Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 08:41 AM EST

PDB ID	:	1ZO3
EMDB ID	:	EMD-1249
Title	:	The P-site and P/E-site tRNA structures fitted to P/I site codon.
Authors	:	Allen, G.S.; Zavialov, A.; Gursky, R.; Ehrenberg, M.; Frank, J.
Deposited on	:	2005-05-12
Resolution	:	13.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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.

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

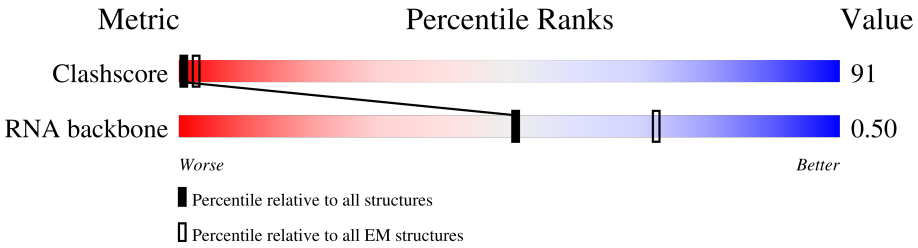
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 13.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	76	33% · 87% 12%
1	B	76	16% · 87% 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3250 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 tRNA.

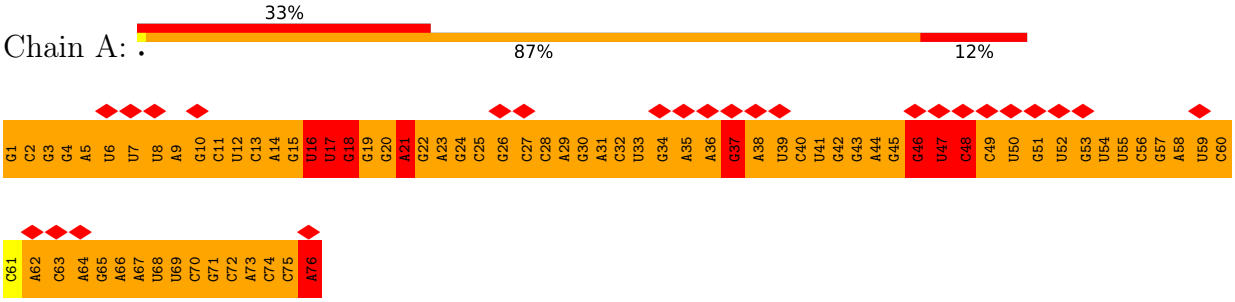
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	76	Total	C	N	O	P	0	0
			1625	725	293	531	76		
1	B	76	Total	C	N	O	P	0	0
			1625	725	293	531	76		

3 Residue-property plots (i)

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

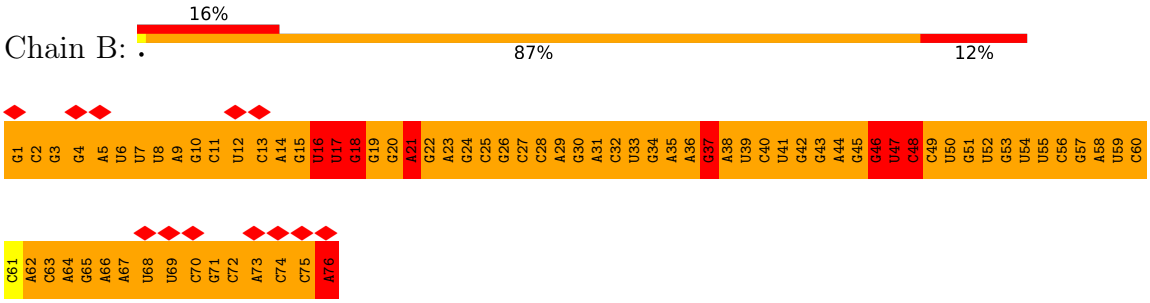
- Molecule 1: tRNA

Chain A:



- Molecule 1: tRNA

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	20283	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	DEFOCUS GROUPS 0.93-3.93 UM	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	-930.00	Depositor
Maximum defocus (nm)	-3930.00	Depositor
Magnification	39000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	142.331	Depositor
Minimum map value	-55.192	Depositor
Average map value	0.138	Depositor
Map value standard deviation	3.177	Depositor
Recommended contour level	7.4	Depositor
Map size (Å)	366.6, 366.6, 366.6	wwPDB
Map dimensions	130, 130, 130	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.82, 2.82, 2.82	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	5.59	278/1817 (15.3%)	6.10	698/2831 (24.7%)
1	B	6.39	280/1817 (15.4%)	6.28	698/2831 (24.7%)
All	All	6.01	558/3634 (15.4%)	6.19	1396/5662 (24.7%)

All (558) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	U	C1'-N1	148.98	3.72	1.48
1	B	39	U	C1'-N1	148.94	3.72	1.48
1	B	1	G	P-OP2	106.09	3.29	1.49
1	A	55	U	C1'-N1	91.85	2.86	1.48
1	B	55	U	C1'-N1	91.80	2.86	1.48
1	B	1	G	P-O5'	59.06	2.18	1.59
1	B	1	G	P-OP1	51.42	2.36	1.49
1	A	75	C	O3'-P	29.95	1.97	1.61
1	B	75	C	O3'-P	29.90	1.97	1.61
1	A	22	G	N3-C4	13.38	1.44	1.35
1	B	22	G	N3-C4	13.36	1.44	1.35
1	B	51	G	N3-C4	13.33	1.44	1.35
1	B	20	G	N3-C4	13.32	1.44	1.35
1	A	19	G	N3-C4	13.31	1.44	1.35
1	B	19	G	N3-C4	13.31	1.44	1.35
1	A	51	G	N3-C4	13.31	1.44	1.35
1	B	18	G	N3-C4	13.29	1.44	1.35
1	B	45	G	N3-C4	13.29	1.44	1.35
1	A	20	G	N3-C4	13.26	1.44	1.35
1	A	45	G	N3-C4	13.25	1.44	1.35
1	A	18	G	N3-C4	13.18	1.44	1.35
1	B	71	G	N3-C4	13.13	1.44	1.35
1	A	71	G	N3-C4	13.12	1.44	1.35
1	A	57	G	N3-C4	13.10	1.44	1.35
1	B	43	G	N3-C4	13.10	1.44	1.35
1	A	43	G	N3-C4	13.09	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	57	G	N3-C4	13.07	1.44	1.35
1	A	26	G	N3-C4	13.07	1.44	1.35
1	B	4	G	N3-C4	13.05	1.44	1.35
1	A	30	G	N3-C4	13.05	1.44	1.35
1	B	1	G	N3-C4	13.05	1.44	1.35
1	B	24	G	N3-C4	13.04	1.44	1.35
1	B	42	G	N3-C4	13.04	1.44	1.35
1	B	30	G	N3-C4	13.03	1.44	1.35
1	A	10	G	N3-C4	13.03	1.44	1.35
1	A	42	G	N3-C4	13.02	1.44	1.35
1	B	26	G	N3-C4	13.00	1.44	1.35
1	A	24	G	N3-C4	12.98	1.44	1.35
1	A	1	G	N3-C4	12.97	1.44	1.35
1	A	4	G	N3-C4	12.96	1.44	1.35
1	B	10	G	N3-C4	12.95	1.44	1.35
1	B	46	G	N3-C4	12.94	1.44	1.35
1	B	65	G	N3-C4	12.92	1.44	1.35
1	A	46	G	N3-C4	12.88	1.44	1.35
1	A	65	G	N3-C4	12.86	1.44	1.35
1	B	15	G	N3-C4	12.81	1.44	1.35
1	B	34	G	N3-C4	12.81	1.44	1.35
1	A	34	G	N3-C4	12.80	1.44	1.35
1	A	15	G	N3-C4	12.79	1.44	1.35
1	A	53	G	N3-C4	12.78	1.44	1.35
1	B	53	G	N3-C4	12.75	1.44	1.35
1	B	37	G	N3-C4	12.75	1.44	1.35
1	A	37	G	N3-C4	12.75	1.44	1.35
1	B	3	G	N3-C4	12.60	1.44	1.35
1	A	3	G	N3-C4	12.52	1.44	1.35
1	B	61	C	C2-N3	11.87	1.45	1.35
1	A	61	C	C2-N3	11.86	1.45	1.35
1	B	32	C	C2-N3	11.61	1.45	1.35
1	A	56	C	C2-N3	11.59	1.45	1.35
1	B	56	C	C2-N3	11.57	1.45	1.35
1	A	11	C	C2-N3	11.57	1.45	1.35
1	A	32	C	C2-N3	11.56	1.45	1.35
1	A	75	C	C2-N3	11.56	1.45	1.35
1	A	48	C	C2-N3	11.54	1.45	1.35
1	B	11	C	C2-N3	11.52	1.45	1.35
1	B	75	C	C2-N3	11.48	1.45	1.35
1	B	48	C	C2-N3	11.48	1.45	1.35
1	B	74	C	C2-N3	11.48	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	C	C2-N3	11.46	1.45	1.35
1	A	25	C	C2-N3	11.45	1.45	1.35
1	B	25	C	C2-N3	11.41	1.44	1.35
1	B	60	C	C2-N3	11.39	1.44	1.35
1	A	49	C	C2-N3	11.38	1.44	1.35
1	B	40	C	C2-N3	11.37	1.44	1.35
1	A	60	C	C2-N3	11.35	1.44	1.35
1	B	72	C	C2-N3	11.34	1.44	1.35
1	A	40	C	C2-N3	11.34	1.44	1.35
1	B	49	C	C2-N3	11.34	1.44	1.35
1	B	63	C	C2-N3	11.31	1.44	1.35
1	A	27	C	C2-N3	11.31	1.44	1.35
1	A	72	C	C2-N3	11.30	1.44	1.35
1	A	63	C	C2-N3	11.29	1.44	1.35
1	A	2	C	C2-N3	11.29	1.44	1.35
1	B	27	C	C2-N3	11.27	1.44	1.35
1	B	2	C	C2-N3	11.21	1.44	1.35
1	A	28	C	C2-N3	11.16	1.44	1.35
1	B	70	C	C2-N3	11.13	1.44	1.35
1	A	70	C	C2-N3	11.11	1.44	1.35
1	B	28	C	C2-N3	11.10	1.44	1.35
1	A	13	C	C2-N3	11.02	1.44	1.35
1	B	13	C	C2-N3	11.01	1.44	1.35
1	A	57	G	N9-C8	-10.62	1.30	1.37
1	B	57	G	N9-C8	-10.61	1.30	1.37
1	B	45	G	N9-C8	-10.45	1.30	1.37
1	A	45	G	N9-C8	-10.43	1.30	1.37
1	A	18	G	N9-C8	-10.35	1.30	1.37
1	B	18	G	N9-C8	-10.30	1.30	1.37
1	B	46	G	N9-C8	-10.29	1.30	1.37
1	B	15	G	N9-C8	-10.27	1.30	1.37
1	A	15	G	N9-C8	-10.27	1.30	1.37
1	A	30	G	N9-C8	-10.26	1.30	1.37
1	B	30	G	N9-C8	-10.25	1.30	1.37
1	B	4	G	N9-C8	-10.24	1.30	1.37
1	A	46	G	N9-C8	-10.22	1.30	1.37
1	A	4	G	N9-C8	-10.18	1.30	1.37
1	B	53	G	N9-C8	-10.15	1.30	1.37
1	A	53	G	N9-C8	-10.13	1.30	1.37
1	B	19	G	N9-C8	-10.12	1.30	1.37
1	A	1	G	N9-C8	-10.11	1.30	1.37
1	A	51	G	N9-C8	-10.10	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	G	N9-C8	-10.08	1.30	1.37
1	A	34	G	N9-C8	-10.07	1.30	1.37
1	B	51	G	N9-C8	-10.07	1.30	1.37
1	A	19	G	N9-C8	-10.07	1.30	1.37
1	B	22	G	N9-C8	-10.06	1.30	1.37
1	B	34	G	N9-C8	-10.06	1.30	1.37
1	B	65	G	N9-C8	-10.04	1.30	1.37
1	A	10	G	N9-C8	-10.03	1.30	1.37
1	A	22	G	N9-C8	-10.03	1.30	1.37
1	A	65	G	N9-C8	-10.03	1.30	1.37
1	A	3	G	N9-C8	-10.02	1.30	1.37
1	B	3	G	N9-C8	-10.02	1.30	1.37
1	B	1	G	N9-C8	-10.01	1.30	1.37
1	B	42	G	N9-C8	-9.99	1.30	1.37
1	A	20	G	N9-C8	-9.96	1.30	1.37
1	A	42	G	N9-C8	-9.95	1.30	1.37
1	B	37	G	N9-C8	-9.94	1.30	1.37
1	B	10	G	N9-C8	-9.94	1.30	1.37
1	B	20	G	N9-C8	-9.90	1.30	1.37
1	B	43	G	N9-C8	-9.88	1.30	1.37
1	B	24	G	N9-C8	-9.87	1.30	1.37
1	A	24	G	N9-C8	-9.81	1.30	1.37
1	A	43	G	N9-C8	-9.76	1.31	1.37
1	A	71	G	N9-C8	-9.71	1.31	1.37
1	A	26	G	N9-C8	-9.63	1.31	1.37
1	B	71	G	N9-C8	-9.61	1.31	1.37
1	B	26	G	N9-C8	-9.57	1.31	1.37
1	A	32	C	N3-C4	-9.57	1.27	1.33
1	B	32	C	N3-C4	-9.56	1.27	1.33
1	A	70	C	N3-C4	-9.45	1.27	1.33
1	B	70	C	N3-C4	-9.45	1.27	1.33
1	A	28	C	N3-C4	-9.43	1.27	1.33
1	B	28	C	N3-C4	-9.40	1.27	1.33
1	A	25	C	N3-C4	-9.37	1.27	1.33
1	B	25	C	N3-C4	-9.32	1.27	1.33
1	A	61	C	N3-C4	-9.31	1.27	1.33
1	B	11	C	N3-C4	-9.30	1.27	1.33
1	B	61	C	N3-C4	-9.27	1.27	1.33
1	A	11	C	N3-C4	-9.25	1.27	1.33
1	B	13	C	N3-C4	-9.17	1.27	1.33
1	A	13	C	N3-C4	-9.14	1.27	1.33
1	B	60	C	N3-C4	-9.14	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	49	C	N3-C4	-9.13	1.27	1.33
1	A	49	C	N3-C4	-9.11	1.27	1.33
1	A	60	C	N3-C4	-9.10	1.27	1.33
1	A	56	C	N3-C4	-9.08	1.27	1.33
1	B	72	C	N3-C4	-9.05	1.27	1.33
1	B	56	C	N3-C4	-9.03	1.27	1.33
1	A	72	C	N3-C4	-8.99	1.27	1.33
1	B	27	C	N3-C4	-8.93	1.27	1.33
1	A	48	C	N3-C4	-8.92	1.27	1.33
1	A	2	C	N3-C4	-8.91	1.27	1.33
1	B	74	C	N3-C4	-8.89	1.27	1.33
1	B	40	C	N3-C4	-8.88	1.27	1.33
1	A	40	C	N3-C4	-8.84	1.27	1.33
1	A	27	C	N3-C4	-8.83	1.27	1.33
1	A	74	C	N3-C4	-8.83	1.27	1.33
1	A	75	C	N3-C4	-8.79	1.27	1.33
1	B	48	C	N3-C4	-8.77	1.27	1.33
1	B	2	C	N3-C4	-8.75	1.27	1.33
1	B	63	C	N3-C4	-8.74	1.27	1.33
1	A	63	C	N3-C4	-8.72	1.27	1.33
1	B	73	A	N7-C5	-8.70	1.34	1.39
1	A	73	A	N7-C5	-8.68	1.34	1.39
1	B	75	C	N3-C4	-8.67	1.27	1.33
1	A	14	A	N9-C8	-8.59	1.30	1.37
1	B	14	A	N9-C8	-8.58	1.30	1.37
1	A	71	G	N7-C5	8.56	1.44	1.39
1	B	71	G	N7-C5	8.56	1.44	1.39
1	A	29	A	N9-C8	-8.55	1.30	1.37
1	A	71	G	N9-C4	-8.54	1.31	1.38
1	B	58	A	N9-C8	-8.54	1.30	1.37
1	A	43	G	N9-C4	-8.52	1.31	1.38
1	B	19	G	N9-C4	-8.52	1.31	1.38
1	A	19	G	N9-C4	-8.52	1.31	1.38
1	B	44	A	N9-C8	-8.49	1.30	1.37
1	B	71	G	N9-C4	-8.49	1.31	1.38
1	B	24	G	N9-C4	-8.48	1.31	1.38
1	A	24	G	N9-C4	-8.46	1.31	1.38
1	A	26	G	N9-C4	-8.47	1.31	1.38
1	A	43	G	N7-C5	8.46	1.44	1.39
1	B	29	A	N9-C8	-8.46	1.30	1.37
1	A	58	A	N9-C8	-8.46	1.30	1.37
1	B	42	G	N9-C4	-8.45	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	A	N7-C5	-8.45	1.34	1.39
1	B	43	G	N9-C4	-8.45	1.31	1.38
1	B	18	G	N9-C4	-8.45	1.31	1.38
1	B	31	A	N7-C5	-8.44	1.34	1.39
1	A	44	A	N9-C8	-8.44	1.30	1.37
1	A	45	G	N7-C5	8.44	1.44	1.39
1	A	42	G	N9-C4	-8.42	1.31	1.38
1	A	10	G	N9-C4	-8.41	1.31	1.38
1	B	29	A	N7-C5	-8.41	1.34	1.39
1	A	18	G	N9-C4	-8.41	1.31	1.38
1	B	9	A	N9-C8	-8.41	1.31	1.37
1	A	31	A	N7-C5	-8.40	1.34	1.39
1	A	64	A	N7-C5	-8.40	1.34	1.39
1	A	29	A	N7-C5	-8.40	1.34	1.39
1	A	57	G	N9-C4	-8.40	1.31	1.38
1	B	10	G	N9-C4	-8.39	1.31	1.38
1	A	51	G	N7-C5	8.39	1.44	1.39
1	B	9	A	N7-C5	-8.38	1.34	1.39
1	A	9	A	N7-C5	-8.38	1.34	1.39
1	B	26	G	N9-C4	-8.38	1.31	1.38
1	B	51	G	N7-C5	8.37	1.44	1.39
1	B	14	A	N7-C5	-8.37	1.34	1.39
1	B	43	G	N7-C5	8.37	1.44	1.39
1	B	1	G	N7-C5	8.36	1.44	1.39
1	A	4	G	N9-C4	-8.35	1.31	1.38
1	B	45	G	N7-C5	8.35	1.44	1.39
1	B	57	G	N9-C4	-8.35	1.31	1.38
1	A	22	G	N9-C4	-8.35	1.31	1.38
1	A	65	G	N9-C4	-8.35	1.31	1.38
1	B	4	G	N9-C4	-8.35	1.31	1.38
1	B	57	G	N7-C5	8.34	1.44	1.39
1	B	31	A	N9-C8	-8.33	1.31	1.37
1	A	73	A	N9-C8	-8.33	1.31	1.37
1	B	65	G	N7-C5	8.32	1.44	1.39
1	A	24	G	N7-C5	8.32	1.44	1.39
1	B	22	G	N9-C4	-8.31	1.31	1.38
1	B	64	A	N7-C5	-8.30	1.34	1.39
1	A	9	A	N9-C8	-8.30	1.31	1.37
1	A	66	A	N9-C8	-8.30	1.31	1.37
1	A	10	G	N7-C5	8.29	1.44	1.39
1	B	73	A	N9-C8	-8.29	1.31	1.37
1	A	57	G	N7-C5	8.29	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	G	N7-C5	8.29	1.44	1.39
1	B	46	G	N9-C4	-8.29	1.31	1.38
1	B	35	A	N7-C5	-8.28	1.34	1.39
1	B	10	G	N7-C5	8.28	1.44	1.39
1	B	15	G	N7-C5	8.28	1.44	1.39
1	A	46	G	N9-C4	-8.27	1.31	1.38
1	B	37	G	N7-C5	8.27	1.44	1.39
1	A	1	G	N7-C5	8.27	1.44	1.39
1	B	19	G	N7-C5	8.27	1.44	1.39
1	A	34	G	N9-C4	-8.25	1.31	1.38
