



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:35 AM UTC

PDB ID : 9Y74 / pdb_00009y74
Title : [22L-7B C|A] 22 bp L-DNA tensegrity triangle that propagates via blunt-end stacking with C stacking on A at the interface
Authors : Horvath, A.; Woloszyn, K.; Vecchioni, S.; Ohayon, Y.P.; Sha, R.
Deposited on : 2025-09-09
Resolution : 8.76 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

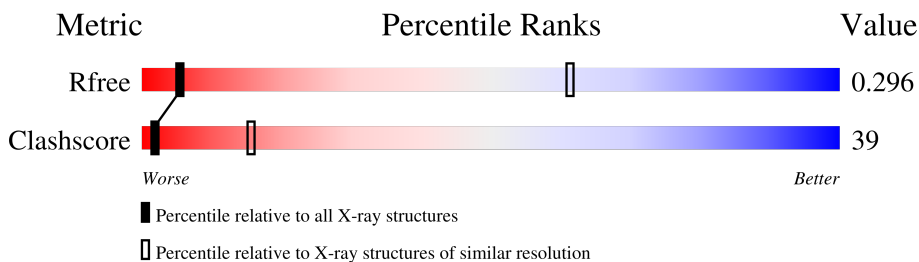
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.76 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)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1168 (11.50-4.00)
Clashscore	190562	1001 (11.50-4.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	A	22	5%	95%
2	B	7	14%	86%
3	C	7	14%	86%
4	D	8	12%	88%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	ODT	A	111	-	X	-	-
4	ODT	D	102	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ODT	D	105	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 896 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 DNA chain called DNA (5'-D*(0DC)P*(0DG)P*(0DA)P*(0DT)P*(0DG)P*(0DC)P*(0DC)P*(0DT)P*(0DG)P*(0DT)P*(0DA)P*(0DC)P*(0DG)(0DG)P*(0DA)P*(0DC)P*(0DA)P*(0DG)P*(0DA)P*(0DT)P*(0DC)P*(0DA))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	22	Total	C	N	O	P	0	0	0
			449	214	86	128	21			

- Molecule 2 is a DNA chain called DNA (5'-D(P*(0DC)P*(0DC)P*(0DG)P*(0DT)P*(0DA)P*(0DC)P*(0DA))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	P	0	0	0
			141	67	26	41	7			

- Molecule 3 is a DNA chain called DNA (5'-D(P*(0DG)P*(0DG)P*(0DC)P*(0DA)P*(0DT)P*(0DC)P*(0DG))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	7	Total	C	N	O	P	0	0	0
			145	68	28	42	7			

- Molecule 4 is a DNA chain called DNA (5'-D*(0DT)P*(0DG)P*(0DA)P*(0DT)P*(0DC)P*(0DT)P*(0DG)P*(0DT))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	8	Total	C	N	O	P	0	0	0
			161	79	26	49	7			

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: DNA (5'-D*(0DC)P*(0DG)P*(0DA)P*(0DT)P*(0DG)P*(0DC)P*(0DC)P*(0DT)P*(0DG)P*(0DT)P*(0DA)P*(0DC)P*(0DG)(0DG)P*(0DA)P*(0DC)P*(0DA)P*(0DG)P*(0DA)P*(0DT)P*(0DC)P*(0DA))-3')

Chain A:  5% 95%

G104	G105	A106	T107	G108	G109	C110	T111	G112	T113	A114	C115	G116	G117	A118	C119	A120	G121	A122	T123	C124	A125
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- Molecule 2: DNA (5'-D(P*(0DC)P*(0DC)P*(0DG)P*(0DT)P*(0DA)P*(0DC)P*(0DA))-3')

Chain B:  14% 86%

G119	C120	G121	T122	A123	C124	A125
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- Molecule 3: DNA (5'-D(P*(0DG)P*(0DG)P*(0DC)P*(0DA)P*(0DT)P*(0DC)P*(0DG))-3')

Chain C:  14% 86%

G209	G210	C211	A212	T213	C214	G215
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- Molecule 4: DNA (5'-D*(0DT)P*(0DG)P*(0DA)P*(0DT)P*(0DC)P*(0DT)P*(0DG)P*(0DT))-3')

Chain D:  12% 88%

T102	G103	A104	T105	C106	T107	G108	T109
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4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	130.40Å 130.40Å 61.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.47 – 8.76 56.47 – 8.76	Depositor EDS
% Data completeness (in resolution range)	83.8 (56.47-8.76) 78.8 (56.47-8.76)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 8.36Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.237 , 0.317 0.235 , 0.296	Depositor DCC
R_{free} test set	16 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	-40.3	Xtriage
Anisotropy	1.498	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	-0.12 , 129.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.07$, $\langle L^2 \rangle = 0.01$	Xtriage
Estimated twinning fraction	0.231 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	896	wwPDB-VP
Average B, all atoms (Å ²)	358.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7941e-03.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0DC, 0DT, 0DA, 0DG

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	449	0	238	29	0
2	B	141	0	75	10	0
3	C	145	0	77	9	0
4	D	161	0	86	14	0
All	All	896	0	476	52	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 39.

All (52) 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)
4:D:107:0DT:H73	4:D:107:0DT:H72	1.58	0.85
3:C:209:0DG:H2'	3:C:210:0DG:H8	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:107:0DT:H72	4:D:107:0DT:H71	1.58	0.84
4:D:107:0DT:H73	4:D:107:0DT:H71	1.58	0.83
1:A:125:0DA:H2A	4:D:102:0DT:O2	1.82	0.79
1:A:105:0DG:H2''	1:A:106:0DA:H8A	1.68	0.73
1:A:119:0DC:H1'	1:A:120:0DA:N7A	2.03	0.73
1:A:105:0DG:H8	1:A:105:0DG:O5'	1.90	0.72
3:C:210:0DG:H2''	3:C:211:0DC:H5	1.70	0.72
1:A:114:0DA:N1A	2:B:122:0DT:N3	2.36	0.68
1:A:114:0DA:H2''	1:A:115:0DC:H5	1.76	0.68
3:C:212:0DA:H2'	3:C:213:0DT:H71	1.77	0.66
1:A:116:0DG:H2''	1:A:117:0DG:C8	2.31	0.61
1:A:125:0DA:N1A	4:D:102:0DT:N3	2.44	0.61
1:A:119:0DC:H1'	1:A:120:0DA:C8A	2.30	0.61
2:B:119:0DC:C6	4:D:109:0DT:H2''	2.31	0.60
3:C:209:0DG:H2'	3:C:210:0DG:C8	2.32	0.56
3:C:209:0DG:H2''	3:C:210:0DG:H5''	1.86	0.56
4:D:102:0DT:H4'	4:D:103:0DG:H5''	1.87	0.56
1:A:114:0DA:H2A	2:B:122:0DT:O2	2.06	0.55
3:C:210:0DG:H2''	3:C:211:0DC:C5	2.36	0.55
2:B:122:0DT:OP1	2:B:122:0DT:H6	2.06	0.55
1:A:119:0DC:H5'	1:A:120:0DA:H5'	1.89	0.55
1:A:122:0DA:H5''	1:A:122:0DA:H8A	1.88	0.55
1:A:110:0DC:H2''	1:A:111:0DT:C6	2.38	0.54
1:A:118:0DA:N1A	4:D:109:0DT:N3	2.41	0.54
1:A:108:0DG:H2''	1:A:109:0DC:H5'	1.88	0.54
2:B:121:0DG:H2''	2:B:122:0DT:H71	1.91	0.53
1:A:105:0DG:H2''	1:A:106:0DA:H5''	1.89	0.53
2:B:119:0DC:H1'	4:D:109:0DT:O3'	2.09	0.52
2:B:119:0DC:P	2:B:120:0DC:H6	2.49	0.52
4:D:108:0DG:H2''	4:D:109:0DT:H5'	1.93	0.51
1:A:105:0DG:H2''	1:A:106:0DA:C8A	2.36	0.51
1:A:112:0DG:H2''	1:A:113:0DT:O4'	2.12	0.50
1:A:122:0DA:H2'	1:A:123:0DT:H71	1.93	0.49
1:A:104:0DC:H6	1:A:104:0DC:O5'	2.13	0.49
1:A:116:0DG:H1'	1:A:117:0DG:O4'	2.13	0.48
1:A:114:0DA:H2''	1:A:115:0DC:C5	2.41	0.48
4:D:104:0DA:N3A	4:D:105:0DT:H5''	2.29	0.48
1:A:116:0DG:H4'	1:A:117:0DG:H5''	1.96	0.48
4:D:102:0DT:H1'	4:D:103:0DG:C4	2.45	0.47
1:A:106:0DA:H2'	1:A:107:0DT:H71	1.96	0.46
2:B:123:0DA:H1'	2:B:124:0DC:C6	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:0DA:N6A	3:C:213:0DT:O4	2.36	0.45
1:A:118:0DA:H2A	4:D:109:0DT:O2	2.17	0.44
2:B:120:0DC:H1'	2:B:121:0DG:H5''	1.99	0.44
3:C:211:0DC:H2''	3:C:212:0DA:C8A	2.48	0.44
1:A:124:0DC:C2	4:D:103:0DG:H21	2.21	0.43
1:A:117:0DG:H4'	1:A:118:0DA:OP2	2.18	0.42
3:C:214:0DC:H2'	3:C:214:0DC:H6	1.76	0.41
2:B:120:0DC:H6	2:B:120:0DC:H2'	1.81	0.41
1:A:106:0DA:C2'	1:A:107:0DT:H71	2.50	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](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

