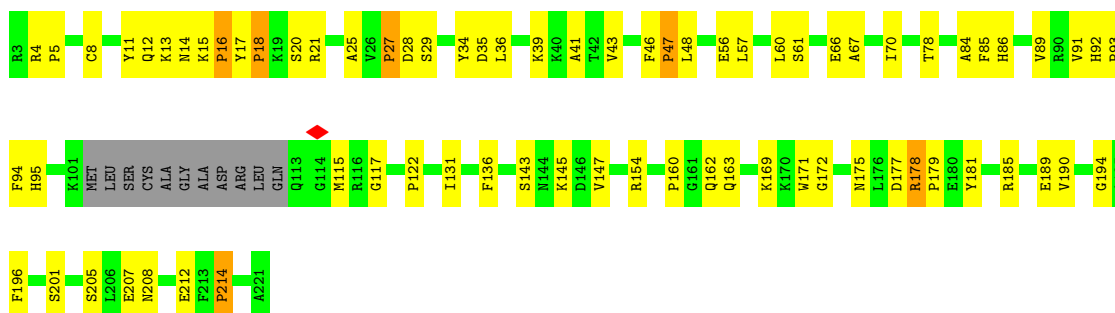
- Molecule 15: Ribosomal protein L10a

Chain B: 17% 67% 30%



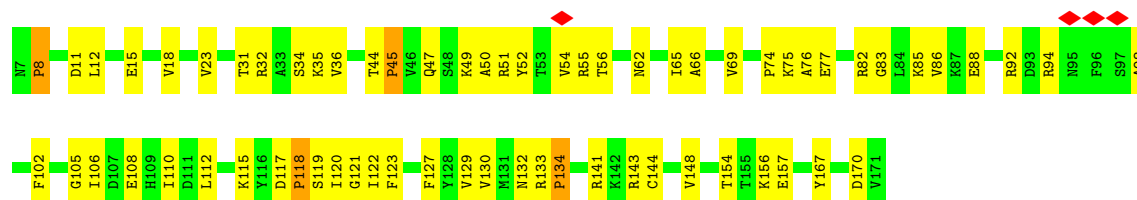
- Molecule 16: Ribosomal protein L10

Chain J: 61% 31% 5%

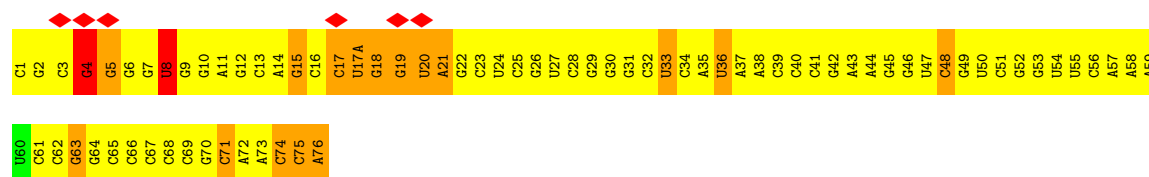
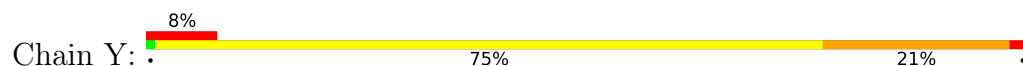


- Molecule 17: Ribosomal protein L11

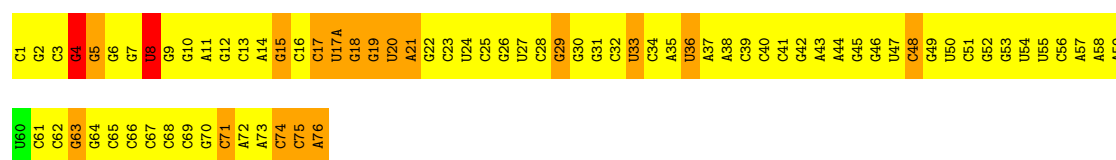
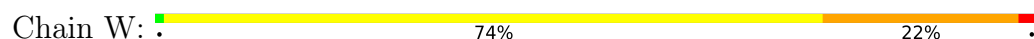
Chain k: 60% 38%



- Molecule 18: tRNA



- Molecule 18: tRNA



- Molecule 19: mRNA fragment



There are no outlier residues recorded for this chain.

- Molecule 20: mRNA fragment



There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23347	Depositor
Resolution determination method	Not provided	
CTF correction method	CTF CORRECTION OF EACH DEFOCUS GROUP VOLUME PRIOR TO BACK PROJECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	65520	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	17103.236	Depositor
Minimum map value	-2542.373	Depositor
Average map value	275.672	Depositor
Map value standard deviation	1215.576	Depositor
Recommended contour level	1000.0	Depositor
Map size ( $\text{\AA}$ )	453.6, 453.6, 453.6	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.52, 2.52, 2.52	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	a	0.69	2/1151 (0.2%)	0.99	8/1793 (0.4%)
2	c	0.63	0/404	0.91	1/627 (0.2%)
3	d	0.49	0/174	0.84	0/270
4	g	0.60	0/737	0.87	2/1146 (0.2%)
5	G	0.52	0/307	0.82	0/476
6	f	0.58	0/504	0.87	0/785
7	h	0.45	0/2650	0.74	1/4127 (0.0%)
8	S	0.39	0/1003	0.66	1/1342 (0.1%)
9	L	0.43	0/1114	0.74	0/1485
10	X	0.35	0/566	0.71	0/753
11	2	1.10	4/2677 (0.1%)	1.68	69/4170 (1.7%)
12	3	0.19	0/290	0.43	0/450
13	9	1.04	0/457	2.15	29/710 (4.1%)
14	7	1.07	2/1174 (0.2%)	2.34	33/1825 (1.8%)
15	B	0.34	0/1054	0.63	9/1468 (0.6%)
16	J	0.66	0/1025	0.89	8/1424 (0.6%)
17	k	0.56	0/809	0.86	5/1122 (0.4%)
18	W	2.74	133/1832 (7.3%)	2.54	183/2855 (6.4%)
18	Y	2.74	134/1832 (7.3%)	2.54	181/2855 (6.3%)
19	y	0.41	0/65	0.70	0/98
20	w	0.40	0/49	0.79	0/74
All	All	1.34	275/19874 (1.4%)	1.56	530/29855 (1.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	3
3	d	0	1
4	g	0	2
7	h	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
17	k	0	1
18	W	0	5
18	Y	0	5
All	All	0	19