1	B	65	G	N9-C4	-8.25	1.31	1.38
1	A	19	G	N7-C5	8.25	1.44	1.39
1	B	20	G	N9-C4	-8.25	1.31	1.38
1	A	31	A	N9-C8	-8.24	1.31	1.37
1	B	24	G	N7-C5	8.24	1.44	1.39
1	B	66	A	N9-C8	-8.24	1.31	1.37
1	B	15	G	N9-C4	-8.24	1.31	1.38
1	A	20	G	N9-C4	-8.23	1.31	1.38
1	B	42	G	N7-C5	8.23	1.44	1.39
1	A	37	G	N7-C5	8.22	1.44	1.39
1	A	51	G	N9-C4	-8.22	1.31	1.38
1	A	42	G	N7-C5	8.21	1.44	1.39
1	B	51	G	N9-C4	-8.20	1.31	1.38
1	B	34	G	N9-C4	-8.19	1.31	1.38
1	A	22	G	N7-C5	8.19	1.44	1.39
1	A	35	A	N7-C5	-8.19	1.34	1.39
1	B	53	G	N9-C4	-8.19	1.31	1.38
1	A	15	G	N9-C4	-8.19	1.31	1.38
1	A	58	A	N7-C5	-8.18	1.34	1.39
1	A	53	G	N9-C4	-8.18	1.31	1.38
1	B	58	A	N7-C5	-8.18	1.34	1.39
1	A	20	G	N7-C5	8.16	1.44	1.39
1	B	1	G	N9-C4	-8.16	1.31	1.38
1	B	76	A	N9-C8	-8.16	1.31	1.37
1	B	21	A	N9-C8	-8.15	1.31	1.37
1	A	26	G	N7-C5	8.14	1.44	1.39
1	A	15	G	N7-C5	8.14	1.44	1.39
1	A	21	A	N9-C8	-8.14	1.31	1.37
1	B	20	G	N7-C5	8.14	1.44	1.39
1	A	38	A	N7-C5	-8.13	1.34	1.39
1	A	64	A	N9-C8	-8.13	1.31	1.37
1	A	76	A	N7-C5	-8.13	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	A	N9-C8	-8.13	1.31	1.37
1	B	76	A	N7-C5	-8.12	1.34	1.39
1	A	1	G	N9-C4	-8.12	1.31	1.38
1	B	26	G	N7-C5	8.11	1.44	1.39
1	B	23	A	N7-C5	-8.11	1.34	1.39
1	A	67	A	N7-C5	-8.10	1.34	1.39
1	B	22	G	N7-C5	8.10	1.44	1.39
1	A	36	A	N9-C8	-8.10	1.31	1.37
1	A	36	A	N7-C5	-8.09	1.34	1.39
1	A	3	G	N7-C5	8.09	1.44	1.39
1	B	36	A	N9-C8	-8.09	1.31	1.37
1	A	45	G	N9-C4	-8.08	1.31	1.38
1	B	67	A	N7-C5	-8.08	1.34	1.39
1	A	30	G	N9-C4	-8.07	1.31	1.38
1	A	37	G	N9-C4	-8.07	1.31	1.38
1	A	3	G	N9-C4	-8.06	1.31	1.38
1	B	62	A	N9-C8	-8.06	1.31	1.37
1	A	35	A	N9-C8	-8.06	1.31	1.37
1	B	38	A	N9-C8	-8.06	1.31	1.37
1	B	18	G	N7-C5	8.05	1.44	1.39
1	B	37	G	N9-C4	-8.05	1.31	1.38
1	B	45	G	N9-C4	-8.05	1.31	1.38
1	B	64	A	N9-C8	-8.05	1.31	1.37
1	B	3	G	N7-C5	8.05	1.44	1.39
1	B	3	G	N9-C4	-8.04	1.31	1.38
1	A	23	A	N9-C8	-8.04	1.31	1.37
1	B	5	A	N7-C5	-8.04	1.34	1.39
1	A	23	A	N7-C5	-8.04	1.34	1.39
1	B	36	A	N7-C5	-8.03	1.34	1.39
1	B	38	A	N7-C5	-8.03	1.34	1.39
1	A	46	G	N7-C5	8.02	1.44	1.39
1	A	62	A	N9-C8	-8.02	1.31	1.37
1	B	23	A	N9-C8	-8.02	1.31	1.37
1	B	30	G	N9-C4	-8.01	1.31	1.38
1	A	38	A	N9-C8	-8.00	1.31	1.37
1	A	18	G	N7-C5	8.00	1.44	1.39
1	B	21	A	N7-C5	-7.98	1.34	1.39
1	B	35	A	N9-C8	-7.98	1.31	1.37
1	A	62	A	N7-C5	-7.98	1.34	1.39
1	B	34	G	N7-C5	7.98	1.44	1.39
1	B	62	A	N7-C5	-7.97	1.34	1.39
1	A	21	A	N7-C5	-7.96	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	A	N7-C5	-7.94	1.34	1.39
1	B	5	A	N9-C8	-7.92	1.31	1.37
1	B	46	G	N7-C5	7.91	1.44	1.39
1	A	34	G	N7-C5	7.90	1.44	1.39
1	B	67	A	N9-C8	-7.85	1.31	1.37
1	A	5	A	N9-C8	-7.84	1.31	1.37
1	B	4	G	N7-C5	7.83	1.44	1.39
1	A	4	G	N7-C5	7.80	1.44	1.39
1	A	67	A	N9-C8	-7.78	1.31	1.37
1	B	53	G	N7-C5	7.77	1.44	1.39
1	B	44	A	N7-C5	-7.75	1.34	1.39
1	A	53	G	N7-C5	7.72	1.43	1.39
1	B	30	G	N7-C5	7.70	1.43	1.39
1	A	44	A	N7-C5	-7.69	1.34	1.39
1	A	30	G	N7-C5	7.65	1.43	1.39
1	A	66	A	N7-C5	-7.57	1.34	1.39
1	B	66	A	N7-C5	-7.52	1.34	1.39
1	A	22	G	C8-N7	-7.50	1.26	1.30
1	B	71	G	C8-N7	-7.44	1.26	1.30
1	B	22	G	C8-N7	-7.41	1.26	1.30
1	A	71	G	C8-N7	-7.36	1.26	1.30
1	A	1	G	C8-N7	-7.30	1.26	1.30
1	B	37	G	C8-N7	-7.26	1.26	1.30
1	B	43	G	C8-N7	-7.26	1.26	1.30
1	A	4	G	C8-N7	-7.26	1.26	1.30
1	A	26	G	C8-N7	-7.25	1.26	1.30
1	B	24	G	C8-N7	-7.24	1.26	1.30
1	A	24	G	C8-N7	-7.24	1.26	1.30
1	B	42	G	C8-N7	-7.24	1.26	1.30
1	A	43	G	C8-N7	-7.22	1.26	1.30
1	B	4	G	C8-N7	-7.22	1.26	1.30
1	B	1	G	C8-N7	-7.20	1.26	1.30
1	A	37	G	C8-N7	-7.20	1.26	1.30
1	B	45	G	C5-C4	-7.18	1.33	1.38
1	A	42	G	C8-N7	-7.17	1.26	1.30
1	B	26	G	C8-N7	-7.17	1.26	1.30
1	A	3	G	C8-N7	-7.15	1.26	1.30
1	A	65	G	C8-N7	-7.15	1.26	1.30
1	B	65	G	C5-C4	-7.14	1.33	1.38
1	B	3	G	C8-N7	-7.14	1.26	1.30
1	B	18	G	C8-N7	-7.14	1.26	1.30
1	A	18	G	C8-N7	-7.13	1.26	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	G	C5-C4	-7.13	1.33	1.38
1	B	37	G	C5-C4	-7.12	1.33	1.38
1	A	30	G	C8-N7	-7.11	1.26	1.30
1	A	15	G	C8-N7	-7.11	1.26	1.30
1	B	65	G	C8-N7	-7.11	1.26	1.30
1	B	30	G	C8-N7	-7.09	1.26	1.30
1	B	22	G	C5-C4	-7.09	1.33	1.38
1	B	18	G	C5-C4	-7.08	1.33	1.38
1	B	20	G	C8-N7	-7.07	1.26	1.30
1	B	20	G	C5-C4	-7.07	1.33	1.38
1	A	37	G	C5-C4	-7.07	1.33	1.38
1	A	18	G	C5-C4	-7.06	1.33	1.38
1	B	15	G	C8-N7	-7.06	1.26	1.30
1	A	65	G	C5-C4	-7.04	1.33	1.38
1	B	19	G	C5-C4	-7.04	1.33	1.38
1	A	20	G	C5-C4	-7.02	1.33	1.38
1	A	20	G	C8-N7	-7.01	1.26	1.30
1	B	46	G	C8-N7	-7.01	1.26	1.30
1	B	34	G	C8-N7	-7.00	1.26	1.30
1	A	22	G	C5-C4	-7.00	1.33	1.38
1	B	51	G	C5-C4	-6.98	1.33	1.38
1	A	46	G	C8-N7	-6.96	1.26	1.30
1	A	51	G	C5-C4	-6.95	1.33	1.38
1	A	45	G	C8-N7	-6.94	1.26	1.30
1	B	32	C	C4-C5	6.93	1.48	1.43
1	A	34	G	C8-N7	-6.92	1.26	1.30
1	B	45	G	C8-N7	-6.92	1.26	1.30
1	B	10	G	C8-N7	-6.91	1.26	1.30
1	A	10	G	C8-N7	-6.89	1.26	1.30
1	A	19	G	C5-C4	-6.89	1.33	1.38
1	B	43	G	C5-C4	-6.89	1.33	1.38
1	A	43	G	C5-C4	-6.88	1.33	1.38
1	A	32	C	C4-C5	6.87	1.48	1.43
1	A	51	G	C8-N7	-6.84	1.26	1.30
1	A	25	C	C4-C5	6.84	1.48	1.43
1	B	42	G	C5-C4	-6.84	1.33	1.38
1	A	30	G	C5-C4	-6.84	1.33	1.38
1	B	51	G	C8-N7	-6.83	1.26	1.30
1	B	3	G	C5-C4	-6.82	1.33	1.38
1	B	25	C	C4-C5	6.81	1.48	1.43
1	A	19	G	C8-N7	-6.80	1.26	1.30
1	A	11	C	C4-C5	6.79	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	30	G	C5-C4	-6.78	1.33	1.38
1	B	1	G	C5-C4	-6.76	1.33	1.38
1	B	11	C	C4-C5	6.76	1.48	1.43
1	A	3	G	C5-C4	-6.76	1.33	1.38
1	B	53	G	C5-C4	-6.75	1.33	1.38
1	A	1	G	C5-C4	-6.75	1.33	1.38
1	B	15	G	C5-C4	-6.74	1.33	1.38
1	A	42	G	C5-C4	-6.72	1.33	1.38
1	B	19	G	C8-N7	-6.72	1.26	1.30
1	A	15	G	C5-C4	-6.72	1.33	1.38
1	B	57	G	C8-N7	-6.70	1.26	1.30
1	A	10	G	C5-C4	-6.69	1.33	1.38
1	B	70	C	C4-C5	6.69	1.48	1.43
1	B	53	G	C8-N7	-6.69	1.26	1.30
1	B	71	G	C5-C4	-6.69	1.33	1.38
1	A	53	G	C8-N7	-6.68	1.26	1.30
1	A	71	G	C5-C4	-6.68	1.33	1.38
1	B	4	G	C5-C4	-6.68	1.33	1.38
1	A	57	G	C8-N7	-6.66	1.26	1.30
1	A	53	G	C5-C4	-6.64	1.33	1.38
1	A	26	G	C5-C4	-6.63	1.33	1.38
1	A	4	G	C5-C4	-6.62	1.33	1.38
1	B	10	G	C5-C4	-6.62	1.33	1.38
1	A	70	C	C4-C5	6.61	1.48	1.43
1	B	74	C	C4-C5	6.60	1.48	1.43
1	A	61	C	C4-C5	6.58	1.48	1.43
1	B	26	G	C5-C4	-6.58	1.33	1.38
1	A	2	C	C4-C5	6.56	1.48	1.43
1	B	2	C	C4-C5	6.56	1.48	1.43
1	B	13	C	C4-C5	6.53	1.48	1.43
1	B	61	C	C4-C5	6.52	1.48	1.43
1	A	74	C	C4-C5	6.51	1.48	1.43
1	B	24	G	C5-C4	-6.51	1.33	1.38
1	A	13	C	C4-C5	6.51	1.48	1.43
1	A	75	C	C4-C5	6.50	1.48	1.43
1	B	57	G	C5-C4	-6.49	1.33	1.38
1	B	75	C	C4-C5	6.45	1.48	1.43
1	A	24	G	C5-C4	-6.44	1.33	1.38
1	B	49	C	C4-C5	6.42	1.48	1.43
1	B	72	C	C4-C5	6.40	1.48	1.43
1	B	28	C	C4-C5	6.40	1.48	1.43
1	B	62	A	C8-N7	-6.39	1.27	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	G	C5-C4	-6.38	1.33	1.38
1	B	60	C	C4-C5	6.38	1.48	1.43
1	B	34	G	C5-C4	-6.37	1.33	1.38
1	A	34	G	C5-C4	-6.36	1.33	1.38
1	A	28	C	C4-C5	6.36	1.48	1.43
1	A	36	A	C8-N7	-6.36	1.27	1.31
1	A	62	A	C8-N7	-6.35	1.27	1.31
1	A	72	C	C4-C5	6.35	1.48	1.43
1	B	36	A	C8-N7	-6.32	1.27	1.31
1	A	49	C	C4-C5	6.32	1.48	1.43
1	A	60	C	C4-C5	6.30	1.48	1.43
1	A	48	C	C4-C5	6.29	1.48	1.43
1	B	48	C	C4-C5	6.29	1.48	1.43
1	B	46	G	C5-C4	-6.25	1.33	1.38
1	A	56	C	C4-C5	6.24	1.48	1.43
1	A	58	A	C8-N7	-6.22	1.27	1.31
1	B	56	C	C4-C5	6.22	1.48	1.43
1	B	35	A	C8-N7	-6.21	1.27	1.31
1	A	35	A	C8-N7	-6.19	1.27	1.31
1	A	76	A	C8-N7	-6.18	1.27	1.31
1	B	58	A	C8-N7	-6.17	1.27	1.31
1	A	9	A	C8-N7	-6.16	1.27	1.31
1	B	40	C	C4-C5	6.15	1.47	1.43
1	B	63	C	C4-C5	6.14	1.47	1.43
1	A	46	G	C5-C4	-6.14	1.34	1.38
1	A	71	G	C2-N3	-6.14	1.27	1.32
1	B	18	G	C2-N3	-6.14	1.27	1.32
1	B	76	A	C8-N7	-6.13	1.27	1.31
1	A	40	C	C4-C5	6.13	1.47	1.43
1	B	71	G	C2-N3	-6.13	1.27	1.32
1	B	19	G	C2-N3	-6.12	1.27	1.32
1	A	19	G	C2-N3	-6.12	1.27	1.32
1	A	31	A	C8-N7	-6.12	1.27	1.31
1	B	65	G	C2-N3	-6.11	1.27	1.32
1	A	18	G	C2-N3	-6.10	1.27	1.32
1	A	63	C	C4-C5	6.09	1.47	1.43
1	A	29	A	C8-N7	-6.08	1.27	1.31
1	A	10	G	C2-N3	-6.07	1.27	1.32
1	B	9	A	C8-N7	-6.07	1.27	1.31
1	B	29	A	C8-N7	-6.06	1.27	1.31
1	B	10	G	C2-N3	-6.05	1.27	1.32
1	A	15	G	C2-N3	-6.04	1.27	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	G	C2-N3	-6.04	1.27	1.32
1	B	31	A	C8-N7	-6.04	1.27	1.31
1	A	57	G	C2-N3	-6.04	1.27	1.32
1	A	24	G	C2-N3	-6.03	1.27	1.32
1	B	46	G	C2-N3	-6.02	1.27	1.32
1	B	73	A	C8-N7	-6.02	1.27	1.31
1	A	44	A	C8-N7	-6.02	1.27	1.31
1	A	5	A	C8-N7	-6.01	1.27	1.31
1	B	67	A	C8-N7	-6.00	1.27	1.31
1	A	64	A	C8-N7	-5.99	1.27	1.31
1	B	24	G	C2-N3	-5.99	1.27	1.32
1	A	67	A	C8-N7	-5.98	1.27	1.31
1	A	73	A	C8-N7	-5.98	1.27	1.31
1	B	53	G	C2-N3	-5.97	1.27	1.32
1	B	15	G	C2-N3	-5.96	1.27	1.32
1	B	5	A	C8-N7	-5.95	1.27	1.31
1	B	57	G	C2-N3	-5.94	1.27	1.32
1	A	46	G	C2-N3	-5.94	1.27	1.32
1	B	44	A	C8-N7	-5.94	1.27	1.31
1	A	23	A	C8-N7	-5.93	1.27	1.31
1	A	21	A	C8-N7	-5.92	1.27	1.31
1	B	64	A	C8-N7	-5.92	1.27	1.31
1	A	37	G	C2-N3	-5.90	1.28	1.32
1	B	21	A	C8-N7	-5.90	1.27	1.31
1	B	37	G	C2-N3	-5.90	1.28	1.32
1	A	53	G	C2-N3	-5.89	1.28	1.32
1	B	38	A	C8-N7	-5.89	1.27	1.31
1	A	30	G	C2-N3	-5.89	1.28	1.32
1	B	45	G	C2-N3	-5.88	1.28	1.32
1	A	45	G	C2-N3	-5.87	1.28	1.32
1	A	66	A	C8-N7	-5.84	1.27	1.31
1	B	27	C	C4-C5	5.84	1.47	1.43
1	A	38	A	C8-N7	-5.84	1.27	1.31
1	A	27	C	C4-C5	5.83	1.47	1.43
1	B	26	G	C2-N3	-5.83	1.28	1.32
1	A	26	G	C2-N3	-5.82	1.28	1.32
1	B	66	A	C8-N7	-5.81	1.27	1.31
1	A	14	A	C8-N7	-5.80	1.27	1.31
1	B	23	A	C8-N7	-5.80	1.27	1.31
1	B	30	G	C2-N3	-5.79	1.28	1.32
1	A	1	G	C2-N3	-5.78	1.28	1.32
1	B	14	A	C8-N7	-5.77	1.27	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4	G	C2-N3	-5.77	1.28	1.32
1	A	4	G	C2-N3	-5.74	1.28	1.32
1	B	1	G	C2-N3	-5.73	1.28	1.32
1	A	3	G	C2-N3	-5.73	1.28	1.32
1	B	43	G	C2-N3	-5.72	1.28	1.32
1	B	51	G	C2-N3	-5.72	1.28	1.32
1	B	3	G	C2-N3	-5.71	1.28	1.32
1	B	20	G	C2-N3	-5.71	1.28	1.32
1	A	20	G	C2-N3	-5.71	1.28	1.32
1	B	22	G	C2-N3	-5.68	1.28	1.32
1	A	51	G	C2-N3	-5.64	1.28	1.32
1	A	43	G	C2-N3	-5.64	1.28	1.32
1	A	22	G	C2-N3	-5.61	1.28	1.32
1	B	34	G	C2-N3	-5.51	1.28	1.32
1	A	34	G	C2-N3	-5.50	1.28	1.32
1	B	42	G	C2-N3	-5.49	1.28	1.32
1	A	42	G	C2-N3	-5.48	1.28	1.32
1	B	27	C	N1-C2	-5.18	1.34	1.40
1	A	51	G	C6-N1	-5.14	1.35	1.39
1	A	27	C	N1-C2	-5.13	1.35	1.40
1	B	51	G	C6-N1	-5.12	1.35	1.39
1	B	61	C	N1-C2	-5.12	1.35	1.40
1	A	61	C	N1-C2	-5.12	1.35	1.40
1	A	57	G	C6-N1	-5.05	1.36	1.39
1	A	11	C	N1-C2	-5.03	1.35	1.40
1	B	74	C	N1-C2	-5.02	1.35	1.40
1	A	18	G	C5-C6	5.02	1.47	1.42
1	B	11	C	N1-C2	-5.01	1.35	1.40