44 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	0DA	B	125	2	20,23,24	3.80	10 (50%)	28,33,36	2.98	14 (50%)
1	0DA	A	106	1	20,23,24	3.81	10 (50%)	28,33,36	2.86	13 (46%)
3	0DT	C	213	3	18,21,22	5.43	14 (77%)	25,30,33	2.55	9 (36%)
1	0DT	A	107	1	18,21,22	5.38	15 (83%)	25,30,33	2.56	9 (36%)
1	0DT	A	113	1	18,21,22	5.36	15 (83%)	25,30,33	2.58	10 (40%)
1	0DA	A	118	1	20,23,24	3.75	8 (40%)	28,33,36	2.90	13 (46%)
2	0DC	B	124	1,2	17,20,21	4.36	13 (76%)	23,28,31	1.12	2 (8%)
1	0DC	A	104	1,3	17,17,21	4.34	13 (76%)	24,24,31	1.35	4 (16%)
4	0DG	D	103	1,4	21,24,25	3.68	14 (66%)	30,35,38	2.29	11 (36%)
1	0DC	A	119	1	17,20,21	4.41	14 (82%)	23,28,31	1.60	2 (8%)
2	0DC	B	120	1,2	17,20,21	4.27	13 (76%)	23,28,31	0.86	0
4	0DC	D	106	1,4	17,20,21	4.54	14 (82%)	23,28,31	1.43	2 (8%)
2	0DT	B	122	2	18,21,22	5.26	14 (77%)	25,30,33	2.50	8 (32%)
1	0DA	A	125	1	20,23,24	3.82	10 (50%)	28,33,36	2.97	13 (46%)
1	0DC	A	110	1,3	17,20,21	4.35	13 (76%)	23,28,31	1.75	6 (26%)
1	0DA	A	122	1	20,23,24	3.76	8 (40%)	28,33,36	3.05	13 (46%)
1	0DG	A	108	1,3	21,24,25	3.77	14 (66%)	30,35,38	2.26	10 (33%)
3	0DG	C	215	1,3	21,24,25	3.81	14 (66%)	30,35,38	2.60	11 (36%)
4	0DA	D	104	4	20,23,24	3.72	9 (45%)	28,33,36	3.12	15 (53%)
1	0DT	A	123	1	18,21,22	5.34	14 (77%)	25,30,33	2.30	9 (36%)
1	0DG	A	121	1,4	21,24,25	3.77	14 (66%)	30,35,38	2.26	10 (33%)
1	0DC	A	115	1,2	17,20,21	4.40	14 (82%)	23,28,31	1.56	3 (13%)
1	0DT	A	111	1	18,21,22	5.30	14 (77%)	25,30,33	2.54	9 (36%)
4	0DT	D	105	4	18,21,22	5.28	14 (77%)	25,30,33	2.59	12 (48%)
2	0DC	B	119	1,2	17,20,21	4.38	13 (76%)	23,28,31	1.94	5 (21%)
1	0DG	A	112	1,2	21,24,25	3.67	14 (66%)	30,35,38	2.26	12 (40%)
3	0DG	C	210	1,3	21,24,25	3.72	13 (61%)	30,35,38	2.37	13 (43%)
3	0DG	C	209	1,3	21,24,25	3.83	14 (66%)	30,35,38	2.27	10 (33%)
1	0DA	A	114	1	20,23,24	3.70	8 (40%)	28,33,36	2.97	13 (46%)
2	0DG	B	121	1,2	21,24,25	3.81	14 (66%)	30,35,38	2.80	13 (43%)
1	0DG	A	117	1,2	21,24,25	3.74	13 (61%)	30,35,38	2.59	16 (53%)
2	0DA	B	123	2	20,23,24	3.82	10 (50%)	28,33,36	3.14	12 (42%)
1	0DG	A	105	1,3	21,24,25	3.79	14 (66%)	30,35,38	2.21	8 (26%)
3	0DA	C	212	3	20,23,24	3.74	9 (45%)	28,33,36	2.99	13 (46%)
3	0DC	C	214	1,3	17,20,21	4.40	14 (82%)	23,28,31	1.62	5 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ODG	D	108	4	21,24,25	3.81	13 (61%)	30,35,38	2.60	12 (40%)
1	ODA	A	120	1	20,23,24	3.83	9 (45%)	28,33,36	3.13	13 (46%)
4	ODT	D	109	4	18,21,22	5.26	14 (77%)	25,30,33	2.27	8 (32%)
1	ODC	A	124	1,4	17,20,21	4.29	13 (76%)	23,28,31	1.09	1 (4%)
1	ODC	A	109	1,3	17,20,21	4.33	14 (82%)	23,28,31	1.24	2 (8%)
4	ODT	D	102	4	18,18,22	5.26	14 (77%)	26,26,33	2.65	10 (38%)
4	ODT	D	107	4	18,21,22	5.40	14 (77%)	25,30,33	2.74	11 (44%)
1	ODG	A	116	1,2	21,24,25	3.72	13 (61%)	30,35,38	2.28	9 (30%)
3	ODC	C	211	1,3	17,20,21	4.43	14 (82%)	23,28,31	1.33	4 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ODA	B	125	2	-	2/7/21/22	0/3/3/3
1	ODA	A	106	1	-	2/7/21/22	0/3/3/3
3	ODT	C	213	3	-	2/7/21/22	0/2/2/2
1	ODT	A	107	1	-	2/7/21/22	0/2/2/2
1	ODT	A	113	1	-	3/7/21/22	0/2/2/2
1	ODA	A	118	1	-	3/7/21/22	0/3/3/3
2	ODC	B	124	1,2	-	0/7/21/22	0/2/2/2
1	ODC	A	104	1,3	-	2/6/18/22	0/2/2/2
4	ODG	D	103	1,4	-	1/7/21/22	0/3/3/3
1	ODC	A	119	1	-	7/7/21/22	0/2/2/2
2	ODC	B	120	1,2	-	4/7/21/22	0/2/2/2
4	ODC	D	106	1,4	-	2/7/21/22	0/2/2/2
2	ODT	B	122	2	-	5/7/21/22	0/2/2/2
1	ODA	A	125	1	-	3/7/21/22	0/3/3/3
1	ODC	A	110	1,3	-	2/7/21/22	0/2/2/2
1	ODA	A	122	1	-	2/7/21/22	0/3/3/3
1	ODG	A	108	1,3	-	2/7/21/22	0/3/3/3
3	ODG	C	215	1,3	-	2/7/21/22	0/3/3/3
4	ODA	D	104	4	-	5/7/21/22	0/3/3/3
1	ODT	A	123	1	-	2/7/21/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ODG	A	121	1,4	-	2/7/21/22	0/3/3/3
1	ODC	A	115	1,2	-	2/7/21/22	0/2/2/2
1	ODT	A	111	1	-	7/7/21/22	0/2/2/2
4	ODT	D	105	4	-	6/7/21/22	0/2/2/2
2	ODC	B	119	1,2	-	4/7/21/22	0/2/2/2
1	ODG	A	112	1,2	-	3/7/21/22	0/3/3/3
3	ODG	C	210	1,3	-	2/7/21/22	0/3/3/3
3	ODG	C	209	1,3	-	3/7/21/22	0/3/3/3
1	ODA	A	114	1	-	2/7/21/22	0/3/3/3
2	ODG	B	121	1,2	-	2/7/21/22	0/3/3/3
1	ODG	A	117	1,2	-	3/7/21/22	0/3/3/3
2	ODA	B	123	2	-	1/7/21/22	0/3/3/3
1	ODG	A	105	1,3	-	0/7/21/22	0/3/3/3
3	ODA	C	212	3	-	7/7/21/22	0/3/3/3
3	ODC	C	214	1,3	-	3/7/21/22	0/2/2/2
4	ODG	D	108	4	-	2/7/21/22	0/3/3/3
1	ODA	A	120	1	-	0/7/21/22	0/3/3/3
4	ODT	D	109	4	-	6/7/21/22	0/2/2/2
1	ODC	A	124	1,4	-	6/7/21/22	0/2/2/2
1	ODC	A	109	1,3	-	2/7/21/22	0/2/2/2
4	ODT	D	102	4	-	6/6/18/22	0/2/2/2
4	ODT	D	107	4	-	0/7/21/22	0/2/2/2
1	ODG	A	116	1,2	-	2/7/21/22	0/3/3/3
3	ODC	C	211	1,3	-	6/7/21/22	0/2/2/2