All (275) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	59	A	N9-C4	-13.26	1.29	1.37
18	W	59	A	N9-C4	-13.23	1.29	1.37
18	Y	2	G	C8-N7	-13.20	1.23	1.30
18	W	2	G	C8-N7	-13.15	1.23	1.30
18	W	40	C	N1-C6	-12.03	1.29	1.37
18	Y	40	C	N1-C6	-11.94	1.29	1.37
14	7	2845	A	C6-N1	-10.99	1.27	1.35
18	W	22	G	N7-C5	-10.55	1.32	1.39
18	Y	22	G	N7-C5	-10.43	1.32	1.39
18	W	72	A	N9-C4	-10.03	1.31	1.37
18	Y	72	A	N9-C4	-9.96	1.31	1.37
18	W	49	G	N9-C8	-9.53	1.31	1.37
18	Y	49	G	N9-C8	-9.52	1.31	1.37
18	Y	24	U	C4-O4	-9.35	1.16	1.23
18	W	24	U	C4-O4	-9.30	1.16	1.23
18	Y	16	C	N1-C6	-9.26	1.31	1.37
18	Y	49	G	N7-C5	-9.15	1.33	1.39
18	W	49	G	N7-C5	-9.14	1.33	1.39
18	W	16	C	N1-C6	-9.08	1.31	1.37
18	W	57	A	N7-C5	-8.94	1.33	1.39
18	Y	57	A	N7-C5	-8.93	1.33	1.39
18	Y	10	G	C5-C6	-8.72	1.33	1.42
18	W	10	G	C5-C6	-8.71	1.33	1.42
18	Y	30	G	C2'-C1'	-8.68	1.43	1.53
18	W	30	G	C2'-C1'	-8.63	1.43	1.53
18	W	48	C	C2-N3	-8.58	1.28	1.35
18	Y	48	C	C2-N3	-8.53	1.28	1.35
18	W	9	G	N7-C5	-8.53	1.34	1.39
18	Y	9	G	N7-C5	-8.41	1.34	1.39
18	W	51	C	C2-N3	-8.34	1.29	1.35
18	Y	51	C	C2-N3	-8.23	1.29	1.35
18	Y	21	A	N9-C4	-8.19	1.32	1.37
18	W	21	A	N9-C4	-8.17	1.32	1.37
18	W	27	U	C2-N3	-8.16	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	27	U	C2-N3	-8.08	1.32	1.37
18	W	61	C	C5-C6	-8.01	1.27	1.34
18	Y	61	C	C5-C6	-7.99	1.27	1.34
18	Y	3	C	N3-C4	-7.88	1.28	1.33
18	W	3	C	N3-C4	-7.85	1.28	1.33
18	Y	31	G	C8-N7	-7.78	1.26	1.30
18	W	15	G	C6-N1	-7.71	1.34	1.39
18	W	31	G	C8-N7	-7.71	1.26	1.30
18	Y	15	G	C6-N1	-7.67	1.34	1.39
18	W	33	U	C2-N3	-7.59	1.32	1.37
18	Y	33	U	C2-N3	-7.58	1.32	1.37
18	Y	39	C	C4-N4	-7.57	1.27	1.33
18	W	39	C	C4-N4	-7.57	1.27	1.33
18	Y	65	C	C4-C5	-7.57	1.36	1.43
18	W	62	C	C4-C5	-7.57	1.36	1.43
18	Y	69	C	C2-N3	-7.54	1.29	1.35
18	W	65	C	C4-C5	-7.52	1.36	1.43
18	W	35	A	N7-C5	-7.51	1.34	1.39
18	W	58	A	N3-C4	-7.51	1.30	1.34
18	Y	62	C	C4-C5	-7.50	1.36	1.43
18	W	57	A	N9-C4	-7.46	1.33	1.37
18	W	69	C	C2-N3	-7.46	1.29	1.35
18	Y	57	A	N9-C4	-7.41	1.33	1.37
18	W	36	U	C3'-C2'	-7.40	1.44	1.52
18	Y	58	A	N3-C4	-7.38	1.30	1.34
18	Y	36	U	C3'-C2'	-7.36	1.44	1.52
18	Y	35	A	N7-C5	-7.32	1.34	1.39
18	W	73	A	C5-C4	-7.31	1.33	1.38
18	Y	67	C	P-O5'	-7.29	1.52	1.59
18	Y	71	C	N1-C2	-7.29	1.32	1.40
18	Y	73	A	C5-C4	-7.28	1.33	1.38
18	W	71	C	N1-C2	-7.23	1.32	1.40
18	Y	69	C	N3-C4	7.19	1.39	1.33
18	W	67	C	P-O5'	-7.17	1.52	1.59
18	W	69	C	N3-C4	7.17	1.39	1.33
18	Y	53	G	N7-C5	-7.17	1.34	1.39
18	W	38	A	C8-N7	-7.10	1.26	1.31
18	W	53	G	N7-C5	-7.08	1.34	1.39
18	Y	38	A	C8-N7	-7.08	1.26	1.31
18	W	43	A	N3-C4	-7.08	1.30	1.34
18	W	39	C	N1-C6	-7.07	1.32	1.37
18	Y	30	G	C6-O6	-7.03	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	W	22	G	C4'-C3'	-7.02	1.45	1.53
18	Y	22	G	C4'-C3'	-7.00	1.45	1.53
18	Y	39	C	N1-C6	-6.98	1.32	1.37
18	Y	43	A	N3-C4	-6.97	1.30	1.34
18	W	19	G	C2-N3	-6.97	1.27	1.32
18	Y	10	G	P-O5'	-6.93	1.52	1.59
18	W	30	G	C6-O6	-6.92	1.18	1.24
18	Y	19	G	C2-N3	-6.92	1.27	1.32
18	W	45	G	N9-C4	-6.90	1.32	1.38
18	W	10	G	P-O5'	-6.89	1.52	1.59
18	Y	45	G	N9-C4	-6.85	1.32	1.38
18	W	18	G	N9-C4	-6.85	1.32	1.38
18	Y	63	G	C5-C6	-6.78	1.35	1.42
18	W	63	G	C5-C6	-6.78	1.35	1.42
18	Y	18	G	N9-C4	-6.78	1.32	1.38
18	Y	30	G	N3-C4	-6.74	1.30	1.35
18	Y	34	C	N1-C6	-6.74	1.33	1.37
18	W	30	G	N3-C4	-6.73	1.30	1.35
18	Y	7	G	P-O5'	-6.71	1.53	1.59
18	W	7	G	P-O5'	-6.67	1.53	1.59
18	W	32	C	N3-C4	-6.66	1.29	1.33
18	Y	32	C	N3-C4	-6.65	1.29	1.33
18	W	58	A	P-O5'	-6.62	1.53	1.59
18	W	17(A)	U	C2-N3	-6.61	1.33	1.37
18	W	17	C	C2'-C1'	-6.60	1.46	1.53
18	Y	17	C	C2'-C1'	-6.60	1.46	1.53
18	Y	59	A	C8-N7	-6.59	1.26	1.31
18	W	25	C	C2-O2	-6.58	1.18	1.24
18	Y	58	A	P-O5'	-6.57	1.53	1.59
18	Y	17(A)	U	C2-N3	-6.57	1.33	1.37
18	W	34	C	N1-C6	-6.53	1.33	1.37
18	Y	72	A	N9-C8	-6.53	1.32	1.37
18	W	12	G	N7-C5	-6.51	1.35	1.39
18	Y	25	C	C2-O2	-6.51	1.18	1.24
18	W	12	G	C8-N7	-6.50	1.27	1.30
18	W	16	C	C4-C5	6.48	1.48	1.43
18	Y	41	C	C2-O2	-6.48	1.18	1.24
18	Y	12	G	C8-N7	-6.48	1.27	1.30
18	W	59	A	C8-N7	-6.46	1.27	1.31
18	W	72	A	N9-C8	-6.45	1.32	1.37
18	W	41	C	C2-O2	-6.44	1.18	1.24
18	Y	16	C	C4-C5	6.43	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	W	18	G	C3'-C2'	-6.41	1.45	1.52
18	Y	12	G	N7-C5	-6.40	1.35	1.39
18	W	8	U	C4-C5	-6.39	1.37	1.43
18	Y	8	U	C4-C5	-6.39	1.37	1.43
18	W	64	G	C6-N1	-6.37	1.35	1.39
18	W	56	C	C4'-C3'	-6.35	1.46	1.53
18	Y	64	G	C6-N1	-6.35	1.35	1.39
18	Y	18	G	C3'-C2'	-6.34	1.45	1.52
18	Y	8	U	C2-O2	-6.34	1.16	1.22
18	W	5	G	C8-N7	-6.33	1.27	1.30
18	W	12	G	N3-C4	-6.33	1.31	1.35
18	Y	56	C	C4'-C3'	-6.33	1.46	1.53
18	W	8	U	C2-O2	-6.33	1.16	1.22
18	Y	18	G	C5-C4	-6.27	1.33	1.38
18	Y	32	C	C3'-C2'	-6.26	1.45	1.52
18	Y	41	C	C4-N4	-6.26	1.28	1.33
18	W	41	C	C4-N4	-6.25	1.28	1.33
18	W	44	A	C5-C4	-6.24	1.34	1.38
18	W	32	C	C3'-C2'	-6.24	1.45	1.52
18	Y	12	G	N3-C4	-6.24	1.31	1.35
18	W	18	G	C5-C4	-6.22	1.33	1.38
18	Y	5	G	C8-N7	-6.20	1.27	1.30
18	Y	33	U	C4'-C3'	-6.20	1.46	1.53
18	Y	44	A	C5-C4	-6.19	1.34	1.38
18	W	3	C	C4-C5	-6.18	1.38	1.43
11	2	2283	G	N9-C8	6.17	1.42	1.37
18	W	33	U	C4'-C3'	-6.15	1.46	1.53
18	Y	3	C	C4-C5	-6.13	1.38	1.43
18	Y	34	C	C4-C5	-6.10	1.38	1.43
18	W	72	A	N7-C5	-6.10	1.35	1.39
18	W	34	C	C4-C5	-6.04	1.38	1.43
18	Y	63	G	P-O5'	-5.99	1.53	1.59
18	Y	72	A	N7-C5	-5.98	1.35	1.39
18	W	44	A	C8-N7	-5.98	1.27	1.31
18	Y	3	C	C3'-C2'	-5.97	1.46	1.52
18	Y	42	G	C8-N7	-5.97	1.27	1.30
18	Y	73	A	C8-N7	-5.96	1.27	1.31
18	Y	36	U	C2-O2	-5.93	1.17	1.22
18	W	73	A	C8-N7	-5.93	1.27	1.31
18	Y	14	A	C6-N1	-5.93	1.31	1.35
18	Y	44	A	C8-N7	-5.92	1.27	1.31
18	Y	11	A	N1-C2	-5.91	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	W	63	G	P-O5'	-5.89	1.53	1.59
18	W	14	A	C6-N1	-5.89	1.31	1.35
18	Y	76	A	C8-N7	-5.88	1.27	1.31
18	W	14	A	P-O5'	-5.88	1.53	1.59
18	Y	63	G	C8-N7	-5.88	1.27	1.30
18	W	42	G	C8-N7	-5.88	1.27	1.30
18	W	3	C	C3'-C2'	-5.87	1.46	1.52
18	W	36	U	C2-O2	-5.86	1.17	1.22
18	W	76	A	C8-N7	-5.86	1.27	1.31
18	W	58	A	N9-C8	-5.84	1.33	1.37
18	W	11	A	N1-C2	-5.84	1.29	1.34
18	Y	14	A	P-O5'	-5.84	1.53	1.59
18	W	43	A	N7-C5	-5.83	1.35	1.39
18	W	63	G	C8-N7	-5.83	1.27	1.30
18	W	11	A	P-O5'	-5.82	1.53	1.59
18	Y	36	U	P-O5'	-5.81	1.53	1.59
18	Y	58	A	N9-C8	-5.80	1.33	1.37
18	Y	71	C	C4-C5	-5.80	1.38	1.43
18	W	9	G	C8-N7	-5.80	1.27	1.30
18	Y	46	G	N1-C2	-5.79	1.33	1.37
18	W	36	U	P-O5'	-5.78	1.53	1.59
18	Y	11	A	P-O5'	-5.77	1.53	1.59
18	Y	11	A	O4'-C1'	-5.77	1.34	1.41
18	Y	9	G	C8-N7	-5.76	1.27	1.30
18	W	21	A	C2-N3	-5.75	1.28	1.33
18	W	46	G	N1-C2	-5.75	1.33	1.37
18	Y	25	C	C4'-C3'	-5.74	1.46	1.52
18	W	58	A	N1-C2	-5.72	1.29	1.34
18	W	71	C	C4-C5	-5.72	1.38	1.43
18	W	11	A	O4'-C1'	-5.72	1.34	1.41
18	Y	43	A	N7-C5	-5.71	1.35	1.39
18	Y	58	A	N1-C2	-5.71	1.29	1.34
18	Y	21	A	C2-N3	-5.70	1.28	1.33
18	Y	21	A	C5-C6	-5.67	1.35	1.41
18	W	25	C	C4'-C3'	-5.66	1.46	1.52
18	Y	30	G	C4'-C3'	-5.63	1.47	1.52
18	W	21	A	C5-C6	-5.62	1.35	1.41
18	W	30	G	C4'-C3'	-5.60	1.47	1.52
18	Y	9	G	N9-C8	-5.59	1.33	1.37
18	W	45	G	C6-N1	-5.58	1.35	1.39
18	Y	45	G	C6-N1	-5.54	1.35	1.39
18	Y	45	G	C1'-N9	-5.53	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	W	9	G	N9-C8	-5.52	1.33	1.37
18	Y	55	U	C5-C6	-5.51	1.29	1.34
18	Y	28	C	C4'-C3'	-5.50	1.47	1.52
18	W	70	G	C8-N7	-5.50	1.27	1.30
18	W	45	G	C1'-N9	-5.49	1.39	1.46
18	Y	70	G	C8-N7	-5.47	1.27	1.30
18	W	17(A)	U	C2-O2	-5.46	1.17	1.22
18	W	28	C	C4'-C3'	-5.44	1.47	1.52
18	W	55	U	C5-C6	-5.41	1.29	1.34
18	W	56	C	N3-C4	-5.40	1.30	1.33
1	a	565	G	N9-C4	5.39	1.42	1.38
18	Y	11	A	C8-N7	-5.39	1.27	1.31
18	W	27	U	C4'-C3'	5.39	1.59	1.53
18	Y	27	U	C4'-C3'	5.38	1.59	1.53
18	Y	56	C	C5-C6	-5.37	1.30	1.34
18	W	61	C	C4'-C3'	-5.35	1.47	1.52
18	W	64	G	C8-N7	-5.35	1.27	1.30
18	Y	64	G	C8-N7	-5.35	1.27	1.30
18	Y	17(A)	U	C2-O2	-5.34	1.17	1.22
18	Y	62	C	C4'-C3'	-5.34	1.47	1.52
18	Y	46	G	C3'-C2'	-5.34	1.46	1.52
18	Y	61	C	C4'-C3'	-5.33	1.47	1.52
18	W	62	C	C4'-C3'	-5.32	1.47	1.52
18	Y	43	A	C5-C6	-5.30	1.36	1.41
18	Y	57	A	N9-C8	-5.29	1.33	1.37
18	W	57	A	N9-C8	-5.28	1.33	1.37
18	W	56	C	C5-C6	-5.28	1.30	1.34
18	Y	14	A	C1'-N9	-5.27	1.39	1.46
18	W	43	A	C5-C6	-5.27	1.36	1.41
18	W	32	C	N1-C2	-5.27	1.34	1.40
18	Y	56	C	N3-C4	-5.26	1.30	1.33
18	W	46	G	C3'-C2'	-5.26	1.47	1.52
18	Y	53	G	C2-N3	-5.25	1.28	1.32
18	W	45	G	N3-C4	-5.24	1.31	1.35
18	W	14	A	C1'-N9	-5.24	1.39	1.46
18	W	11	A	C8-N7	-5.23	1.27	1.31
18	Y	45	G	N3-C4	-5.22	1.31	1.35
18	Y	74	C	C4'-O4'	-5.22	1.38	1.45
18	W	74	C	C4'-O4'	-5.21	1.38	1.45
18	W	50	U	N3-C4	-5.20	1.33	1.38
18	Y	73	A	N1-C2	-5.19	1.29	1.34
18	Y	59	A	C6-N6	-5.19	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	W	22	G	C3'-C2'	-5.19	1.47	1.52
18	W	23	C	C4'-C3'	-5.18	1.47	1.52
18	Y	50	U	N3-C4	-5.18	1.33	1.38
11	2	2302	G	C6-N1	-5.17	1.35	1.39
18	Y	22	G	C3'-C2'	-5.17	1.47	1.52
18	Y	23	C	C4'-C3'	-5.17	1.47	1.52
18	W	22	G	N9-C8	-5.17	1.34	1.37
18	Y	32	C	N1-C2	-5.15	1.35	1.40
18	W	53	G	C2-N3	-5.15	1.28	1.32
18	W	11	A	C5-C4	-5.14	1.35	1.38
18	Y	46	G	N9-C4	-5.14	1.33	1.38
18	W	18	G	N9-C8	5.14	1.41	1.37
18	W	59	A	C6-N6	-5.13	1.29	1.33
11	2	2279	A	N7-C5	-5.12	1.36	1.39
18	Y	49	G	N3-C4	-5.11	1.31	1.35
18	W	73	A	N1-C2	-5.10	1.29	1.34
18	Y	19	G	C6-O6	-5.10	1.19	1.24
18	Y	37	A	C2-N3	-5.10	1.28	1.33
18	Y	22	G	N9-C8	-5.09	1.34	1.37
18	W	46	G	N9-C4	-5.09	1.33	1.38
1	a	565	G	C2-N3	5.07	1.36	1.32
18	Y	26	G	C8-N7	-5.06	1.27	1.30
18	W	19	G	C6-O6	-5.06	1.19	1.24
18	W	40	C	P-O5'	-5.05	1.54	1.59
18	Y	40	C	P-O5'	-5.04	1.54	1.59
18	W	29	G	N7-C5	-5.04	1.36	1.39
18	W	37	A	C2-N3	-5.04	1.29	1.33
18	Y	18	G	N9-C8	5.03	1.41	1.37
14	7	2830	G	N3-C4	-5.02	1.31	1.35
18	Y	15	G	N1-C2	5.01	1.41	1.37
11	2	2283	G	C8-N7	5.00	1.33	1.30