All (1396) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	U	C6-N1-C1'	-83.89	3.75	121.20
1	B	55	U	C6-N1-C1'	-83.89	3.75	121.20
1	B	39	U	C6-N1-C1'	-73.68	18.05	121.20
1	A	39	U	C6-N1-C1'	-73.67	18.06	121.20
1	A	55	U	C5-C6-N1	-50.83	97.29	122.70
1	B	55	U	C5-C6-N1	-50.77	97.32	122.70
1	B	1	G	O5'-P-OP2	-50.64	49.93	110.70
1	B	1	G	OP1-P-OP2	-47.98	47.63	119.60
1	B	1	G	O5'-P-OP1	-36.28	67.17	110.70
1	B	55	U	C6-N1-C2	29.00	138.40	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	U	C6-N1-C2	28.97	138.38	121.00
1	A	10	G	C4-C5-N7	-24.60	100.96	110.80
1	B	10	G	C4-C5-N7	-24.57	100.97	110.80
1	A	22	G	C4-C5-N7	-24.35	101.06	110.80
1	A	20	G	C4-C5-N7	-24.34	101.07	110.80
1	A	45	G	C4-C5-N7	-24.33	101.07	110.80
1	A	46	G	C4-C5-N7	-24.28	101.09	110.80
1	A	18	G	C4-C5-N7	-24.28	101.09	110.80
1	B	18	G	C4-C5-N7	-24.28	101.09	110.80
1	B	20	G	C4-C5-N7	-24.27	101.09	110.80
1	A	19	G	C4-C5-N7	-24.23	101.11	110.80
1	B	22	G	C4-C5-N7	-24.23	101.11	110.80
1	B	46	G	C4-C5-N7	-24.23	101.11	110.80
1	B	45	G	C4-C5-N7	-24.22	101.11	110.80
1	A	24	G	C4-C5-N7	-24.22	101.11	110.80
1	B	24	G	C4-C5-N7	-24.21	101.11	110.80
1	A	42	G	C4-C5-N7	-24.18	101.13	110.80
1	B	42	G	C4-C5-N7	-24.18	101.13	110.80
1	B	19	G	C4-C5-N7	-24.16	101.13	110.80
1	B	57	G	C4-C5-N7	-24.15	101.14	110.80
1	A	51	G	C4-C5-N7	-24.14	101.14	110.80
1	B	51	G	C4-C5-N7	-24.12	101.15	110.80
1	B	71	G	C4-C5-N7	-24.12	101.15	110.80
1	B	37	G	C4-C5-N7	-24.12	101.15	110.80
1	A	37	G	C4-C5-N7	-24.12	101.15	110.80
1	A	57	G	C4-C5-N7	-24.11	101.16	110.80
1	B	15	G	C4-C5-N7	-24.11	101.16	110.80
1	B	43	G	C4-C5-N7	-24.10	101.16	110.80
1	A	43	G	C4-C5-N7	-24.10	101.16	110.80
1	A	71	G	C4-C5-N7	-24.08	101.17	110.80
1	A	15	G	C4-C5-N7	-24.03	101.19	110.80
1	A	26	G	C4-C5-N7	-24.01	101.19	110.80
1	B	26	G	C4-C5-N7	-23.94	101.22	110.80
1	B	1	G	C4-C5-N7	-23.92	101.23	110.80
1	A	3	G	C4-C5-N7	-23.91	101.24	110.80
1	A	1	G	C4-C5-N7	-23.89	101.24	110.80
1	B	3	G	C4-C5-N7	-23.89	101.25	110.80
1	A	34	G	C4-C5-N7	-23.86	101.25	110.80
1	B	34	G	C4-C5-N7	-23.86	101.26	110.80
1	A	65	G	C4-C5-N7	-23.81	101.27	110.80
1	B	4	G	C4-C5-N7	-23.80	101.28	110.80
1	A	4	G	C4-C5-N7	-23.78	101.29	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	53	G	C4-C5-N7	-23.77	101.29	110.80
1	B	65	G	C4-C5-N7	-23.73	101.31	110.80
1	B	53	G	C4-C5-N7	-23.69	101.32	110.80
1	A	30	G	C4-C5-N7	-23.49	101.40	110.80
1	B	30	G	C4-C5-N7	-23.46	101.42	110.80
1	A	55	U	C4-C5-C6	23.23	133.63	119.70
1	B	55	U	C4-C5-C6	23.19	133.62	119.70
1	B	39	U	O4'-C1'-N1	-21.03	91.37	108.20
1	A	39	U	O4'-C1'-N1	-21.02	91.39	108.20
1	B	55	U	C2-N3-C4	-20.12	114.93	127.00
1	A	55	U	C2-N3-C4	-20.07	114.96	127.00
1	A	46	G	N3-C4-C5	-19.59	118.81	128.60
1	B	46	G	N3-C4-C5	-19.54	118.83	128.60
1	A	34	G	N3-C4-C5	-19.45	118.88	128.60
1	B	34	G	N3-C4-C5	-19.45	118.88	128.60
1	B	43	G	N3-C4-C5	-19.38	118.91	128.60
1	A	43	G	N3-C4-C5	-19.36	118.92	128.60
1	A	10	G	N3-C4-C5	-19.26	118.97	128.60
1	B	10	G	N3-C4-C5	-19.21	119.00	128.60
1	A	24	G	N3-C4-C5	-19.16	119.02	128.60
1	B	24	G	N3-C4-C5	-19.12	119.04	128.60
1	B	51	G	N3-C4-C5	-19.11	119.04	128.60
1	B	42	G	N3-C4-C5	-19.09	119.05	128.60
1	A	26	G	N3-C4-C5	-19.09	119.06	128.60
1	A	51	G	N3-C4-C5	-19.09	119.06	128.60
1	A	30	G	N3-C4-C5	-19.06	119.07	128.60
1	A	18	G	N3-C4-C5	-19.05	119.07	128.60
1	A	65	G	N3-C4-C5	-19.05	119.08	128.60
1	B	1	G	N3-C4-C5	-19.04	119.08	128.60
1	B	18	G	N3-C4-C5	-19.04	119.08	128.60
1	B	30	G	N3-C4-C5	-19.03	119.08	128.60
1	A	42	G	N3-C4-C5	-19.02	119.09	128.60
1	A	57	G	N3-C4-C5	-19.00	119.10	128.60
1	B	65	G	N3-C4-C5	-18.99	119.11	128.60
1	A	22	G	N3-C4-C5	-18.98	119.11	128.60
1	A	1	G	N3-C4-C5	-18.98	119.11	128.60
1	B	26	G	N3-C4-C5	-18.96	119.12	128.60
1	B	57	G	N3-C4-C5	-18.95	119.13	128.60
1	B	71	G	N3-C4-C5	-18.93	119.14	128.60
1	B	22	G	N3-C4-C5	-18.92	119.14	128.60
1	A	71	G	N3-C4-C5	-18.90	119.15	128.60
1	A	20	G	N3-C4-C5	-18.75	119.22	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	20	G	N3-C4-C5	-18.74	119.23	128.60
1	B	4	G	N3-C4-C5	-18.70	119.25	128.60
1	A	45	G	N3-C4-C5	-18.68	119.26	128.60
1	A	4	G	N3-C4-C5	-18.67	119.27	128.60
1	B	45	G	N3-C4-C5	-18.61	119.30	128.60
1	B	3	G	N3-C4-C5	-18.60	119.30	128.60
1	A	3	G	N3-C4-C5	-18.58	119.31	128.60
1	A	37	G	N3-C4-C5	-18.42	119.39	128.60
1	A	53	G	N3-C4-C5	-18.41	119.39	128.60
1	B	15	G	N3-C4-C5	-18.41	119.39	128.60
1	B	37	G	N3-C4-C5	-18.39	119.41	128.60
1	B	53	G	N3-C4-C5	-18.37	119.41	128.60
1	A	15	G	N3-C4-C5	-18.35	119.42	128.60
1	A	19	G	N3-C4-C5	-18.15	119.53	128.60
1	B	19	G	N3-C4-C5	-18.08	119.56	128.60
1	B	43	G	C2-N3-C4	17.07	120.44	111.90
1	A	57	G	C2-N3-C4	17.03	120.42	111.90
1	B	57	G	C2-N3-C4	17.01	120.40	111.90
1	A	43	G	C2-N3-C4	16.99	120.39	111.90
1	B	34	G	C2-N3-C4	16.92	120.36	111.90
1	A	34	G	C2-N3-C4	16.92	120.36	111.90
1	B	10	G	C2-N3-C4	16.89	120.35	111.90
1	A	10	G	C2-N3-C4	16.88	120.34	111.90
1	A	24	G	C2-N3-C4	16.84	120.32	111.90
1	B	24	G	C2-N3-C4	16.80	120.30	111.90
1	A	65	G	C2-N3-C4	16.80	120.30	111.90
1	B	65	G	C2-N3-C4	16.75	120.27	111.90
1	A	30	G	C2-N3-C4	16.74	120.27	111.90
1	A	46	G	C2-N3-C4	16.70	120.25	111.90
1	A	15	G	C2-N3-C4	16.68	120.24	111.90
1	B	46	G	C2-N3-C4	16.67	120.24	111.90
1	B	30	G	C2-N3-C4	16.67	120.24	111.90
1	B	15	G	C2-N3-C4	16.65	120.22	111.90
1	A	26	G	C2-N3-C4	16.64	120.22	111.90
1	B	71	G	C2-N3-C4	16.63	120.22	111.90
1	A	18	G	C2-N3-C4	16.63	120.21	111.90
1	A	71	G	C2-N3-C4	16.61	120.21	111.90
1	B	42	G	C2-N3-C4	16.59	120.19	111.90
1	B	3	G	C2-N3-C4	16.58	120.19	111.90
1	A	42	G	C2-N3-C4	16.57	120.19	111.90
1	B	26	G	C2-N3-C4	16.57	120.19	111.90
1	B	18	G	C2-N3-C4	16.57	120.18	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3	G	C2-N3-C4	16.56	120.18	111.90
1	A	22	G	C2-N3-C4	16.56	120.18	111.90
1	A	45	G	C2-N3-C4	16.56	120.18	111.90
1	A	37	G	C2-N3-C4	16.55	120.17	111.90
1	B	45	G	C2-N3-C4	16.55	120.17	111.90
1	B	53	G	C2-N3-C4	16.53	120.17	111.90
1	A	1	G	C2-N3-C4	16.52	120.16	111.90
1	B	22	G	C2-N3-C4	16.52	120.16	111.90
1	B	20	G	C2-N3-C4	16.50	120.15	111.90
1	A	53	G	C2-N3-C4	16.50	120.15	111.90
1	B	1	G	C2-N3-C4	16.48	120.14	111.90
1	B	37	G	C2-N3-C4	16.47	120.13	111.90
1	A	20	G	C2-N3-C4	16.45	120.12	111.90
1	A	4	G	C2-N3-C4	16.42	120.11	111.90
1	B	51	G	C2-N3-C4	16.39	120.09	111.90
1	B	4	G	C2-N3-C4	16.38	120.09	111.90
1	A	51	G	C2-N3-C4	16.31	120.05	111.90
1	A	19	G	C2-N3-C4	16.21	120.01	111.90
1	B	19	G	C2-N3-C4	16.14	119.97	111.90
1	A	20	G	N9-C4-C5	15.59	111.64	105.40
1	B	20	G	N9-C4-C5	15.58	111.63	105.40
1	A	10	G	N9-C4-C5	15.56	111.62	105.40
1	B	10	G	N9-C4-C5	15.46	111.59	105.40
1	A	45	G	N9-C4-C5	15.46	111.58	105.40
1	A	22	G	N9-C4-C5	15.42	111.57	105.40
1	B	45	G	N9-C4-C5	15.39	111.56	105.40
1	B	22	G	N9-C4-C5	15.35	111.54	105.40
1	B	51	G	N9-C4-C5	15.34	111.53	105.40
1	B	18	G	N9-C4-C5	15.31	111.53	105.40
1	A	18	G	N9-C4-C5	15.31	111.53	105.40
1	A	51	G	N9-C4-C5	15.30	111.52	105.40
1	A	43	G	N9-C4-C5	15.23	111.49	105.40
1	B	43	G	N9-C4-C5	15.18	111.47	105.40
1	B	19	G	N9-C4-C5	15.16	111.47	105.40
1	A	19	G	N9-C4-C5	15.15	111.46	105.40
1	B	42	G	N9-C4-C5	15.13	111.45	105.40
1	B	37	G	N9-C4-C5	15.10	111.44	105.40
1	A	42	G	N9-C4-C5	15.09	111.44	105.40
1	A	26	G	N9-C4-C5	15.08	111.43	105.40
1	A	37	G	N9-C4-C5	15.05	111.42	105.40
1	B	64	A	C2-N3-C4	15.03	118.11	110.60
1	A	64	A	C2-N3-C4	15.01	118.11	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	24	G	N9-C4-C5	15.01	111.41	105.40
1	B	26	G	N9-C4-C5	15.01	111.40	105.40
1	B	24	G	N9-C4-C5	15.00	111.40	105.40
1	B	65	G	N9-C4-C5	14.99	111.39	105.40
1	B	15	G	N9-C4-C5	14.98	111.39	105.40
1	A	65	G	N9-C4-C5	14.97	111.39	105.40
1	B	1	G	N9-C4-C5	14.94	111.38	105.40
1	B	71	G	N9-C4-C5	14.89	111.36	105.40
1	B	46	G	N9-C4-C5	14.86	111.34	105.40
1	A	71	G	N9-C4-C5	14.86	111.34	105.40
1	A	46	G	N9-C4-C5	14.85	111.34	105.40
1	A	76	A	C2-N3-C4	14.85	118.02	110.60
1	A	15	G	N9-C4-C5	14.83	111.33	105.40
1	A	38	A	C2-N3-C4	14.82	118.01	110.60
1	A	1	G	N9-C4-C5	14.81	111.33	105.40
1	B	38	A	C2-N3-C4	14.81	118.00	110.60
1	A	5	A	C2-N3-C4	14.79	117.99	110.60
1	B	76	A	C2-N3-C4	14.79	117.99	110.60
1	B	5	A	C2-N3-C4	14.76	117.98	110.60
1	B	57	G	N9-C4-C5	14.74	111.30	105.40
1	A	44	A	C2-N3-C4	14.69	117.94	110.60
1	B	35	A	C2-N3-C4	14.68	117.94	110.60
1	A	14	A	C2-N3-C4	14.68	117.94	110.60
1	B	58	A	C2-N3-C4	14.68	117.94	110.60
1	B	3	G	N9-C4-C5	14.66	111.26	105.40
1	A	67	A	C2-N3-C4	14.65	117.93	110.60
1	B	44	A	C2-N3-C4	14.65	117.92	110.60
1	B	67	A	C2-N3-C4	14.64	117.92	110.60
1	B	73	A	C2-N3-C4	14.63	117.91	110.60
1	A	57	G	N9-C4-C5	14.62	111.25	105.40
1	A	58	A	C2-N3-C4	14.62	117.91	110.60
1	A	73	A	C2-N3-C4	14.62	117.91	110.60
1	B	29	A	C2-N3-C4	14.62	117.91	110.60
1	A	3	G	N9-C4-C5	14.61	111.24	105.40
1	A	35	A	C2-N3-C4	14.60	117.90	110.60
1	B	14	A	C2-N3-C4	14.59	117.90	110.60
1	A	29	A	C2-N3-C4	14.56	117.88	110.60
1	B	53	G	N9-C4-C5	14.56	111.22	105.40
1	A	23	A	C2-N3-C4	14.56	117.88	110.60
1	B	23	A	C2-N3-C4	14.55	117.88	110.60
1	B	34	G	N9-C4-C5	14.55	111.22	105.40
1	A	53	G	N9-C4-C5	14.53	111.21	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	34	G	N9-C4-C5	14.52	111.21	105.40
1	A	66	A	C2-N3-C4	14.49	117.84	110.60
1	B	4	G	N9-C4-C5	14.48	111.19	105.40
1	B	66	A	C2-N3-C4	14.47	117.84	110.60
1	A	9	A	C2-N3-C4	14.44	117.82	110.60
1	B	9	A	C2-N3-C4	14.42	117.81	110.60
1	A	4	G	N9-C4-C5	14.41	111.16	105.40
1	A	31	A	C2-N3-C4	14.39	117.79	110.60
1	B	36	A	C2-N3-C4	14.37	117.78	110.60
1	A	36	A	C2-N3-C4	14.35	117.78	110.60
1	A	30	G	N9-C4-C5	14.34	111.14	105.40
1	B	31	A	C2-N3-C4	14.34	117.77	110.60
1	B	30	G	N9-C4-C5	14.33	111.13	105.40
1	B	62	A	C2-N3-C4	14.23	117.72	110.60
1	A	62	A	C2-N3-C4	14.17	117.69	110.60
1	A	21	A	C2-N3-C4	14.13	117.67	110.60
1	B	55	U	C2-N1-C1'	14.13	134.65	117.70
1	A	55	U	C2-N1-C1'	14.11	134.63	117.70
1	B	21	A	C2-N3-C4	14.03	117.62	110.60
1	A	34	G	C5-C6-O6	-13.93	120.24	128.60
1	B	34	G	C5-C6-O6	-13.91	120.26	128.60
1	B	67	A	N1-C2-N3	-13.76	122.42	129.30
1	A	67	A	N1-C2-N3	-13.74	122.43	129.30
1	A	5	A	N1-C2-N3	-13.70	122.45	129.30
1	B	66	A	N1-C2-N3	-13.68	122.46	129.30
1	A	15	G	C6-C5-N7	13.67	138.60	130.40
1	B	30	G	C5-C6-O6	-13.66	120.40	128.60
1	B	15	G	C6-C5-N7	13.65	138.59	130.40
1	B	5	A	N1-C2-N3	-13.64	122.48	129.30
1	A	66	A	N1-C2-N3	-13.62	122.49	129.30
1	A	19	G	C6-C5-N7	13.62	138.57	130.40
1	A	30	G	C5-C6-O6	-13.61	120.44	128.60
1	B	36	A	N1-C2-N3	-13.59	122.51	129.30
1	B	19	G	C6-C5-N7	13.57	138.54	130.40
1	A	36	A	N1-C2-N3	-13.56	122.52	129.30
1	A	37	G	C6-C5-N7	13.56	138.53	130.40
1	B	37	G	C6-C5-N7	13.53	138.52	130.40
1	B	65	G	C5-C6-O6	-13.51	120.49	128.60
1	B	23	A	N1-C2-N3	-13.47	122.57	129.30
1	B	64	A	N1-C2-N3	-13.46	122.57	129.30
1	A	65	G	C5-C6-O6	-13.45	120.53	128.60
1	B	45	G	C6-C5-N7	13.43	138.46	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	23	A	N1-C2-N3	-13.42	122.59	129.30
1	A	45	G	C6-C5-N7	13.42	138.45	130.40
1	A	64	A	N1-C2-N3	-13.42	122.59	129.30
1	A	20	G	C6-C5-N7	13.42	138.45	130.40
1	A	29	A	N1-C2-N3	-13.42	122.59	129.30
1	B	29	A	N1-C2-N3	-13.41	122.59	129.30
1	B	20	G	C6-C5-N7	13.41	138.44	130.40
1	A	14	A	N1-C2-N3	-13.39	122.61	129.30
1	A	51	G	C5-C6-O6	-13.38	120.57	128.60
1	B	51	G	C5-C6-O6	-13.38	120.58	128.60
1	B	10	G	C6-C5-N7	13.37	138.42	130.40
1	A	38	A	N1-C2-N3	-13.33	122.64	129.30
1	A	53	G	C6-C5-N7	13.32	138.39	130.40
1	A	10	G	C6-C5-N7	13.31	138.39	130.40
1	A	18	G	C6-C5-N7	13.29	138.38	130.40
1	B	22	G	C5-C6-O6	-13.29	120.62	128.60
1	B	71	G	C6-C5-N7	13.29	138.38	130.40
1	B	53	G	C6-C5-N7	13.29	138.37	130.40
1	A	71	G	C6-C5-N7	13.29	138.37	130.40
1	B	18	G	C6-C5-N7	13.28	138.37	130.40
1	B	14	A	N1-C2-N3	-13.27	122.67	129.30
1	A	57	G	C6-C5-N7	13.26	138.36	130.40
1	B	9	A	N1-C2-N3	-13.25	122.67	129.30
1	B	1	G	C5-C6-O6	-13.25	120.65	128.60
1	A	9	A	N1-C2-N3	-13.24	122.68	129.30
1	A	22	G	C5-C6-O6	-13.24	120.65	128.60
1	B	43	G	C5-C6-O6	-13.24	120.65	128.60
1	A	22	G	C6-C5-N7	13.24	138.34	130.40
1	B	57	G	C6-C5-N7	13.24	138.34	130.40
1	B	22	G	C6-C5-N7	13.23	138.34	130.40
1	B	38	A	N1-C2-N3	-13.23	122.69	129.30
1	A	1	G	C5-C6-O6	-13.22	120.67	128.60
1	A	21	A	N1-C2-N3	-13.21	122.69	129.30
1	A	3	G	C6-C5-N7	13.19	138.31	130.40
1	B	21	A	N1-C2-N3	-13.19	122.70	129.30
1	A	43	G	C5-C6-O6	-13.17	120.70	128.60
1	A	76	A	N1-C2-N3	-13.17	122.71	129.30
1	B	3	G	C6-C5-N7	13.16	138.30	130.40
1	A	62	A	N1-C2-N3	-13.14	122.73	129.30
1	B	62	A	N1-C2-N3	-13.14	122.73	129.30
1	B	71	G	C5-C6-O6	-13.13	120.72	128.60
1	A	71	G	C5-C6-O6	-13.11	120.73	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	31	A	N1-C2-N3	-13.10	122.75	129.30
1	B	76	A	N1-C2-N3	-13.10	122.75	129.30
1	A	42	G	C6-C5-N7	13.10	138.26	130.40
1	B	58	A	N1-C2-N3	-13.10	122.75	129.30
1	A	73	A	N1-C2-N3	-13.09	122.75	129.30
1	B	31	A	N1-C2-N3	-13.09	122.76	129.30
1	B	24	G	C6-C5-N7	13.07	138.24	130.40
1	B	53	G	C5-C6-O6	-13.07	120.76	128.60
1	A	24	G	C6-C5-N7	13.06	138.24	130.40
1	A	58	A	N1-C2-N3	-13.06	122.77	129.30
1	A	53	G	C5-C6-O6	-13.06	120.76	128.60
1	B	26	G	C5-C6-O6	-13.06	120.76	128.60
1	A	4	G	C5-C6-O6	-13.03	120.78	128.60
1	B	4	G	C5-C6-O6	-13.03	120.78	128.60
1	A	42	G	C5-C6-O6	-13.03	120.78	128.60
1	A	3	G	C5-C6-O6	-13.02	120.79	128.60
1	B	73	A	N1-C2-N3	-13.01	122.79	129.30
1	A	4	G	C6-C5-N7	13.00	138.20	130.40
1	A	1	G	C6-C5-N7	13.00	138.20	130.40
1	B	42	G	C6-C5-N7	12.99	138.19	130.40
1	A	26	G	C5-C6-O6	-12.98	120.81	128.60
1	A	51	G	C6-C5-N7	12.98	138.19	130.40
1	B	51	G	C6-C5-N7	12.97	138.18	130.40
1	B	37	G	C5-C6-O6	-12.96	120.82	128.60
1	B	3	G	C5-C6-O6	-12.95	120.83	128.60
1	B	4	G	C6-C5-N7	12.95	138.17	130.40
1	B	1	G	C6-C5-N7	12.95	138.17	130.40
1	B	43	G	C6-C5-N7	12.94	138.17	130.40
1	A	37	G	C5-C6-O6	-12.94	120.83	128.60
1	A	44	A	N1-C2-N3	-12.94	122.83	129.30
1	B	46	G	C6-C5-N7	12.94	138.17	130.40
1	A	46	G	C6-C5-N7	12.94	138.16	130.40
1	B	35	A	N1-C2-N3	-12.94	122.83	129.30
1	B	44	A	N1-C2-N3	-12.93	122.83	129.30
1	A	65	G	C6-C5-N7	12.93	138.16	130.40
1	A	35	A	N1-C2-N3	-12.91	122.84	129.30
1	B	26	G	C6-C5-N7	12.91	138.15	130.40
1	A	43	G	C6-C5-N7	12.90	138.14	130.40
1	B	46	G	C5-C6-O6	-12.90	120.86	128.60
1	B	65	G	C6-C5-N7	12.89	138.14	130.40
1	B	42	G	C5-C6-O6	-12.89	120.86	128.60