All (559) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	213	ODT	C2'-C3'	-12.31	1.21	1.52
1	A	111	ODT	C2'-C3'	-12.04	1.22	1.52
4	D	107	ODT	C2'-C3'	-11.94	1.22	1.52
2	B	122	ODT	C2'-C3'	-11.93	1.22	1.52
4	D	109	ODT	C2'-C3'	-11.92	1.22	1.52
4	D	102	ODT	C2'-C3'	-11.84	1.22	1.52
1	A	123	ODT	C2'-C3'	-11.67	1.23	1.52
1	A	107	ODT	C2'-C3'	-11.46	1.23	1.52
4	D	105	ODT	C2'-C3'	-11.35	1.24	1.52
1	A	113	ODT	C2'-C3'	-11.00	1.24	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	0DT	C6-C5	9.98	1.50	1.34
4	D	105	0DT	C6-C5	9.88	1.50	1.34
1	A	113	0DT	C6-C5	9.77	1.50	1.34
1	A	123	0DT	C6-C5	9.53	1.50	1.34
2	B	122	0DT	C6-C5	9.52	1.50	1.34
4	D	109	0DT	C6-C5	9.45	1.50	1.34
4	D	102	0DT	C6-C5	9.39	1.49	1.34
1	A	111	0DT	C6-C5	9.28	1.49	1.34
3	C	213	0DT	C6-C5	9.26	1.49	1.34
4	D	107	0DT	C6-C5	9.23	1.49	1.34
3	C	212	0DA	O4'-C1'	9.17	1.62	1.42
1	A	125	0DA	O4'-C1'	9.12	1.62	1.42
1	A	122	0DA	O4'-C1'	9.06	1.62	1.42
1	A	106	0DA	O4'-C1'	9.04	1.62	1.42
1	A	120	0DA	O4'-C1'	9.03	1.62	1.42
2	B	123	0DA	O4'-C1'	8.87	1.62	1.42
1	A	118	0DA	O4'-C1'	8.87	1.62	1.42
1	A	114	0DA	O4'-C1'	8.82	1.62	1.42
2	B	125	0DA	O4'-C1'	8.81	1.62	1.42
4	D	104	0DA	O4'-C1'	8.73	1.61	1.42
4	D	102	0DT	O4'-C4'	-8.15	1.26	1.45
1	A	122	0DA	C6A-N6A	7.98	1.54	1.34
4	D	105	0DT	O4'-C4'	-7.95	1.27	1.45
2	B	122	0DT	O4'-C4'	-7.91	1.27	1.45
1	A	120	0DA	C6A-N6A	7.85	1.54	1.34
1	A	107	0DT	O4'-C4'	-7.80	1.27	1.45
1	A	114	0DA	C6A-N6A	7.79	1.54	1.34
1	A	113	0DT	C2-N1	7.79	1.50	1.38
3	C	212	0DA	C6A-N6A	7.75	1.54	1.34
1	A	125	0DA	C6A-N6A	7.70	1.53	1.34
1	A	123	0DT	O4'-C4'	-7.68	1.27	1.45
1	A	118	0DA	C6A-N6A	7.66	1.53	1.34
4	D	109	0DT	O4'-C4'	-7.65	1.28	1.45
4	D	104	0DA	C6A-N6A	7.63	1.53	1.34
3	C	209	0DG	C4-N3	7.62	1.51	1.34
2	B	120	0DC	O4'-C4'	-7.61	1.28	1.45
3	C	213	0DT	O4'-C4'	-7.59	1.28	1.45
2	B	121	0DG	O4'-C4'	-7.57	1.28	1.45
2	B	123	0DA	O4'-C4'	-7.57	1.28	1.45
1	A	111	0DT	O4'-C4'	-7.56	1.28	1.45
2	B	125	0DA	C6A-N6A	7.56	1.53	1.34
3	C	215	0DG	C4-N3	7.55	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	0DA	O4'-C4'	-7.53	1.28	1.45
4	D	107	0DT	O4'-C4'	-7.52	1.28	1.45
1	A	124	0DC	O4'-C4'	-7.51	1.28	1.45
4	D	107	0DT	C2-N1	7.51	1.50	1.38
1	A	119	0DC	O4'-C4'	-7.50	1.28	1.45
1	A	106	0DA	C6A-N6A	7.47	1.53	1.34
2	B	119	0DC	O4'-C4'	-7.43	1.28	1.45
2	B	123	0DA	C6A-N6A	7.41	1.53	1.34
4	D	108	0DG	O4'-C4'	-7.39	1.28	1.45
1	A	106	0DA	O4'-C4'	-7.36	1.28	1.45
1	A	113	0DT	O4'-C4'	-7.36	1.28	1.45
3	C	211	0DC	O4'-C4'	-7.36	1.28	1.45
1	A	122	0DA	O4'-C4'	-7.34	1.28	1.45
4	D	104	0DA	O4'-C4'	-7.31	1.28	1.45
3	C	212	0DA	O4'-C4'	-7.31	1.28	1.45
1	A	115	0DC	C2-N3	7.31	1.50	1.36
4	D	106	0DC	C2-N3	7.31	1.50	1.36
2	B	124	0DC	O4'-C4'	-7.30	1.28	1.45
1	A	121	0DG	O4'-C4'	-7.30	1.28	1.45
1	A	109	0DC	O4'-C4'	-7.29	1.28	1.45
1	A	105	0DG	C4-N3	7.27	1.50	1.34
1	A	117	0DG	O4'-C4'	-7.25	1.28	1.45
1	A	120	0DA	O4'-C4'	-7.25	1.28	1.45
4	D	107	0DT	C2-N3	7.21	1.50	1.38
1	A	118	0DA	O4'-C4'	-7.21	1.29	1.45
4	D	108	0DG	C4-N3	7.20	1.50	1.34
3	C	213	0DT	C2-N1	7.18	1.49	1.38
4	D	103	0DG	O4'-C4'	-7.17	1.29	1.45
4	D	106	0DC	O4'-C4'	-7.16	1.29	1.45
1	A	108	0DG	O4'-C4'	-7.15	1.29	1.45
3	C	214	0DC	O4'-C4'	-7.13	1.29	1.45
3	C	209	0DG	O4'-C4'	-7.13	1.29	1.45
2	B	125	0DA	O4'-C4'	-7.12	1.29	1.45
1	A	116	0DG	C4-N3	7.12	1.50	1.34
1	A	110	0DC	O4'-C4'	-7.12	1.29	1.45
1	A	104	0DC	O4'-C4'	-7.09	1.29	1.45
3	C	215	0DG	O4'-C4'	-7.07	1.29	1.45
3	C	214	0DC	C2-N3	7.05	1.50	1.36
2	B	119	0DC	C2-N3	7.05	1.50	1.36
3	C	210	0DG	C4-N3	7.05	1.50	1.34
3	C	210	0DG	O4'-C4'	-7.02	1.29	1.45
1	A	107	0DT	C2-N1	7.00	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	0DC	O4'-C4'	-6.99	1.29	1.45
3	C	211	0DC	C2-N3	6.98	1.50	1.36
1	A	121	0DG	C4-N3	6.97	1.50	1.34
1	A	123	0DT	C2-N1	6.94	1.49	1.38
1	A	108	0DG	C4-N3	6.93	1.50	1.34
1	A	116	0DG	O4'-C4'	-6.93	1.29	1.45
2	B	125	0DA	C2'-C1'	-6.91	1.33	1.52
1	A	105	0DG	O4'-C4'	-6.91	1.29	1.45
1	A	110	0DC	C2-N3	6.87	1.50	1.36
2	B	121	0DG	C4-N3	6.85	1.49	1.34
1	A	114	0DA	O4'-C4'	-6.84	1.29	1.45
1	A	120	0DA	C2'-C1'	-6.82	1.33	1.52
2	B	123	0DA	C2'-C1'	-6.81	1.33	1.52
1	A	106	0DA	C2'-C1'	-6.78	1.34	1.52
1	A	119	0DC	C2-N3	6.76	1.49	1.36
1	A	109	0DC	C2-N3	6.74	1.49	1.36
1	A	125	0DA	C2'-C1'	-6.72	1.34	1.52
1	A	104	0DC	C2-N3	6.70	1.49	1.36
1	A	112	0DG	O4'-C4'	-6.69	1.30	1.45
4	D	104	0DA	C2'-C1'	-6.66	1.34	1.52
1	A	112	0DG	C4-N3	6.66	1.49	1.34
1	A	113	0DT	C2-N3	6.65	1.49	1.38
1	A	117	0DG	C4-N3	6.64	1.49	1.34
3	C	213	0DT	C2-N3	6.63	1.49	1.38
1	A	114	0DA	C2'-C1'	-6.62	1.34	1.52
1	A	107	0DT	C2-N3	6.60	1.49	1.38
1	A	119	0DC	C6-C5	6.59	1.50	1.35
2	B	124	0DC	C6-C5	6.58	1.50	1.35
1	A	118	0DA	C2'-C1'	-6.55	1.34	1.52
3	C	209	0DG	C2-N2	6.54	1.49	1.34
4	D	106	0DC	C6-C5	6.53	1.50	1.35
3	C	212	0DA	C2'-C1'	-6.52	1.34	1.52
1	A	111	0DT	C2-N1	6.51	1.48	1.38
4	D	108	0DG	C2-N2	6.50	1.49	1.34
2	B	124	0DC	C2-N3	6.50	1.49	1.36
1	A	122	0DA	C2'-C1'	-6.48	1.34	1.52
1	A	123	0DT	C2-N3	6.48	1.49	1.38
2	B	122	0DT	C2-N3	6.43	1.49	1.38
3	C	211	0DC	C6-C5	6.42	1.50	1.35
4	D	105	0DT	C2-N1	6.40	1.48	1.38
1	A	124	0DC	C2-N3	6.40	1.49	1.36
3	C	215	0DG	C2-N2	6.39	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	0DG	C2-N2	6.38	1.49	1.34