All (530) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	7	2845	A	N1-C6-N6	39.32	142.19	118.60
14	7	2845	A	C6-N1-C2	38.58	141.75	118.60
14	7	2845	A	C5-C6-N1	-33.94	100.73	117.70
14	7	2845	A	N1-C2-N3	-22.70	117.95	129.30
13	9	2681	U	C2-N1-C1'	14.58	135.19	117.70
18	Y	54	U	C5-C6-N1	13.56	129.48	122.70
18	W	54	U	C5-C6-N1	13.48	129.44	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	9	2681	U	C6-N1-C1'	-13.14	102.80	121.20
18	Y	43	A	C8-N9-C4	-12.70	100.72	105.80
18	W	43	A	C8-N9-C4	-12.68	100.73	105.80
14	7	2845	A	C5-C6-N6	-12.67	113.56	123.70
18	Y	43	A	N1-C2-N3	-11.53	123.53	129.30
18	W	43	A	N1-C2-N3	-11.53	123.54	129.30
18	Y	43	A	C2-N3-C4	10.92	116.06	110.60
18	W	43	A	C2-N3-C4	10.91	116.05	110.60
18	Y	37	A	C5-N7-C8	10.87	109.33	103.90
18	W	37	A	C5-N7-C8	10.81	109.31	103.90
18	W	74	C	N3-C4-C5	-10.59	117.66	121.90
18	Y	74	C	N3-C4-C5	-10.46	117.72	121.90
11	2	2195	C	N3-C4-C5	10.38	126.05	121.90
18	W	37	A	N7-C8-N9	-10.12	108.74	113.80
18	Y	37	A	N7-C8-N9	-10.08	108.76	113.80
11	2	2289	U	C2-N3-C4	-10.07	120.96	127.00
13	9	2681	U	C5-C4-O4	-10.04	119.88	125.90
18	W	31	G	C5-C6-O6	-9.96	122.62	128.60
18	Y	31	G	C5-C6-O6	-9.90	122.66	128.60
11	2	2245	C	C6-N1-C2	-9.86	116.36	120.30
11	2	2283	G	C8-N9-C4	-9.85	102.46	106.40
18	W	18	G	C5-C6-N1	9.52	116.26	111.50
18	Y	18	G	C5-C6-N1	9.50	116.25	111.50
11	2	2278	C	N1-C2-O2	9.47	124.58	118.90
18	W	72	A	C5-C6-N1	9.46	122.43	117.70
18	Y	12	G	C2-N3-C4	9.46	116.63	111.90
18	W	12	G	C2-N3-C4	9.44	116.62	111.90
13	9	2671	A	C5-C6-N6	-9.37	116.21	123.70
18	Y	72	A	C5-C6-N1	9.30	122.35	117.70
18	Y	61	C	N3-C4-C5	-9.29	118.18	121.90
18	W	61	C	N3-C4-C5	-9.26	118.20	121.90
18	W	1	C	C6-N1-C2	-9.22	116.61	120.30
18	Y	1	C	C6-N1-C2	-9.13	116.65	120.30
18	W	18	G	C5-C6-O6	-9.02	123.19	128.60
18	W	31	G	C2-N3-C4	8.97	116.39	111.90
18	Y	18	G	C5-C6-O6	-8.96	123.22	128.60
18	Y	31	G	C2-N3-C4	8.96	116.38	111.90
18	W	66	C	C6-N1-C2	8.95	123.88	120.30
11	2	2277	C	C5-C6-N1	-8.95	116.53	121.00
18	Y	66	C	C6-N1-C2	8.88	123.85	120.30
14	7	2835	U	C2-N1-C1'	8.88	128.35	117.70
18	W	76	A	N1-C6-N6	8.80	123.88	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	h	1714	U	N1-C1'-C2'	8.79	125.42	114.00
18	Y	76	A	N1-C6-N6	8.74	123.84	118.60
11	2	2247	G	C5-C6-O6	-8.71	123.37	128.60
18	Y	43	A	N9-C4-C5	8.70	109.28	105.80
18	W	6	G	C4-C5-N7	8.66	114.26	110.80
11	2	2302	G	N1-C6-O6	-8.64	114.72	119.90
18	W	43	A	N9-C4-C5	8.61	109.24	105.80
18	Y	6	G	C4-C5-N7	8.58	114.23	110.80
13	9	2683	U	C5-C4-O4	-8.49	120.81	125.90
14	7	2828	G	N1-C6-O6	8.47	124.98	119.90
18	Y	49	G	N7-C8-N9	8.47	117.33	113.10
14	7	2867	C	N1-C2-O2	-8.46	113.82	118.90
18	Y	68	C	C6-N1-C2	-8.44	116.92	120.30
14	7	2828	G	C5-C6-O6	-8.40	123.56	128.60
11	2	2283	G	N3-C2-N2	-8.38	114.03	119.90
18	W	68	C	C6-N1-C2	-8.38	116.95	120.30
18	Y	16	C	C6-N1-C2	8.38	123.65	120.30
18	W	49	G	N7-C8-N9	8.36	117.28	113.10
18	W	51	C	C2-N3-C4	8.36	124.08	119.90
18	Y	51	C	C2-N3-C4	8.29	124.05	119.90
11	2	2247	G	C4-C5-N7	8.28	114.11	110.80
14	7	2837	A	N1-C6-N6	-8.28	113.63	118.60
18	W	16	C	C6-N1-C2	8.28	123.61	120.30
18	W	18	G	C5-N7-C8	-8.27	100.17	104.30
18	Y	18	G	C5-N7-C8	-8.26	100.17	104.30
11	2	2303	A	C8-N9-C4	8.23	109.09	105.80
18	W	2	G	N9-C4-C5	-8.11	102.16	105.40
18	Y	2	G	N9-C4-C5	-8.09	102.17	105.40
18	W	9	G	C5-N7-C8	7.96	108.28	104.30
18	W	9	G	C4-C5-N7	-7.94	107.62	110.80
18	Y	9	G	C4-C5-N7	-7.93	107.63	110.80
18	Y	70	G	C4-C5-N7	-7.92	107.63	110.80
18	Y	63	G	N3-C4-N9	7.91	130.75	126.00
18	W	63	G	N3-C4-N9	7.90	130.74	126.00
18	Y	15	G	N1-C6-O6	-7.88	115.17	119.90
18	Y	59	A	C8-N9-C4	7.86	108.94	105.80
18	W	15	G	N1-C6-O6	-7.86	115.19	119.90
18	Y	9	G	C5-N7-C8	7.85	108.22	104.30
18	Y	76	A	C5-C6-N1	-7.84	113.78	117.70
18	W	59	A	C8-N9-C4	7.84	108.94	105.80
13	9	2671	A	N1-C6-N6	7.82	123.29	118.60
18	W	70	G	C4-C5-N7	-7.81	107.68	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	21	A	C2-N3-C4	7.80	114.50	110.60
18	Y	6	G	C5-C6-O6	-7.79	123.93	128.60
11	2	2283	G	N1-C6-O6	7.76	124.56	119.90
11	2	2290	C	N1-C2-O2	-7.75	114.25	118.90
18	W	21	A	C2-N3-C4	7.74	114.47	110.60
18	W	76	A	C5-C6-N1	-7.72	113.84	117.70
14	7	2851	A	N1-C6-N6	-7.70	113.98	118.60
18	Y	73	A	N7-C8-N9	-7.70	109.95	113.80
18	W	52	G	C5-C6-N1	7.69	115.34	111.50
18	W	6	G	C5-C6-O6	-7.69	123.99	128.60
18	Y	54	U	C4-C5-C6	-7.68	115.09	119.70
14	7	2835	U	C5-C4-O4	-7.67	121.30	125.90
18	Y	52	G	C5-C6-N1	7.66	115.33	111.50
18	W	18	G	C4-C5-N7	7.66	113.86	110.80
18	W	54	U	C4-C5-C6	-7.62	115.12	119.70
18	Y	18	G	C4-C5-N7	7.60	113.84	110.80
18	Y	17	C	C5-C6-N1	7.60	124.80	121.00
11	2	2247	G	C6-C5-N7	-7.59	125.84	130.40
18	Y	38	A	N9-C4-C5	-7.58	102.77	105.80
11	2	2277	C	C2-N3-C4	-7.58	116.11	119.90
18	Y	62	C	C6-N1-C2	7.58	123.33	120.30
18	W	73	A	N7-C8-N9	-7.56	110.02	113.80
18	W	62	C	C6-N1-C2	7.55	123.32	120.30
14	7	2835	U	N3-C4-O4	7.55	124.68	119.40
18	Y	62	C	C4-C5-C6	7.54	121.17	117.40
18	W	17	C	C5-C6-N1	7.53	124.77	121.00
18	W	62	C	C4-C5-C6	7.53	121.17	117.40
18	Y	72	A	N1-C6-N6	-7.52	114.09	118.60
11	2	2283	G	N3-C4-N9	-7.50	121.50	126.00
18	W	72	A	N1-C6-N6	-7.50	114.10	118.60
18	W	38	A	N9-C4-C5	-7.49	102.80	105.80
18	W	4	G	O4'-C1'-N9	7.48	114.18	108.20
11	2	2201	G	N1-C6-O6	7.47	124.38	119.90
13	9	2683	U	C2-N1-C1'	7.47	126.66	117.70
18	Y	4	G	O4'-C1'-N9	7.42	114.13	108.20
18	W	5	G	N9-C4-C5	-7.38	102.45	105.40
17	k	8	PRO	N-CA-CB	7.38	112.15	103.30
18	Y	24	U	C5-C4-O4	7.38	130.32	125.90
11	2	2241	U	C5-C4-O4	7.37	130.32	125.90
13	9	2679	A	N1-C6-N6	7.37	123.02	118.60
18	Y	62	C	C5-C6-N1	-7.34	117.33	121.00
18	W	5	G	C8-N9-C4	7.33	109.33	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	5	G	N9-C4-C5	-7.33	102.47	105.40
18	Y	49	G	C8-N9-C4	-7.32	103.47	106.40
18	W	8	U	C6-N1-C2	-7.31	116.61	121.00
18	W	24	U	C5-C4-O4	7.31	130.29	125.90
18	W	62	C	C5-C6-N1	-7.30	117.35	121.00
13	9	2683	U	C6-N1-C1'	-7.28	111.01	121.20
18	W	17	C	C3'-C2'-C1'	7.27	107.32	101.50
18	Y	17	C	C3'-C2'-C1'	7.26	107.31	101.50
11	2	2302	G	C6-C5-N7	7.24	134.75	130.40
13	9	2681	U	N1-C2-N3	-7.24	110.56	114.90
18	Y	5	G	C8-N9-C4	7.24	109.29	106.40
18	Y	55	U	C5-C6-N1	7.22	126.31	122.70
18	W	53	G	C6-N1-C2	7.21	129.43	125.10
18	Y	8	U	C6-N1-C2	-7.19	116.69	121.00
18	W	49	G	C8-N9-C4	-7.16	103.53	106.40
18	Y	53	G	C6-N1-C2	7.16	129.40	125.10
18	W	55	U	C5-C6-N1	7.12	126.26	122.70
11	2	2267	C	N1-C2-O2	-7.12	114.63	118.90
13	9	2673	A	C5-C6-N6	-7.10	118.02	123.70
13	9	2669	G	C6-C5-N7	-7.08	126.15	130.40
11	2	2247	G	N1-C6-O6	7.03	124.12	119.90
18	Y	6	G	N9-C4-C5	-7.02	102.59	105.40
18	W	6	G	N9-C4-C5	-6.99	102.60	105.40
18	W	31	G	N1-C2-N3	-6.96	119.72	123.90
4	g	1172	G	N9-C1'-C2'	6.91	122.98	114.00
18	Y	12	G	C5-C6-N1	6.91	114.95	111.50
18	Y	31	G	N1-C2-N3	-6.91	119.76	123.90
11	2	2248	C	N1-C2-O2	-6.87	114.78	118.90
18	Y	31	G	N3-C4-N9	6.87	130.12	126.00
18	W	31	G	N3-C4-N9	6.86	130.12	126.00
11	2	2283	G	N7-C8-N9	6.83	116.52	113.10
18	W	12	G	C5-C6-N1	6.82	114.91	111.50
2	c	981	A	N9-C1'-C2'	6.82	122.86	114.00
13	9	2681	U	N3-C4-O4	6.82	124.17	119.40
11	2	2277	C	N1-C2-O2	-6.81	114.82	118.90
18	W	61	C	C4-C5-C6	6.77	120.79	117.40
1	a	588	A	N9-C1'-C2'	6.76	122.79	114.00
14	7	2824	G	C6-N1-C2	6.76	129.16	125.10
14	7	2830	G	C5-C6-N1	-6.74	108.13	111.50
13	9	2669	G	C4-C5-N7	6.73	113.49	110.80
11	2	2304	C	C6-N1-C2	-6.70	117.62	120.30
18	Y	61	C	C4-C5-C6	6.69	120.74	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	W	23	C	O4'-C1'-N1	6.67	113.54	108.20
18	Y	23	C	O4'-C1'-N1	6.66	113.53	108.20
1	a	559	C	N1-C1'-C2'	6.63	122.62	114.00
18	W	75	C	C4-C5-C6	6.58	120.69	117.40
18	Y	61	C	N3-C4-N4	6.56	122.59	118.00
18	Y	75	C	C4-C5-C6	6.55	120.68	117.40
18	W	28	C	O4'-C1'-N1	6.54	113.43	108.20
11	2	2289	U	N3-C4-C5	6.54	118.52	114.60
18	W	61	C	N3-C4-N4	6.54	122.58	118.00
11	2	2278	C	N1-C2-N3	-6.53	114.63	119.20
18	Y	28	C	O4'-C1'-N1	6.51	113.41	108.20
11	2	2277	C	C6-N1-C2	6.50	122.90	120.30
18	W	1	C	C5-C6-N1	6.49	124.25	121.00
18	W	22	G	O4'-C1'-N9	6.49	113.39	108.20
18	Y	22	G	O4'-C1'-N9	6.48	113.38	108.20
18	W	15	G	N3-C4-C5	-6.46	125.37	128.60
18	Y	55	U	N1-C2-N3	-6.46	111.03	114.90
14	7	2845	A	C2-N3-C4	-6.45	107.38	110.60
18	W	66	C	C2-N3-C4	6.44	123.12	119.90
18	Y	1	C	C5-C6-N1	6.42	124.21	121.00
18	Y	68	C	C5-C6-N1	6.41	124.20	121.00
17	k	45	PRO	N-CA-CB	6.41	110.99	103.30
15	B	56	PRO	N-CA-CB	6.40	110.98	103.30
14	7	2847	A	C8-N9-C4	-6.40	103.24	105.80
1	a	565	G	N3-C2-N2	6.37	124.36	119.90
18	W	55	U	N1-C2-N3	-6.36	111.08	114.90
18	Y	1	C	C5-C4-N4	6.35	124.64	120.20
18	Y	66	C	C2-N3-C4	6.35	123.07	119.90
18	Y	15	G	N3-C4-C5	-6.34	125.43	128.60
18	W	37	A	C5-C6-N1	-6.34	114.53	117.70
18	W	68	C	C5-C6-N1	6.34	124.17	121.00
18	Y	75	C	O5'-P-OP1	-6.33	100.00	105.70
18	W	52	G	C4-C5-C6	-6.33	115.00	118.80
14	7	2865	U	N1-C2-O2	-6.32	118.38	122.80
18	Y	37	A	C5-C6-N1	-6.32	114.54	117.70
18	W	15	G	C5-C6-O6	6.32	132.39	128.60
11	2	2218	G	C5-C6-N1	6.31	114.66	111.50
18	Y	52	G	C4-C5-C6	-6.31	115.01	118.80
18	W	1	C	C5-C4-N4	6.31	124.62	120.20
18	Y	15	G	C5-C6-O6	6.29	132.38	128.60
18	W	75	C	O5'-P-OP1	-6.29	100.04	105.70
18	W	26	G	C2-N3-C4	-6.28	108.76	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	64	G	N3-C2-N2	-6.27	115.51	119.90
18	W	64	G	N3-C2-N2	-6.27	115.51	119.90
11	2	2248	C	C6-N1-C2	6.27	122.81	120.30
18	Y	4	G	N9-C4-C5	6.26	107.90	105.40
14	7	2857	C	N3-C4-C5	6.25	124.40	121.90
4	g	1172	G	C2'-C3'-O3'	6.25	123.70	113.70
18	W	4	G	N9-C4-C5	6.25	107.90	105.40
18	W	65	C	N1-C2-O2	-6.24	115.15	118.90
16	J	179	PRO	N-CA-CB	6.22	110.76	103.30
13	9	2681	U	N1-C2-O2	6.20	127.14	122.80
11	2	2278	C	C6-N1-C1'	-6.20	113.37	120.80
18	Y	76	A	C4-C5-C6	6.19	120.09	117.00
11	2	2278	C	C2-N1-C1'	6.18	125.60	118.80
18	Y	26	G	C2-N3-C4	-6.18	108.81	111.90
1	a	574	A	N9-C1'-C2'	6.17	122.03	114.00
18	W	76	A	C4-C5-C6	6.16	120.08	117.00
18	W	76	A	C4-C5-N7	-6.14	107.63	110.70
16	J	47	PRO	N-CA-CB	6.14	110.67	103.30
14	7	2837	A	C8-N9-C4	6.12	108.25	105.80
18	W	72	A	C4-C5-C6	-6.12	113.94	117.00
11	2	2280	A	C8-N9-C4	-6.12	103.35	105.80
18	Y	65	C	N1-C2-O2	-6.12	115.23	118.90
13	9	2669	G	N9-C4-C5	-6.12	102.95	105.40
14	7	2837	A	N7-C8-N9	-6.11	110.75	113.80
18	Y	20	U	N1-C2-O2	6.11	127.07	122.80
18	W	71	C	N1-C2-N3	-6.10	114.93	119.20
18	Y	71	C	N1-C2-N3	-6.09	114.94	119.20
18	W	19	G	C8-N9-C4	6.08	108.83	106.40
18	W	37	A	C8-N9-C4	6.08	108.23	105.80
18	W	13	C	C5-C4-N4	-6.08	115.94	120.20
18	Y	69	C	N1-C1'-C2'	-6.07	105.32	112.00
18	W	71	C	C2-N3-C4	6.06	122.93	119.90
18	Y	76	A	C4-C5-N7	-6.05	107.67	110.70
15	B	61	PRO	N-CA-CB	6.05	110.56	103.30
18	W	69	C	N1-C1'-C2'	-6.04	105.35	112.00
11	2	2289	U	C5-C6-N1	-6.04	119.68	122.70
18	Y	13	C	C5-C4-N4	-6.04	115.97	120.20
15	B	135	PRO	N-CA-CB	6.04	110.54	103.30
18	Y	19	G	C8-N9-C4	6.04	108.81	106.40
11	2	2278	C	C2-N3-C4	6.03	122.91	119.90
14	7	2869	U	N3-C2-O2	-6.02	117.98	122.20
18	Y	57	A	C5-C6-N1	6.02	120.71	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	W	20	U	N1-C2-O2	6.02	127.01	122.80
18	Y	72	A	C4-C5-C6	-6.02	113.99	117.00
11	2	2196	C	C6-N1-C2	-6.01	117.89	120.30
18	Y	12	G	C5-C6-O6	-6.01	124.99	128.60
15	B	121	PRO	N-CA-CB	6.01	110.51	103.30