1	A	34	G	C6-C5-N7	12.89	138.13	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	46	G	C5-C6-O6	-12.88	120.87	128.60
1	B	34	G	C6-C5-N7	12.88	138.13	130.40
1	A	15	G	C5-C6-O6	-12.87	120.88	128.60
1	A	26	G	C6-C5-N7	12.86	138.11	130.40
1	B	15	G	C5-C6-O6	-12.84	120.89	128.60
1	B	30	G	C6-C5-N7	12.79	138.08	130.40
1	A	30	G	C6-C5-N7	12.79	138.07	130.40
1	B	10	G	C5-C6-O6	-12.75	120.95	128.60
1	A	10	G	C5-C6-O6	-12.72	120.97	128.60
1	B	45	G	C5-C6-O6	-12.70	120.98	128.60
1	A	57	G	C5-C6-O6	-12.62	121.03	128.60
1	A	19	G	C5-C6-O6	-12.61	121.03	128.60
1	A	45	G	C5-C6-O6	-12.61	121.04	128.60
1	B	19	G	C5-C6-O6	-12.60	121.04	128.60
1	A	24	G	C5-C6-O6	-12.59	121.05	128.60
1	B	24	G	C5-C6-O6	-12.58	121.05	128.60
1	B	20	G	C5-C6-O6	-12.57	121.06	128.60
1	B	57	G	C5-C6-O6	-12.57	121.06	128.60
1	A	20	G	C5-C6-O6	-12.53	121.08	128.60
1	A	14	A	C5-N7-C8	12.52	110.16	103.90
1	B	14	A	C5-N7-C8	12.44	110.12	103.90
1	B	31	A	C5-N7-C8	12.39	110.10	103.90
1	A	31	A	C5-N7-C8	12.35	110.08	103.90
1	A	18	G	C5-C6-O6	-12.35	121.19	128.60
1	B	73	A	C5-N7-C8	12.35	110.07	103.90
1	A	67	A	C5-N7-C8	12.34	110.07	103.90
1	B	67	A	C5-N7-C8	12.34	110.07	103.90
1	A	58	A	C5-N7-C8	12.34	110.07	103.90
1	A	73	A	C5-N7-C8	12.33	110.07	103.90
1	B	76	A	C5-N7-C8	12.30	110.05	103.90
1	A	21	A	C5-N7-C8	12.30	110.05	103.90
1	B	58	A	C5-N7-C8	12.29	110.05	103.90
1	B	21	A	C5-N7-C8	12.29	110.05	103.90
1	B	18	G	C5-C6-O6	-12.29	121.23	128.60
1	B	29	A	C5-N7-C8	12.28	110.04	103.90
1	A	9	A	C5-N7-C8	12.26	110.03	103.90
1	A	64	A	C5-N7-C8	12.25	110.03	103.90
1	A	76	A	C5-N7-C8	12.25	110.02	103.90
1	A	62	A	C5-N7-C8	12.23	110.02	103.90
1	B	64	A	C5-N7-C8	12.22	110.01	103.90
1	B	35	A	C5-N7-C8	12.21	110.01	103.90
1	A	29	A	C5-N7-C8	12.19	109.99	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	75	C	P-O3'-C3'	-12.19	105.08	119.70
1	B	75	C	P-O3'-C3'	-12.19	105.08	119.70
1	A	5	A	C5-N7-C8	12.18	109.99	103.90
1	A	35	A	C5-N7-C8	12.18	109.99	103.90
1	B	9	A	C5-N7-C8	12.15	109.98	103.90
1	B	62	A	C5-N7-C8	12.15	109.97	103.90
1	B	36	A	C5-N7-C8	12.14	109.97	103.90
1	A	36	A	C5-N7-C8	12.10	109.95	103.90
1	B	5	A	C5-N7-C8	12.07	109.94	103.90
1	B	23	A	C5-N7-C8	12.05	109.93	103.90
1	A	38	A	C5-N7-C8	12.01	109.90	103.90
1	A	23	A	C5-N7-C8	11.99	109.89	103.90
1	B	44	A	C5-N7-C8	11.98	109.89	103.90
1	A	44	A	C5-N7-C8	11.96	109.88	103.90
1	B	38	A	C5-N7-C8	11.95	109.88	103.90
1	B	66	A	C5-N7-C8	11.58	109.69	103.90
1	A	66	A	C5-N7-C8	11.57	109.69	103.90
1	A	50	U	C5-C4-O4	-11.19	119.19	125.90
1	A	11	C	N3-C4-C5	-11.18	117.43	121.90
1	B	11	C	N3-C4-C5	-11.16	117.44	121.90
1	B	50	U	C5-C4-O4	-11.14	119.21	125.90
1	B	39	U	C2-N1-C1'	-11.14	104.33	117.70
1	A	39	U	C2-N1-C1'	-11.14	104.33	117.70
1	B	75	C	N3-C4-C5	-11.13	117.45	121.90
1	A	23	A	C4-C5-C6	11.12	122.56	117.00
1	B	69	U	C5-C4-O4	-11.12	119.23	125.90
1	B	23	A	C4-C5-C6	11.11	122.55	117.00
1	A	75	C	N3-C4-C5	-11.10	117.46	121.90
1	B	32	C	N3-C4-C5	-11.09	117.46	121.90
1	A	69	U	C5-C4-O4	-11.09	119.25	125.90
1	A	25	C	N3-C4-C5	-11.07	117.47	121.90
1	B	54	U	C5-C4-O4	-11.04	119.28	125.90
1	A	32	C	N3-C4-C5	-11.03	117.49	121.90
1	B	48	C	N3-C4-C5	-11.02	117.49	121.90
1	A	54	U	C5-C4-O4	-11.02	119.29	125.90
1	B	41	U	C5-C4-O4	-11.01	119.29	125.90
1	A	72	C	N3-C4-C5	-11.00	117.50	121.90
1	B	72	C	N3-C4-C5	-11.00	117.50	121.90
1	B	25	C	N3-C4-C5	-10.98	117.51	121.90
1	A	41	U	C5-C4-O4	-10.97	119.32	125.90
1	A	44	A	C4-C5-C6	10.95	122.47	117.00
1	B	49	C	N3-C4-C5	-10.95	117.52	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	17	U	C5-C4-O4	-10.94	119.33	125.90
1	B	64	A	C4-C5-C6	10.94	122.47	117.00
1	A	48	C	N3-C4-C5	-10.94	117.52	121.90
1	A	12	U	C5-C4-O4	-10.93	119.34	125.90
1	B	13	C	N3-C4-C5	-10.92	117.53	121.90
1	B	17	U	C5-C4-O4	-10.92	119.35	125.90
1	B	12	U	C5-C4-O4	-10.91	119.36	125.90
1	A	14	A	C4-C5-N7	-10.90	105.25	110.70
1	B	44	A	C4-C5-C6	10.89	122.45	117.00
1	B	14	A	C4-C5-N7	-10.88	105.26	110.70
1	A	13	C	N3-C4-C5	-10.87	117.55	121.90
1	A	56	C	N3-C4-C5	-10.87	117.55	121.90
1	A	35	A	C4-C5-C6	10.87	122.43	117.00
1	A	44	A	C4-C5-N7	-10.86	105.27	110.70
1	B	35	A	C4-C5-C6	10.85	122.43	117.00
1	A	74	C	N3-C4-C5	-10.85	117.56	121.90
1	B	59	U	C5-C4-O4	-10.85	119.39	125.90
1	A	64	A	C4-C5-C6	10.84	122.42	117.00
1	B	44	A	C4-C5-N7	-10.83	105.28	110.70
1	A	59	U	C5-C4-O4	-10.82	119.41	125.90
1	A	66	A	C4-C5-C6	10.82	122.41	117.00
1	B	70	C	N3-C4-C5	-10.82	117.57	121.90
1	B	56	C	N3-C4-C5	-10.81	117.57	121.90
1	A	49	C	N3-C4-C5	-10.80	117.58	121.90
1	A	60	C	N3-C4-C5	-10.81	117.58	121.90
1	A	70	C	N3-C4-C5	-10.81	117.58	121.90
1	B	16	U	C5-C4-O4	-10.80	119.42	125.90
1	B	38	A	C4-C5-C6	10.80	122.40	117.00
1	A	38	A	C4-C5-C6	10.78	122.39	117.00
1	B	74	C	N3-C4-C5	-10.78	117.59	121.90
1	B	66	A	C4-C5-C6	10.77	122.38	117.00
1	B	47	U	C5-C4-O4	-10.76	119.44	125.90
1	A	16	U	C5-C4-O4	-10.76	119.44	125.90
1	B	52	U	C5-C4-O4	-10.75	119.45	125.90
1	A	52	U	C5-C4-O4	-10.74	119.45	125.90
1	B	60	C	N3-C4-C5	-10.74	117.60	121.90
1	B	58	A	C4-C5-N7	-10.74	105.33	110.70
1	B	36	A	C4-C5-N7	-10.73	105.33	110.70
1	B	7	U	C5-C4-O4	-10.72	119.47	125.90
1	A	47	U	C5-C4-O4	-10.72	119.47	125.90
1	A	58	A	C4-C5-N7	-10.71	105.34	110.70
1	B	6	U	C5-C4-O4	-10.71	119.47	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	5	A	C4-C5-C6	10.70	122.35	117.00
1	B	2	C	N3-C4-C5	-10.70	117.62	121.90
1	A	68	U	C5-C4-O4	-10.69	119.48	125.90
1	A	5	A	C4-C5-N7	-10.69	105.36	110.70
1	A	6	U	C5-C4-O4	-10.68	119.49	125.90
1	A	7	U	C5-C4-O4	-10.68	119.49	125.90
1	A	21	A	C4-C5-N7	-10.68	105.36	110.70
1	B	5	A	C4-C5-C6	10.66	122.33	117.00
1	B	33	U	C5-C4-O4	-10.66	119.50	125.90
1	A	28	C	N3-C4-C5	-10.66	117.64	121.90
1	A	76	A	C4-C5-N7	-10.66	105.37	110.70
1	B	76	A	C4-C5-N7	-10.65	105.38	110.70
1	B	68	U	C5-C4-O4	-10.65	119.51	125.90
1	A	36	A	C4-C5-N7	-10.63	105.38	110.70
1	B	28	C	N3-C4-C5	-10.62	117.65	121.90
1	B	23	A	C4-C5-N7	-10.62	105.39	110.70
1	B	10	G	C5-N7-C8	10.61	109.61	104.30
1	A	33	U	C5-C4-O4	-10.61	119.54	125.90
1	A	63	C	N3-C4-C5	-10.60	117.66	121.90
1	B	21	A	C4-C5-N7	-10.59	105.41	110.70
1	A	67	A	C4-C5-N7	-10.59	105.41	110.70
1	A	23	A	C4-C5-N7	-10.58	105.41	110.70
1	B	5	A	C4-C5-N7	-10.56	105.42	110.70
1	A	62	A	C4-C5-C6	10.55	122.28	117.00
1	B	37	G	C5-N7-C8	10.55	109.58	104.30
1	B	67	A	C4-C5-N7	-10.55	105.42	110.70
1	B	73	A	C4-C5-N7	-10.55	105.42	110.70
1	A	2	C	N3-C4-C5	-10.55	117.68	121.90
1	A	35	A	C4-C5-N7	-10.55	105.42	110.70
1	B	62	A	C4-C5-C6	10.55	122.27	117.00
1	B	73	A	C4-C5-C6	10.55	122.27	117.00
1	A	10	G	C5-N7-C8	10.55	109.57	104.30
1	B	64	A	C4-C5-N7	-10.54	105.43	110.70
1	A	8	U	C5-C4-O4	-10.53	119.58	125.90
1	A	62	A	C4-C5-N7	-10.53	105.43	110.70
1	A	73	A	C4-C5-C6	10.53	122.26	117.00
1	A	73	A	C4-C5-N7	-10.52	105.44	110.70
1	A	3	G	C5-N7-C8	10.52	109.56	104.30
1	A	67	A	C4-C5-C6	10.52	122.26	117.00
1	A	21	A	C4-C5-C6	10.52	122.26	117.00
1	B	63	C	N3-C4-C5	-10.51	117.69	121.90
1	B	35	A	C4-C5-N7	-10.51	105.44	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	21	A	C4-C5-C6	10.51	122.25	117.00
1	A	64	A	C4-C5-N7	-10.51	105.45	110.70
1	A	37	G	C5-N7-C8	10.50	109.55	104.30
1	B	3	G	C5-N7-C8	10.50	109.55	104.30
1	B	62	A	C4-C5-N7	-10.50	105.45	110.70
1	B	31	A	C4-C5-N7	-10.50	105.45	110.70
1	B	58	A	C4-C5-C6	10.50	122.25	117.00
1	A	53	G	C5-N7-C8	10.50	109.55	104.30
1	B	8	U	C5-C4-O4	-10.49	119.61	125.90
1	A	9	A	C4-C5-N7	-10.47	105.47	110.70
1	B	71	G	C5-N7-C8	10.46	109.53	104.30
1	A	19	G	C5-N7-C8	10.46	109.53	104.30
1	A	20	G	C5-N7-C8	10.44	109.52	104.30
1	B	9	A	C4-C5-N7	-10.44	105.48	110.70
1	A	31	A	C4-C5-N7	-10.43	105.48	110.70
1	B	20	G	C5-N7-C8	10.43	109.51	104.30
1	A	46	G	C5-N7-C8	10.42	109.51	104.30
1	A	58	A	C4-C5-C6	10.41	122.21	117.00
1	B	24	G	C5-N7-C8	10.41	109.50	104.30
1	A	27	C	N3-C4-C5	-10.41	117.74	121.90
1	B	67	A	C4-C5-C6	10.41	122.20	117.00
1	B	76	A	C4-C5-C6	10.40	122.20	117.00
1	A	22	G	C5-N7-C8	10.40	109.50	104.30
1	B	29	A	C4-C5-N7	-10.40	105.50	110.70
1	B	38	A	C4-C5-N7	-10.40	105.50	110.70
1	A	38	A	C4-C5-N7	-10.39	105.50	110.70
1	A	42	G	C5-N7-C8	10.39	109.50	104.30
1	B	19	G	C5-N7-C8	10.39	109.50	104.30
1	A	24	G	C5-N7-C8	10.39	109.49	104.30
1	A	76	A	C4-C5-C6	10.38	122.19	117.00
1	A	4	G	C5-N7-C8	10.38	109.49	104.30
1	B	9	A	C4-C5-C6	10.38	122.19	117.00
1	A	34	G	C5-N7-C8	10.38	109.49	104.30
1	B	22	G	C5-N7-C8	10.38	109.49	104.30
1	B	46	G	C5-N7-C8	10.38	109.49	104.30
1	B	53	G	C5-N7-C8	10.37	109.49	104.30
1	A	29	A	C4-C5-N7	-10.37	105.51	110.70
1	A	44	A	N3-C4-C5	-10.37	119.54	126.80
1	A	71	G	C5-N7-C8	10.36	109.48	104.30
1	B	18	G	C5-N7-C8	10.36	109.48	104.30
1	A	18	G	C5-N7-C8	10.36	109.48	104.30
1	B	26	G	C5-N7-C8	10.36	109.48	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	42	G	C5-N7-C8	10.36	109.48	104.30
1	B	44	A	N3-C4-C5	-10.35	119.55	126.80
1	B	64	A	N3-C4-C5	-10.35	119.56	126.80
1	A	26	G	C5-N7-C8	10.34	109.47	104.30
1	B	4	G	C5-N7-C8	10.33	109.46	104.30
1	B	34	G	C5-N7-C8	10.33	109.46	104.30
1	B	14	A	C4-C5-C6	10.32	122.16	117.00
1	B	36	A	C4-C5-C6	10.31	122.16	117.00
1	A	64	A	N3-C4-C5	-10.31	119.58	126.80
1	B	29	A	C4-C5-C6	10.30	122.15	117.00
1	A	14	A	C4-C5-C6	10.30	122.15	117.00
1	B	27	C	N3-C4-C5	-10.30	117.78	121.90
1	A	9	A	C4-C5-C6	10.28	122.14	117.00
1	B	66	A	C4-C5-N7	-10.28	105.56	110.70
1	A	66	A	C4-C5-N7	-10.27	105.56	110.70
1	A	15	G	C5-N7-C8	10.26	109.43	104.30
1	A	55	U	C5-C4-O4	-10.26	119.74	125.90
1	A	61	C	N3-C4-C5	-10.26	117.80	121.90
1	A	29	A	C4-C5-C6	10.26	122.13	117.00
1	A	30	G	C5-N7-C8	10.25	109.42	104.30
1	A	35	A	N3-C4-C5	-10.25	119.63	126.80
1	B	43	G	C5-N7-C8	10.25	109.42	104.30
1	B	35	A	N3-C4-C5	-10.24	119.63	126.80
1	B	61	C	N3-C4-C5	-10.24	117.80	121.90
1	B	40	C	N3-C4-C5	-10.23	117.81	121.90
1	A	43	G	C5-N7-C8	10.22	109.41	104.30
1	A	40	C	N3-C4-C5	-10.22	117.81	121.90
1	A	51	G	C5-N7-C8	10.21	109.41	104.30
1	A	36	A	C4-C5-C6	10.21	122.11	117.00
1	A	45	G	C5-N7-C8	10.21	109.40	104.30
1	B	51	G	C5-N7-C8	10.20	109.40	104.30
1	B	15	G	C5-N7-C8	10.20	109.40	104.30
1	B	30	G	C5-N7-C8	10.19	109.39	104.30
1	B	55	U	C5-C4-O4	-10.18	119.79	125.90
1	B	45	G	C5-N7-C8	10.17	109.39	104.30
1	A	1	G	C5-N7-C8	10.15	109.37	104.30
1	A	23	A	N3-C4-C5	-10.13	119.71	126.80
1	B	1	G	C5-N7-C8	10.13	109.36	104.30
1	A	57	G	C5-N7-C8	10.12	109.36	104.30
1	B	23	A	N3-C4-C5	-10.12	119.72	126.80
1	B	57	G	C5-N7-C8	10.12	109.36	104.30
1	A	76	A	N3-C4-C5	-10.08	119.74	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	58	A	N3-C4-C5	-10.08	119.75	126.80
1	A	65	G	C5-N7-C8	10.07	109.33	104.30
1	B	76	A	N3-C4-C5	-10.07	119.75	126.80
1	A	39	U	C5-C4-O4	-10.05	119.87	125.90
1	B	31	A	C4-C5-C6	10.04	122.02	117.00
1	A	58	A	N3-C4-C5	-10.01	119.79	126.80
1	A	38	A	N3-C4-C5	-10.00	119.80	126.80
1	B	38	A	N3-C4-C5	-10.00	119.80	126.80
1	A	31	A	C4-C5-C6	10.00	122.00	117.00
1	B	39	U	C5-C4-O4	-10.00	119.90	125.90
1	B	65	G	C5-N7-C8	10.00	109.30	104.30
1	B	14	A	N3-C4-C5	-9.98	119.82	126.80
1	A	14	A	N3-C4-C5	-9.97	119.82	126.80
1	B	73	A	N3-C4-C5	-9.97	119.82	126.80
1	A	73	A	N3-C4-C5	-9.92	119.85	126.80
1	A	5	A	N3-C4-C5	-9.92	119.86	126.80
1	B	5	A	N3-C4-C5	-9.89	119.88	126.80
1	B	29	A	N3-C4-C5	-9.86	119.90	126.80
1	A	29	A	N3-C4-C5	-9.82	119.93	126.80
1	A	66	A	N3-C4-C5	-9.79	119.95	126.80
1	B	36	A	N3-C4-C5	-9.77	119.96	126.80
1	B	66	A	N3-C4-C5	-9.74	119.98	126.80
1	B	9	A	N3-C4-C5	-9.72	120.00	126.80
1	A	9	A	N3-C4-C5	-9.71	120.00	126.80
1	A	36	A	N3-C4-C5	-9.70	120.01	126.80
1	A	67	A	N3-C4-C5	-9.70	120.01	126.80
1	B	31	A	N3-C4-C5	-9.70	120.01	126.80
1	B	62	A	N3-C4-C5	-9.70	120.01	126.80
1	A	31	A	N3-C4-C5	-9.70	120.01	126.80
1	A	62	A	N3-C4-C5	-9.67	120.03	126.80
1	A	21	A	N3-C4-C5	-9.66	120.04	126.80
1	B	67	A	N3-C4-C5	-9.64	120.05	126.80
1	B	21	A	N3-C4-C5	-9.57	120.10	126.80
1	A	47	U	O4'-C1'-N1	9.39	115.71	108.20
1	B	47	U	O4'-C1'-N1	9.39	115.71	108.20
1	B	8	U	C2-N3-C4	-8.95	121.63	127.00
1	B	16	U	C2-N3-C4	-8.93	121.64	127.00
1	A	16	U	C2-N3-C4	-8.91	121.65	127.00
1	B	39	U	C2-N3-C4	-8.88	121.67	127.00
1	A	8	U	C2-N3-C4	-8.86	121.69	127.00
1	A	39	U	C2-N3-C4	-8.77	121.74	127.00
1	B	54	U	C2-N3-C4	-8.76	121.75	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	54	U	C2-N3-C4	-8.73	121.76	127.00
1	B	52	U	C2-N3-C4	-8.68	121.79	127.00
1	B	6	U	C2-N3-C4	-8.68	121.79	127.00
1	A	6	U	C2-N3-C4	-8.66	121.81	127.00
1	A	52	U	C2-N3-C4	-8.63	121.82	127.00
1	A	59	U	C2-N3-C4	-8.63	121.82	127.00
1	B	59	U	C2-N3-C4	-8.63	121.82	127.00
1	B	17	U	C2-N3-C4	-8.56	121.86	127.00
1	A	17	U	C2-N3-C4	-8.54	121.87	127.00
1	B	44	A	N3-C4-N9	8.54	134.23	127.40
1	A	64	A	N3-C4-N9	8.53	134.23	127.40
1	B	50	U	C2-N3-C4	-8.51	121.89	127.00
1	A	44	A	N3-C4-N9	8.51	134.20	127.40
1	B	64	A	N3-C4-N9	8.48	134.19	127.40
1	A	50	U	C2-N3-C4	-8.46	121.92	127.00
1	B	47	U	C2-N3-C4	-8.44	121.94	127.00
1	A	47	U	C2-N3-C4	-8.43	121.94	127.00
1	B	29	A	N3-C4-N9	8.40	134.12	127.40
1	A	29	A	N3-C4-N9	8.36	134.09	127.40
1	A	69	U	C2-N3-C4	-8.34	121.99	127.00
1	B	69	U	C2-N3-C4	-8.33	122.00	127.00
1	B	35	A	N3-C4-N9	8.29	134.03	127.40
1	A	35	A	N3-C4-N9	8.29	134.03	127.40
1	B	58	A	N3-C4-N9	8.26	134.01	127.40
1	A	41	U	C2-N3-C4	-8.23	122.06	127.00
1	A	58	A	N3-C4-N9	8.23	133.99	127.40
1	A	75	C	OP1-P-O3'	8.23	123.31	105.20
1	B	75	C	OP1-P-O3'	8.23	123.31	105.20
1	B	7	U	C2-N3-C4	-8.23	122.06	127.00
1	B	76	A	N3-C4-N9	8.22	133.98	127.40
1	A	68	U	C2-N3-C4	-8.22	122.07	127.00
1	A	31	A	N3-C4-N9	8.21	133.97	127.40
1	A	14	A	N3-C4-N9	8.20	133.96	127.40
1	B	14	A	N3-C4-N9	8.20	133.96	127.40
1	B	38	A	N3-C4-N9	8.19	133.95	127.40
1	B	41	U	C2-N3-C4	-8.19	122.08	127.00
1	A	76	A	N3-C4-N9	8.19	133.95	127.40
1	A	38	A	N3-C4-N9	8.19	133.95	127.40
1	B	33	U	C2-N3-C4	-8.18	122.09	127.00
1	A	7	U	C2-N3-C4	-8.17	122.10	127.00
1	B	31	A	N3-C4-N9	8.17	133.93	127.40
1	A	33	U	C2-N3-C4	-8.15	122.11	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	68	U	C2-N3-C4	-8.14	122.12	127.00
1	A	23	A	N3-C4-N9	8.13	133.91	127.40
1	A	73	A	N3-C4-N9	8.12	133.90	127.40
1	B	73	A	N3-C4-N9	8.12	133.90	127.40
1	A	12	U	C2-N3-C4	-8.11	122.13	127.00
1	B	12	U	C2-N3-C4	-8.11	122.13	127.00
1	B	23	A	N3-C4-N9	8.07	133.86	127.40
1	A	9	A	N3-C4-N9	8.02	133.82	127.40
1	B	36	A	N3-C4-N9	8.01	133.81	127.40
1	A	36	A	N3-C4-N9	8.01	133.81	127.40