4	D	103	0DG	C4-N3	6.37	1.48	1.34
2	B	121	0DG	C2-N2	6.37	1.49	1.34
3	C	215	0DG	C2-N3	6.37	1.48	1.33
1	A	121	0DG	C2-N2	6.36	1.49	1.34
2	B	120	0DC	C2-N3	6.27	1.48	1.36
3	C	214	0DC	C6-C5	6.27	1.49	1.35
1	A	108	0DG	C2-N2	6.27	1.48	1.34
4	D	102	0DT	C2-N3	6.27	1.48	1.38
2	B	119	0DC	C6-C5	6.26	1.49	1.35
1	A	110	0DC	C6-C5	6.26	1.49	1.35
1	A	109	0DC	C6-C5	6.24	1.49	1.35
3	C	209	0DG	C2-N3	6.23	1.48	1.33
4	D	109	0DT	C2-N3	6.23	1.48	1.38
4	D	109	0DT	C2-N1	6.22	1.48	1.38
3	C	210	0DG	C2-N2	6.22	1.48	1.34
1	A	124	0DC	C6-C5	6.21	1.49	1.35
2	B	120	0DC	C6-C5	6.21	1.49	1.35
1	A	117	0DG	C2-N2	6.19	1.48	1.34
1	A	115	0DC	C6-C5	6.14	1.49	1.35
1	A	116	0DG	C2-N2	6.14	1.48	1.34
1	A	112	0DG	C2-N2	6.13	1.48	1.34
1	A	105	0DG	C2-N3	6.12	1.48	1.33
4	D	108	0DG	C2-N3	6.08	1.47	1.33
1	A	111	0DT	C2-N3	6.01	1.48	1.38
4	D	105	0DT	C2-N3	5.97	1.48	1.38
1	A	116	0DG	C2-N3	5.97	1.47	1.33
1	A	104	0DC	C6-C5	5.91	1.48	1.35
4	D	103	0DG	C2-N2	5.91	1.48	1.34
3	C	210	0DG	C2-N3	5.91	1.47	1.33
1	A	121	0DG	C2-N3	5.88	1.47	1.33
1	A	124	0DC	C1'-N1	-5.87	1.33	1.48
4	D	103	0DG	C1'-N9	-5.86	1.33	1.48
1	A	108	0DG	C2-N3	5.86	1.47	1.33
1	A	117	0DG	C1'-N9	-5.84	1.33	1.48
1	A	112	0DG	C2-N3	5.76	1.47	1.33
2	B	121	0DG	C1'-N9	-5.75	1.33	1.48
2	B	120	0DC	C1'-N1	-5.73	1.33	1.48
3	C	214	0DC	C2-N1	5.69	1.52	1.40
3	C	210	0DG	C1'-N9	-5.65	1.33	1.48
4	D	106	0DC	C2-N1	5.65	1.51	1.40
1	A	121	0DG	C1'-N9	-5.63	1.33	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	0DC	C4-N3	5.57	1.45	1.34
4	D	102	0DT	C1'-N1	-5.56	1.34	1.48
2	B	124	0DC	C4-N3	5.55	1.45	1.34
1	A	116	0DG	C1'-N9	-5.50	1.34	1.48
2	B	119	0DC	C3'-C4'	5.46	1.67	1.53
4	D	102	0DT	C2-N1	5.46	1.47	1.38
3	C	215	0DG	C1'-N9	-5.45	1.34	1.48
1	A	105	0DG	C1'-N9	-5.44	1.34	1.48
2	B	122	0DT	C2-N1	5.44	1.47	1.38
3	C	209	0DG	C1'-N9	-5.43	1.34	1.48
2	B	122	0DT	C1'-N1	-5.40	1.34	1.48
4	D	109	0DT	C1'-N1	-5.35	1.34	1.48
4	D	106	0DC	C4-N3	5.35	1.45	1.34
1	A	104	0DC	C4-N3	5.35	1.45	1.34
1	A	111	0DT	C1'-N1	-5.34	1.34	1.48
1	A	124	0DC	C4-N3	5.33	1.45	1.34
3	C	213	0DT	C3'-C4'	5.32	1.67	1.53
1	A	117	0DG	C2-N3	5.28	1.46	1.33
1	A	110	0DC	C2-N1	5.28	1.51	1.40
1	A	109	0DC	C4-N3	5.28	1.45	1.34
1	A	115	0DC	C2-N1	5.25	1.51	1.40
3	C	211	0DC	C2-N1	5.24	1.51	1.40
1	A	104	0DC	C2-N1	5.24	1.51	1.40
1	A	109	0DC	C2-N1	5.24	1.51	1.40
1	A	119	0DC	C4-N3	5.23	1.44	1.34
1	A	112	0DG	C1'-N9	-5.23	1.34	1.48
1	A	108	0DG	C1'-N9	-5.22	1.35	1.48
2	B	121	0DG	C2-N3	5.18	1.45	1.33
4	D	108	0DG	C1'-N9	-5.18	1.35	1.48
3	C	213	0DT	C1'-N1	-5.17	1.35	1.48
1	A	121	0DG	C3'-C4'	5.16	1.66	1.53
3	C	214	0DC	C4-N3	5.16	1.44	1.34
1	A	113	0DT	C3'-C4'	5.15	1.66	1.53
1	A	110	0DC	C1'-N1	-5.14	1.35	1.48
2	B	119	0DC	C4-N3	5.14	1.44	1.34
2	B	124	0DC	C3'-C4'	5.13	1.66	1.53
1	A	112	0DG	C3'-C4'	5.13	1.66	1.53
3	C	211	0DC	C4-N3	5.12	1.44	1.34
1	A	109	0DC	C1'-N1	-5.11	1.35	1.48
1	A	111	0DT	C3'-C4'	5.11	1.66	1.53
1	A	119	0DC	C2-N1	5.11	1.50	1.40
4	D	106	0DC	C4-N4	5.11	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	0DC	C3'-C4'	5.10	1.66	1.53
1	A	104	0DC	C1'-N1	-5.10	1.35	1.48
4	D	106	0DC	C3'-C4'	5.10	1.66	1.53
2	B	120	0DC	C4-N3	5.08	1.44	1.34
1	A	116	0DG	C3'-C4'	5.07	1.66	1.53
1	A	108	0DG	C3'-C4'	5.06	1.66	1.53
1	A	108	0DG	O4'-C1'	5.06	1.53	1.42
4	D	105	0DT	C3'-C4'	5.05	1.66	1.53
4	D	103	0DG	C2-N3	5.05	1.45	1.33
1	A	123	0DT	C3'-C4'	5.04	1.66	1.53
1	A	123	0DT	C1'-N1	-5.03	1.35	1.48
2	B	119	0DC	C2-N1	5.01	1.50	1.40
1	A	119	0DC	C4-N4	5.00	1.46	1.33
4	D	103	0DG	O4'-C1'	4.98	1.53	1.42
2	B	124	0DC	C1'-N1	-4.98	1.35	1.48
1	A	115	0DC	C4-N4	4.97	1.45	1.33
4	D	102	0DT	C3'-C4'	4.97	1.66	1.53
1	A	115	0DC	C4-N3	4.97	1.44	1.34
3	C	211	0DC	C4-N4	4.96	1.45	1.33
4	D	105	0DT	C1'-N1	-4.96	1.35	1.48
4	D	103	0DG	C3'-C4'	4.96	1.66	1.53
1	A	105	0DG	C3'-C4'	4.95	1.66	1.53
4	D	108	0DG	C3'-C4'	4.95	1.66	1.53
1	A	107	0DT	C6-N1	4.94	1.46	1.38
3	C	211	0DC	C3'-C4'	4.94	1.66	1.53
3	C	214	0DC	C4-N4	4.92	1.45	1.33
3	C	209	0DG	C3'-C4'	4.90	1.65	1.53
4	D	107	0DT	C1'-N1	-4.89	1.35	1.48
1	A	110	0DC	C4-N4	4.89	1.45	1.33
1	A	117	0DG	C3'-C4'	4.88	1.65	1.53
3	C	210	0DG	O4'-C1'	4.86	1.53	1.42
1	A	113	0DT	C6-N1	4.84	1.46	1.38
1	A	104	0DC	C3'-C4'	4.84	1.65	1.53
4	D	108	0DG	O4'-C1'	4.83	1.53	1.42
4	D	107	0DT	C3'-C4'	4.83	1.65	1.53
3	C	215	0DG	C3'-C4'	4.83	1.65	1.53
2	B	119	0DC	C4-N4	4.83	1.45	1.33
1	A	115	0DC	C3'-C4'	4.81	1.65	1.53
3	C	209	0DG	O4'-C1'	4.81	1.53	1.42
1	A	107	0DT	C3'-C4'	4.80	1.65	1.53
1	A	112	0DG	O4'-C1'	4.80	1.53	1.42
2	B	120	0DC	C3'-C4'	4.79	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	214	0DC	C1'-N1	-4.79	1.36	1.48
1	A	109	0DC	C4-N4	4.78	1.45	1.33
2	B	121	0DG	C3'-C4'	4.78	1.65	1.53
1	A	115	0DC	C1'-N1	-4.78	1.36	1.48
1	A	104	0DC	C4-N4	4.75	1.45	1.33
2	B	124	0DC	C4-N4	4.75	1.45	1.33
1	A	105	0DG	O4'-C1'	4.75	1.53	1.42
3	C	210	0DG	C3'-C4'	4.71	1.65	1.53
1	A	124	0DC	C4-N4	4.70	1.45	1.33
1	A	116	0DG	O4'-C1'	4.68	1.52	1.42
2	B	121	0DG	O4'-C1'	4.65	1.52	1.42
3	C	215	0DG	O4'-C1'	4.64	1.52	1.42
3	C	214	0DC	C3'-C4'	4.63	1.65	1.53
4	D	105	0DT	C6-N1	4.62	1.45	1.38
1	A	124	0DC	C3'-C4'	4.60	1.65	1.53
1	A	111	0DT	C6-N1	4.60	1.45	1.38