11	2	2194	G	C8-N9-C4	6.01	108.80	106.40
11	2	2283	G	C5-N7-C8	-6.01	101.30	104.30
18	Y	37	A	C8-N9-C4	6.00	108.20	105.80
14	7	2835	U	C6-N1-C1'	-6.00	112.81	121.20
13	9	2669	G	C4-N9-C1'	6.00	134.29	126.50
13	9	2669	G	N3-C4-N9	5.99	129.60	126.00
18	W	21	A	N3-C4-N9	5.99	132.19	127.40
18	W	56	C	C5-C4-N4	-5.99	116.01	120.20
18	W	74	C	C3'-C2'-C1'	5.99	106.29	101.50
18	Y	10	G	C8-N9-C4	5.98	108.79	106.40
18	Y	74	C	C3'-C2'-C1'	5.98	106.29	101.50
18	Y	56	C	C5-C4-N4	-5.97	116.02	120.20
18	Y	63	G	C6-C5-N7	-5.97	126.82	130.40
18	Y	61	C	C2-N3-C4	5.96	122.88	119.90
18	Y	71	C	C2-N3-C4	5.96	122.88	119.90
18	Y	44	A	N9-C4-C5	-5.96	103.42	105.80
18	W	8	U	C2-N3-C4	5.95	130.57	127.00
18	W	10	G	C8-N9-C4	5.95	108.78	106.40
15	B	126	PRO	N-CA-CB	5.94	110.43	103.30
18	W	63	G	C6-C5-N7	-5.94	126.84	130.40
18	W	22	G	N3-C4-C5	5.93	131.56	128.60
14	7	2868	U	N3-C2-O2	5.92	126.35	122.20
18	W	12	G	C5-C6-O6	-5.92	125.05	128.60
18	W	18	G	O4'-C1'-N9	-5.92	103.46	108.20
18	Y	18	G	O4'-C1'-N9	-5.91	103.47	108.20
18	Y	8	U	C2-N3-C4	5.90	130.54	127.00
18	W	57	A	C5-C6-N1	5.90	120.65	117.70
18	Y	21	A	N3-C4-N9	5.90	132.12	127.40
18	W	61	C	C2-N3-C4	5.89	122.84	119.90
18	W	12	G	N9-C4-C5	-5.88	103.05	105.40
18	W	59	A	N1-C2-N3	-5.88	126.36	129.30
11	2	2303	A	N9-C4-C5	-5.88	103.45	105.80
15	B	43	PRO	N-CA-CB	5.88	110.36	103.30
18	Y	22	G	N3-C4-C5	5.86	131.53	128.60
15	B	137	PRO	N-CA-CB	5.86	110.33	103.30
13	9	2671	A	C6-N1-C2	-5.85	115.09	118.60
14	7	2867	C	N3-C2-O2	5.85	125.99	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	2201	G	C5-C6-O6	-5.84	125.09	128.60
18	W	44	A	O4'-C1'-N9	-5.84	103.52	108.20
15	B	212	PRO	N-CA-CB	5.84	110.31	103.30
18	Y	59	A	N1-C2-N3	-5.83	126.38	129.30
17	k	74	PRO	N-CA-CB	5.83	110.30	103.30
18	W	66	C	N1-C2-N3	-5.83	115.12	119.20
15	B	59	PRO	N-CA-CB	5.82	110.28	103.30
11	2	2241	U	C6-N1-C1'	5.80	129.32	121.20
18	Y	44	A	O4'-C1'-N9	-5.80	103.56	108.20
18	Y	70	G	C5-N7-C8	5.80	107.20	104.30
11	2	2302	G	C5-C6-N1	5.80	114.40	111.50
13	9	2669	G	C8-N9-C1'	-5.80	119.47	127.00
18	W	44	A	N9-C4-C5	-5.79	103.48	105.80
18	W	18	G	C2-N3-C4	5.78	114.79	111.90
16	J	122	PRO	N-CA-CB	5.78	110.24	103.30
18	Y	48	C	N1-C2-O2	-5.78	115.43	118.90
1	a	558	G	N9-C1'-C2'	5.78	121.51	114.00
18	Y	51	C	C4'-C3'-C2'	5.78	108.38	102.60
18	W	51	C	C4'-C3'-C2'	5.78	108.38	102.60
18	W	48	C	N1-C2-O2	-5.78	115.44	118.90
16	J	18	PRO	N-CA-CB	5.77	110.23	103.30
18	Y	50	U	N3-C4-O4	-5.76	115.37	119.40
11	2	2283	G	N1-C2-N2	5.75	121.37	116.20
18	Y	66	C	N1-C2-N3	-5.75	115.18	119.20
11	2	2290	C	C2-N3-C4	-5.75	117.03	119.90
18	W	55	U	O4'-C1'-N1	5.74	112.79	108.20
18	W	58	A	N9-C4-C5	-5.73	103.51	105.80
11	2	2302	G	N3-C4-N9	-5.73	122.56	126.00
18	W	10	G	N9-C4-C5	-5.73	103.11	105.40
18	W	70	G	C5-N7-C8	5.72	107.16	104.30
18	W	64	G	N1-C2-N3	5.72	127.33	123.90
18	Y	12	G	N9-C4-C5	-5.72	103.11	105.40
18	Y	64	G	N1-C2-N3	5.72	127.33	123.90
18	Y	55	U	O4'-C1'-N1	5.71	112.77	108.20
18	Y	71	C	C6-N1-C2	5.71	122.58	120.30
11	2	2283	G	C2-N3-C4	-5.71	109.05	111.90
18	Y	18	G	C2-N3-C4	5.71	114.75	111.90
14	7	2837	A	C4-C5-N7	-5.70	107.85	110.70
18	W	50	U	N3-C4-O4	-5.69	115.42	119.40
18	W	6	G	C5-N7-C8	-5.68	101.46	104.30
18	Y	58	A	N9-C4-C5	-5.68	103.53	105.80
11	2	2290	C	N3-C4-C5	5.68	124.17	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	2248	C	N3-C2-O2	5.67	125.87	121.90
1	a	565	G	N1-C2-N2	-5.67	111.10	116.20
18	W	50	U	C4-C5-C6	-5.67	116.30	119.70
18	Y	44	A	C4-C5-N7	5.67	113.53	110.70
18	Y	10	G	N9-C4-C5	-5.66	103.14	105.40
18	Y	13	C	O4'-C1'-N1	-5.66	103.67	108.20
18	W	71	C	C6-N1-C2	5.66	122.56	120.30
18	Y	18	G	C4-C5-C6	-5.65	115.41	118.80
18	W	18	G	C4-C5-C6	-5.65	115.41	118.80
1	a	552	C	N1-C1'-C2'	5.64	121.34	114.00
16	J	16	PRO	N-CA-CB	5.64	110.07	103.30
18	Y	8	U	N3-C4-C5	-5.64	111.21	114.60
18	W	8	U	N3-C4-C5	-5.64	111.22	114.60
11	2	2301	U	C6-N1-C2	5.64	124.38	121.00
18	Y	6	G	C5-N7-C8	-5.63	101.48	104.30
18	Y	50	U	C4-C5-C6	-5.63	116.32	119.70
16	J	214	PRO	N-CA-CB	5.62	110.05	103.30
18	Y	73	A	C8-N9-C4	5.62	108.05	105.80
18	W	10	G	C4-C5-N7	5.62	113.05	110.80
13	9	2679	A	N9-C4-C5	-5.60	103.56	105.80
18	W	13	C	O4'-C1'-N1	-5.60	103.72	108.20
11	2	2196	C	N3-C4-C5	5.59	124.14	121.90
18	W	44	A	C4-C5-N7	5.59	113.50	110.70
11	2	2197	C	N3-C2-O2	5.58	125.81	121.90
13	9	2668	U	C2-N1-C1'	5.58	124.40	117.70
18	Y	10	G	C4-C5-N7	5.58	113.03	110.80
18	Y	75	C	N1-C2-O2	-5.57	115.56	118.90
11	2	2300	G	C8-N9-C1'	-5.56	119.77	127.00
18	W	73	A	C8-N9-C4	5.56	108.03	105.80
18	Y	63	G	N3-C4-C5	-5.56	125.82	128.60
11	2	2246	G	C5-C6-N1	5.56	114.28	111.50
14	7	2853	A	N1-C6-N6	5.56	121.93	118.60
18	W	63	G	N7-C8-N9	5.55	115.88	113.10
18	Y	63	G	N7-C8-N9	5.55	115.88	113.10
18	Y	42	G	N1-C6-O6	-5.54	116.58	119.90
18	Y	64	G	C6-N1-C2	-5.53	121.78	125.10
11	2	2241	U	N1-C2-N3	5.52	118.21	114.90
11	2	2301	U	N3-C2-O2	5.52	126.06	122.20
18	W	65	C	N3-C2-O2	5.52	125.76	121.90
18	W	31	G	C5-N7-C8	5.52	107.06	104.30
18	W	13	C	N3-C4-N4	5.51	121.86	118.00
18	Y	13	C	N3-C4-N4	5.51	121.86	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	53	G	C5-C6-N1	-5.50	108.75	111.50
18	W	21	A	C1'-O4'-C4'	-5.50	105.50	109.90
18	W	75	C	N1-C2-O2	-5.50	115.60	118.90
18	Y	64	G	C8-N9-C4	-5.49	104.20	106.40
18	W	44	A	C2-N3-C4	-5.49	107.86	110.60
18	W	64	G	C6-N1-C2	-5.49	121.81	125.10
17	k	134	PRO	N-CA-CB	5.49	109.88	103.30
18	Y	21	A	C1'-O4'-C4'	-5.49	105.51	109.90
18	Y	4	G	N9-C1'-C2'	-5.48	105.97	112.00
18	Y	6	G	C4-C5-C6	-5.48	115.51	118.80
18	Y	44	A	C2-N3-C4	-5.48	107.86	110.60
18	W	4	G	N9-C1'-C2'	-5.48	105.97	112.00
18	W	74	C	C4-C5-C6	5.47	120.14	117.40
18	W	6	G	C4-C5-C6	-5.47	115.52	118.80
14	7	2830	G	C2-N3-C4	-5.47	109.17	111.90
18	W	17(A)	U	C2-N3-C4	5.47	130.28	127.00
18	Y	20	U	N3-C4-O4	-5.46	115.58	119.40
11	2	2274	U	N3-C2-O2	-5.45	118.38	122.20
18	W	23	C	N3-C4-C5	-5.45	119.72	121.90
18	W	53	G	C5-C6-N1	-5.45	108.77	111.50
11	2	2195	C	C5-C4-N4	-5.45	116.39	120.20
18	W	72	A	C6-C5-N7	5.45	136.11	132.30
18	W	63	G	N3-C4-C5	-5.44	125.88	128.60
18	W	64	G	C8-N9-C4	-5.44	104.22	106.40
18	Y	18	G	C3'-C2'-C1'	5.43	105.85	101.50
18	Y	12	G	N3-C4-N9	5.43	129.26	126.00
18	Y	17(A)	U	C2-N3-C4	5.42	130.25	127.00
18	W	12	G	N3-C4-N9	5.42	129.25	126.00
18	Y	65	C	N3-C2-O2	5.42	125.69	121.90
11	2	2289	U	C5-C4-O4	-5.42	122.65	125.90
18	W	18	G	C3'-C2'-C1'	5.42	105.83	101.50
13	9	2671	A	C5-C6-N1	5.41	120.41	117.70
18	W	42	G	N1-C6-O6	-5.41	116.65	119.90
11	2	2301	U	N1-C2-O2	-5.41	119.01	122.80
11	2	2283	G	N3-C4-C5	5.41	131.30	128.60
18	Y	50	U	N3-C4-C5	5.41	117.84	114.60
18	Y	31	G	C5-C6-N1	5.40	114.20	111.50
18	Y	23	C	N3-C4-C5	-5.40	119.74	121.90
18	Y	74	C	N3-C4-N4	5.39	121.78	118.00
18	W	50	U	N3-C4-C5	5.39	117.83	114.60
11	2	2194	G	N7-C8-N9	-5.39	110.41	113.10
18	Y	68	C	N1-C2-N3	5.39	122.97	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	72	A	C6-C5-N7	5.39	136.07	132.30
18	Y	31	G	C5-N7-C8	5.38	106.99	104.30
18	W	71	C	C4-C5-C6	-5.38	114.71	117.40
14	7	2869	U	C2-N1-C1'	5.37	124.15	117.70
18	W	5	G	N7-C8-N9	-5.37	110.42	113.10
18	W	17	C	C4-C5-C6	-5.37	114.72	117.40
18	W	20	U	N3-C4-O4	-5.37	115.64	119.40
18	Y	65	C	C4-C5-C6	5.36	120.08	117.40
18	Y	74	C	C4-C5-C6	5.35	120.08	117.40
18	W	74	C	N3-C4-N4	5.35	121.75	118.00
18	Y	43	A	N7-C8-N9	5.35	116.47	113.80
18	W	68	C	N1-C2-N3	5.35	122.94	119.20
18	Y	67	C	C6-N1-C2	-5.34	118.16	120.30
18	Y	5	G	N7-C8-N9	-5.34	110.43	113.10
18	Y	17	C	C4-C5-C6	-5.34	114.73	117.40
17	k	118	PRO	N-CA-CB	5.33	109.70	103.30
18	Y	3	C	C5-C6-N1	-5.33	118.33	121.00
18	Y	70	G	C6-C5-N7	5.33	133.60	130.40
18	W	59	A	N1-C6-N6	-5.33	115.41	118.60
18	W	43	A	N7-C8-N9	5.32	116.46	113.80
18	Y	15	G	C6-N1-C2	-5.31	121.91	125.10
11	2	2275	A	C5-C6-N1	-5.31	115.05	117.70
11	2	2303	A	C5-C6-N1	5.31	120.36	117.70
11	2	2247	G	C5-N7-C8	-5.30	101.65	104.30
14	7	2859	U	N3-C2-O2	5.29	125.91	122.20
18	W	31	G	C5-C6-N1	5.29	114.15	111.50
18	Y	59	A	N1-C6-N6	-5.29	115.43	118.60
18	W	65	C	C4-C5-C6	5.29	120.05	117.40
13	9	2671	A	N9-C4-C5	-5.28	103.69	105.80
18	Y	71	C	C4-C5-C6	-5.28	114.76	117.40
18	W	71	C	C5'-C4'-C3'	-5.28	107.55	116.00
18	Y	71	C	C5'-C4'-C3'	-5.28	107.55	116.00
18	Y	37	A	C4-C5-C6	5.28	119.64	117.00
18	W	15	G	C6-N1-C2	-5.26	121.94	125.10
18	W	21	A	N3-C4-C5	-5.26	123.12	126.80
18	Y	44	A	C5-N7-C8	-5.25	101.27	103.90
18	W	74	C	C2-N3-C4	5.25	122.53	119.90
18	W	70	G	C6-C5-N7	5.25	133.55	130.40
18	W	38	A	N7-C8-N9	5.25	116.42	113.80
11	2	2246	G	N3-C4-N9	5.25	129.15	126.00
18	Y	21	A	N3-C4-C5	-5.25	123.13	126.80
13	9	2683	U	C2-N3-C4	-5.24	123.86	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	W	31	G	N1-C6-O6	5.24	123.05	119.90
18	W	4	G	C3'-C2'-C1'	5.24	105.69	101.50
18	W	37	A	C4-C5-C6	5.24	119.62	117.00
18	W	3	C	C5-C6-N1	-5.23	118.38	121.00
18	Y	24	U	P-O5'-C5'	-5.23	112.53	120.90
18	Y	21	A	N1-C6-N6	-5.23	115.46	118.60
18	W	44	A	C5-N7-C8	-5.23	101.28	103.90
18	W	4	G	C5'-C4'-C3'	-5.22	107.64	116.00
18	W	21	A	N1-C6-N6	-5.22	115.47	118.60
18	W	24	U	P-O5'-C5'	-5.22	112.55	120.90
18	Y	38	A	N7-C8-N9	5.21	116.41	113.80
18	W	24	U	N3-C2-O2	-5.21	118.56	122.20
18	W	67	C	C6-N1-C2	-5.20	118.22	120.30
18	Y	20	U	O4'-C1'-N1	5.20	112.36	108.20
18	Y	32	C	N1-C2-O2	-5.20	115.78	118.90
18	W	20	U	O4'-C1'-N1	5.19	112.35	108.20
18	Y	24	U	N3-C2-O2	-5.19	118.57	122.20
18	Y	4	G	C5'-C4'-C3'	-5.18	107.71	116.00
18	Y	74	C	C2-N3-C4	5.18	122.49	119.90
18	Y	4	G	C3'-C2'-C1'	5.16	105.63	101.50
18	Y	53	G	C4-C5-N7	5.15	112.86	110.80
13	9	2671	A	N3-C4-N9	5.14	131.52	127.40
18	W	14	A	C6-N1-C2	5.14	121.69	118.60
18	W	71	C	C4'-C3'-C2'	-5.14	97.46	102.60
18	Y	14	A	C6-N1-C2	5.14	121.69	118.60
18	Y	31	G	N3-C4-C5	-5.14	126.03	128.60
11	2	2215	A	C2-N3-C4	-5.14	108.03	110.60
18	W	69	C	C2-N3-C4	5.13	122.47	119.90
18	Y	71	C	C4'-C3'-C2'	-5.13	97.47	102.60
18	W	31	G	N3-C4-C5	-5.12	126.04	128.60
18	Y	17(A)	U	N1-C2-O2	5.12	126.38	122.80
18	Y	56	C	N3-C4-C5	5.12	123.95	121.90
18	W	17(A)	U	N1-C2-O2	5.12	126.38	122.80
16	J	27	PRO	N-CA-CB	5.12	109.44	103.30
18	W	32	C	N1-C2-O2	-5.11	115.83	118.90
13	9	2672	G	C4-C5-N7	5.11	112.84	110.80
18	Y	31	G	N1-C6-O6	5.09	122.96	119.90
18	W	56	C	N3-C4-C5	5.08	123.93	121.90
13	9	2685	C	C2-N1-C1'	5.08	124.38	118.80
18	W	26	G	N3-C4-N9	-5.08	122.95	126.00
11	2	2281	A	C4-C5-C6	5.07	119.53	117.00
18	W	10	G	C5-C6-O6	-5.07	125.56	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Y	11	A	N1-C6-N6	5.06	121.64	118.60
16	J	178	ARG	N-CA-C	5.05	124.65	111.00
18	Y	69	C	C2-N3-C4	5.05	122.43	119.90
14	7	2828	G	C8-N9-C1'	-5.05	120.44	127.00
18	W	63	G	N9-C4-C5	-5.05	103.38	105.40
8	S	131	THR	N-CA-C	5.04	124.61	111.00
14	7	2869	U	C6-N1-C2	-5.04	117.97	121.00
18	W	2	G	N3-C4-N9	5.03	129.02	126.00
18	W	11	A	N1-C6-N6	5.03	121.62	118.60
18	Y	73	A	C5-N7-C8	5.03	106.42	103.90
18	W	53	G	C4-C5-N7	5.03	112.81	110.80
1	a	559	C	O4'-C1'-N1	5.03	112.22	108.20
18	Y	4	G	C4-C5-N7	-5.02	108.79	110.80
11	2	2261	G	N1-C6-O6	5.02	122.91	119.90
18	Y	59	A	N9-C4-C5	-5.01	103.80	105.80
13	9	2672	G	N9-C4-C5	-5.01	103.40	105.40
14	7	2824	G	C5-C6-N1	-5.01	109.00	111.50
18	W	1	C	N1-C1'-C2'	5.00	120.50	114.00
11	2	2290	C	C5-C6-N1	-5.00	118.50	121.00