1	B	9	A	N3-C4-N9	7.99	133.79	127.40
1	B	62	A	N3-C4-N9	7.97	133.78	127.40
1	A	62	A	N3-C4-N9	7.95	133.76	127.40
1	B	5	A	N3-C4-N9	7.91	133.73	127.40
1	A	21	A	N3-C4-N9	7.89	133.71	127.40
1	A	5	A	N3-C4-N9	7.87	133.70	127.40
1	B	21	A	N3-C4-N9	7.85	133.68	127.40
1	B	34	G	C5-C6-N1	7.84	115.42	111.50
1	A	66	A	N3-C4-N9	7.83	133.66	127.40
1	A	34	G	C5-C6-N1	7.82	115.41	111.50
1	B	1	G	P-O5'-C5'	-7.77	108.47	120.90
1	B	66	A	N3-C4-N9	7.76	133.61	127.40
1	B	67	A	N3-C4-N9	7.76	133.61	127.40
1	A	67	A	N3-C4-N9	7.75	133.60	127.40
1	B	29	A	N1-C6-N6	7.59	123.15	118.60
1	B	19	G	N7-C8-N9	-7.58	109.31	113.10
1	B	71	G	C5-C6-N1	7.57	115.29	111.50
1	A	71	G	C5-C6-N1	7.55	115.27	111.50
1	A	29	A	N1-C6-N6	7.54	123.12	118.60
1	A	19	G	N7-C8-N9	-7.54	109.33	113.10
1	B	65	G	N1-C6-O6	7.50	124.40	119.90
1	A	53	G	N7-C8-N9	-7.49	109.36	113.10
1	A	30	G	N1-C6-O6	7.45	124.37	119.90
1	B	30	G	N1-C6-O6	7.45	124.37	119.90
1	B	30	G	C5-C6-N1	7.45	115.22	111.50
1	B	49	C	N3-C4-N4	7.44	123.21	118.00
1	A	51	G	C5-C6-N1	7.44	115.22	111.50
1	B	45	G	C5-C6-N1	7.44	115.22	111.50
1	B	51	G	C5-C6-N1	7.44	115.22	111.50
1	B	8	U	N1-C2-N3	7.43	119.36	114.90
1	A	53	G	C5-C6-N1	7.42	115.21	111.50
1	A	34	G	N1-C6-O6	7.42	124.35	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1	G	N1-C6-O6	7.42	124.35	119.90
1	B	53	G	N7-C8-N9	-7.41	109.40	113.10
1	B	53	G	C5-C6-N1	7.41	115.20	111.50
1	B	43	G	C5-C6-N1	7.41	115.20	111.50
1	A	65	G	N1-C6-O6	7.40	124.34	119.90
1	A	8	U	N1-C2-N3	7.40	119.34	114.90
1	A	37	G	C5-C6-N1	7.40	115.20	111.50
1	A	49	C	N3-C4-N4	7.39	123.17	118.00
1	A	25	C	N3-C4-N4	7.39	123.17	118.00
1	A	30	G	C5-C6-N1	7.38	115.19	111.50
1	A	35	A	N1-C6-N6	7.38	123.03	118.60
1	A	43	G	C5-C6-N1	7.38	115.19	111.50
1	B	25	C	N3-C4-N4	7.37	123.16	118.00
1	B	34	G	N1-C6-O6	7.37	124.32	119.90
1	A	45	G	C5-C6-N1	7.35	115.18	111.50
1	A	20	G	C5-C6-N1	7.35	115.18	111.50
1	A	1	G	N1-C6-O6	7.33	124.30	119.90
1	B	71	G	N7-C8-N9	-7.33	109.43	113.10
1	B	35	A	N1-C6-N6	7.33	123.00	118.60
1	A	32	C	N3-C4-N4	7.32	123.13	118.00
1	B	37	G	C5-C6-N1	7.32	115.16	111.50
1	B	32	C	N3-C4-N4	7.31	123.12	118.00
1	A	71	G	N7-C8-N9	-7.31	109.45	113.10
1	B	20	G	C5-C6-N1	7.31	115.15	111.50
1	A	3	G	N7-C8-N9	-7.30	109.45	113.10
1	B	10	G	N7-C8-N9	-7.30	109.45	113.10
1	B	22	G	C5-C6-N1	7.30	115.15	111.50
1	A	23	A	N1-C6-N6	7.29	122.97	118.60
1	A	3	G	N1-C6-O6	7.28	124.27	119.90
1	B	3	G	N7-C8-N9	-7.28	109.46	113.10
1	B	37	G	N7-C8-N9	-7.28	109.46	113.10
1	B	5	A	N1-C6-N6	7.28	122.97	118.60
1	A	22	G	C5-C6-N1	7.27	115.14	111.50
1	B	31	A	N1-C6-N6	7.27	122.96	118.60
1	A	65	G	C5-C6-N1	7.26	115.13	111.50
1	B	26	G	N1-C6-O6	7.26	124.25	119.90
1	A	5	A	N1-C6-N6	7.24	122.94	118.60
1	A	10	G	N7-C8-N9	-7.24	109.48	113.10
1	B	23	A	N1-C6-N6	7.24	122.94	118.60
1	A	37	G	N7-C8-N9	-7.24	109.48	113.10
1	A	57	G	C5-C6-N1	7.23	115.12	111.50
1	B	57	G	C5-C6-N1	7.23	115.12	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	28	C	N3-C4-N4	7.23	123.06	118.00
1	B	28	C	N3-C4-N4	7.23	123.06	118.00
1	A	4	G	C5-C6-N1	7.22	115.11	111.50
1	A	26	G	N1-C6-O6	7.22	124.23	119.90
1	B	65	G	C5-C6-N1	7.21	115.11	111.50
1	B	3	G	N1-C6-O6	7.21	124.23	119.90
1	B	22	G	N1-C6-O6	7.21	124.23	119.90
1	A	4	G	N7-C8-N9	-7.21	109.50	113.10
1	B	4	G	C5-C6-N1	7.20	115.10	111.50
1	B	13	C	N3-C4-N4	7.20	123.04	118.00
1	B	39	U	N1-C2-N3	7.19	119.22	114.90
1	A	31	A	N1-C6-N6	7.19	122.91	118.60
1	A	9	A	OP1-P-OP2	-7.18	108.83	119.60
1	A	22	G	N1-C6-O6	7.18	124.21	119.90
1	A	51	G	N1-C6-O6	7.18	124.21	119.90
1	A	15	G	C5-C6-N1	7.18	115.09	111.50
1	B	51	G	N1-C6-O6	7.18	124.21	119.90
1	A	34	G	N7-C8-N9	-7.17	109.52	113.10
1	A	42	G	N7-C8-N9	-7.16	109.52	113.10
1	A	18	G	OP1-P-OP2	-7.16	108.86	119.60
1	B	18	G	N7-C8-N9	-7.16	109.52	113.10
1	A	39	U	N1-C2-N3	7.16	119.19	114.90
1	B	4	G	N7-C8-N9	-7.16	109.52	113.10
1	B	70	C	N3-C4-N4	7.15	123.00	118.00
1	B	9	A	OP1-P-OP2	-7.15	108.88	119.60
1	B	44	A	N1-C6-N6	7.15	122.89	118.60
1	B	42	G	N7-C8-N9	-7.14	109.53	113.10
1	B	18	G	OP1-P-OP2	-7.14	108.89	119.60
1	B	46	G	C5-C6-N1	7.13	115.07	111.50
1	B	24	G	N7-C8-N9	-7.13	109.53	113.10
1	A	70	C	N3-C4-N4	7.13	122.99	118.00
1	A	13	C	N3-C4-N4	7.13	122.99	118.00
1	B	11	C	N3-C4-N4	7.13	122.99	118.00
1	B	15	G	C5-C6-N1	7.13	115.06	111.50
1	A	11	C	N3-C4-N4	7.12	122.99	118.00
1	A	73	A	N1-C6-N6	7.12	122.87	118.60
1	B	73	A	N1-C6-N6	7.12	122.87	118.60
1	A	19	G	C5-C6-N1	7.12	115.06	111.50
1	A	43	G	N7-C8-N9	-7.12	109.54	113.10
1	A	42	G	N1-C6-O6	7.12	124.17	119.90
1	A	44	A	N1-C6-N6	7.11	122.87	118.60
1	B	26	G	N7-C8-N9	-7.11	109.54	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	46	G	C5-C6-N1	7.11	115.05	111.50
1	B	19	G	C5-C6-N1	7.10	115.05	111.50
1	B	16	U	N1-C2-N3	7.10	119.16	114.90
1	A	18	G	N7-C8-N9	-7.10	109.55	113.10
1	A	16	U	N1-C2-N3	7.10	119.16	114.90
1	A	26	G	N7-C8-N9	-7.10	109.55	113.10
1	A	20	G	N7-C8-N9	-7.10	109.55	113.10
1	B	20	G	N7-C8-N9	-7.09	109.55	113.10
1	A	42	G	C5-C6-N1	7.09	115.04	111.50
1	A	21	A	N1-C6-N6	7.09	122.85	118.60
1	A	24	G	N7-C8-N9	-7.08	109.56	113.10
1	A	57	G	N7-C8-N9	-7.08	109.56	113.10
1	A	61	C	N3-C4-N4	7.08	122.95	118.00
1	A	62	A	N1-C6-N6	7.08	122.85	118.60
1	B	24	G	C5-C6-N1	7.08	115.04	111.50
1	A	30	G	N7-C8-N9	-7.07	109.56	113.10
1	A	1	G	C5-C6-N1	7.07	115.03	111.50
1	B	43	G	N1-C6-O6	7.07	124.14	119.90
1	A	51	G	N7-C8-N9	-7.07	109.57	113.10
1	B	43	G	N7-C8-N9	-7.07	109.57	113.10
1	B	62	A	N1-C6-N6	7.07	122.84	118.60
1	B	58	A	OP1-P-OP2	-7.06	109.01	119.60
1	A	64	A	N1-C6-N6	7.06	122.83	118.60
1	B	42	G	C5-C6-N1	7.05	115.03	111.50
1	B	34	G	N7-C8-N9	-7.05	109.57	113.10
1	B	61	C	N3-C4-N4	7.05	122.93	118.00
1	A	58	A	OP1-P-OP2	-7.04	109.03	119.60
1	B	51	G	N7-C8-N9	-7.04	109.58	113.10
1	B	57	G	N7-C8-N9	-7.04	109.58	113.10
1	B	38	A	N1-C6-N6	7.03	122.82	118.60
1	B	21	A	N1-C6-N6	7.03	122.82	118.60
1	B	4	G	N1-C6-O6	7.03	124.12	119.90
1	B	45	G	OP1-P-OP2	-7.03	109.06	119.60
1	A	43	G	N1-C6-O6	7.02	124.11	119.90
1	A	75	C	N3-C4-N4	7.02	122.92	118.00
1	A	38	A	N1-C6-N6	7.02	122.81	118.60
1	B	64	A	N1-C6-N6	7.02	122.81	118.60
1	A	27	C	N3-C4-N4	7.01	122.91	118.00
1	B	42	G	N1-C6-O6	7.01	124.11	119.90
1	A	4	G	N1-C6-O6	7.01	124.11	119.90
1	A	65	G	N7-C8-N9	-7.01	109.59	113.10
1	A	18	G	C5-C6-N1	7.01	115.00	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	48	C	OP1-P-OP2	-7.01	109.09	119.60
1	A	24	G	C5-C6-N1	7.00	115.00	111.50
1	A	45	G	OP1-P-OP2	-7.00	109.09	119.60
1	A	2	C	N3-C4-N4	7.00	122.90	118.00
1	B	2	C	N3-C4-N4	7.00	122.90	118.00
1	B	27	C	N3-C4-N4	7.00	122.90	118.00
1	B	75	C	N3-C4-N4	7.00	122.90	118.00
1	B	18	G	C5-C6-N1	7.00	115.00	111.50
1	B	1	G	C5-C6-N1	7.00	115.00	111.50
1	A	72	C	N3-C4-N4	6.99	122.90	118.00
1	B	10	G	C5-C6-N1	6.99	115.00	111.50
1	B	40	C	N3-C4-N4	6.99	122.89	118.00
1	A	48	C	OP1-P-OP2	-6.98	109.12	119.60
1	B	22	G	N7-C8-N9	-6.98	109.61	113.10
1	A	40	C	N3-C4-N4	6.97	122.88	118.00
1	B	30	G	N7-C8-N9	-6.97	109.61	113.10
1	B	72	C	N3-C4-N4	6.97	122.88	118.00
1	A	15	G	N7-C8-N9	-6.97	109.61	113.10
1	A	27	C	OP1-P-OP2	-6.97	109.15	119.60
1	B	26	G	C5-C6-N1	6.96	114.98	111.50
1	B	27	C	OP1-P-OP2	-6.96	109.15	119.60
1	A	46	G	N1-C6-O6	6.96	124.08	119.90
1	A	68	U	OP1-P-OP2	-6.96	109.16	119.60
1	B	65	G	N7-C8-N9	-6.96	109.62	113.10
1	B	68	U	OP1-P-OP2	-6.96	109.17	119.60
1	A	10	G	N1-C6-O6	6.96	124.07	119.90
1	A	39	U	OP1-P-OP2	-6.95	109.17	119.60
1	B	46	G	N1-C6-O6	6.95	124.07	119.90
1	A	36	A	OP1-P-OP2	-6.94	109.19	119.60
1	A	8	U	OP1-P-OP2	-6.94	109.19	119.60
1	A	46	G	N7-C8-N9	-6.94	109.63	113.10
1	B	8	U	OP1-P-OP2	-6.94	109.20	119.60
1	A	19	G	OP1-P-OP2	-6.93	109.20	119.60
1	B	55	U	OP1-P-OP2	-6.93	109.20	119.60
1	B	73	A	OP1-P-OP2	-6.93	109.20	119.60
1	A	73	A	OP1-P-OP2	-6.93	109.21	119.60
1	A	55	U	OP1-P-OP2	-6.93	109.21	119.60
1	B	36	A	OP1-P-OP2	-6.93	109.21	119.60
1	B	4	G	OP1-P-OP2	-6.92	109.21	119.60
1	B	19	G	OP1-P-OP2	-6.92	109.21	119.60
1	A	22	G	N7-C8-N9	-6.92	109.64	113.10
1	B	15	G	N7-C8-N9	-6.92	109.64	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	10	G	C5-C6-N1	6.92	114.96	111.50
1	A	21	A	OP1-P-OP2	-6.92	109.22	119.60
1	B	10	G	N1-C6-O6	6.92	124.05	119.90
1	A	26	G	C5-C6-N1	6.91	114.96	111.50
1	B	16	U	OP1-P-OP2	-6.91	109.23	119.60
1	B	39	U	OP1-P-OP2	-6.91	109.23	119.60
1	A	16	U	OP1-P-OP2	-6.91	109.23	119.60
1	B	21	A	OP1-P-OP2	-6.91	109.24	119.60
1	A	4	G	OP1-P-OP2	-6.91	109.24	119.60
1	B	40	C	OP1-P-OP2	-6.90	109.25	119.60
1	B	56	C	N3-C4-N4	6.90	122.83	118.00
1	B	50	U	OP1-P-OP2	-6.90	109.25	119.60
1	A	67	A	OP1-P-OP2	-6.90	109.26	119.60
1	A	45	G	N7-C8-N9	-6.89	109.65	113.10
1	B	53	G	N1-C6-O6	6.89	124.04	119.90
1	B	15	G	N1-C6-O6	6.89	124.03	119.90
1	B	3	G	C5-C6-N1	6.89	114.94	111.50
1	B	45	G	N7-C8-N9	-6.89	109.66	113.10
1	A	3	G	C5-C6-N1	6.88	114.94	111.50
1	B	46	G	N7-C8-N9	-6.88	109.66	113.10
1	B	74	C	N3-C4-N4	6.88	122.82	118.00
1	B	67	A	OP1-P-OP2	-6.88	109.28	119.60
1	A	40	C	OP1-P-OP2	-6.88	109.28	119.60
1	A	53	G	N1-C6-O6	6.88	124.03	119.90
1	A	56	C	N3-C4-N4	6.88	122.81	118.00
1	B	12	U	OP1-P-OP2	-6.88	109.29	119.60
1	A	50	U	OP1-P-OP2	-6.87	109.29	119.60
1	A	74	C	N3-C4-N4	6.87	122.81	118.00
1	A	74	C	OP1-P-OP2	-6.87	109.29	119.60
1	B	76	A	N1-C6-N6	6.87	122.72	118.60
1	A	15	G	N1-C6-O6	6.87	124.02	119.90
1	B	24	G	OP1-P-OP2	-6.87	109.29	119.60
1	B	74	C	OP1-P-OP2	-6.87	109.29	119.60
1	B	2	C	OP1-P-OP2	-6.87	109.30	119.60
1	A	2	C	OP1-P-OP2	-6.87	109.30	119.60
1	A	24	G	OP1-P-OP2	-6.87	109.30	119.60
1	B	35	A	OP1-P-OP2	-6.87	109.30	119.60
1	B	31	A	OP1-P-OP2	-6.86	109.31	119.60
1	B	37	G	OP1-P-OP2	-6.86	109.31	119.60
1	B	63	C	N3-C4-N4	6.86	122.80	118.00
1	B	7	U	OP1-P-OP2	-6.86	109.31	119.60
1	B	37	G	N1-C6-O6	6.86	124.02	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	12	U	OP1-P-OP2	-6.85	109.32	119.60
1	A	51	G	OP1-P-OP2	-6.85	109.32	119.60
1	B	51	G	OP1-P-OP2	-6.85	109.32	119.60
1	A	63	C	N3-C4-N4	6.85	122.80	118.00
1	A	25	C	OP1-P-OP2	-6.85	109.33	119.60
1	B	48	C	C4-C5-C6	6.85	120.82	117.40
1	B	47	U	OP1-P-OP2	-6.85	109.33	119.60
1	B	53	G	OP1-P-OP2	-6.84	109.33	119.60
1	B	67	A	N1-C6-N6	6.84	122.71	118.60
1	B	33	U	OP1-P-OP2	-6.84	109.33	119.60
1	B	62	A	OP1-P-OP2	-6.84	109.34	119.60
1	B	66	A	N1-C6-N6	6.84	122.71	118.60
1	A	7	U	OP1-P-OP2	-6.84	109.34	119.60
1	A	31	A	OP1-P-OP2	-6.84	109.34	119.60
1	A	47	U	OP1-P-OP2	-6.84	109.34	119.60
1	A	35	A	OP1-P-OP2	-6.84	109.35	119.60
1	A	54	U	OP1-P-OP2	-6.83	109.35	119.60
1	A	5	A	OP1-P-OP2	-6.83	109.35	119.60
1	A	37	G	OP1-P-OP2	-6.83	109.35	119.60
1	B	25	C	OP1-P-OP2	-6.83	109.35	119.60
1	A	66	A	N1-C6-N6	6.83	122.70	118.60
1	A	67	A	N1-C6-N6	6.83	122.70	118.60
1	A	62	A	OP1-P-OP2	-6.83	109.36	119.60
1	B	41	U	OP1-P-OP2	-6.83	109.36	119.60
1	A	71	G	N1-C6-O6	6.83	124.00	119.90
1	A	57	G	OP1-P-OP2	-6.82	109.36	119.60
1	B	1	G	N7-C8-N9	-6.82	109.69	113.10
1	B	48	C	N3-C4-N4	6.82	122.78	118.00
1	B	54	U	OP1-P-OP2	-6.82	109.37	119.60
1	B	71	G	N1-C6-O6	6.82	123.99	119.90
1	A	48	C	N3-C4-N4	6.82	122.77	118.00
1	A	33	U	OP1-P-OP2	-6.82	109.37	119.60
1	A	44	A	OP1-P-OP2	-6.82	109.38	119.60
1	A	53	G	OP1-P-OP2	-6.82	109.38	119.60
1	B	36	A	N1-C6-N6	6.82	122.69	118.60
1	B	57	G	OP1-P-OP2	-6.82	109.37	119.60
1	A	36	A	N1-C6-N6	6.82	122.69	118.60
1	A	41	U	OP1-P-OP2	-6.82	109.38	119.60
1	A	43	G	OP1-P-OP2	-6.82	109.38	119.60
1	B	70	C	OP1-P-OP2	-6.81	109.38	119.60
1	A	70	C	OP1-P-OP2	-6.81	109.39	119.60
1	B	5	A	OP1-P-OP2	-6.81	109.38	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	38	A	OP1-P-OP2	-6.80	109.40	119.60
1	B	42	G	OP1-P-OP2	-6.80	109.39	119.60
1	B	43	G	OP1-P-OP2	-6.80	109.40	119.60
1	A	6	U	OP1-P-OP2	-6.80	109.40	119.60
1	A	76	A	OP1-P-OP2	-6.80	109.40	119.60
1	A	75	C	OP1-P-OP2	-6.80	109.41	119.60
1	B	44	A	OP1-P-OP2	-6.80	109.40	119.60
1	A	52	U	OP1-P-OP2	-6.79	109.41	119.60
1	B	38	A	OP1-P-OP2	-6.79	109.42	119.60
1	A	26	G	OP1-P-OP2	-6.79	109.42	119.60
1	A	66	A	OP1-P-OP2	-6.79	109.42	119.60
1	B	6	U	OP1-P-OP2	-6.79	109.42	119.60
1	B	26	G	OP1-P-OP2	-6.79	109.42	119.60
1	A	42	G	OP1-P-OP2	-6.78	109.42	119.60
1	B	75	C	OP1-P-OP2	-6.78	109.43	119.60
1	B	76	A	OP1-P-OP2	-6.78	109.42	119.60
1	A	1	G	N7-C8-N9	-6.78	109.71	113.10
1	A	72	C	OP1-P-OP2	-6.78	109.43	119.60
1	B	20	G	OP1-P-OP2	-6.78	109.43	119.60
1	B	60	C	N3-C4-N4	6.78	122.75	118.00
1	B	72	C	OP1-P-OP2	-6.78	109.43	119.60
1	B	14	A	OP1-P-OP2	-6.78	109.43	119.60
1	A	32	C	OP1-P-OP2	-6.78	109.44	119.60
1	A	37	G	N1-C6-O6	6.78	123.97	119.90
1	A	59	U	N1-C2-N3	6.78	118.97	114.90
1	A	63	C	OP1-P-OP2	-6.77	109.44	119.60
1	B	69	U	OP1-P-OP2	-6.77	109.44	119.60
1	A	69	U	OP1-P-OP2	-6.77	109.44	119.60
1	B	52	U	OP1-P-OP2	-6.77	109.44	119.60
1	A	20	G	OP1-P-OP2	-6.77	109.45	119.60
1	A	14	A	OP1-P-OP2	-6.77	109.45	119.60
1	A	60	C	N3-C4-N4	6.77	122.74	118.00
1	B	63	C	OP1-P-OP2	-6.77	109.45	119.60
1	B	66	A	OP1-P-OP2	-6.77	109.45	119.60
1	A	58	A	N1-C6-N6	6.76	122.66	118.60
1	B	23	A	OP1-P-OP2	-6.76	109.46	119.60
1	A	29	A	OP1-P-OP2	-6.76	109.46	119.60
1	A	48	C	C4-C5-C6	6.76	120.78	117.40
1	B	34	G	OP1-P-OP2	-6.76	109.46	119.60
1	A	76	A	N1-C6-N6	6.75	122.65	118.60
1	B	32	C	OP1-P-OP2	-6.75	109.47	119.60
1	A	60	C	C4-C5-C6	6.75	120.78	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	24	G	N1-C6-O6	6.75	123.95	119.90
1	A	34	G	OP1-P-OP2	-6.75	109.48	119.60
1	A	23	A	OP1-P-OP2	-6.75	109.48	119.60
1	B	60	C	OP1-P-OP2	-6.74	109.48	119.60
1	B	11	C	OP1-P-OP2	-6.74	109.49	119.60
1	B	9	A	N1-C6-N6	6.74	122.64	118.60
1	B	28	C	OP1-P-OP2	-6.74	109.49	119.60
1	A	28	C	OP1-P-OP2	-6.74	109.49	119.60
1	B	29	A	OP1-P-OP2	-6.74	109.50	119.60
1	B	65	G	OP1-P-OP2	-6.74	109.50	119.60
1	A	60	C	OP1-P-OP2	-6.73	109.51	119.60
1	A	47	U	N1-C2-N3	6.73	118.94	114.90
1	A	11	C	OP1-P-OP2	-6.73	109.51	119.60
1	A	71	G	OP1-P-OP2	-6.72	109.51	119.60
1	B	60	C	C4-C5-C6	6.72	120.76	117.40
1	A	3	G	OP1-P-OP2	-6.72	109.52	119.60
1	A	65	G	OP1-P-OP2	-6.72	109.53	119.60
1	B	59	U	N1-C2-N3	6.71	118.93	114.90
1	B	64	A	OP1-P-OP2	-6.71	109.53	119.60
1	B	49	C	OP1-P-OP2	-6.71	109.53	119.60
1	B	56	C	OP1-P-OP2	-6.71	109.53	119.60
1	B	71	G	OP1-P-OP2	-6.71	109.54	119.60
1	B	58	A	N1-C6-N6	6.70	122.62	118.60
1	A	49	C	OP1-P-OP2	-6.70	109.55	119.60
1	A	1	G	OP1-P-OP2	-6.70	109.55	119.60
1	B	3	G	OP1-P-OP2	-6.70	109.55	119.60
1	A	64	A	OP1-P-OP2	-6.70	109.55	119.60