1	A	123	0DT	C6-N1	4.58	1.45	1.38
1	A	117	0DG	O4'-C1'	4.57	1.52	1.42
1	A	109	0DC	C3'-C4'	4.55	1.65	1.53
1	A	119	0DC	C1'-N1	-4.55	1.36	1.48
2	B	120	0DC	C4-N4	4.53	1.44	1.33
1	A	110	0DC	C3'-C4'	4.49	1.64	1.53
4	D	106	0DC	O4'-C1'	4.48	1.52	1.42
2	B	119	0DC	C1'-N1	-4.47	1.36	1.48
2	B	122	0DT	C3'-C4'	4.47	1.64	1.53
4	D	106	0DC	O3'-C3'	4.46	1.52	1.43
1	A	107	0DT	C1'-N1	-4.45	1.36	1.48
1	A	115	0DC	O4'-C1'	4.42	1.52	1.42
4	D	109	0DT	C3'-C4'	4.41	1.64	1.53
1	A	104	0DC	O4'-C1'	4.40	1.52	1.42
3	C	214	0DC	O4'-C1'	4.39	1.52	1.42
3	C	211	0DC	C1'-N1	-4.37	1.37	1.48
4	D	102	0DT	C6-N1	4.36	1.45	1.38
4	D	109	0DT	C6-N1	4.36	1.45	1.38
3	C	211	0DC	O4'-C1'	4.33	1.52	1.42
1	A	121	0DG	O4'-C1'	4.32	1.52	1.42
2	B	124	0DC	C2-N1	4.31	1.49	1.40
3	C	213	0DT	C6-N1	4.30	1.45	1.38
4	D	106	0DC	C1'-N1	-4.29	1.37	1.48
4	D	109	0DT	O4'-C1'	4.27	1.51	1.42
4	D	107	0DT	O4'-C1'	4.25	1.51	1.42
2	B	122	0DT	C6-N1	4.23	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	0DT	O4'-C1'	4.22	1.51	1.42
1	A	115	0DC	O3'-C3'	4.20	1.52	1.43
2	B	124	0DC	O4'-C1'	4.16	1.51	1.42
1	A	107	0DT	O4'-C1'	4.15	1.51	1.42
1	A	110	0DC	O4'-C1'	4.13	1.51	1.42
4	D	107	0DT	C6-N1	4.09	1.45	1.38
2	B	120	0DC	C2-N1	4.07	1.48	1.40
1	A	124	0DC	O4'-C1'	4.06	1.51	1.42
1	A	113	0DT	C1'-N1	-4.06	1.37	1.48
1	A	123	0DT	O4'-C1'	4.01	1.51	1.42
1	A	109	0DC	O4'-C1'	4.01	1.51	1.42
2	B	119	0DC	O4'-C1'	4.00	1.51	1.42
2	B	122	0DT	O4'-C1'	4.00	1.51	1.42
1	A	113	0DT	O3'-C3'	3.97	1.51	1.43
3	C	213	0DT	O4'-C1'	3.97	1.51	1.42
1	A	124	0DC	C2-N1	3.95	1.48	1.40
1	A	104	0DC	O3'-C3'	3.93	1.51	1.43
3	C	211	0DC	O3'-C3'	3.93	1.51	1.43
2	B	120	0DC	O4'-C1'	3.92	1.51	1.42
4	D	107	0DT	C4-N3	3.89	1.46	1.38
1	A	111	0DT	C4-N3	3.86	1.46	1.38
2	B	122	0DT	C4-N3	3.85	1.46	1.38
1	A	119	0DC	O4'-C1'	3.82	1.50	1.42
4	D	102	0DT	O4'-C1'	3.74	1.50	1.42
3	C	213	0DT	O3'-C3'	3.72	1.51	1.43
2	B	124	0DC	O3'-C3'	3.64	1.51	1.43
1	A	113	0DT	C4-N3	3.64	1.45	1.38
1	A	123	0DT	C4-N3	3.64	1.45	1.38
1	A	111	0DT	O4'-C1'	3.63	1.50	1.42
4	D	105	0DT	O4'-C1'	3.59	1.50	1.42
1	A	107	0DT	O3'-C3'	3.59	1.50	1.43
1	A	107	0DT	C4-N3	3.58	1.45	1.38
1	A	119	0DC	C6-N1	3.58	1.46	1.38
4	D	109	0DT	C4-N3	3.57	1.45	1.38
3	C	213	0DT	C4-N3	3.56	1.45	1.38
2	B	124	0DC	C6-N1	3.54	1.46	1.38
2	B	120	0DC	O3'-C3'	3.52	1.50	1.43
4	D	106	0DC	C6-N1	3.52	1.46	1.38
3	C	211	0DC	C6-N1	3.52	1.46	1.38
2	B	125	0DA	O3'-C3'	-3.51	1.36	1.43
3	C	214	0DC	O3'-C3'	3.49	1.50	1.43
1	A	110	0DC	C6-N1	3.47	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	105	0DT	C4-N3	3.47	1.45	1.38
4	D	102	0DT	C4-N3	3.46	1.45	1.38
1	A	104	0DC	C6-N1	3.40	1.46	1.38
2	B	119	0DC	C6-N1	3.38	1.46	1.38
3	C	214	0DC	C6-N1	3.38	1.46	1.38
2	B	121	0DG	O3'-C3'	3.38	1.50	1.43
1	A	109	0DC	C6-N1	3.35	1.46	1.38
4	D	105	0DT	O3'-C3'	3.34	1.50	1.43
4	D	105	0DT	C4-C5	3.33	1.50	1.44
1	A	106	0DA	O3'-C3'	-3.31	1.36	1.43
1	A	123	0DT	O3'-C3'	3.28	1.50	1.43
2	B	119	0DC	O3'-C3'	3.28	1.50	1.43
1	A	119	0DC	O3'-C3'	3.26	1.50	1.43
1	A	111	0DT	O3'-C3'	3.22	1.50	1.43
4	D	102	0DT	C4-C5	3.22	1.50	1.44
1	A	120	0DA	O3'-C3'	-3.20	1.36	1.43
1	A	109	0DC	O3'-C3'	3.18	1.50	1.43
4	D	107	0DT	O3'-C3'	3.17	1.50	1.43
4	D	107	0DT	C4-C5	3.16	1.50	1.44
1	A	115	0DC	C6-N1	3.16	1.45	1.38
1	A	124	0DC	C6-N1	3.12	1.45	1.38
2	B	123	0DA	O3'-C3'	-3.09	1.36	1.43
1	A	113	0DT	C4-C5	3.07	1.49	1.44
2	B	121	0DG	O6-C6	-3.05	1.17	1.23
1	A	110	0DC	O3'-C3'	3.05	1.49	1.43
1	A	123	0DT	C4-C5	3.04	1.49	1.44
1	A	119	0DC	C5-C4	3.03	1.50	1.42
4	D	108	0DG	O3'-C3'	3.03	1.49	1.43
1	A	117	0DG	O3'-C3'	3.02	1.49	1.43
2	B	122	0DT	O3'-C3'	3.01	1.49	1.43
1	A	124	0DC	O3'-C3'	2.98	1.49	1.43
1	A	125	0DA	O3'-C3'	-2.97	1.37	1.43
1	A	108	0DG	O3'-C3'	2.95	1.49	1.43
4	D	109	0DT	O3'-C3'	2.94	1.49	1.43
2	B	120	0DC	C6-N1	2.92	1.45	1.38
1	A	107	0DT	C4-C5	2.92	1.49	1.44
1	A	112	0DG	O3'-C3'	2.89	1.49	1.43
4	D	106	0DC	C5-C4	2.86	1.49	1.42
1	A	109	0DC	C5-C4	2.85	1.49	1.42
1	A	122	0DA	O3'-C3'	-2.85	1.37	1.43
1	A	117	0DG	C6-N1	2.85	1.44	1.38
2	B	124	0DC	C5-C4	2.84	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	0DC	C5-C4	2.83	1.49	1.42
1	A	110	0DC	C5-C4	2.83	1.49	1.42
3	C	213	0DT	C4-C5	2.83	1.49	1.44
2	B	123	0DA	C5A-C4A	-2.82	1.34	1.39
4	D	103	0DG	O3'-C3'	2.81	1.49	1.43
1	A	105	0DG	O3'-C3'	2.80	1.49	1.43
4	D	109	0DT	C4-C5	2.78	1.49	1.44
1	A	108	0DG	C5-C6	2.77	1.54	1.44
4	D	102	0DT	O3'-C3'	2.77	1.49	1.43
4	D	108	0DG	C5-C6	2.75	1.54	1.44
2	B	121	0DG	C6-N1	2.74	1.44	1.38
2	B	125	0DA	C5A-N7A	-2.72	1.34	1.39
1	A	117	0DG	O6-C6	-2.71	1.18	1.23
1	A	114	0DA	C5A-N7A	-2.70	1.34	1.39
1	A	118	0DA	C5A-N7A	-2.69	1.34	1.39
3	C	211	0DC	C5-C4	2.68	1.49	1.42
1	A	106	0DA	C5A-N7A	-2.67	1.34	1.39
1	A	120	0DA	C5A-N7A	-2.67	1.34	1.39
1	A	118	0DA	C5'-C4'	2.67	1.59	1.51
1	A	115	0DC	O2-C2	-2.66	1.18	1.23
1	A	121	0DG	C5-C6	2.66	1.54	1.44
1	A	118	0DA	O3'-C3'	-2.66	1.37	1.43
2	B	120	0DC	O2-C2	-2.65	1.18	1.23
1	A	121	0DG	O3'-C3'	2.63	1.48	1.43
2	B	119	0DC	O2-C2	-2.63	1.18	1.23
3	C	209	0DG	C5-C6	2.63	1.54	1.44
1	A	112	0DG	C2-N1	2.63	1.44	1.37
4	D	103	0DG	O6-C6	-2.62	1.18	1.23
2	B	122	0DT	C4-C5	2.62	1.49	1.44
1	A	111	0DT	C4-C5	2.60	1.49	1.44
1	A	104	0DC	C5-C4	2.60	1.49	1.42