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	W	15	G	Sidechain
18	W	29	G	Sidechain
18	W	33	U	Sidechain
18	W	4	G	Sidechain
18	W	8	U	Sidechain
18	Y	15	G	Sidechain
18	Y	29	G	Sidechain
18	Y	33	U	Sidechain
18	Y	4	G	Sidechain
18	Y	8	U	Sidechain
1	a	547	C	Sidechain
1	a	559	C	Sidechain
1	a	574	A	Sidechain
3	d	1545	A	Sidechain
4	g	1157	U	Sidechain
4	g	1158	U	Sidechain
7	h	1610	G	Sidechain
7	h	1714	U	Sidechain

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Mol	Chain	Res	Type	Group
17	k	51	ARG	Peptide

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	S	123/125 (98%)	90 (73%)	25 (20%)	8 (6%)	1	16
9	L	139/141 (99%)	106 (76%)	18 (13%)	15 (11%)	0	8
10	X	66/68 (97%)	48 (73%)	12 (18%)	6 (9%)	1	11
15	B	211/213 (99%)	76 (36%)	67 (32%)	68 (32%)	0	0
16	J	204/219 (93%)	80 (39%)	52 (26%)	72 (35%)	0	0
17	k	163/165 (99%)	57 (35%)	42 (26%)	64 (39%)	0	0
All	All	906/931 (97%)	457 (50%)	216 (24%)	233 (26%)	0	1

All (233) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	S	15	GLY
9	L	45	ALA
9	L	62	GLN
9	L	87	PRO
9	L	88	MET
9	L	89	ASP
9	L	107	GLY
9	L	108	ARG
9	L	117	PRO
10	X	8	LEU

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Mol	Chain	Res	Type
10	X	64	ALA
15	B	24	LYS
15	B	36	VAL
15	B	39	LYS
15	B	42	ASP
15	B	43	PRO
15	B	55	LEU
15	B	56	PRO
15	B	58	CYS
15	B	59	PRO
15	B	60	ARG
15	B	61	PRO
15	B	109	ALA
15	B	115	VAL
15	B	120	VAL
15	B	122	ARG
15	B	124	LEU
15	B	126	PRO
15	B	127	GLN
15	B	128	LEU
15	B	129	SER
15	B	135	PRO
15	B	143	ASP
15	B	151	VAL
15	B	174	MET
15	B	201	VAL
15	B	207	LYS
15	B	208	SER
15	B	209	SER
15	B	210	MET
15	B	212	PRO
16	J	5	PRO
16	J	11	TYR
16	J	13	LYS
16	J	14	ASN
16	J	16	PRO
16	J	17	TYR
16	J	25	ALA
16	J	29	SER
16	J	34	TYR
16	J	39	LYS
16	J	43	VAL