1	B	46	G	OP1-P-OP2	-6.70	109.56	119.60
1	A	9	A	N1-C6-N6	6.69	122.62	118.60
1	A	56	C	OP1-P-OP2	-6.69	109.56	119.60
1	B	47	U	N1-C2-N3	6.69	118.91	114.90
1	A	46	G	OP1-P-OP2	-6.68	109.57	119.60
1	B	24	G	N1-C6-O6	6.68	123.91	119.90
1	A	52	U	N1-C2-N3	6.68	118.91	114.90
1	A	19	G	N1-C6-O6	6.68	123.91	119.90
1	B	19	G	N1-C6-O6	6.68	123.91	119.90
1	A	30	G	OP1-P-OP2	-6.68	109.58	119.60
1	B	52	U	N1-C2-N3	6.68	118.91	114.90
1	A	15	G	OP1-P-OP2	-6.67	109.59	119.60
1	A	61	C	OP1-P-OP2	-6.67	109.59	119.60
1	B	61	C	OP1-P-OP2	-6.67	109.60	119.60
1	A	59	U	OP1-P-OP2	-6.66	109.61	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	15	G	OP1-P-OP2	-6.66	109.61	119.60
1	B	30	G	OP1-P-OP2	-6.66	109.61	119.60
1	B	59	U	OP1-P-OP2	-6.65	109.62	119.60
1	B	50	U	N1-C2-N3	6.65	118.89	114.90
1	A	50	U	N1-C2-N3	6.65	118.89	114.90
1	A	22	G	OP1-P-OP2	-6.65	109.63	119.60
1	B	22	G	OP1-P-OP2	-6.63	109.66	119.60
1	A	6	U	N1-C2-N3	6.62	118.87	114.90
1	A	68	U	N1-C2-N3	6.61	118.87	114.90
1	B	6	U	N1-C2-N3	6.61	118.87	114.90
1	A	57	G	N1-C6-O6	6.59	123.85	119.90
1	B	14	A	N1-C6-N6	6.59	122.55	118.60
1	B	33	U	N1-C2-N3	6.58	118.85	114.90
1	A	14	A	N1-C6-N6	6.58	122.55	118.60
1	A	33	U	N1-C2-N3	6.57	118.84	114.90
1	B	17	U	OP1-P-OP2	-6.54	109.79	119.60
1	B	57	G	N1-C6-O6	6.54	123.82	119.90
1	A	34	G	N3-C4-N9	6.53	129.91	126.00
1	B	68	U	N1-C2-N3	6.52	118.81	114.90
1	A	17	U	OP1-P-OP2	-6.52	109.82	119.60
1	A	18	G	N1-C6-O6	6.50	123.80	119.90
1	B	34	G	N3-C4-N9	6.50	129.90	126.00
1	B	45	G	N1-C6-O6	6.50	123.80	119.90
1	A	17	U	N1-C2-N3	6.49	118.79	114.90
1	B	10	G	OP1-P-OP2	-6.48	109.87	119.60
1	A	45	G	N1-C6-O6	6.48	123.79	119.90
1	B	20	G	N1-C6-O6	6.48	123.79	119.90
1	A	10	G	OP1-P-OP2	-6.46	109.91	119.60
1	B	18	G	N1-C6-O6	6.45	123.77	119.90
1	B	17	U	N1-C2-N3	6.44	118.76	114.90
1	A	46	G	N3-C4-N9	6.42	129.85	126.00
1	A	69	U	N1-C2-N3	6.40	118.74	114.90
1	B	54	U	N1-C2-N3	6.40	118.74	114.90
1	A	20	G	N1-C6-O6	6.40	123.74	119.90
1	A	54	U	N1-C2-N3	6.39	118.73	114.90
1	A	13	C	OP1-P-OP2	-6.37	110.04	119.60
1	B	46	G	N3-C4-N9	6.37	129.82	126.00
1	B	13	C	OP1-P-OP2	-6.36	110.06	119.60
1	A	72	C	C4-C5-C6	6.35	120.58	117.40
1	B	69	U	N1-C2-N3	6.35	118.71	114.90
1	B	12	U	N1-C2-N3	6.34	118.71	114.90
1	A	12	U	N1-C2-N3	6.34	118.70	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	30	G	N3-C4-N9	6.33	129.79	126.00
1	B	72	C	C4-C5-C6	6.33	120.56	117.40
1	A	74	C	C4-C5-C6	6.32	120.56	117.40
1	B	74	C	N3-C2-O2	-6.31	117.48	121.90
1	B	30	G	N3-C4-N9	6.31	129.79	126.00
1	B	7	U	N1-C2-N3	6.29	118.67	114.90
1	B	74	C	C4-C5-C6	6.29	120.55	117.40
1	A	7	U	N1-C2-N3	6.29	118.67	114.90
1	A	41	U	N1-C2-N3	6.29	118.67	114.90
1	A	74	C	N3-C2-O2	-6.29	117.50	121.90
1	A	21	A	O4'-C1'-N9	6.27	113.22	108.20
1	B	21	A	O4'-C1'-N9	6.27	113.22	108.20
1	B	41	U	N1-C2-N3	6.25	118.65	114.90
1	A	32	C	C4-C5-C6	6.25	120.52	117.40
1	B	32	C	C4-C5-C6	6.25	120.53	117.40
1	A	75	C	N3-C2-O2	-6.24	117.53	121.90
1	B	75	C	N3-C2-O2	-6.23	117.54	121.90
1	A	27	C	N1-C2-O2	6.20	122.62	118.90
1	B	61	C	N3-C2-O2	-6.19	117.56	121.90
1	B	54	U	N3-C4-C5	6.19	118.31	114.60
1	B	46	G	O4'-C1'-N9	6.17	113.14	108.20
1	A	46	G	O4'-C1'-N9	6.17	113.14	108.20
1	A	54	U	N3-C4-C5	6.17	118.30	114.60
1	A	61	C	N3-C2-O2	-6.17	117.58	121.90
1	A	25	C	C4-C5-C6	6.14	120.47	117.40
1	B	27	C	N1-C2-O2	6.14	122.59	118.90
1	B	69	U	N3-C4-C5	6.14	118.29	114.60
1	A	13	C	C4-C5-C6	6.14	120.47	117.40
1	A	56	C	C4-C5-C6	6.14	120.47	117.40
1	B	25	C	C4-C5-C6	6.14	120.47	117.40
1	B	13	C	C4-C5-C6	6.14	120.47	117.40
1	A	27	C	N3-C2-O2	-6.13	117.61	121.90
1	B	40	C	N3-C2-O2	-6.12	117.62	121.90
1	B	2	C	C4-C5-C6	6.12	120.46	117.40
1	B	27	C	N3-C2-O2	-6.11	117.62	121.90
1	A	69	U	N3-C4-C5	6.10	118.26	114.60
1	B	56	C	C4-C5-C6	6.08	120.44	117.40
1	A	57	G	N3-C4-N9	6.08	129.65	126.00
1	A	73	A	N7-C8-N9	-6.08	110.76	113.80
1	A	40	C	N3-C2-O2	-6.08	117.65	121.90
1	A	74	C	N1-C2-O2	6.07	122.54	118.90
1	B	11	C	C4-C5-C6	6.07	120.44	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	11	C	C4-C5-C6	6.07	120.44	117.40
1	B	16	U	N3-C4-C5	6.07	118.24	114.60
1	A	70	C	C4-C5-C6	6.06	120.43	117.40
1	B	21	A	N7-C8-N9	-6.06	110.77	113.80
1	B	73	A	N7-C8-N9	-6.06	110.77	113.80
1	B	74	C	N1-C2-O2	6.05	122.53	118.90
1	A	38	A	N7-C8-N9	-6.05	110.78	113.80
1	A	21	A	N7-C8-N9	-6.04	110.78	113.80
1	B	14	A	N7-C8-N9	-6.04	110.78	113.80
1	B	70	C	C4-C5-C6	6.04	120.42	117.40
1	A	14	A	N7-C8-N9	-6.03	110.78	113.80
1	A	16	U	N3-C4-C5	6.03	118.22	114.60
1	B	43	G	N3-C4-N9	6.03	129.62	126.00
1	A	63	C	C4-C5-C6	6.02	120.41	117.40
1	A	2	C	C4-C5-C6	6.01	120.41	117.40
1	A	75	C	N1-C2-O2	6.01	122.50	118.90
1	A	11	C	N3-C2-O2	-6.00	117.70	121.90
1	B	6	U	N3-C4-C5	5.99	118.19	114.60
1	A	67	A	N7-C8-N9	-5.98	110.81	113.80
1	A	43	G	N3-C4-N9	5.98	129.59	126.00
1	B	64	A	N7-C8-N9	-5.98	110.81	113.80
1	A	8	U	N1-C1'-C2'	-5.97	105.44	112.00
1	B	60	C	N3-C2-O2	-5.96	117.73	121.90
1	B	75	C	N1-C2-O2	5.96	122.48	118.90
1	A	24	G	N3-C4-N9	5.96	129.58	126.00
1	B	11	C	N3-C2-O2	-5.96	117.73	121.90
1	B	8	U	N1-C1'-C2'	-5.96	105.45	112.00
1	B	57	G	N3-C4-N9	5.96	129.58	126.00
1	B	50	U	N3-C4-C5	5.96	118.17	114.60
1	A	4	G	N3-C4-N9	5.95	129.57	126.00
1	A	64	A	N7-C8-N9	-5.95	110.83	113.80
1	A	6	U	N3-C4-C5	5.95	118.17	114.60
1	A	1	G	N3-C4-N9	5.94	129.57	126.00
1	B	31	A	N7-C8-N9	-5.94	110.83	113.80
1	A	61	C	N1-C2-O2	5.94	122.46	118.90
1	B	24	G	N3-C4-N9	5.94	129.56	126.00
1	A	27	C	C4-C5-C6	5.93	120.37	117.40
1	B	52	U	N3-C4-C5	5.93	118.16	114.60
1	B	4	G	N3-C4-N9	5.93	129.56	126.00
1	B	38	A	N7-C8-N9	-5.93	110.83	113.80
1	B	67	A	N7-C8-N9	-5.93	110.83	113.80
1	A	32	C	N3-C2-O2	-5.92	117.75	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	56	C	N3-C2-O2	-5.92	117.75	121.90
1	B	61	C	N1-C2-O2	5.92	122.45	118.90
1	A	50	U	N3-C4-C5	5.92	118.15	114.60
1	B	32	C	N3-C2-O2	-5.92	117.76	121.90
1	A	25	C	N1-C2-O2	5.91	122.45	118.90
1	B	63	C	N1-C2-O2	5.91	122.45	118.90
1	B	63	C	C4-C5-C6	5.91	120.35	117.40
1	A	31	A	N7-C8-N9	-5.91	110.85	113.80
1	B	1	G	N3-C4-N9	5.90	129.54	126.00
1	B	49	C	C4-C5-C6	5.89	120.35	117.40
1	A	65	G	N3-C4-N9	5.89	129.53	126.00
1	A	60	C	N3-C2-O2	-5.89	117.78	121.90
1	A	63	C	N1-C2-O2	5.89	122.43	118.90
1	B	25	C	N1-C2-O2	5.89	122.43	118.90
1	B	35	A	N7-C8-N9	-5.89	110.86	113.80
1	B	59	U	N3-C4-C5	5.89	118.13	114.60
1	A	56	C	N3-C2-O2	-5.88	117.78	121.90
1	B	63	C	N3-C2-O2	-5.88	117.79	121.90
1	A	63	C	N3-C2-O2	-5.88	117.79	121.90
1	A	35	A	N7-C8-N9	-5.87	110.86	113.80
1	A	13	C	N3-C2-O2	-5.87	117.79	121.90
1	B	7	U	N3-C4-C5	5.87	118.12	114.60
1	A	55	U	N1-C2-N3	5.86	118.42	114.90
1	B	55	U	N1-C2-N3	5.86	118.42	114.90
1	A	58	A	N7-C8-N9	-5.86	110.87	113.80
1	B	17	U	N3-C4-C5	5.86	118.11	114.60
1	A	40	C	C4-C5-C6	5.86	120.33	117.40
1	B	58	A	N7-C8-N9	-5.86	110.87	113.80
1	B	70	C	N3-C2-O2	-5.85	117.80	121.90
1	A	26	G	N3-C4-N9	5.85	129.51	126.00
1	B	56	C	N1-C2-O2	5.85	122.41	118.90
1	A	52	U	N3-C4-C5	5.85	118.11	114.60
1	A	59	U	N3-C4-C5	5.85	118.11	114.60
1	A	71	G	N3-C4-N9	5.84	129.51	126.00
1	B	13	C	N3-C2-O2	-5.84	117.81	121.90
1	B	40	C	C4-C5-C6	5.84	120.32	117.40
1	B	13	C	N1-C2-O2	5.84	122.40	118.90
1	B	33	U	N3-C4-C5	5.84	118.10	114.60
1	B	47	U	N3-C4-C5	5.84	118.10	114.60
1	B	71	G	N3-C4-N9	5.84	129.50	126.00
1	A	49	C	C4-C5-C6	5.83	120.32	117.40
1	B	27	C	C4-C5-C6	5.83	120.32	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	65	G	N3-C4-N9	5.83	129.50	126.00
1	A	17	U	N3-C4-C5	5.83	118.10	114.60
1	A	49	C	N3-C2-O2	-5.82	117.82	121.90
1	B	42	G	N3-C4-N9	5.82	129.49	126.00
1	A	13	C	N1-C2-O2	5.82	122.39	118.90
1	A	47	U	N3-C4-C5	5.81	118.09	114.60
1	B	32	C	N1-C2-O2	5.81	122.39	118.90
1	B	60	C	N1-C2-O2	5.81	122.39	118.90
1	A	28	C	C4-C5-C6	5.81	120.30	117.40
1	A	11	C	N1-C2-O2	5.80	122.38	118.90
1	A	70	C	N3-C2-O2	-5.79	117.84	121.90
1	A	7	U	N3-C4-C5	5.79	118.08	114.60
1	A	32	C	N1-C2-O2	5.79	122.37	118.90
1	A	42	G	N3-C4-N9	5.79	129.47	126.00
1	B	26	G	N3-C4-N9	5.79	129.47	126.00
1	A	5	A	N7-C8-N9	-5.79	110.91	113.80
1	B	29	A	N7-C8-N9	-5.79	110.91	113.80
1	B	11	C	N1-C2-O2	5.78	122.37	118.90
1	A	40	C	N1-C2-O2	5.78	122.37	118.90
1	B	40	C	N1-C2-O2	5.78	122.37	118.90
1	A	33	U	N3-C4-C5	5.78	118.07	114.60
1	A	56	C	N1-C2-O2	5.78	122.36	118.90
1	A	60	C	N1-C2-O2	5.77	122.36	118.90
1	B	49	C	N3-C2-O2	-5.77	117.86	121.90
1	A	49	C	N1-C2-O2	5.77	122.36	118.90
1	B	2	C	N3-C2-O2	-5.77	117.86	121.90
1	B	75	C	C4-C5-C6	5.76	120.28	117.40
1	B	76	A	N7-C8-N9	-5.75	110.92	113.80
1	A	2	C	N3-C2-O2	-5.75	117.87	121.90
1	B	5	A	N7-C8-N9	-5.75	110.93	113.80
1	A	3	G	N3-C4-N9	5.75	129.45	126.00
1	A	18	G	O4'-C1'-N9	5.75	112.80	108.20
1	A	75	C	C4-C5-C6	5.74	120.27	117.40
1	B	70	C	N1-C2-O2	5.73	122.34	118.90
1	B	25	C	N3-C2-O2	-5.73	117.89	121.90
1	B	28	C	C4-C5-C6	5.73	120.26	117.40
1	B	3	G	N3-C4-N9	5.73	129.44	126.00
1	A	41	U	N3-C4-C5	5.72	118.03	114.60
1	B	41	U	N3-C4-C5	5.72	118.03	114.60
1	B	49	C	N1-C2-O2	5.72	122.33	118.90
1	A	9	A	N7-C8-N9	-5.71	110.94	113.80
1	A	25	C	N3-C2-O2	-5.71	117.90	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	9	A	N7-C8-N9	-5.71	110.95	113.80
1	A	51	G	N3-C4-N9	5.70	129.42	126.00
1	B	18	G	O4'-C1'-N9	5.70	112.76	108.20
1	B	39	U	N3-C4-C5	5.70	118.02	114.60
1	B	51	G	N3-C4-N9	5.70	129.42	126.00
1	A	29	A	N7-C8-N9	-5.70	110.95	113.80
1	B	10	G	N3-C4-N9	5.70	129.42	126.00
1	B	8	U	N3-C4-C5	5.69	118.01	114.60
1	A	12	U	N3-C4-C5	5.68	118.01	114.60
1	A	57	G	C8-N9-C4	5.68	108.67	106.40
1	A	5	A	C6-N1-C2	5.68	122.01	118.60
1	A	10	G	N3-C4-N9	5.68	129.41	126.00
1	B	5	A	C6-N1-C2	5.68	122.01	118.60
1	A	18	G	N3-C4-N9	5.67	129.40	126.00
1	A	76	A	N7-C8-N9	-5.66	110.97	113.80
1	A	72	C	N3-C2-O2	-5.66	117.94	121.90
1	A	53	G	N3-C4-N9	5.66	129.39	126.00
1	B	12	U	N3-C4-C5	5.66	117.99	114.60
1	A	8	U	N3-C4-C5	5.65	117.99	114.60
1	B	23	A	N7-C8-N9	-5.65	110.97	113.80
1	B	18	G	N3-C4-N9	5.65	129.39	126.00
1	B	36	A	C6-N1-C2	5.65	121.99	118.60
1	A	36	A	C6-N1-C2	5.65	121.99	118.60
1	A	39	U	N3-C4-C5	5.64	117.98	114.60
1	A	68	U	N3-C4-C5	5.63	117.98	114.60
1	A	70	C	N1-C2-O2	5.63	122.28	118.90
1	B	36	A	N7-C8-N9	-5.62	110.99	113.80
1	A	61	C	C4-C5-C6	5.62	120.21	117.40
1	B	61	C	C4-C5-C6	5.61	120.20	117.40
1	B	53	G	N3-C4-N9	5.60	129.36	126.00
1	A	44	A	N7-C8-N9	-5.60	111.00	113.80
1	B	72	C	N3-C2-O2	-5.60	117.98	121.90
1	B	44	A	N7-C8-N9	-5.59	111.00	113.80
1	A	62	A	N7-C8-N9	-5.58	111.01	113.80
1	A	23	A	N7-C8-N9	-5.58	111.01	113.80
1	A	36	A	N7-C8-N9	-5.55	111.03	113.80
1	B	57	G	C8-N9-C4	5.55	108.62	106.40
1	A	22	G	N3-C4-N9	5.54	129.32	126.00
1	B	62	A	N7-C8-N9	-5.54	111.03	113.80
1	B	76	A	O4'-C1'-N9	5.53	112.63	108.20
1	B	22	G	N3-C4-N9	5.53	129.32	126.00
1	B	68	U	N3-C4-C5	5.53	117.92	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	76	A	O4'-C1'-N9	5.52	112.61	108.20
1	A	45	G	N9-C1'-C2'	-5.50	105.95	112.00
1	B	66	A	C6-N1-C2	5.50	121.90	118.60
1	B	68	U	C5'-C4'-C3'	-5.50	107.20	116.00
1	A	68	U	C5'-C4'-C3'	-5.50	107.21	116.00
1	A	15	G	N9-C1'-C2'	-5.49	105.97	112.00
1	B	19	G	C8-N9-C4	5.49	108.59	106.40
1	B	29	A	C6-N1-C2	5.48	121.89	118.60
1	A	53	G	C8-N9-C4	5.48	108.59	106.40
1	B	45	G	N9-C1'-C2'	-5.48	105.97	112.00
1	B	15	G	N9-C1'-C2'	-5.47	105.98	112.00
1	A	66	A	C6-N1-C2	5.46	121.88	118.60
1	A	28	C	N3-C2-O2	-5.46	118.08	121.90
1	A	2	C	N1-C2-O2	5.45	122.17	118.90
1	A	29	A	C6-N1-C2	5.45	121.87	118.60
1	B	21	A	C1'-O4'-C4'	-5.45	105.54	109.90
1	B	28	C	N3-C2-O2	-5.45	118.09	121.90
1	A	28	C	N1-C2-O2	5.44	122.16	118.90
1	B	48	C	N3-C2-O2	-5.44	118.09	121.90
1	A	19	G	C8-N9-C4	5.43	108.57	106.40
1	B	2	C	N1-C2-O2	5.43	122.16	118.90
1	B	53	G	C8-N9-C4	5.42	108.57	106.40
1	A	21	A	C1'-O4'-C4'	-5.42	105.56	109.90
1	A	15	G	N3-C4-N9	5.41	129.24	126.00
1	A	4	G	C8-N9-C4	5.40	108.56	106.40
1	A	48	C	N3-C2-O2	-5.40	118.12	121.90
1	B	66	A	N7-C8-N9	-5.39	111.10	113.80
1	A	71	G	C8-N9-C4	5.39	108.56	106.40
1	A	21	A	C6-N1-C2	5.39	121.83	118.60
1	A	72	C	N1-C2-O2	5.38	122.13	118.90
1	A	66	A	N7-C8-N9	-5.38	111.11	113.80
1	B	28	C	N1-C2-O2	5.38	122.13	118.90
1	A	67	A	C6-N1-C2	5.37	121.82	118.60
1	B	21	A	C6-N1-C2	5.37	121.82	118.60
1	A	64	A	C6-N1-C2	5.37	121.82	118.60
1	B	4	G	C8-N9-C4	5.36	108.54	106.40
1	B	64	A	C6-N1-C2	5.35	121.81	118.60
1	B	67	A	C6-N1-C2	5.35	121.81	118.60
1	B	15	G	N3-C4-N9	5.35	129.21	126.00
1	B	72	C	N1-C2-O2	5.34	122.11	118.90
1	A	23	A	C6-N1-C2	5.33	121.80	118.60
1	B	23	A	C6-N1-C2	5.33	121.80	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	34	G	C8-N9-C4	5.33	108.53	106.40
1	A	37	G	N3-C4-N9	5.32	129.19	126.00
1	A	38	A	C6-N1-C2	5.32	121.79	118.60
1	B	71	G	C8-N9-C4	5.31	108.52	106.40
1	B	38	A	C6-N1-C2	5.27	121.76	118.60
1	A	3	G	C8-N9-C4	5.26	108.51	106.40
1	A	45	G	N3-C4-N9	5.26	129.15	126.00
1	B	37	G	N3-C4-N9	5.25	129.15	126.00
1	B	45	G	N3-C4-N9	5.24	129.15	126.00
1	B	20	G	N3-C4-N9	5.23	129.14	126.00
1	A	14	A	C6-N1-C2	5.23	121.74	118.60
1	A	20	G	N3-C4-N9	5.23	129.14	126.00
1	B	14	A	C6-N1-C2	5.21	121.73	118.60
1	B	34	G	C8-N9-C4	5.21	108.48	106.40
1	A	2	C	C5'-C4'-C3'	-5.20	107.67	116.00
1	B	31	A	C6-N1-C2	5.19	121.72	118.60
1	B	2	C	C5'-C4'-C3'	-5.18	107.71	116.00
1	B	3	G	C8-N9-C4	5.18	108.47	106.40
1	A	30	G	C8-N9-C4	5.18	108.47	106.40
1	A	31	A	C6-N1-C2	5.15	121.69	118.60
1	B	9	A	C6-N1-C2	5.12	121.67	118.60
1	A	9	A	C6-N1-C2	5.11	121.67	118.60
1	B	30	G	C8-N9-C4	5.11	108.44	106.40
1	A	48	C	N1-C2-O2	5.11	121.97	118.90
1	B	24	G	C8-N9-C4	5.11	108.44	106.40
1	B	48	C	N1-C2-O2	5.09	121.96	118.90
1	A	46	G	C8-N9-C4	5.08	108.43	106.40
1	A	24	G	C8-N9-C4	5.07	108.43	106.40
1	A	59	U	C5'-C4'-C3'	-5.07	107.89	116.00
1	B	59	U	C5'-C4'-C3'	-5.06	107.90	116.00
1	A	15	G	C8-N9-C4	5.06	108.42	106.40
1	A	55	U	N3-C4-O4	5.06	122.94	119.40
1	B	76	A	C6-N1-C2	5.04	121.63	118.60
1	A	42	G	C8-N9-C4	5.04	108.42	106.40
1	A	16	U	O4'-C1'-N1	5.03	112.23	108.20
1	B	44	A	C6-N1-C2	5.03	121.62	118.60
1	A	19	G	N3-C4-N9	5.02	129.01	126.00
1	B	42	G	C8-N9-C4	5.02	108.41	106.40
1	B	16	U	O4'-C1'-N1	5.02	112.22	108.20
1	A	65	G	C8-N9-C4	5.01	108.41	106.40
1	B	15	G	C8-N9-C4	5.01	108.41	106.40
1	A	62	A	C6-N1-C2	5.01	121.60	118.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1625	0	811	298	0
1	B	1625	0	814	296	0
All	All	3250	0	1625	438	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 91.