4	D	103	0DG	C6-N1	2.59	1.43	1.38
3	C	215	0DG	C5-C6	2.59	1.54	1.44
3	C	209	0DG	C2-N1	2.58	1.43	1.37
1	A	112	0DG	C5-N7	-2.57	1.33	1.39
1	A	116	0DG	O6-C6	-2.57	1.18	1.23
3	C	210	0DG	C5-C6	2.56	1.54	1.44
1	A	124	0DC	O2-C2	-2.56	1.18	1.23
1	A	121	0DG	C2-N1	2.56	1.43	1.37
1	A	115	0DC	C5-C4	2.55	1.48	1.42
3	C	215	0DG	C2-N1	2.54	1.43	1.37
1	A	111	0DT	O4-C4	-2.54	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	0DA	O3'-C3'	-2.53	1.38	1.43
1	A	105	0DG	C2-N1	2.53	1.43	1.37
3	C	209	0DG	O3'-C3'	2.53	1.48	1.43
1	A	122	0DA	C5A-N7A	-2.51	1.34	1.39
4	D	102	0DT	O2-C2	-2.51	1.18	1.23
1	A	117	0DG	C5-C6	2.51	1.53	1.44
1	A	112	0DG	C5-C6	2.51	1.53	1.44
3	C	214	0DC	C5-C4	2.51	1.48	1.42
1	A	105	0DG	O6-C6	-2.51	1.18	1.23
3	C	212	0DA	C5A-N7A	-2.50	1.34	1.39
1	A	105	0DG	C5-N7	-2.50	1.34	1.39
3	C	211	0DC	O2-C2	-2.50	1.19	1.23
4	D	108	0DG	C6-N1	2.50	1.43	1.38
3	C	210	0DG	O6-C6	-2.49	1.18	1.23
2	B	123	0DA	C4A-N9A	-2.48	1.32	1.37
3	C	213	0DT	O4-C4	-2.48	1.18	1.23
2	B	119	0DC	C5-C4	2.47	1.48	1.42
1	A	108	0DG	C6-N1	2.47	1.43	1.38
4	D	104	0DA	O3'-C3'	-2.47	1.38	1.43
4	D	108	0DG	C2-N1	2.47	1.43	1.37
1	A	116	0DG	C5-N7	-2.46	1.34	1.39
3	C	210	0DG	C2-N1	2.46	1.43	1.37
1	A	121	0DG	C6-N1	2.46	1.43	1.38
1	A	119	0DC	O2-C2	-2.45	1.19	1.23
2	B	120	0DC	C5-C4	2.45	1.48	1.42
1	A	116	0DG	O3'-C3'	2.45	1.48	1.43
3	C	215	0DG	C2'-C1'	2.44	1.59	1.52
1	A	106	0DA	C8A-N9A	-2.44	1.33	1.37
1	A	125	0DA	C5'-C4'	2.43	1.58	1.51
1	A	108	0DG	C2-N1	2.43	1.43	1.37
1	A	116	0DG	C2-N1	2.42	1.43	1.37
4	D	104	0DA	C5A-N7A	-2.42	1.34	1.39
2	B	125	0DA	C5'-C4'	2.42	1.58	1.51
3	C	211	0DC	C2'-C1'	2.42	1.58	1.52
4	D	103	0DG	C2-N1	2.42	1.43	1.37
1	A	120	0DA	C8A-N9A	-2.40	1.33	1.37
3	C	215	0DG	O3'-C3'	2.40	1.48	1.43
1	A	105	0DG	C2'-C1'	2.39	1.58	1.52
1	A	108	0DG	O6-C6	-2.39	1.19	1.23
4	D	106	0DC	C2'-C1'	2.39	1.58	1.52
2	B	125	0DA	C3'-C4'	2.39	1.59	1.53
4	D	108	0DG	O6-C6	-2.38	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	103	0DG	C5-C6	2.38	1.53	1.44
3	C	209	0DG	C6-N1	2.36	1.43	1.38
2	B	122	0DT	O2-C2	-2.36	1.18	1.23
3	C	215	0DG	O6-C6	-2.35	1.19	1.23
1	A	117	0DG	C2-N1	2.35	1.43	1.37
2	B	121	0DG	C5-C6	2.34	1.53	1.44
4	D	103	0DG	C4-N9	-2.34	1.32	1.38
1	A	109	0DC	O2-C2	-2.34	1.19	1.23
4	D	109	0DT	O4-C4	-2.33	1.19	1.23
4	D	105	0DT	O2-C2	-2.33	1.18	1.23
1	A	125	0DA	C5A-N7A	-2.33	1.34	1.39
2	B	124	0DC	O2-C2	-2.32	1.19	1.23
1	A	120	0DA	C2A-N1A	2.32	1.38	1.33
1	A	114	0DA	C5'-C4'	2.31	1.58	1.51
2	B	121	0DG	C4-N9	-2.30	1.32	1.38
1	A	116	0DG	C5-C6	2.30	1.53	1.44
3	C	209	0DG	O6-C6	-2.29	1.19	1.23
3	C	210	0DG	C6-N1	2.29	1.43	1.38
4	D	102	0DT	O4-C4	-2.29	1.19	1.23
1	A	113	0DT	O4-C4	-2.28	1.19	1.23
4	D	104	0DA	C5A-C4A	-2.28	1.35	1.39
1	A	105	0DG	C5-C6	2.28	1.52	1.44
3	C	214	0DC	C2'-C1'	2.28	1.58	1.52
1	A	107	0DT	O2-C2	-2.28	1.19	1.23
2	B	123	0DA	C5A-N7A	-2.27	1.34	1.39
1	A	104	0DC	O2-C2	-2.27	1.19	1.23
3	C	214	0DC	O2-C2	-2.26	1.19	1.23
4	D	109	0DT	O2-C2	-2.26	1.19	1.23
1	A	113	0DT	C2'-C1'	2.26	1.58	1.52
1	A	125	0DA	C4A-N9A	-2.25	1.33	1.37
1	A	107	0DT	C2'-C1'	2.25	1.58	1.52
1	A	112	0DG	O6-C6	-2.25	1.19	1.23
2	B	121	0DG	C2'-C1'	2.24	1.58	1.52
1	A	123	0DT	O4-C4	-2.23	1.19	1.23
1	A	108	0DG	C2'-C1'	2.23	1.58	1.52
2	B	122	0DT	O4-C4	-2.23	1.19	1.23
3	C	215	0DG	C5-N7	-2.22	1.34	1.39
3	C	212	0DA	O3'-C3'	-2.21	1.38	1.43
4	D	106	0DC	O2-C2	-2.21	1.19	1.23
1	A	117	0DG	C4-N9	-2.21	1.32	1.38
1	A	121	0DG	O6-C6	-2.20	1.19	1.23
3	C	213	0DT	O2-C2	-2.20	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	105	0DT	O4-C4	-2.20	1.19	1.23
3	C	215	0DG	C6-N1	2.19	1.43	1.38
3	C	212	0DA	C3'-C4'	2.18	1.58	1.53
1	A	115	0DC	C2'-C1'	2.18	1.58	1.52
1	A	106	0DA	C5A-C4A	-2.17	1.35	1.39
1	A	112	0DG	C2'-C1'	2.15	1.58	1.52
4	D	104	0DA	C3'-C4'	2.15	1.58	1.53
1	A	114	0DA	C3'-C4'	2.14	1.58	1.53
1	A	107	0DT	O4-C4	-2.14	1.19	1.23
1	A	105	0DG	C6-N1	2.14	1.42	1.38
4	D	107	0DT	O2-C2	-2.14	1.19	1.23
1	A	112	0DG	C6-N1	2.13	1.42	1.38
3	C	210	0DG	O3'-C3'	2.13	1.47	1.43
2	B	121	0DG	C2-N1	2.13	1.42	1.37
1	A	123	0DT	O2-C2	-2.12	1.19	1.23
1	A	113	0DT	O2-C2	-2.12	1.19	1.23
1	A	119	0DC	C2'-C1'	2.10	1.58	1.52
2	B	123	0DA	C5'-C4'	2.10	1.57	1.51
4	D	104	0DA	C5'-C4'	2.10	1.57	1.51
2	B	125	0DA	C5A-C4A	-2.10	1.35	1.39
3	C	210	0DG	C5-N7	-2.09	1.34	1.39
1	A	125	0DA	C5A-C4A	-2.08	1.35	1.39
1	A	108	0DG	C5-N7	-2.08	1.34	1.39
1	A	125	0DA	C3'-C4'	2.08	1.58	1.53
1	A	120	0DA	C5'-C4'	2.08	1.57	1.51
1	A	118	0DA	C3'-C4'	2.08	1.58	1.53
1	A	116	0DG	C2'-C1'	2.08	1.58	1.52
3	C	209	0DG	C5-N7	-2.07	1.34	1.39
1	A	106	0DA	C2A-N1A	2.07	1.37	1.33
1	A	110	0DC	O2-C2	-2.07	1.19	1.23
1	A	111	0DT	O2-C2	-2.06	1.19	1.23
2	B	123	0DA	C3'-C4'	2.06	1.58	1.53
1	A	121	0DG	C5-N7	-2.06	1.34	1.39
1	A	121	0DG	C2'-C1'	2.06	1.57	1.52
3	C	209	0DG	C2'-C1'	2.05	1.57	1.52
1	A	109	0DC	C2'-C1'	2.04	1.57	1.52
4	D	108	0DG	C5-N7	-2.04	1.35	1.39
1	A	122	0DA	C5'-C4'	2.04	1.57	1.51
1	A	122	0DA	C2A-N1A	2.03	1.37	1.33
3	C	212	0DA	C5'-C4'	2.03	1.57	1.51
2	B	125	0DA	C2A-N1A	2.02	1.37	1.33
3	C	212	0DA	C2A-N1A	2.02	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	103	0DG	C5-N7	-2.01	1.35	1.39
4	D	107	0DT	O4-C4	-2.01	1.19	1.23
1	A	106	0DA	C5'-C4'	2.01	1.57	1.51