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Mol	Chain	Res	Type
16	J	46	PHE
16	J	48	LEU
16	J	57	LEU
16	J	61	SER
16	J	70	ILE
16	J	92	HIS
16	J	115	MET
16	J	136	PHE
16	J	145	LYS
16	J	147	VAL
16	J	160	PRO
16	J	162	GLN
16	J	169	LYS
16	J	178	ARG
16	J	190	VAL
16	J	201	SER
16	J	208	ASN
17	k	8	PRO
17	k	15	GLU
17	k	18	VAL
17	k	23	VAL
17	k	32	ARG
17	k	34	SER
17	k	45	PRO
17	k	47	GLN
17	k	49	LYS
17	k	50	ALA
17	k	52	TYR
17	k	54	VAL
17	k	55	ARG
17	k	56	THR
17	k	62	ASN
17	k	65	ILE
17	k	66	ALA
17	k	69	VAL
17	k	76	ALA
17	k	85	LYS
17	k	86	VAL
17	k	88	GLU
17	k	102	PHE
17	k	108	GLU
17	k	110	ILE

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Mol	Chain	Res	Type
17	k	115	LYS
17	k	118	PRO
17	k	120	ILE
17	k	122	ILE
17	k	129	VAL
17	k	132	ASN
17	k	133	ARG
17	k	134	PRO
17	k	143	ARG
17	k	148	VAL
17	k	154	THR
8	S	31	GLU
8	S	33	LEU
9	L	35	GLY
9	L	54	GLU
9	L	76	ARG
9	L	138	LYS
10	X	24	LYS
15	B	25	LYS
15	B	26	ARG
15	B	41	TYR
15	B	44	GLN
15	B	47	LYS
15	B	67	ILE
15	B	77	ALA
15	B	96	ASN
15	B	117	ILE
15	B	123	LEU
15	B	169	VAL
15	B	193	LEU
15	B	194	LEU
15	B	196	LYS
15	B	197	ASN
15	B	204	LEU
15	B	206	VAL
16	J	12	GLN
16	J	21	ARG
16	J	28	ASP
16	J	35	ASP
16	J	36	LEU
16	J	78	THR
16	J	84	ALA

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Mol	Chain	Res	Type
16	J	86	HIS
16	J	93	PRO
16	J	95	HIS
16	J	143	SER
16	J	175	ASN
16	J	177	ASP
16	J	185	ARG
16	J	189	GLU
16	J	196	PHE
16	J	207	GLU
17	k	11	ASP
17	k	31	THR
17	k	77	GLU
17	k	82	ARG
17	k	83	GLY
17	k	92	ARG
17	k	94	ARG
17	k	112	LEU
17	k	121	GLY
17	k	123	PHE
17	k	127	PHE
17	k	141	ARG
17	k	170	ASP
8	S	130	PRO
9	L	91	CYS
9	L	109	GLN
10	X	60	PRO
15	B	22	GLU
15	B	49	PHE
15	B	57	ASN
15	B	101	LYS
15	B	102	LYS
15	B	152	ARG
15	B	202	GLY
16	J	15	LYS
16	J	47	PRO
16	J	56	GLU
16	J	85	PHE
16	J	94	PHE
16	J	181	TYR
16	J	205	SER
16	J	214	PRO

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Mol	Chain	Res	Type
17	k	35	LYS
17	k	119	SER
17	k	156	LYS
17	k	167	TYR
10	X	25	ASP
15	B	27	ASN
15	B	107	TYR
15	B	132	GLY
15	B	155	ILE
15	B	165	LEU
15	B	189	PHE
15	B	213	ALA
16	J	20	SER
16	J	60	LEU
16	J	66	GLU
16	J	91	VAL
16	J	154	ARG
16	J	163	GLN
17	k	98	ALA
17	k	106	ILE
17	k	144	CYS
8	S	123	GLU
10	X	26	LYS
15	B	5	THR
15	B	45	ARG
15	B	92	LYS
15	B	108	ASN
15	B	154	THR
16	J	8	CYS
16	J	41	ALA
16	J	67	ALA
16	J	171	TRP
16	J	212	GLU
17	k	12	LEU
17	k	44	THR
17	k	130	VAL
8	S	85	TYR
17	k	36	VAL
17	k	75	LYS
17	k	157	GLU
8	S	104	GLY
16	J	4	ARG

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Mol	Chain	Res	Type
16	J	172	GLY
16	J	194	GLY
15	B	69	GLY
9	L	110	GLY
15	B	65	ILE
16	J	18	PRO
16	J	117	GLY
16	J	131	ILE
17	k	105	GLY
17	k	117	ASP
8	S	53	GLY
16	J	27	PRO
16	J	89	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	S	105/105 (100%)	101 (96%)	4 (4%)	33	57
9	L	113/113 (100%)	102 (90%)	11 (10%)	8	27
10	X	57/57 (100%)	55 (96%)	2 (4%)	36	59
All	All	275/275 (100%)	258 (94%)	17 (6%)	22	43

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	S	66	ARG
8	S	83	THR
8	S	85	TYR
8	S	124	PHE
9	L	9	ILE
9	L	19	ARG
9	L	33	LEU
9	L	55	LYS
9	L	69	LYS

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Mol	Chain	Res	Type
9	L	81	LYS
9	L	82	ILE
9	L	89	ASP
9	L	92	LEU
9	L	106	LEU
9	L	132	LEU
10	X	34	ARG
10	X	62	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
8	S	29	ASN
8	S	84	HIS
8	S	133	HIS
9	L	62	GLN
9	L	78	ASN
9	L	98	ASN
10	X	42	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	47/48 (97%)	15 (31%)	0
11	2	111/112 (99%)	54 (48%)	9 (8%)
12	3	11/12 (91%)	6 (54%)	1 (9%)
13	9	18/19 (94%)	13 (72%)	1 (5%)
14	7	49/50 (98%)	29 (59%)	5 (10%)
18	W	76/77 (98%)	17 (22%)	0
18	Y	76/77 (98%)	17 (22%)	0
19	y	2/3 (66%)	0	0
2	c	16/17 (94%)	4 (25%)	0
20	w	1/2 (50%)	0	0
3	d	6/7 (85%)	2 (33%)	0
4	g	30/31 (96%)	8 (26%)	0
5	G	12/13 (92%)	2 (16%)	1 (8%)
6	f	20/21 (95%)	5 (25%)	0
7	h	110/111 (99%)	12 (10%)	0
All	All	585/600 (97%)	184 (31%)	17 (2%)



All (184) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	544	G
1	a	547	C
1	a	548	A
1	a	552	C
1	a	553	A
1	a	554	U
1	a	559	C
1	a	560	C
1	a	568	G
1	a	573	A
1	a	574	A
1	a	575	U
1	a	576	U
1	a	577	C
1	a	588	A
2	c	975	G
2	c	976	A
2	c	978	C
2	c	982	U
3	d	1545	A
3	d	1546	G
4	g	1155	A
4	g	1158	U
4	g	1163	U
4	g	1165	A
4	g	1166	A
4	g	1168	A
4	g	1169	C
4	g	1172	G
5	G	1430	C
5	G	1431	A
6	f	1242	G
6	f	1245	G
6	f	1246	C
6	f	1247	A
6	f	1256	C
7	h	1608	C
7	h	1609	C
7	h	1624	G
7	h	1649	U
7	h	1651	G
7	h	1652	A

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Mol	Chain	Res	Type
7	h	1661	G
7	h	1674	A
7	h	1710	G
7	h	1713	G
7	h	1714	U
7	h	1715	A
11	2	2195	C
11	2	2201	G
11	2	2205	U
11	2	2206	G
11	2	2207	A
11	2	2208	A
11	2	2209	U
11	2	2210	G
11	2	2211	U
11	2	2215	A
11	2	2222	A
11	2	2223	A
11	2	2224	A
11	2	2227	C
11	2	2237	C
11	2	2244	A
11	2	2247	G
11	2	2248	C
11	2	2249	G
11	2	2250	G
11	2	2252	A
11	2	2254	U
11	2	2255	A
11	2	2256	A
11	2	2257	C
11	2	2259	A
11	2	2260	U
11	2	2261	G
11	2	2262	A
11	2	2263	C
11	2	2264	U
11	2	2266	U
11	2	2270	A
11	2	2272	G
11	2	2273	G
11	2	2275	A

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Mol	Chain	Res	Type
11	2	2276	G
11	2	2277	C
11	2	2280	A
11	2	2281	A
11	2	2282	U
11	2	2283	G
11	2	2286	U
11	2	2288	G
11	2	2290	C
11	2	2291	A
11	2	2292	U
11	2	2295	A
11	2	2296	A
11	2	2297	U
11	2	2298	U
11	2	2299	A
11	2	2300	G
11	2	2303	A
12	3	2479	C
12	3	2484	A
12	3	2485	A
12	3	2486	A
12	3	2487	U
12	3	2488	A
13	9	2671	A
13	9	2672	G
13	9	2675	C
13	9	2676	A
13	9	2677	G
13	9	2678	A
13	9	2679	A
13	9	2681	U
13	9	2682	C
13	9	2683	U
13	9	2684	C
13	9	2685	C
13	9	2686	A
14	7	2825	C
14	7	2826	U
14	7	2828	G
14	7	2829	U
14	7	2830	G

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Mol	Chain	Res	Type
14	7	2833	A
14	7	2834	G
14	7	2835	U
14	7	2836	C
14	7	2838	A
14	7	2839	G
14	7	2840	C
14	7	2842	U
14	7	2843	U
14	7	2844	C
14	7	2845	A
14	7	2846	U
14	7	2847	A
14	7	2849	C
14	7	2850	G
14	7	2851	A
14	7	2852	C
14	7	2859	U
14	7	2860	U
14	7	2867	C
14	7	2870	C
14	7	2871	G
14	7	2872	A
14	7	2873	U
18	Y	4	G
18	Y	5	G
18	Y	8	U
18	Y	17	C
18	Y	17(A)	U
18	Y	18	G
18	Y	19	G
18	Y	20	U
18	Y	21	A
18	Y	36	U
18	Y	47	U
18	Y	48	C
18	Y	63	G
18	Y	71	C
18	Y	74	C
18	Y	75	C
18	Y	76	A
18	W	4	G

*Continued on next page...*

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Mol	Chain	Res	Type
18	W	5	G
18	W	8	U
18	W	17	C
18	W	17(A)	U
18	W	18	G
18	W	19	G
18	W	20	U
18	W	21	A
18	W	36	U
18	W	47	U
18	W	48	C
18	W	63	G
18	W	71	C
18	W	74	C
18	W	75	C
18	W	76	A

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	G	1430	C
11	2	2211	U
11	2	2251	G
11	2	2254	U
11	2	2255	A
11	2	2270	A
11	2	2280	A
11	2	2281	A
11	2	2290	C
11	2	2297	U
12	3	2487	U
13	9	2684	C
14	7	2834	G
14	7	2850	G
14	7	2851	A
14	7	2859	U
14	7	2872	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](#)

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](#)

There are no chain breaks in this entry.

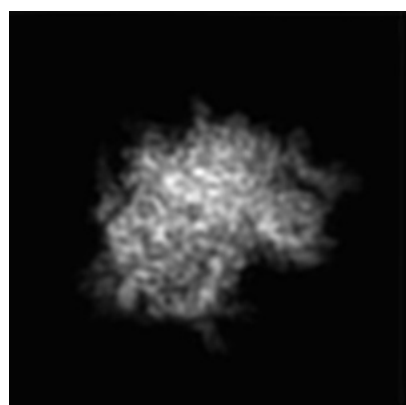
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5329. These allow visual inspection of the internal detail of the map and identification of artifacts.