All (438) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:U:C4	1:B:34:G:H2'	1.18	1.64
1:A:37:G:C6	1:B:36:A:C2	2.04	1.45
1:A:33:U:C6	1:B:33:U:O2'	1.70	1.42
1:A:33:U:H1'	1:B:35:A:N6	1.41	1.36
1:A:32:C:C6	1:B:33:U:N3	1.70	1.35
1:A:39:U:H1'	1:B:37:G:O2'	1.24	1.34
1:A:33:U:C4	1:B:34:G:C2'	2.09	1.33
1:A:42:G:H3'	1:B:28:C:C5'	1.35	1.33
1:A:33:U:O4	1:B:34:G:C2'	1.77	1.32
1:A:33:U:C1'	1:B:35:A:H62	1.43	1.29
1:A:31:A:H3'	1:B:33:U:O4	1.24	1.27
1:A:42:G:C3'	1:B:28:C:C5'	2.10	1.27
1:A:42:G:OP1	1:B:27:C:H2'	1.15	1.27
1:A:33:U:C6	1:B:33:U:C2'	2.19	1.25
1:A:36:A:OP2	1:B:35:A:H1'	1.19	1.25
1:A:34:G:H5"	1:B:34:G:OP1	1.07	1.24
1:A:41:U:P	1:B:27:C:OP2	1.96	1.23
1:A:42:G:P	1:B:27:C:H2'	1.78	1.23
1:A:42:G:O3'	1:B:28:C:C4'	1.84	1.23
1:A:34:G:C5'	1:B:34:G:OP1	1.86	1.22
1:A:42:G:C3'	1:B:28:C:H5"	1.67	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:C:O3'	1:A:76:A:P	1.97	1.22
1:A:37:G:O6	1:B:36:A:C2	1.92	1.22
1:B:75:C:O3'	1:B:76:A:P	1.97	1.21
1:A:41:U:OP1	1:B:27:C:OP2	1.65	1.15
1:A:35:A:C8	1:B:34:G:N7	2.16	1.14
1:A:37:G:O6	1:B:36:A:N1	1.81	1.14
1:A:36:A:H2'	1:A:37:G:H5"	1.15	1.13
1:A:39:U:C2'	1:B:37:G:O3'	1.97	1.12
1:A:37:G:N7	1:B:35:A:H2	1.45	1.12
1:A:36:A:OP2	1:B:35:A:C1'	1.97	1.12
1:A:33:U:O4	1:B:34:G:H2'	0.94	1.11
1:A:41:U:OP2	1:B:27:C:OP2	1.66	1.10
1:A:35:A:H2'	1:B:34:G:N1	1.62	1.09
1:A:33:U:C1'	1:B:35:A:N6	2.07	1.09
1:A:40:C:C5	1:B:37:G:O5'	1.88	1.06
1:A:32:C:H6	1:B:33:U:N3	1.14	1.06
1:A:42:G:OP1	1:B:27:C:C2'	2.03	1.05
1:A:37:G:N7	1:B:35:A:C2	2.24	1.04
1:A:32:C:C6	1:B:36:A:OP2	1.96	1.03
1:A:33:U:H1'	1:B:35:A:C6	1.78	1.03
1:A:74:C:H2'	1:A:75:C:C6	1.95	1.02
1:B:1:G:O5'	1:B:1:G:P	2.18	1.02
1:B:74:C:H2'	1:B:75:C:C6	1.95	1.01
1:A:33:U:H6	1:B:33:U:C2'	1.60	1.01
1:A:39:U:H1'	1:B:37:G:C2'	1.80	1.00
1:A:33:U:N3	1:B:34:G:C4	1.91	0.99
1:A:35:A:H2'	1:B:34:G:C6	1.95	0.99
1:A:42:G:O3'	1:B:28:C:H4'	1.20	0.98
1:A:42:G:P	1:B:27:C:C2'	2.52	0.98
1:A:18:G:N2	1:A:57:G:H2'	1.78	0.98
1:A:37:G:N1	1:B:36:A:C2	2.31	0.98
1:A:31:A:C3'	1:B:33:U:O4	2.12	0.97
1:B:18:G:N2	1:B:57:G:H2'	1.78	0.97
1:A:39:U:C1'	1:B:37:G:O2'	2.12	0.97
1:A:37:G:O6	1:B:36:A:C6	2.18	0.96
1:B:36:A:H2'	1:B:37:G:H5"	1.15	0.96
1:A:39:U:O2'	1:B:38:A:P	2.24	0.95
1:A:33:U:C5	1:B:33:U:H2'	2.01	0.95
1:A:32:C:C2	1:B:35:A:C8	2.56	0.94
1:A:35:A:C8	1:B:34:G:C5	2.56	0.94
1:A:33:U:C3'	1:B:33:U:O2'	2.16	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:A:C2'	1:A:37:G:H5"	1.98	0.92
1:A:33:U:N3	1:B:34:G:N9	1.90	0.92
1:A:33:U:H3'	1:B:33:U:O2'	1.69	0.91
1:A:33:U:C1'	1:B:35:A:C6	2.47	0.91
1:A:20:G:H21	1:A:22:G:H5'	1.35	0.91
1:A:32:C:C2	1:B:35:A:C4	2.59	0.90
1:A:32:C:O2	1:B:35:A:C5	2.24	0.90
1:A:33:U:H6	1:B:33:U:O2'	1.23	0.90
1:A:32:C:N3	1:B:35:A:C4	2.15	0.89
1:A:33:U:C6	1:B:33:U:H2'	2.06	0.89
1:A:31:A:H2'	1:B:36:A:OP2	1.72	0.89
1:B:20:G:H21	1:B:22:G:H5'	1.35	0.88
1:A:20:G:H2'	1:A:21:A:H5"	1.54	0.88
1:B:20:G:H2'	1:B:21:A:H5"	1.54	0.88
1:A:32:C:H6	1:B:36:A:OP2	1.58	0.85
1:A:32:C:H2'	1:A:33:U:C6	2.12	0.85
1:A:42:G:OP2	1:B:27:C:C2'	2.10	0.85
1:B:1:G:P	1:B:1:G:OP1	2.36	0.84
1:B:32:C:H2'	1:B:33:U:C6	2.12	0.84
1:A:39:U:O2'	1:B:37:G:O3'	1.95	0.83
1:A:38:A:N1	1:B:37:G:C8	2.42	0.82
1:B:68:U:H2'	1:B:69:U:H6	1.44	0.82
1:A:68:U:H2'	1:A:69:U:H6	1.44	0.81
1:A:66:A:H2'	1:A:67:A:H8	1.46	0.81
1:A:35:A:H8	1:B:34:G:N7	1.75	0.81
1:B:47:U:C6	1:B:47:U:H5"	2.16	0.80
1:B:63:C:H2'	1:B:64:A:H8	1.46	0.80
1:A:39:U:H2'	1:B:37:G:O3'	1.80	0.80
1:B:66:A:H2'	1:B:67:A:H8	1.46	0.80
1:A:47:U:H5"	1:A:47:U:C6	2.16	0.80
1:A:63:C:H2'	1:A:64:A:H8	1.46	0.79
1:A:31:A:C2	1:B:37:G:OP2	2.35	0.79
1:A:32:C:O2	1:B:35:A:C4	2.36	0.79
1:B:20:G:N2	1:B:22:G:H5'	1.98	0.78
1:A:42:G:H3'	1:B:28:C:H5"	0.79	0.78
1:A:39:U:C1'	1:B:37:G:O3'	2.32	0.77
1:A:20:G:N2	1:A:22:G:H5'	1.98	0.77
1:B:75:C:C3'	1:B:76:A:P	2.72	0.77
1:B:14:A:H2'	1:B:15:G:H8	1.49	0.77
1:A:75:C:C3'	1:A:76:A:P	2.72	0.77
1:A:32:C:O4'	1:B:33:U:C2	2.29	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:A:H2'	1:A:15:G:H8	1.49	0.77
1:A:33:U:N3	1:B:34:G:H2'	1.95	0.77
1:A:74:C:H2'	1:A:75:C:H6	1.47	0.77
1:B:74:C:H2'	1:B:75:C:H6	1.47	0.77
1:A:33:U:H6	1:B:33:U:C1'	1.97	0.76
1:B:20:G:C2'	1:B:21:A:H5"	2.16	0.76
1:A:35:A:C2'	1:B:34:G:C6	2.66	0.76
1:A:43:G:P	1:B:28:C:H4'	2.25	0.75
1:A:33:U:C5	1:B:33:U:O2	2.39	0.75
1:B:32:C:H2'	1:B:33:U:H6	1.51	0.75
1:B:44:A:H2'	1:B:45:G:H8	1.52	0.74
1:A:16:U:H3	1:A:60:C:H1'	1.53	0.74
1:A:20:G:C2'	1:A:21:A:H5"	2.16	0.73
1:B:16:U:H3	1:B:60:C:H1'	1.53	0.73
1:A:37:G:N1	1:B:36:A:H2	1.86	0.73
1:A:33:U:C5	1:B:33:U:C2	2.77	0.72
1:A:44:A:H2'	1:A:45:G:H8	1.53	0.72
1:A:37:G:C6	1:B:36:A:N3	2.57	0.72
1:A:33:U:C1'	1:B:33:U:O2'	2.37	0.72
1:A:31:A:C2'	1:B:36:A:OP2	2.33	0.72
1:A:6:U:H2'	1:A:7:U:C6	2.25	0.71
1:B:6:U:H2'	1:B:7:U:C6	2.25	0.71
1:A:35:A:H8	1:B:34:G:C8	2.08	0.71
1:A:31:A:H3'	1:B:33:U:C4	2.22	0.70
1:B:28:C:H2'	1:B:29:A:H8	1.56	0.70
1:A:28:C:H2'	1:A:29:A:H8	1.56	0.69
1:A:68:U:H2'	1:A:69:U:C6	2.27	0.69
1:A:33:U:C5	1:B:33:U:C2'	2.63	0.69
1:B:37:G:H2'	1:B:38:A:H8	1.58	0.69
1:A:44:A:H2'	1:A:45:G:C8	2.28	0.69
1:B:14:A:H2'	1:B:15:G:C8	2.29	0.68
1:B:44:A:H2'	1:B:45:G:C8	2.28	0.68
1:A:74:C:H2'	1:A:75:C:C5	2.29	0.68
1:A:6:U:H2'	1:A:7:U:H6	1.58	0.68
1:A:37:G:H2'	1:A:38:A:H8	1.58	0.68
1:B:9:A:H61	1:B:22:G:H2'	1.59	0.68
1:A:32:C:H2'	1:A:33:U:H6	1.51	0.67
1:A:33:U:H2'	1:B:34:G:C8	2.30	0.67
1:A:34:G:H2'	1:A:35:A:O4'	1.94	0.67
1:A:9:A:H61	1:A:22:G:H2'	1.59	0.67
1:B:6:U:H2'	1:B:7:U:H6	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:C:H2'	1:B:75:C:C5	2.29	0.67
1:A:14:A:H2'	1:A:15:G:C8	2.29	0.67
1:A:33:U:O4'	1:B:35:A:N6	2.18	0.66
1:B:68:U:H2'	1:B:69:U:C6	2.27	0.66
1:A:43:G:OP2	1:B:28:C:C5'	2.44	0.66
1:A:33:U:H5	1:B:33:U:C2	2.13	0.66
1:A:32:C:C2	1:B:35:A:N9	2.36	0.65
1:B:36:A:C2'	1:B:37:G:H5"	1.97	0.65
1:A:47:U:N3	1:A:50:U:H5"	2.12	0.64
1:B:31:A:O2'	1:B:32:C:H5'	1.97	0.64
1:A:16:U:N3	1:A:60:C:H1'	2.13	0.63
1:B:47:U:N3	1:B:50:U:H5"	2.12	0.63
1:A:39:U:O2'	1:B:38:A:OP1	2.14	0.63
1:B:11:C:H2'	1:B:12:U:C6	2.33	0.63
1:B:10:G:H2'	1:B:11:C:C6	2.33	0.63
1:B:63:C:H2'	1:B:64:A:C8	2.30	0.63
1:A:63:C:H2'	1:A:64:A:C8	2.30	0.63
1:A:66:A:H2'	1:A:67:A:C8	2.33	0.63
1:B:8:U:H5'	1:B:49:C:OP2	1.99	0.63
1:A:33:U:C2'	1:B:33:U:O2'	2.46	0.63
1:A:34:G:OP2	1:B:33:U:O3'	2.17	0.63
1:B:16:U:N3	1:B:60:C:H1'	2.14	0.63
1:A:10:G:H2'	1:A:11:C:C6	2.33	0.62
1:A:33:U:C5	1:B:35:A:O5'	2.53	0.62
1:A:37:G:C6	1:B:36:A:N1	2.49	0.62
1:A:8:U:H5'	1:A:49:C:OP2	1.98	0.62
1:A:43:G:OP2	1:B:28:C:H5"	2.00	0.62
1:B:66:A:H2'	1:B:67:A:C8	2.33	0.61
1:A:25:C:O2'	1:A:26:G:H5'	2.00	0.61
1:A:37:G:H2'	1:A:38:A:C8	2.35	0.61
1:B:25:C:O2'	1:B:26:G:H5'	2.00	0.61
1:B:1:G:P	1:B:1:G:HO5'	2.22	0.61
1:B:37:G:H2'	1:B:38:A:C8	2.35	0.61
1:A:1:G:O2'	1:A:2:C:H5'	2.01	0.61
1:A:33:U:O4	1:B:35:A:O5'	2.17	0.60
1:A:41:U:H3'	1:B:28:C:OP2	2.01	0.60
1:B:39:U:H2'	1:B:40:C:C6	2.36	0.60
1:B:54:U:O2'	1:B:55:U:H5'	2.01	0.60
1:B:72:C:H2'	1:B:73:A:H8	1.64	0.60
1:A:42:G:O2'	1:B:29:A:OP1	2.07	0.60
1:A:39:U:H2'	1:A:40:C:C6	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:G:H2'	1:B:4:G:H8	1.67	0.60
1:A:3:G:H2'	1:A:4:G:H8	1.67	0.60
1:A:10:G:O2'	1:A:11:C:H5'	2.02	0.60
1:A:18:G:H1'	1:A:57:G:N2	2.17	0.60
1:B:68:U:H6	1:B:68:U:O5'	1.85	0.60
1:A:8:U:H5'	1:A:49:C:P	2.42	0.60
1:B:1:G:O2'	1:B:2:C:H5'	2.01	0.60
1:A:72:C:H2'	1:A:73:A:H8	1.65	0.60
1:A:33:U:C6	1:B:33:U:C1'	2.79	0.59
1:A:54:U:O2'	1:A:55:U:H5'	2.01	0.59
1:B:18:G:H1'	1:B:57:G:N2	2.17	0.59
1:A:23:A:H2'	1:A:24:G:C8	2.37	0.59
1:A:33:U:O5'	1:B:33:U:O2'	2.18	0.59
1:B:8:U:H4'	1:B:48:C:H4'	1.85	0.59
1:B:10:G:O2'	1:B:11:C:H5'	2.02	0.59
1:A:19:G:H5"	1:A:60:C:H42	1.67	0.59
1:B:23:A:H2'	1:B:24:G:C8	2.37	0.59
1:A:8:U:H4'	1:A:48:C:H4'	1.85	0.59
1:A:68:U:H6	1:A:68:U:O5'	1.85	0.59
1:B:8:U:H5'	1:B:49:C:P	2.42	0.59
1:B:47:U:H5"	1:B:47:U:H6	1.67	0.59
1:B:19:G:H5"	1:B:60:C:H42	1.67	0.58
1:A:47:U:H5"	1:A:47:U:H6	1.67	0.58
1:A:26:G:H2'	1:A:27:C:C6	2.38	0.58
1:A:37:G:O6	1:B:36:A:C5	2.56	0.58
1:B:26:G:H2'	1:B:27:C:C6	2.38	0.58
1:A:33:U:C4	1:B:34:G:C3'	2.87	0.58
1:A:53:G:O2'	1:A:54:U:H5'	2.04	0.58
1:A:31:A:C3'	1:B:33:U:C4	2.85	0.58
1:A:64:A:H2'	1:A:65:G:H8	1.69	0.58
1:B:30:G:O2'	1:B:31:A:H5'	2.04	0.57
1:B:53:G:O2'	1:B:54:U:H5'	2.04	0.57
1:A:32:C:C5	1:B:33:U:N3	2.59	0.57
1:A:56:C:O2'	1:A:57:G:H5'	2.04	0.57
1:A:62:A:H2'	1:A:63:C:C6	2.40	0.57
1:A:30:G:O2'	1:A:31:A:H5'	2.04	0.57
1:A:71:G:O2'	1:A:72:C:H5'	2.05	0.57
1:A:23:A:H2'	1:A:24:G:H8	1.70	0.57
1:B:23:A:H2'	1:B:24:G:H8	1.70	0.57
1:B:56:C:O2'	1:B:57:G:H5'	2.05	0.57
1:B:62:A:H2'	1:B:63:C:C6	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:G:O2'	1:B:72:C:H5'	2.05	0.57
1:A:20:G:C3'	1:A:21:A:H5"	2.35	0.57
1:A:43:G:H2'	1:A:44:A:C8	2.40	0.56
1:B:64:A:H2'	1:B:65:G:H8	1.69	0.56
1:A:11:C:H2'	1:A:12:U:C6	2.40	0.56
1:A:33:U:C6	1:B:33:U:O2	2.59	0.56
1:A:42:G:O3'	1:B:28:C:C5'	2.40	0.56
1:A:33:U:C1'	1:B:33:U:HO2'	2.18	0.56
1:A:33:U:N1	1:B:33:U:O2'	2.24	0.56
1:A:35:A:C8	1:B:34:G:C8	2.83	0.56
1:A:40:C:O2'	1:A:41:U:H5'	2.06	0.56
1:B:20:G:C3'	1:B:21:A:H5"	2.35	0.56
1:B:43:G:H2'	1:B:44:A:C8	2.40	0.56
1:A:67:A:O2'	1:A:68:U:H5'	2.06	0.55
1:B:51:G:H2'	1:B:52:U:C6	2.42	0.55
1:A:33:U:C4'	1:B:33:U:O2'	2.54	0.55
1:B:40:C:O2'	1:B:41:U:H5'	2.06	0.55
1:B:41:U:H2'	1:B:42:G:H8	1.72	0.55
1:A:37:G:O6	1:B:35:A:N1	2.40	0.55
1:A:41:U:H2'	1:A:42:G:H8	1.72	0.55
1:B:67:A:O2'	1:B:68:U:H5'	2.06	0.55
1:B:39:U:H2'	1:B:40:C:H6	1.73	0.54
1:A:51:G:H2'	1:A:52:U:C6	2.42	0.54
1:A:33:U:O4	1:B:34:G:O2'	2.24	0.54
1:A:35:A:N9	1:B:34:G:C5	2.76	0.54
1:A:30:G:C6	1:B:36:A:H5"	2.43	0.53
1:A:43:G:P	1:B:28:C:C5'	2.95	0.53
1:A:39:U:H2'	1:A:40:C:H6	1.73	0.53
1:A:32:C:OP2	1:B:33:U:O4	2.21	0.53
1:A:29:A:O2'	1:A:30:G:H5'	2.08	0.53
1:B:29:A:O2'	1:B:30:G:H5'	2.08	0.53
1:B:35:A:O2'	1:B:36:A:H5'	2.09	0.53
1:A:75:C:C2'	1:A:76:A:P	2.97	0.53
1:A:38:A:O2'	1:A:39:U:H5'	2.09	0.53
1:B:49:C:H2'	1:B:50:U:H6	1.74	0.53
1:B:75:C:C2'	1:B:76:A:P	2.97	0.53
1:A:32:C:C2	1:B:35:A:C5	2.90	0.53
1:B:38:A:O2'	1:B:39:U:H5'	2.09	0.52
1:A:43:G:P	1:B:28:C:H5"	2.49	0.52
1:B:2:C:H2'	1:B:3:G:C8	2.44	0.52
1:A:33:U:C2'	1:B:33:U:HO2'	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:U:H3’	1:B:33:U:O3’	2.10	0.52
1:A:49:C:H2’	1:A:50:U:H6	1.74	0.52
1:B:18:G:H1’	1:B:57:G:C2	2.45	0.52
1:A:18:G:H1’	1:A:57:G:C2	2.45	0.52
1:B:1:G:P	1:B:1:G:C5’	2.97	0.52
1:B:19:G:N2	1:B:57:G:H1’	2.25	0.52
1:A:2:C:H2’	1:A:3:G:C8	2.44	0.52
1:A:33:U:O4’	1:B:33:U:O2’	2.28	0.52
1:A:19:G:N2	1:A:57:G:H1’	2.25	0.51
1:A:27:C:H2’	1:A:28:C:C6	2.43	0.51
1:B:47:U:H3	1:B:50:U:H5”	1.74	0.51
1:B:52:U:O2’	1:B:53:G:H5’	2.10	0.51
1:A:35:A:O2’	1:A:36:A:H5’	2.09	0.51
1:A:73:A:O2’	1:A:74:C:H5’	2.10	0.51
1:A:33:U:H5	1:B:35:A:O5’	1.93	0.51
1:A:36:A:H2’	1:A:37:G:C5’	2.11	0.51
1:A:52:U:O2’	1:A:53:G:H5’	2.10	0.51
1:B:73:A:O2’	1:B:74:C:H5’	2.10	0.51
1:B:14:A:C2	1:B:15:G:H1’	2.46	0.51
1:A:18:G:H22	1:A:57:G:H2’	1.71	0.51
1:B:47:U:C6	1:B:47:U:C5’	2.91	0.51
1:B:55:U:O4	1:B:57:G:H3’	2.10	0.51
1:A:24:G:O2’	1:A:25:C:H5’	2.11	0.51
1:A:33:U:C5	1:B:34:G:H3’	2.46	0.51
1:A:47:U:C6	1:A:47:U:C5’	2.91	0.50
1:A:33:U:C4	1:B:34:G:N9	2.70	0.50
1:A:55:U:O4	1:A:57:G:H3’	2.10	0.50
1:A:33:U:OP2	1:B:33:U:C6	2.65	0.50
1:A:37:G:O6	1:B:36:A:N3	2.39	0.50
1:A:14:A:C2	1:A:15:G:H1’	2.46	0.50
1:B:47:U:H6	1:B:47:U:C5’	2.25	0.50
1:B:24:G:O2’	1:B:25:C:H5’	2.11	0.50
1:A:47:U:H3	1:A:50:U:H5”	1.74	0.50
1:A:47:U:H6	1:A:47:U:C5’	2.25	0.50
1:A:35:A:OP2	1:B:33:U:O2’	2.27	0.49
1:B:58:A:H1’	1:B:60:C:OP2	2.11	0.49
1:B:58:A:H4’	1:B:59:U:OP1	2.12	0.49
1:A:58:A:H1’	1:A:60:C:OP2	2.11	0.49
1:B:10:G:H2’	1:B:11:C:H6	1.77	0.49
1:B:20:G:H2’	1:B:21:A:C5’	2.35	0.49
1:A:38:A:C6	1:B:37:G:C8	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:U:H6	1:B:33:U:H1'	1.73	0.49
1:A:9:A:N6	1:A:22:G:H2'	2.27	0.49
1:A:10:G:H2'	1:A:11:C:H6	1.77	0.49
1:A:18:G:H21	1:A:57:G:H2'	1.73	0.49
1:A:39:U:O2'	1:B:38:A:H5'	2.12	0.48
1:B:9:A:N6	1:B:22:G:H2'	2.26	0.48
1:B:37:G:O2'	1:B:38:A:H5'	2.14	0.48
1:B:18:G:H22	1:B:57:G:H2'	1.71	0.48
1:B:64:A:O2'	1:B:65:G:H5'	2.14	0.48
1:B:11:C:H2'	1:B:12:U:H6	1.78	0.48
1:B:35:A:C4	1:B:36:A:C8	3.02	0.48
1:B:4:G:H1	1:B:69:U:H3	1.62	0.47
1:A:31:A:C2	1:B:37:G:H5'	2.48	0.47
1:B:3:G:C6	1:B:71:G:C6	3.02	0.47
1:A:33:U:C2'	1:B:34:G:N7	2.76	0.47
1:A:37:G:O6	1:B:36:A:C4	2.66	0.47
1:A:64:A:O2'	1:A:65:G:H5'	2.14	0.47
1:A:44:A:H2'	1:A:45:G:O4'	2.14	0.47
1:A:58:A:H4'	1:A:59:U:OP1	2.12	0.47
1:A:5:A:H2'	1:A:6:U:C6	2.50	0.47
1:A:3:G:C6	1:A:71:G:C6	3.02	0.47
1:B:33:U:H2'	1:B:35:A:OP2	2.14	0.47
1:A:35:A:C4	1:A:36:A:C8	3.02	0.47
1:A:37:G:O2'	1:A:38:A:H5'	2.14	0.47
1:A:33:U:N3	1:B:34:G:C1'	2.76	0.47
1:B:4:G:C6	1:B:70:C:N3	2.83	0.47
1:A:4:G:C6	1:A:70:C:N3	2.83	0.47
1:A:33:U:C4'	1:B:35:A:H62	2.25	0.47
1:A:43:G:OP2	1:B:28:C:H5'	2.14	0.47
1:A:17:U:O3'	1:A:18:G:H3'	2.15	0.46
1:B:18:G:P	1:B:18:G:H3'	2.55	0.46
1:A:31:A:N1	1:B:37:G:OP2	2.48	0.46
1:A:33:U:H2'	1:A:35:A:OP2	2.14	0.46
1:B:5:A:H2'	1:B:6:U:C6	2.50	0.46
1:A:31:A:H2'	1:B:33:U:C4	2.51	0.46
1:A:34:G:O5'	1:B:34:G:OP1	2.33	0.46
1:B:67:A:H2'	1:B:68:U:C6	2.50	0.46
1:A:4:G:H1	1:A:69:U:H3	1.62	0.46
1:A:39:U:O2'	1:B:38:A:C5'	2.63	0.46
1:A:20:G:H3'	1:A:21:A:H5"	1.98	0.46
1:A:72:C:O2'	1:A:73:A:H5'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:A:H2'	1:A:68:U:C6	2.50	0.46
1:B:44:A:H2'	1:B:45:G:O4'	2.14	0.46
1:B:72:C:O2'	1:B:73:A:H5'	2.16	0.46
1:A:18:G:H3'	1:A:18:G:P	2.55	0.46
1:A:26:G:H2'	1:A:27:C:H6	1.80	0.46
1:A:41:U:H2'	1:A:42:G:C8	2.51	0.46
1:A:65:G:O2'	1:A:66:A:H5'	2.16	0.46
1:A:2:C:H2'	1:A:3:G:H8	1.81	0.45
1:A:33:U:OP2	1:B:33:U:H6	1.98	0.45
1:A:39:U:H1'	1:B:37:G:O3'	2.01	0.45
1:A:51:G:C6	1:A:64:A:C6	3.04	0.45
1:A:33:U:C4	1:B:35:A:O5'	2.69	0.45
1:A:38:A:H2'	1:A:39:U:H6	1.81	0.45
1:B:2:C:H2'	1:B:3:G:H8	1.81	0.45
1:B:17:U:O3'	1:B:18:G:H3'	2.15	0.45
1:A:36:A:C2'	1:A:37:G:C5'	2.84	0.45
1:A:43:G:P	1:B:28:C:C4'	2.98	0.45
1:B:41:U:H2'	1:B:42:G:C8	2.51	0.45
1:A:39:U:H1'	1:B:37:G:HO2'	1.63	0.45
1:B:65:G:O2'	1:B:66:A:H5'	2.16	0.45
1:B:51:G:C6	1:B:64:A:C6	3.04	0.45
1:A:30:G:O6	1:B:36:A:O3'	2.35	0.44
1:B:13:C:O2'	1:B:14:A:H5'	2.17	0.44
1:A:5:A:O2'	1:A:6:U:H5'	2.18	0.44
1:A:20:G:H2'	1:A:21:A:C5'	2.35	0.44
1:A:13:C:O2'	1:A:14:A:H5'	2.17	0.44
1:A:33:U:P	1:B:32:C:O2'	2.76	0.44
1:B:4:G:C2	1:B:5:A:C4	3.05	0.44
1:B:26:G:H2'	1:B:27:C:H6	1.80	0.44
1:A:32:C:O4'	1:B:33:U:N3	2.51	0.44
1:B:20:G:H3'	1:B:21:A:H5"	1.98	0.44
1:B:38:A:H2'	1:B:39:U:H6	1.81	0.44
1:A:14:A:O2'	1:A:15:G:H5'	2.17	0.44
1:A:29:A:C6	1:A:42:G:C6	3.06	0.43
1:B:33:U:C6	1:B:35:A:OP2	2.71	0.43
1:A:18:G:C6	1:A:58:A:C5	3.06	0.43
1:A:57:G:O2'	1:A:58:A:H5'	2.18	0.43
1:B:5:A:O2'	1:B:6:U:H5'	2.18	0.43
1:B:14:A:O2'	1:B:15:G:H5'	2.17	0.43
1:B:29:A:C6	1:B:42:G:C6	3.06	0.43
1:A:4:G:C2	1:A:5:A:C4	3.05	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:G:C6	1:B:58:A:C5	3.06	0.43
1:A:33:U:C6	1:A:35:A:OP2	2.71	0.43
1:A:68:U:O2'	1:A:69:U:H5'	2.19	0.43
1:B:68:U:O2'	1:B:69:U:H5'	2.19	0.43
1:A:62:A:O2'	1:A:63:C:H5'	2.18	0.43
1:B:14:A:H2'	1:B:15:G:O4'	2.19	0.42
1:B:57:G:O2'	1:B:58:A:H5'	2.19	0.42
1:B:62:A:O2'	1:B:63:C:H5'	2.18	0.42
1:A:14:A:H2'	1:A:15:G:O4'	2.19	0.42
1:A:36:A:O4'	1:B:34:G:N1	2.52	0.42
1:B:30:G:C6	1:B:31:A:C5	3.08	0.42
1:B:49:C:O2'	1:B:50:U:H5'	2.19	0.42
1:A:49:C:O2'	1:A:50:U:H5'	2.19	0.42
1:A:51:G:C5	1:A:52:U:C4	3.07	0.42
1:B:51:G:C5	1:B:52:U:C4	3.07	0.42
1:A:42:G:OP1	1:B:28:C:O4'	2.37	0.42
1:B:55:U:H2'	1:B:56:C:H3'	2.02	0.42
1:A:8:U:H2'	1:A:46:G:N2	2.35	0.42
1:A:18:G:H4'	1:A:19:G:OP1	2.20	0.42
1:B:8:U:H2'	1:B:46:G:N2	2.35	0.42
1:A:39:U:O2'	1:A:40:C:H5'	2.20	0.42
1:B:18:G:H4'	1:B:19:G:OP1	2.20	0.42
1:B:19:G:H5"	1:B:60:C:N4	2.33	0.42
1:A:31:A:H2	1:B:37:G:H5'	1.83	0.41
1:A:55:U:H2'	1:A:56:C:H3'	2.02	0.41
1:B:14:A:C4	1:B:15:G:C8	3.09	0.41
1:A:30:G:C6	1:A:31:A:C5	3.07	0.41
1:A:33:U:N3	1:B:34:G:C2'	2.63	0.41
1:A:25:C:H2'	1:A:26:G:O4'	2.21	0.41
1:A:32:C:C2	1:B:35:A:N7	2.86	0.41
1:B:42:G:H2'	1:B:43:G:H8	1.86	0.41
1:A:42:G:H2'	1:A:43:G:H8	1.86	0.41
1:B:18:G:H2'	1:B:18:G:OP1	2.21	0.41
1:A:28:C:H2'	1:A:29:A:C8	2.46	0.41
1:A:8:U:O2	1:A:21:A:H2	2.04	0.41
1:A:33:U:C2'	1:B:34:G:C8	3.02	0.41
1:B:42:G:O2'	1:B:43:G:H5'	2.21	0.41
1:B:49:C:H2'	1:B:50:U:C6	2.55	0.41
1:A:18:G:H2'	1:A:18:G:OP1	2.21	0.41
1:B:18:G:H21	1:B:57:G:H2'	1.73	0.41
1:B:32:C:O2'	1:B:33:U:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:U:O2'	1:B:40:C:H5'	2.20	0.41
1:A:14:A:C4	1:A:15:G:C8	3.09	0.41
1:A:32:C:O2'	1:A:33:U:H5'	2.20	0.41
1:A:51:G:O2'	1:A:52:U:H5'	2.21	0.41
1:A:11:C:H6	1:A:11:C:O5'	2.04	0.40
1:A:49:C:H2'	1:A:50:U:C6	2.55	0.40
1:A:26:G:O2'	1:A:27:C:H5'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein molecules in this entry.