All (398) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	0DA	N6A-C6A-N1A	-7.70	101.22	118.38
1	A	125	0DA	N6A-C6A-N1A	-7.50	101.66	118.38
1	A	120	0DA	N6A-C6A-N1A	-7.48	101.71	118.38
3	C	212	0DA	N6A-C6A-N1A	-7.35	102.01	118.38
2	B	123	0DA	N6A-C6A-N1A	-7.29	102.13	118.38
4	D	104	0DA	N6A-C6A-N1A	-7.10	102.55	118.38
1	A	114	0DA	N6A-C6A-N1A	-7.06	102.65	118.38
2	B	121	0DG	C1'-N9-C8	6.99	143.59	127.91
1	A	106	0DA	N6A-C6A-N1A	-6.83	103.16	118.38
1	A	118	0DA	N6A-C6A-N1A	-6.81	103.21	118.38
3	C	215	0DG	C5-C4-N3	-6.80	117.57	128.39
2	B	121	0DG	C1'-N9-C4	-6.69	107.45	125.50
4	D	107	0DT	C4-N3-C2	-6.52	118.80	127.34
3	C	209	0DG	C5-C4-N3	-6.41	118.18	128.39
1	A	105	0DG	C5-C4-N3	-6.36	118.27	128.39
2	B	125	0DA	N6A-C6A-N1A	-6.36	104.22	118.38
1	A	122	0DA	C5A-C6A-N6A	6.35	139.01	123.29
1	A	125	0DA	C5A-C6A-N6A	6.34	138.98	123.29
1	A	116	0DG	C5-C4-N3	-6.29	118.39	128.39
1	A	108	0DG	C5-C4-N3	-6.26	118.43	128.39
1	A	117	0DG	C1'-N9-C8	6.21	141.84	127.91
1	A	112	0DG	C5-C4-N3	-6.19	118.53	128.39
4	D	108	0DG	C5-C4-N3	-6.17	118.57	128.39
3	C	213	0DT	C4-N3-C2	-6.15	119.27	127.34
1	A	117	0DG	C1'-N9-C4	-6.06	109.16	125.50
4	D	102	0DT	C4-N3-C2	-6.05	119.41	127.34
1	A	107	0DT	C4-N3-C2	-6.00	119.47	127.34
1	A	120	0DA	C5A-C6A-N6A	5.97	138.07	123.29
4	D	105	0DT	C4-N3-C2	-5.90	119.61	127.34
1	A	114	0DA	C5A-C6A-N6A	5.89	137.86	123.29
3	C	212	0DA	C5A-C4A-N3A	-5.86	118.64	126.72
2	B	125	0DA	N1A-C2A-N3A	-5.86	119.72	128.58
4	D	108	0DG	C2'-C1'-N9	5.83	128.40	113.81
1	A	122	0DA	C5A-C4A-N3A	-5.78	118.75	126.72
1	A	121	0DG	C5-C4-N3	-5.73	119.27	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	0DT	C5-C4-N3	5.69	120.27	115.32
1	A	118	0DA	C5A-C6A-N6A	5.67	137.33	123.29
1	A	120	0DA	C5A-C4A-N3A	-5.67	118.91	126.72
1	A	107	0DT	N3-C2-N1	5.65	122.25	114.89
3	C	210	0DG	C5-C4-N3	-5.65	119.40	128.39
3	C	212	0DA	C5A-C6A-N6A	5.64	137.26	123.29
2	B	123	0DA	N9A-C8A-N7A	-5.63	105.95	113.94
4	D	104	0DA	C5A-C6A-N6A	5.62	137.20	123.29
1	A	119	0DC	O4'-C1'-N1	5.59	117.78	107.86
1	A	113	0DT	C4-N3-C2	-5.57	120.04	127.34
3	C	213	0DT	C5-C4-N3	5.56	120.15	115.32
1	A	111	0DT	C4-N3-C2	-5.53	120.09	127.34
3	C	215	0DG	O4'-C1'-N9	5.50	117.63	107.86
1	A	114	0DA	C5A-C4A-N3A	-5.43	119.23	126.72
2	B	123	0DA	C5A-C6A-N6A	5.42	136.70	123.29
4	D	103	0DG	C1'-N9-C8	5.39	140.00	127.91
1	A	123	0DT	C4-N3-C2	-5.37	120.29	127.34
2	B	122	0DT	C4-N3-C2	-5.37	120.30	127.34
4	D	102	0DT	O2-C2-N1	-5.36	115.83	122.80
4	D	103	0DG	C1'-N9-C4	-5.35	111.06	125.50
1	A	120	0DA	N9A-C8A-N7A	-5.33	106.38	113.94
1	A	113	0DT	N3-C2-N1	5.28	121.77	114.89
2	B	123	0DA	N1A-C2A-N3A	-5.28	120.59	128.58
1	A	106	0DA	C5A-C6A-N6A	5.27	136.33	123.29
4	D	109	0DT	C4-N3-C2	-5.27	120.43	127.34
4	D	104	0DA	N9A-C8A-N7A	-5.26	106.48	113.94
4	D	107	0DT	N3-C2-N1	5.24	121.71	114.89
1	A	118	0DA	C5A-C4A-N3A	-5.19	119.57	126.72
2	B	122	0DT	O2-C2-N1	-5.19	116.05	122.80
3	C	209	0DG	C2-N3-C4	5.18	121.21	112.30
4	D	108	0DG	C2-N3-C4	5.14	121.15	112.30
4	D	105	0DT	N3-C2-N1	5.11	121.55	114.89
3	C	215	0DG	C2-N3-C4	5.10	121.08	112.30
4	D	102	0DT	C5-C4-N3	5.10	119.75	115.32
2	B	125	0DA	C5A-C4A-N3A	-5.10	119.70	126.72
2	B	119	0DC	C1'-N1-C2	5.09	126.56	117.83
1	A	108	0DG	C2-N3-C4	5.08	121.05	112.30
2	B	121	0DG	C2-N3-C4	5.08	121.05	112.30
1	A	122	0DA	N1A-C2A-N3A	-5.07	120.91	128.58
1	A	125	0DA	N9A-C8A-N7A	-5.07	106.75	113.94
3	C	215	0DG	N9-C4-N3	5.05	136.04	125.95
4	D	105	0DT	C5-C4-N3	5.03	119.70	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	125	0DA	C5A-C6A-N6A	5.02	135.71	123.29
1	A	106	0DA	C5A-C4A-N3A	-4.99	119.85	126.72
2	B	123	0DA	C4A-N9A-C1'	-4.98	106.52	126.50
4	D	107	0DT	C5-C4-N3	4.92	119.60	115.32
1	A	111	0DT	O4-C4-C5	-4.83	119.39	124.92
1	A	105	0DG	C2-N3-C4	4.82	120.61	112.30
4	D	104	0DA	C5A-C4A-N3A	-4.82	120.08	126.72
3	C	209	0DG	N9-C4-N3	4.82	135.59	125.95
3	C	212	0DA	N1A-C2A-N3A	-4.78	121.35	128.58
4	D	109	0DT	C5-C4-N3	4.77	119.47	115.32
4	D	102	0DT	N3-C2-N1	4.77	121.10	114.89
1	A	106	0DA	N1A-C2A-N3A	-4.77	121.36	128.58
1	A	121	0DG	C2-N3-C4	4.71	120.41	112.30
2	B	125	0DA	N9A-C8A-N7A	-4.71	107.26	113.94
1	A	116	0DG	C2-N3-C4	4.70	120.40	112.30
2	B	122	0DT	O4-C4-C5	-4.70	119.54	124.92
1	A	123	0DT	C5-C4-N3	4.69	119.40	115.32
1	A	105	0DG	N9-C4-N3	4.69	135.32	125.95
2	B	123	0DA	C1'-N9A-C8A	4.69	143.34	126.95
1	A	107	0DT	C5-C4-N3	4.67	119.38	115.32
4	D	104	0DA	N1A-C2A-N3A	-4.65	121.55	128.58
1	A	118	0DA	N1A-C2A-N3A	-4.63	121.57	128.58
1	A	111	0DT	O4'-C1'-N1	4.61	116.05	107.86
2	B	122	0DT	C5-C4-N3	4.61	119.33	115.32
1	A	114	0DA	N9A-C8A-N7A	-4.60	107.41	113.94
1	A	117	0DG	C2-N3-C4	4.60	120.22	112.30
1	A	114	0DA	N1A-C2A-N3A	-4.59	121.63	128.58
3	C	210	0DG	C2-N3-C4	4.59	120.21	112.30
1	A	116	0DG	N9-C4-N3	4.58	135.12	125.95
3	C	213	0DT	N3-C2-N1	4.57	120.84	114.89
1	A	118	0DA	N9A-C8A-N7A	-4.57	107.45	113.94
2	B	122	0DT	N3-C2-N1	4.53	120.78	114.89
1	A	112	0DG	C2-N3-C4	4.51	120.07	112.30
1	A	123	0DT	N3-C2-N1	4.51	120.76	114.89
1	A	110	0DC	O4'-C1'-N1	4.50	115.85	107.86
1	A	113	0DT	C5-C4-N3	4.47	119.21	115.32
3	C	213	0DT	O4-C4-C5	-4.45	119.82	124.92
1	A	106	0DA	N9A-C8A-N7A	-4.42	107.66	113.94
3	C	212	0DA	N9A-C8A-N7A	-4.36	107.75	113.94
2	B	123	0DA	C5A-C4A-N3A	-4.34	120.74	126.72
1	A	122	0DA	N9A-C8A-N7A	-4.34	107.78	113.94
1	A	120	0DA	N1A-C2A-N3A	-4.32	122.04	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	0DG	C5-C4-N3	-4.29	121.56	128.39
4	D	109	0DT	N3-C2-N1	4.27	120.45	114.89
2	B	125	0DA	N3A-C4A-N9A	4.27	134.42	127.17
2	B	123	0DA	C4A-N9A-C8A	4.17	110.12	105.74
3	C	214	0DC	C1'-N1-C2	4.17	124.99	117.83
4	D	103	0DG	C5-C4-N3	-4.16	121.76	128.39
4	D	107	0DT	O4-C4-C5	-4.16	120.16	124.92
3	C	212	0DA	N3A-C4A-N9A	4.13	134.20	127.17
1	A	125	0DA	C4A-N9A-C1'	-4.12	109.96	126.50
4	D	103	0DG	C2-N3-C4	4.11	119.37	112.30
4	D	104	0DA	C4A-N9A-C1'	-4.09	110.11	126.50
1	A	125	0DA	C5A-C4A-N3A	-4.07	121.12	126.72
2	B	121	0DG	C5-C4-N3	-4.00	122.02	128.39
1	A	120	0DA	C5A-N7A-C8A	3.98	109.71	103.45
1	A	120	0DA	N3A-C4A-N9A	3.98	133.94	127.17
4	D	108	0DG	N9-C4-N3	3.96	133.87	125.95
4	D	109	0DT	O4-C4-C5	-3.96	120.39	124.92
1	A	125	0DA	C1'-N9A-C8A	3.96	140.79	126.95
1	A	115	0DC	C1'-N1-C2	3.95	124.61	117.83
1	A	111	0DT	N3-C2-N1	3.94	120.02	114.89
1	A	122	0DA	N3A-C4A-N9A	3.93	133.85	127.17
1	A	124	0DC	C3'-C2'-C1'	-3.91	93.04	102.60
4	D	104	0DA	C1'-N9A-C8A	3.83	140.34	126.95
4	D	102	0DT	C5-C6-N1	-3.82	119.16	123.31
1	A	107	0DT	O4-C4-C5	-3.79	120.58	124.92
1	A	113	0DT	C6-N1-C2	-3.79	117.53	121.30
1	A	112	0DG	N9-C4-N3	3.79	133.52	125.95
1	A	113	0DT	O4-C4-C5	-3.78	120.59	124.92
1	A	106	0DA	N3A-C4A-N9A	3.78	133.60	127.17
1	A	120	0DA	C4A-N9A-C8A	3.78	109.71	105.74
1	A	112	0DG	O4'-C1'-N9	3.77	114.56	107.86
2	B	125	0DA	C4A-N9A-C8A	3.76	109.69	105.74