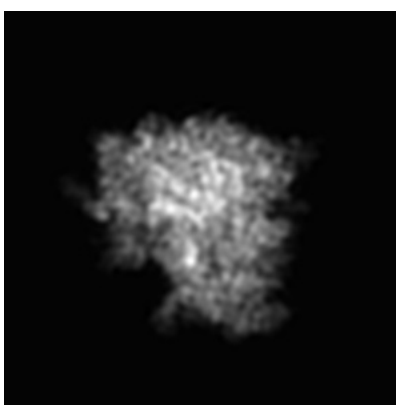
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

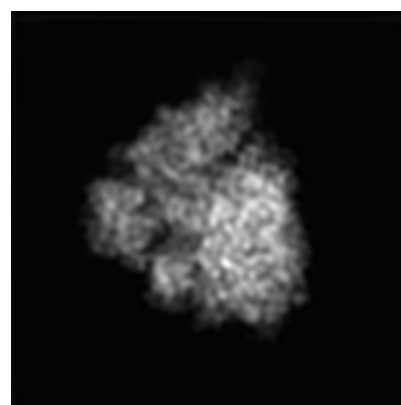
#### 6.1.1 Primary map



X



Y

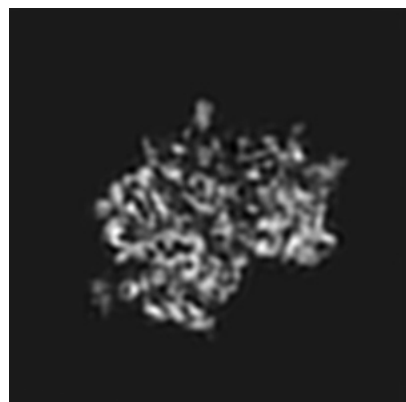


Z

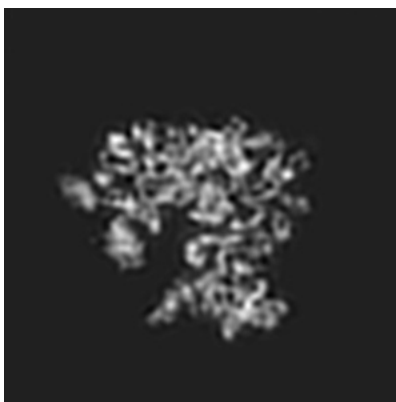
The images above show the map projected in three orthogonal directions.

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

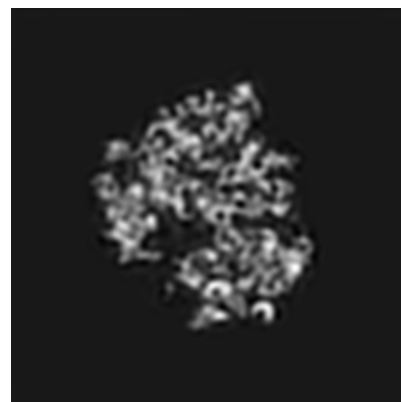
#### 6.2.1 Primary map



X Index: 90



Y Index: 90

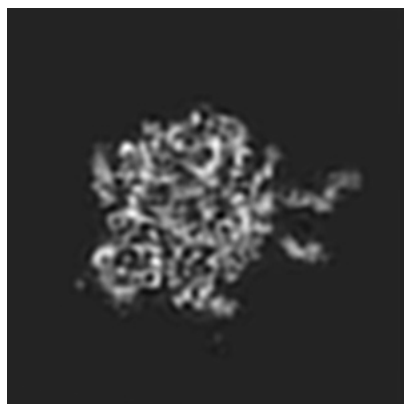


Z Index: 90

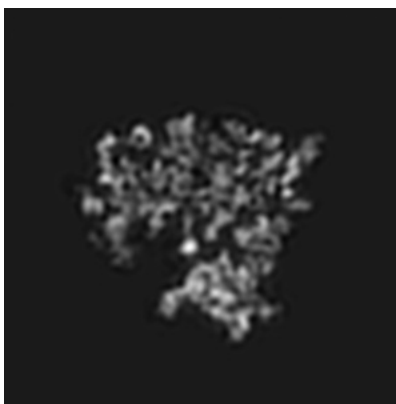
The images above show central slices of the map in three orthogonal directions.

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

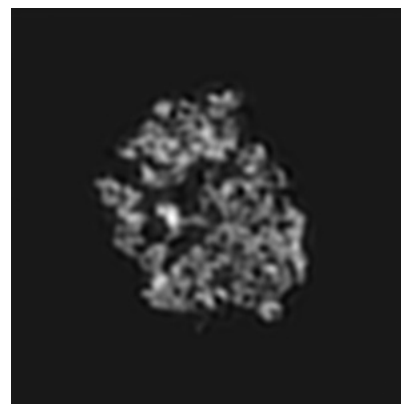
### 6.3.1 Primary map



X Index: 107



Y Index: 85

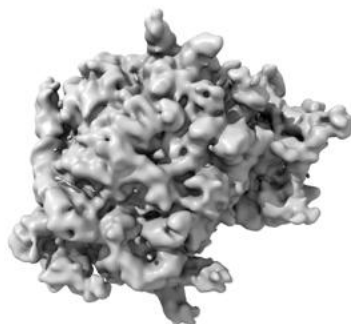


Z Index: 83

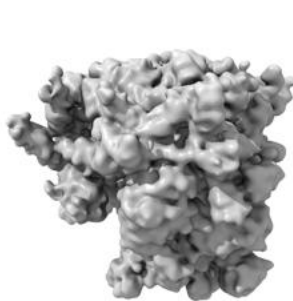
The images above show the largest variance slices of the map in three orthogonal directions.

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

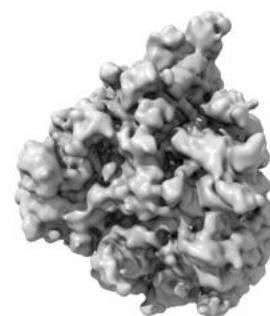
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1000.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



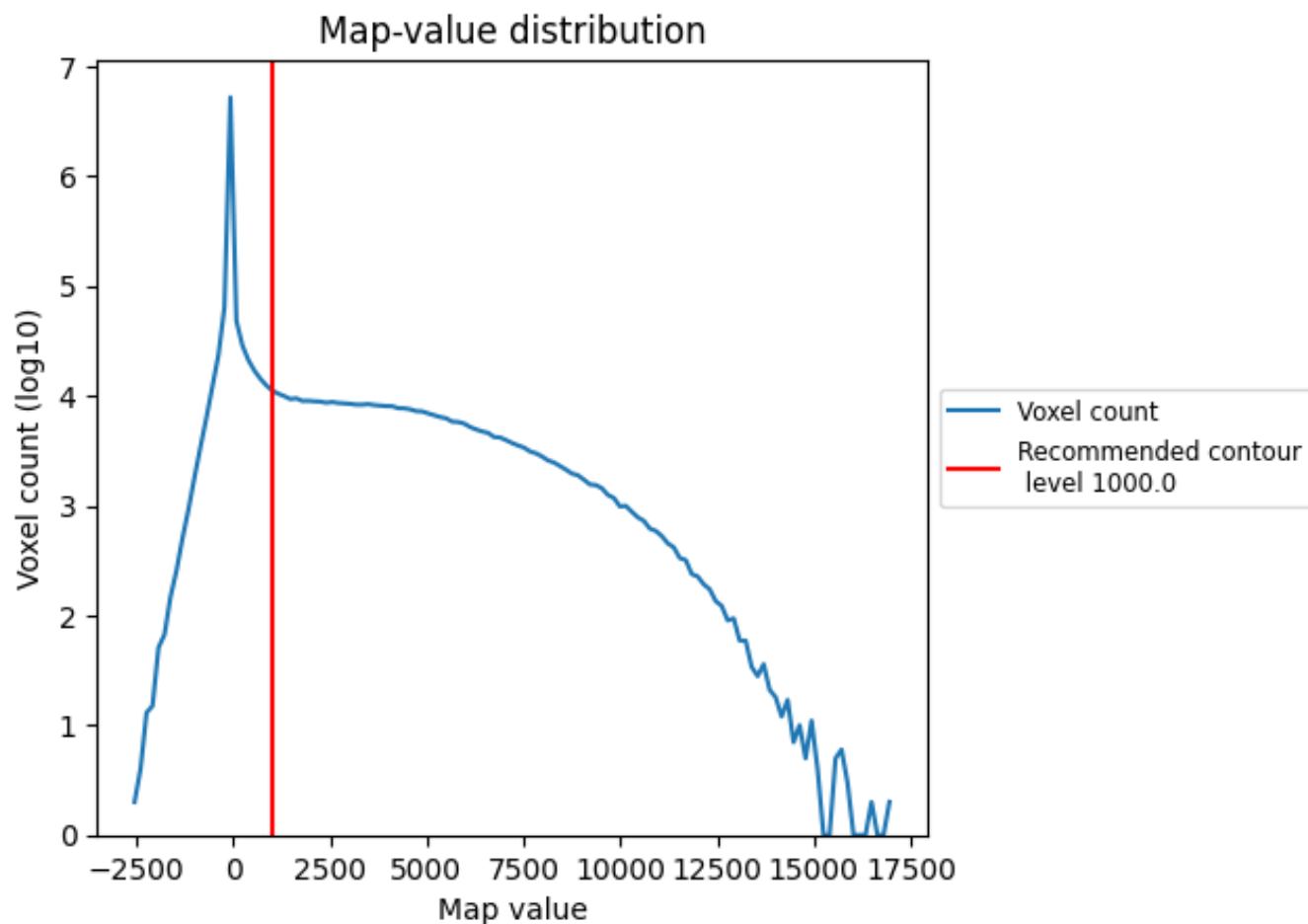
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

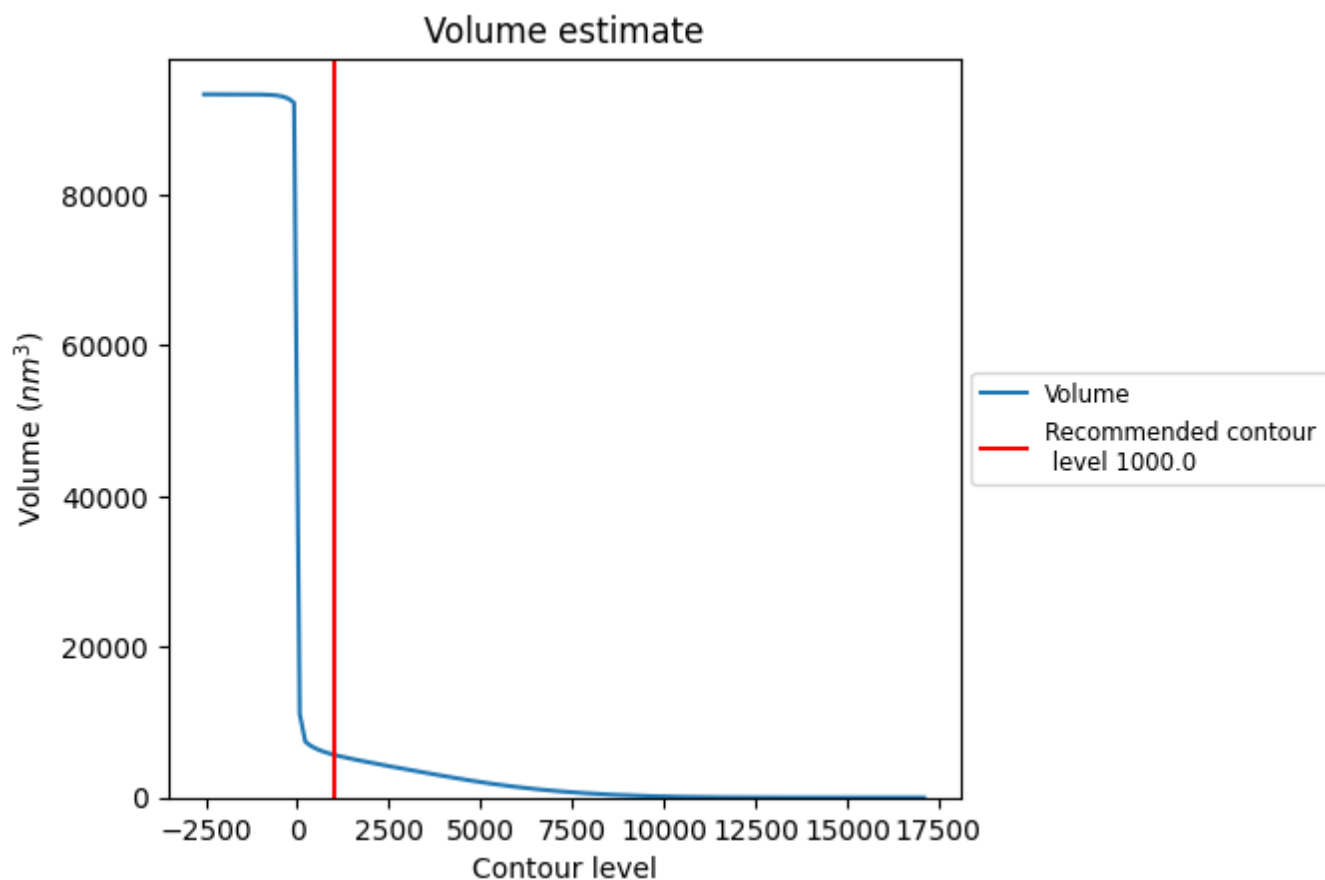
This section contains the results of statistical analysis of the map.