5.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	75/76 (98%)	9 (12%)	4 (5%)
1	B	75/76 (98%)	9 (12%)	4 (5%)
All	All	150/152 (98%)	18 (12%)	8 (5%)

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	16	U
1	A	17	U
1	A	18	G
1	A	21	A
1	A	37	G
1	A	46	G
1	A	47	U
1	A	48	C
1	A	76	A

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Mol	Chain	Res	Type
1	B	16	U
1	B	17	U
1	B	18	G
1	B	21	A
1	B	37	G
1	B	46	G
1	B	47	U
1	B	48	C
1	B	76	A

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	16	U
1	A	17	U
1	A	46	G
1	A	47	U
1	B	16	U
1	B	17	U
1	B	46	G
1	B	47	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
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	75:C	O3'	76:A	P	1.97
1	B	75:C	O3'	76:A	P	1.97

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1249. 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

6.1.1 Primary map

X

Y

Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 65

Y Index: 65

Z Index: 65

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: 54

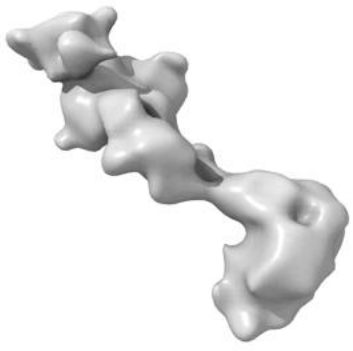
Y Index: 59

Z Index: 68

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

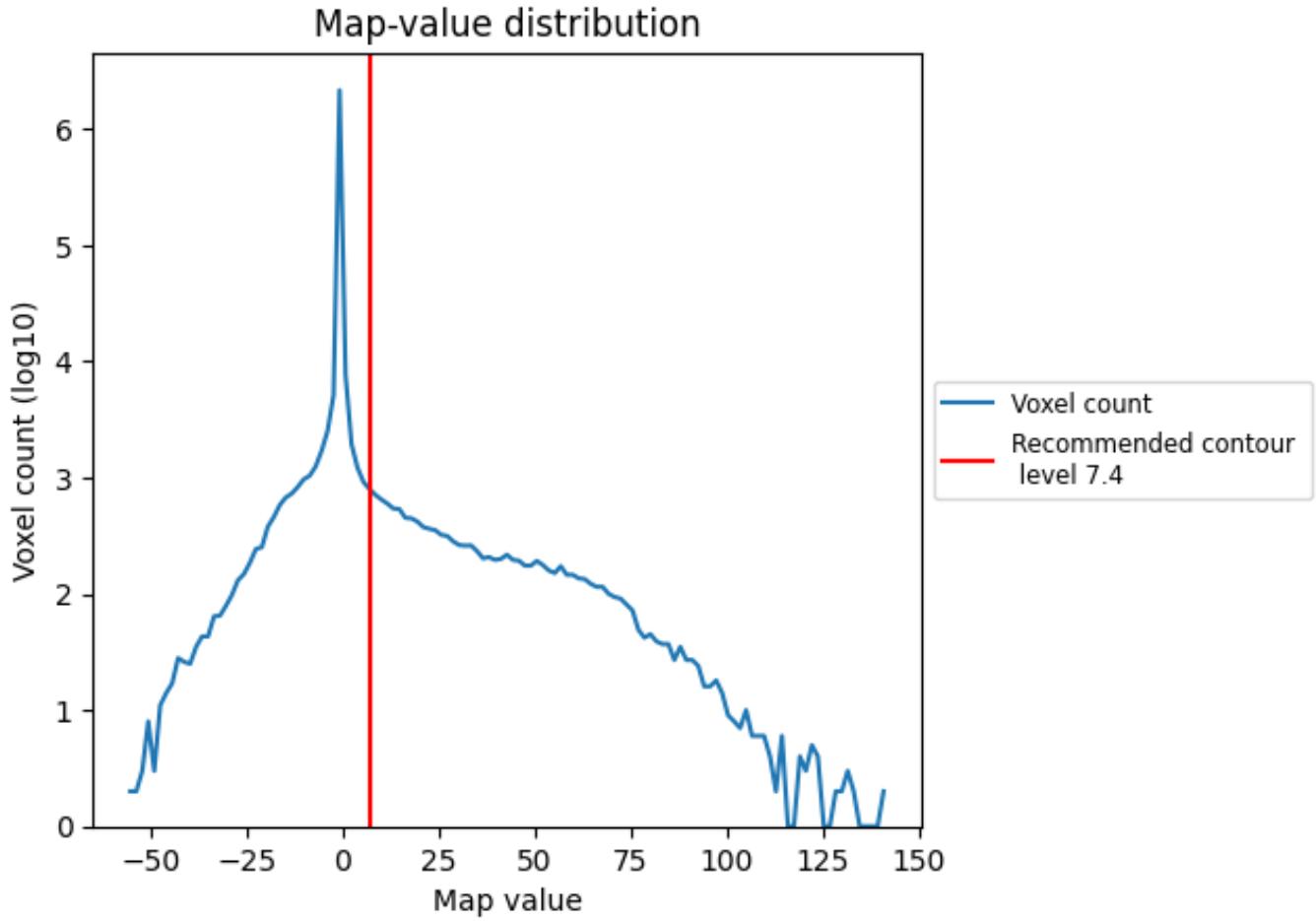
6.5 Mask visualisation (i)

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

7 Map analysis

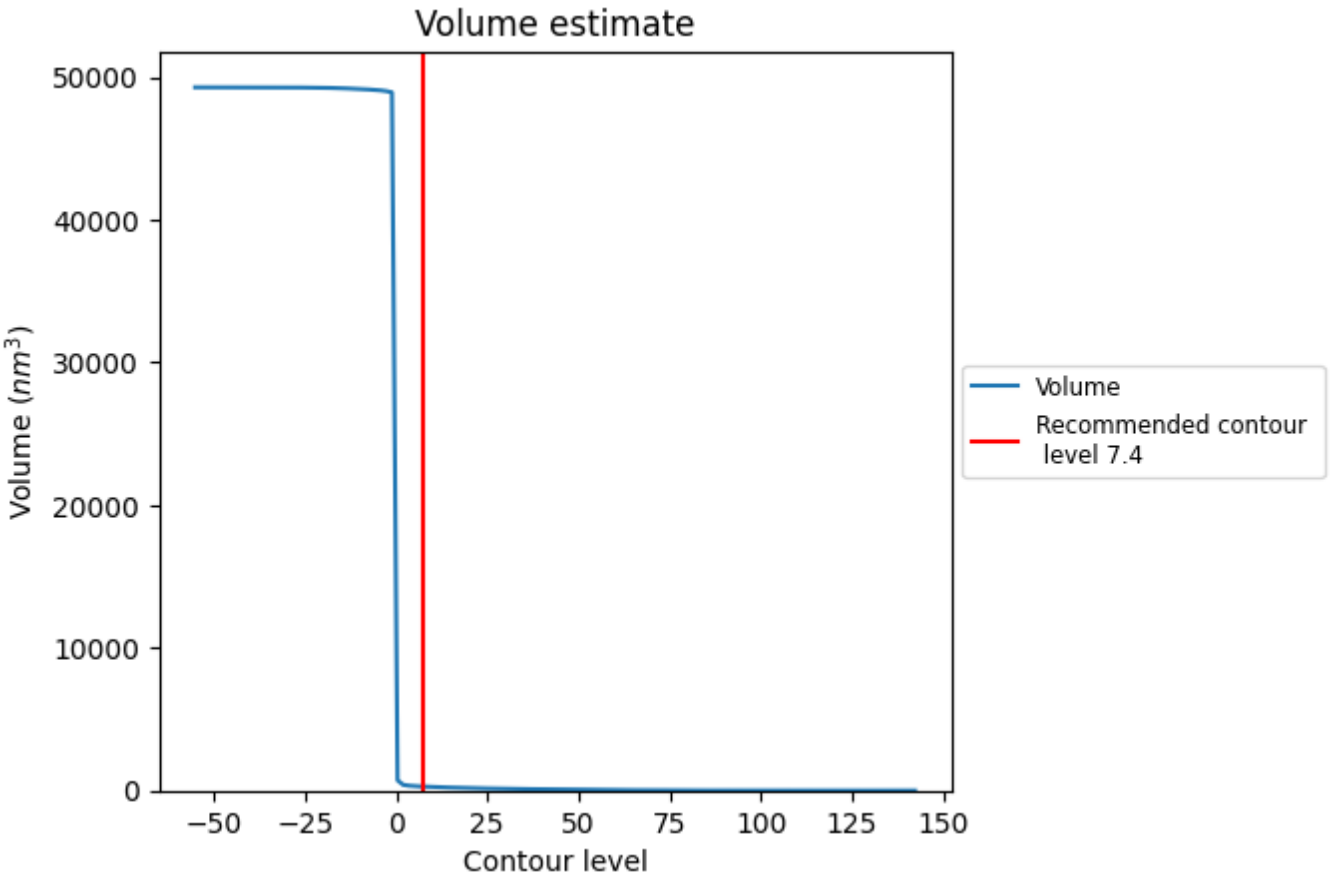
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

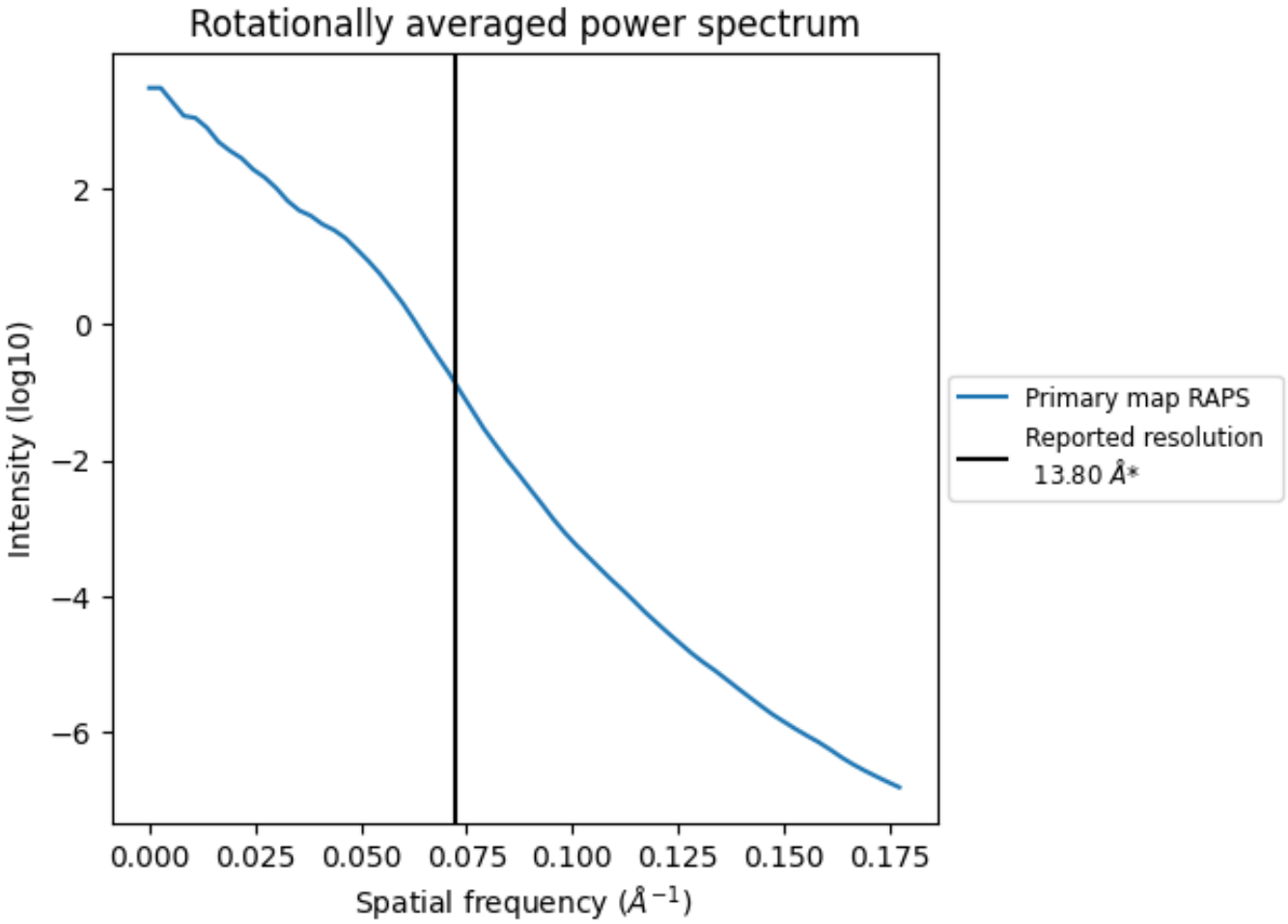
7.2 Volume estimate (i)



The volume at the recommended contour level is 280 nm^3; this corresponds to an approximate mass of 253 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.072 Å^{-1}

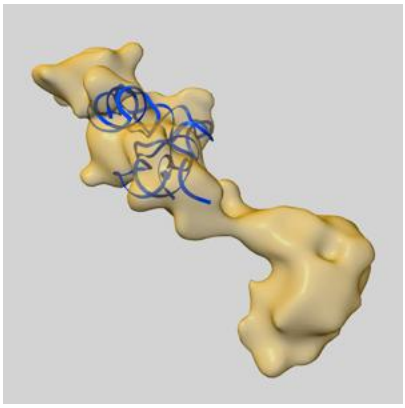
8 Fourier-Shell correlation

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

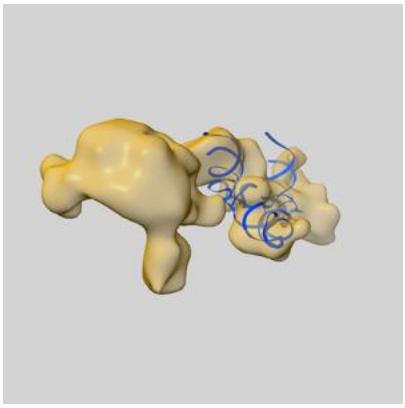
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1249 and PDB model 1ZO3. Per-residue inclusion information can be found in section 3 on page 4.

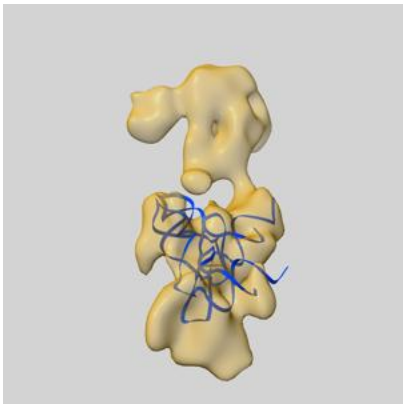
9.1 Map-model overlay



X



Y



Z

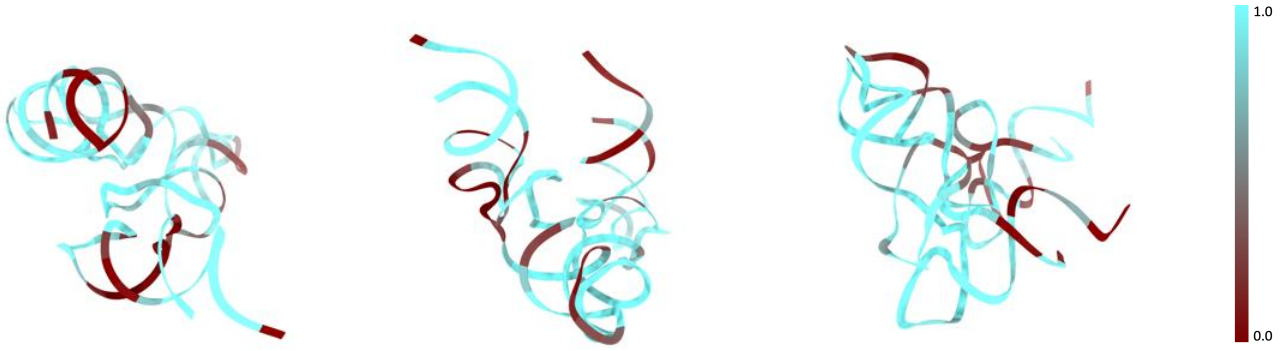
The images above show the 3D surface view of the map at the recommended contour level 7.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

X Y Z

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

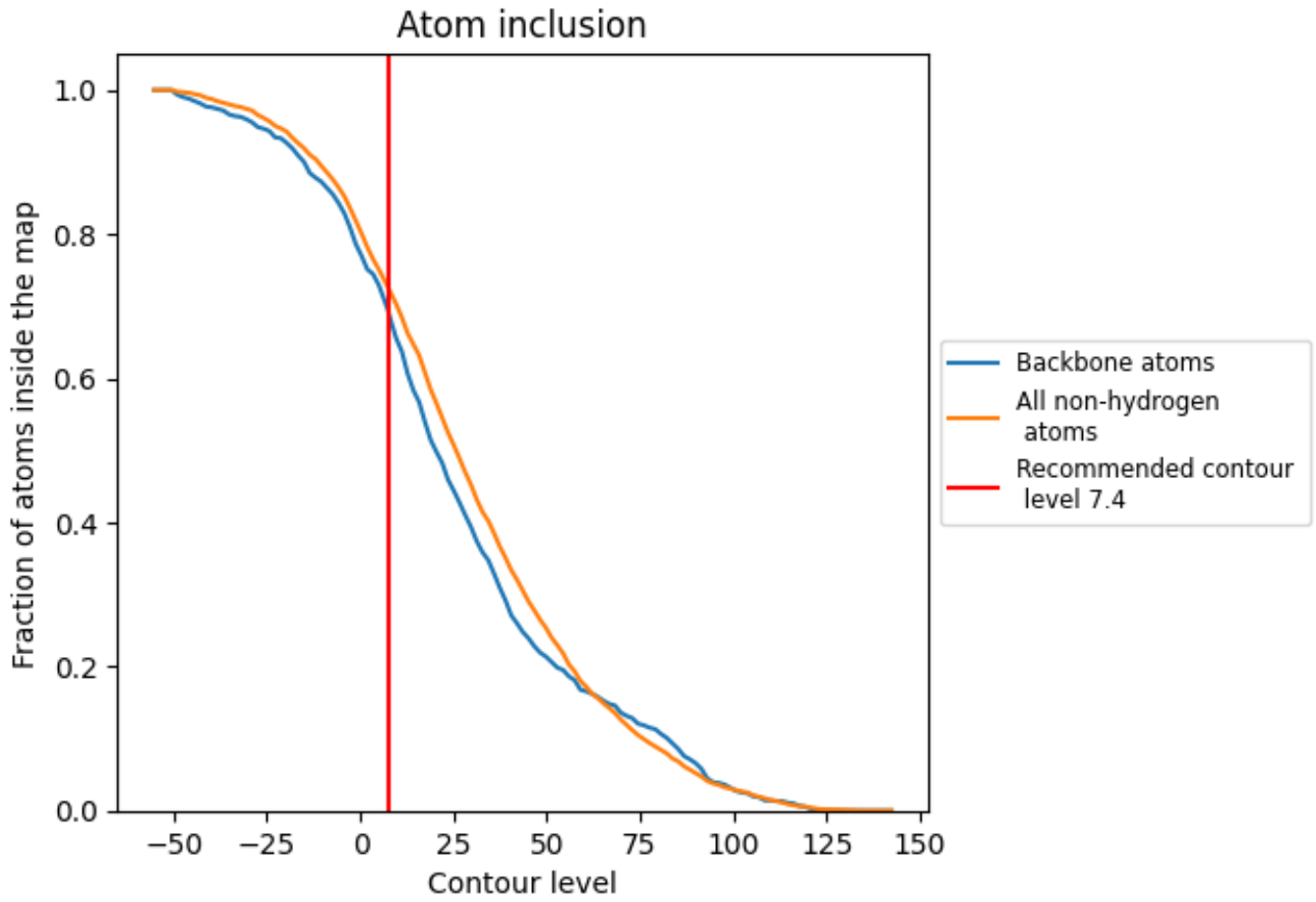
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (7.4).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (7.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7268	0.0250
A	0.6634	0.0130
B	0.7902	0.0360