### 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.

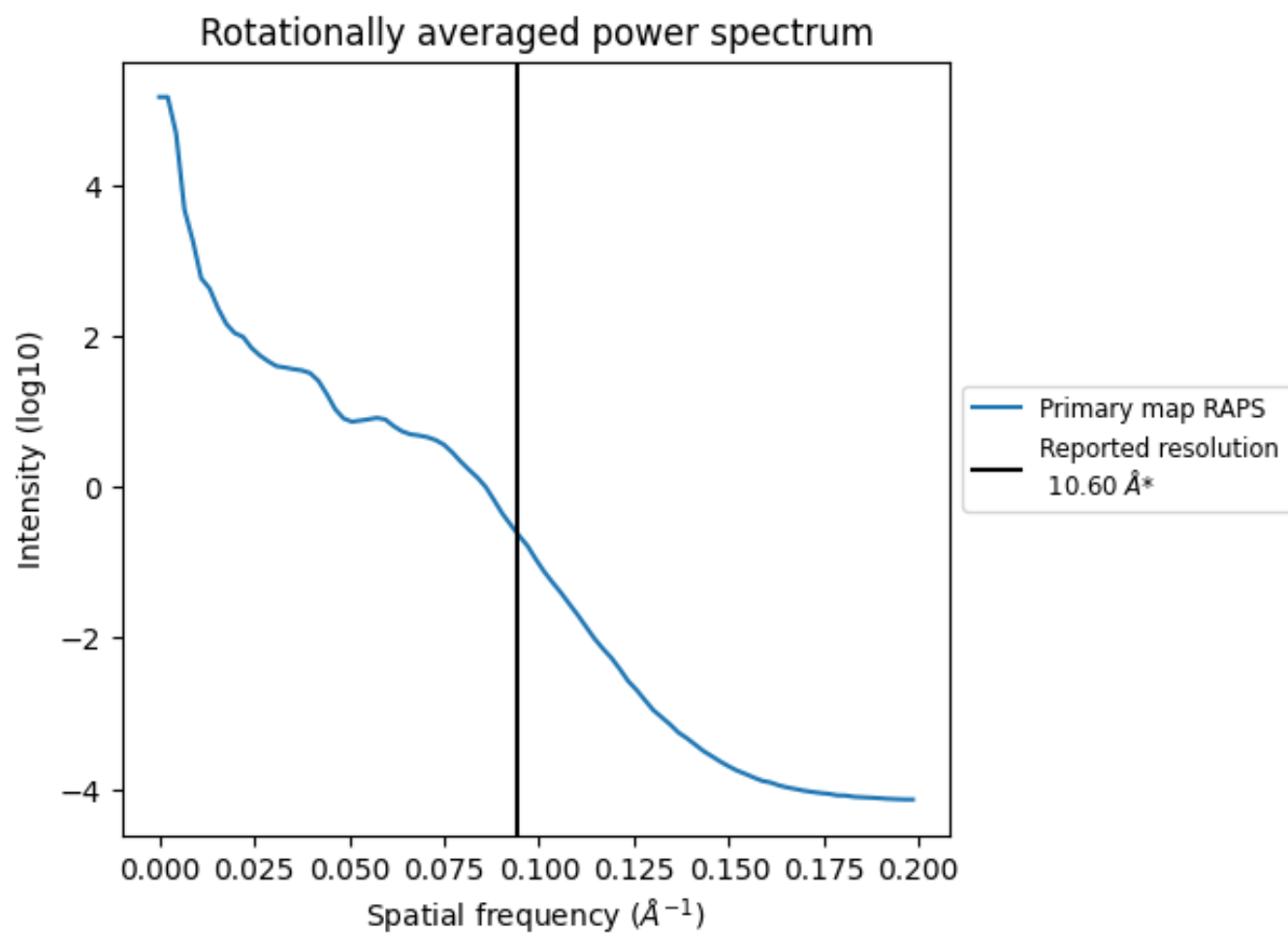
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5682 nm<sup>3</sup>; this corresponds to an approximate mass of 5133 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  $0.094 \text{ \AA}^{-1}$

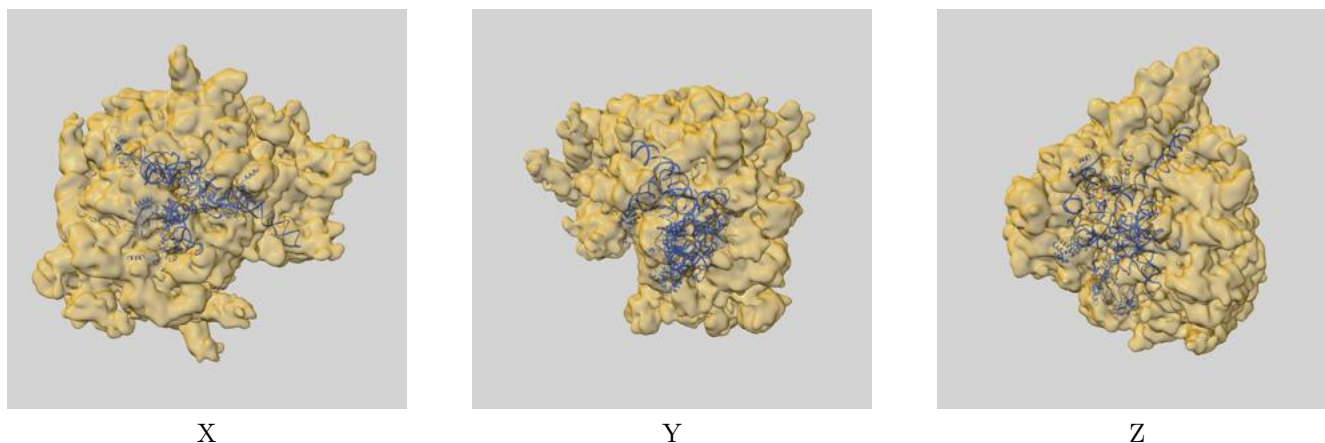
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

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

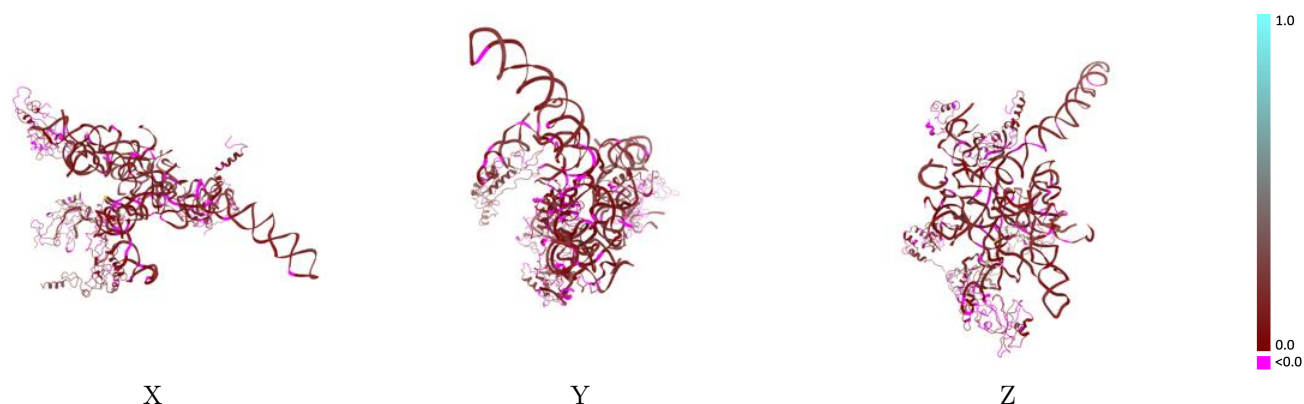
This section contains information regarding the fit between EMDB map EMD-5329 and PDB model 3J0Q. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



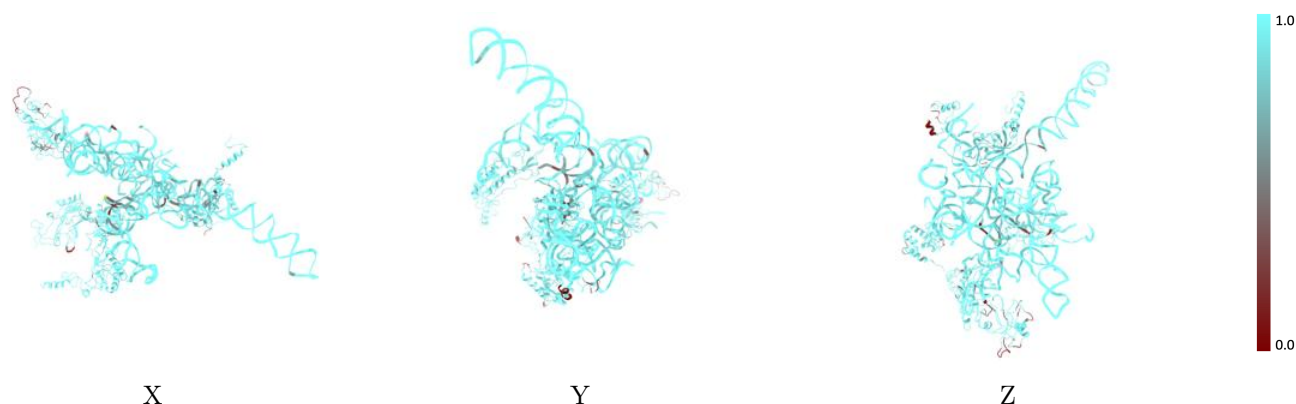
The images above show the 3D surface view of the map at the recommended contour level 1000.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



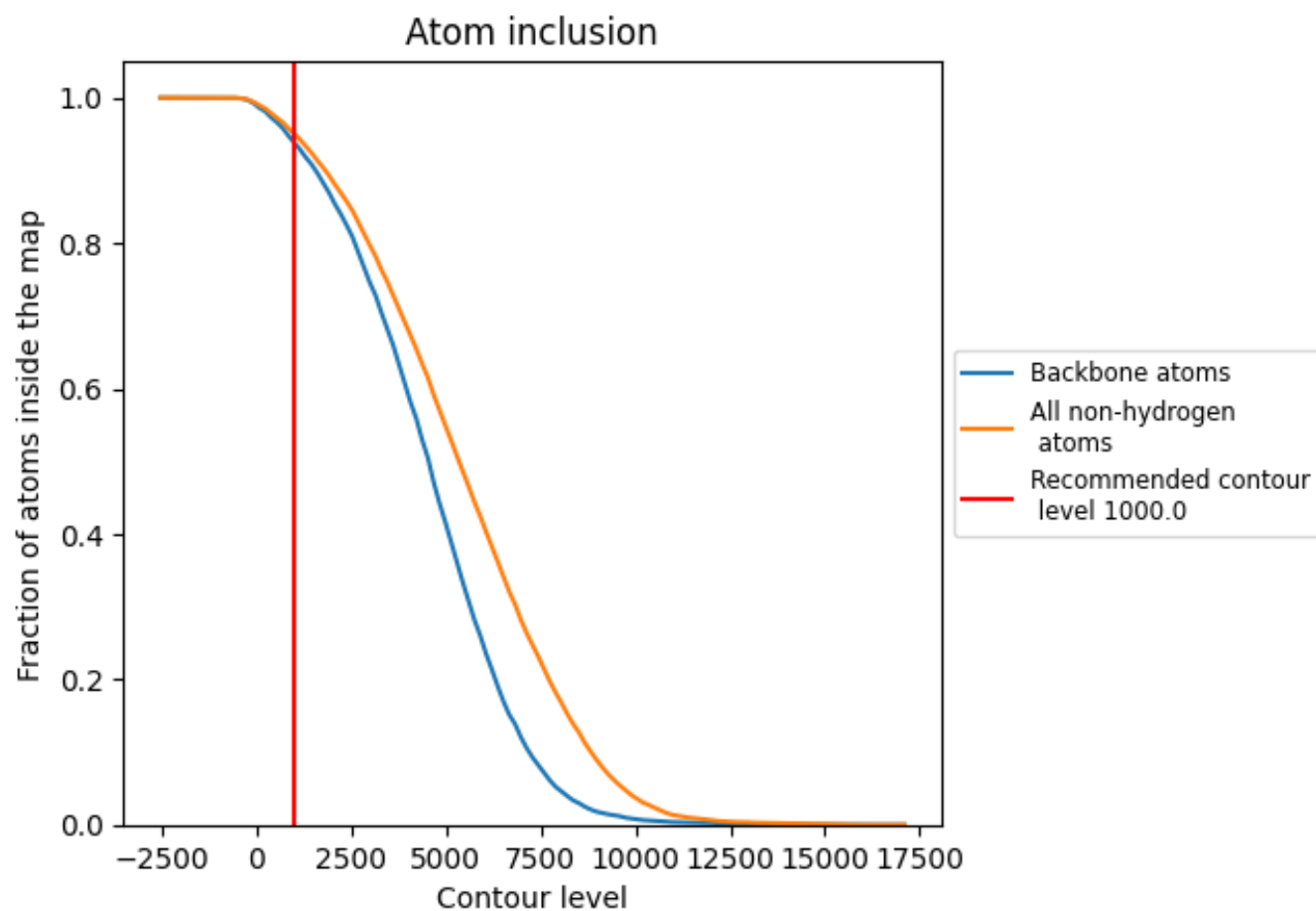
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1000.0).

## 9.4 Atom inclusion [i](#)















































At the recommended contour level, 94% of all backbone atoms, 95% 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 (1000.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9499	 0.0950
2	 0.9787	 0.1170
3	 1.0000	 0.0550
7	 0.9934	 0.1040
9	 0.9975	 0.1260
B	 0.8133	 0.0120
G	 1.0000	 0.1230
J	 0.9932	 0.1220
L	 0.9343	 0.0550
S	 0.9295	 0.0730
W	 0.9780	 0.1260
X	 0.7929	 0.0320
Y	 0.8683	 0.0770
a	 1.0000	 0.1180
c	 0.9917	 0.0990
d	 1.0000	 0.1270
f	 1.0000	 0.1510
g	 0.9970	 0.0850
h	 0.9519	 0.1060
k	 0.9716	 0.1040
w	 0.8409	 -0.0740
y	 0.9833	 0.0890