1	A	108	0DG	N9-C4-N3	3.75	133.45	125.95
3	C	210	0DG	N9-C4-N3	3.73	133.41	125.95
3	C	215	0DG	C2'-C1'-N9	-3.68	104.62	113.81
2	B	121	0DG	C2'-C1'-N9	3.67	122.99	113.81
1	A	125	0DA	N1A-C2A-N3A	-3.66	123.04	128.58
3	C	210	0DG	C1'-N9-C4	-3.64	115.67	125.50
2	B	119	0DC	O4'-C1'-N1	3.64	114.33	107.86
1	A	121	0DG	N9-C4-N3	3.63	133.21	125.95
4	D	105	0DT	C5-C6-N1	-3.62	119.39	123.31
4	D	104	0DA	C4A-N9A-C8A	3.60	109.52	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	107	0DT	O4'-C1'-N1	3.57	114.19	107.86
3	C	210	0DG	C3'-C2'-C1'	-3.55	93.90	102.60
1	A	118	0DA	C4A-N9A-C1'	-3.53	112.34	126.50
3	C	210	0DG	C1'-N9-C8	3.53	135.83	127.91
1	A	106	0DA	C4A-N9A-C8A	3.51	109.43	105.74
1	A	123	0DT	O4-C4-C5	-3.51	120.90	124.92
3	C	212	0DA	C2A-N3A-C4A	3.50	120.37	111.83
1	A	104	0DC	C1'-N1-C2	3.50	123.83	117.83
1	A	110	0DC	O4'-C1'-C2'	-3.47	99.75	106.25
4	D	104	0DA	C5A-N7A-C8A	3.46	108.89	103.45
1	A	114	0DA	C5A-N7A-C8A	3.45	108.88	103.45
1	A	118	0DA	C1'-N9A-C8A	3.43	138.94	126.95
4	D	107	0DT	C6-C5-C4	3.43	120.84	118.02
1	A	122	0DA	C2A-N3A-C4A	3.41	120.17	111.83
1	A	108	0DG	C2-N1-C6	-3.39	118.96	125.11
2	B	123	0DA	C2A-N3A-C4A	3.38	120.08	111.83
4	D	103	0DG	N9-C8-N7	-3.38	107.14	113.40
1	A	114	0DA	N3A-C4A-N9A	3.37	132.91	127.17
1	A	121	0DG	C1'-N9-C4	-3.36	116.44	125.50
1	A	122	0DA	C5A-N7A-C8A	3.35	108.72	103.45
2	B	121	0DG	C5-C6-N1	3.35	121.78	113.25
4	D	108	0DG	C3'-C2'-C1'	-3.35	94.41	102.60
1	A	125	0DA	C4A-N9A-C8A	3.34	109.25	105.74
1	A	114	0DA	C4A-N9A-C1'	-3.33	113.16	126.50
2	B	125	0DA	C2A-N3A-C4A	3.33	119.96	111.83
1	A	118	0DA	N3A-C4A-N9A	3.33	132.82	127.17
2	B	125	0DA	C4A-N9A-C1'	-3.30	113.27	126.50
1	A	106	0DA	C4A-N9A-C1'	-3.29	113.31	126.50
1	A	125	0DA	C5A-N7A-C8A	3.29	108.62	103.45
1	A	107	0DT	C6-N1-C2	-3.28	118.03	121.30
3	C	211	0DC	O4'-C1'-N1	3.28	113.68	107.86
4	D	106	0DC	C1'-N1-C2	3.26	123.43	117.83
1	A	118	0DA	C5A-N7A-C8A	3.25	108.56	103.45
2	B	119	0DC	C1'-N1-C6	-3.25	115.14	121.53
2	B	123	0DA	C5A-N7A-C8A	3.24	108.55	103.45
1	A	107	0DT	C6-C5-C4	3.24	120.69	118.02
3	C	212	0DA	C5A-N7A-C8A	3.24	108.54	103.45
1	A	114	0DA	C1'-N9A-C8A	3.24	138.28	126.95
1	A	117	0DG	N9-C8-N7	-3.23	107.42	113.40
1	A	120	0DA	C2A-N3A-C4A	3.22	119.69	111.83
4	D	104	0DA	C4'-O4'-C1'	-3.22	101.86	109.51
2	B	121	0DG	N9-C8-N7	-3.22	107.43	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	108	0DG	C2-N1-C6	-3.22	119.28	125.11
1	A	121	0DG	C1'-N9-C8	3.21	135.12	127.91
1	A	112	0DG	C2-N1-C6	-3.20	119.30	125.11
3	C	213	0DT	C5-C6-N1	-3.20	119.84	123.31
4	D	104	0DA	C2A-N3A-C4A	3.19	119.63	111.83
1	A	116	0DG	O4'-C1'-N9	3.18	113.51	107.86
1	A	106	0DA	C2A-N3A-C4A	3.14	119.49	111.83
1	A	114	0DA	C2A-N3A-C4A	3.13	119.48	111.83
1	A	107	0DT	O2-C2-N1	-3.12	118.73	122.80
1	A	120	0DA	C4A-N9A-C1'	-3.11	114.03	126.50
1	A	120	0DA	C4A-C5A-N7A	-3.09	107.04	110.58
3	C	215	0DG	C2-N1-C6	-3.09	119.51	125.11
4	D	108	0DG	O4'-C1'-C2'	-3.07	100.51	106.25
2	B	124	0DC	O4'-C1'-N1	3.07	113.31	107.86
4	D	109	0DT	O2-C2-N1	-3.05	118.83	122.80
1	A	118	0DA	C2A-N3A-C4A	3.04	119.26	111.83
2	B	119	0DC	C2'-C1'-N1	3.04	121.41	113.81
1	A	113	0DT	O4'-C1'-C2'	-3.03	100.58	106.25
1	A	121	0DG	N9-C8-N7	-3.01	107.81	113.40
4	D	102	0DT	O4-C4-C5	-3.01	121.47	124.92
3	C	210	0DG	C2-N1-C6	-3.01	119.66	125.11
4	D	105	0DT	O2-C2-N1	-3.00	118.89	122.80
4	D	104	0DA	N3A-C4A-N9A	3.00	132.27	127.17
1	A	120	0DA	C6A-C5A-C4A	2.98	121.25	117.18
3	C	210	0DG	N9-C8-N7	-2.98	107.88	113.40
1	A	109	0DC	C1'-N1-C2	2.97	122.93	117.83
2	B	122	0DT	C1'-N1-C6	2.96	125.72	120.74
1	A	116	0DG	C2-N1-C6	-2.95	119.76	125.11
1	A	121	0DG	C2-N1-C6	-2.94	119.77	125.11
2	B	121	0DG	N1-C2-N3	-2.94	117.95	123.32
1	A	106	0DA	C1'-N9A-C8A	2.94	137.22	126.95
4	D	108	0DG	C5-C6-N1	2.92	120.70	113.25
1	A	117	0DG	C5-C6-N1	2.91	120.66	113.25
3	C	212	0DA	C4A-N9A-C1'	-2.90	114.87	126.50
2	B	125	0DA	C5A-N7A-C8A	2.90	108.01	103.45
1	A	111	0DT	C5-C6-N1	-2.90	120.17	123.31
1	A	113	0DT	O4'-C1'-N1	2.90	113.01	107.86
1	A	107	0DT	C5-C6-N1	-2.90	120.17	123.31
1	A	117	0DG	C2-N1-C6	-2.89	119.87	125.11
2	B	121	0DG	O3'-C3'-C2'	2.89	120.90	110.88
2	B	125	0DA	C1'-N9A-C8A	2.88	137.03	126.95
4	D	105	0DT	C1'-N1-C6	2.88	125.58	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	0DG	C2-N1-C6	-2.87	119.90	125.11
1	A	114	0DA	C4A-C5A-N7A	-2.87	107.31	110.58
1	A	125	0DA	C4A-C5A-N7A	-2.86	107.31	110.58
2	B	125	0DA	C2'-C1'-N9A	-2.86	107.90	114.63
1	A	113	0DT	C6-C5-C4	2.85	120.37	118.02
1	A	108	0DG	C1'-N9-C8	2.84	134.28	127.91
1	A	114	0DA	C6A-C5A-C4A	2.84	121.05	117.18
3	C	212	0DA	C4A-N9A-C8A	2.83	108.71	105.74
3	C	209	0DG	C2-N1-C6	-2.83	119.98	125.11
4	D	103	0DG	C2-N1-C6	-2.82	120.00	125.11
3	C	209	0DG	C5-C6-N1	2.82	120.43	113.25
1	A	118	0DA	C4A-N9A-C8A	2.81	108.69	105.74
1	A	106	0DA	C5A-N7A-C8A	2.81	107.86	103.45
1	A	122	0DA	C4A-N9A-C1'	-2.80	115.27	126.50
1	A	108	0DG	N9-C8-N7	-2.80	108.21	113.40
3	C	215	0DG	C5-C6-N1	2.80	120.37	113.25
1	A	108	0DG	C5-C6-N1	2.79	120.36	113.25
1	A	105	0DG	O6-C6-C5	-2.78	119.18	126.53
4	D	102	0DT	C4'-O4'-C1'	-2.78	102.90	109.51
3	C	214	0DC	O2-C2-N3	-2.78	117.94	122.33
3	C	213	0DT	C6-C5-C4	2.78	120.31	118.02
1	A	117	0DG	O4'-C1'-N9	-2.77	102.94	107.86
1	A	108	0DG	C1'-N9-C4	-2.76	118.06	125.50
4	D	108	0DG	N9-C8-N7	-2.74	108.31	113.40
2	B	125	0DA	O4'-C1'-N9A	2.74	112.89	107.96
1	A	122	0DA	C6A-C5A-C4A	2.74	120.92	117.18
4	D	104	0DA	C4A-C5A-N7A	-2.73	107.45	110.58
1	A	118	0DA	C6A-C5A-C4A	2.73	120.90	117.18
1	A	111	0DT	C4'-O4'-C1'	-2.73	103.03	109.51
3	C	210	0DG	C5-C6-N1	2.72	120.17	113.25
4	D	107	0DT	O2-C2-N1	-2.72	119.26	122.80
4	D	105	0DT	C4'-O4'-C1'	-2.71	103.07	109.51
3	C	212	0DA	C1'-N9A-C8A	2.70	136.40	126.95
1	A	116	0DG	C5-C6-N1	2.70	120.13	113.25
4	D	109	0DT	O4'-C1'-C2'	-2.70	101.20	106.25
4	D	107	0DT	C5-C6-N1	-2.70	120.39	123.31
3	C	213	0DT	O4'-C1'-C2'	-2.69	101.23	106.25
1	A	114	0DA	C4A-N9A-C8A	2.68	108.55	105.74
2	B	124	0DC	C3'-C2'-C1'	-2.68	96.05	102.60
4	D	109	0DT	C5-C6-N1	-2.68	120.41	123.31
1	A	105	0DG	C5-C6-N1	2.66	120.03	113.25
4	D	108	0DG	C1'-N9-C4	-2.66	118.33	125.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	107	0DT	C5M-C5-C6	-2.66	119.26	122.85
4	D	107	0DT	C6-N1-C2	-2.65	118.66	121.30
1	A	117	0DG	C2'-C1'-N9	2.65	120.44	113.81
4	D	104	0DA	O4'-C1'-N9A	2.65	112.72	107.96
4	D	105	0DT	C6-C5-C4	2.64	120.20	118.02
1	A	122	0DA	C1'-N9A-C8A	2.63	136.16	126.95
2	B	121	0DG	C2-N1-C6	-2.63	120.34	125.11
3	C	209	0DG	N9-C8-N7	-2.63	108.53	113.40
1	A	125	0DA	C2A-N3A-C4A	2.63	118.25	111.83
3	C	214	0DC	C1'-N1-C6	-2.62	116.37	121.53
1	A	120	0DA	C1'-N9A-C8A	2.62	136.12	126.95
2	B	123	0DA	N3A-C4A-N9A	2.62	131.62	127.17
1	A	122	0DA	C4A-N9A-C8A	2.61	108.47	105.74
4	D	102	0DT	C6-C5-C4	2.60	120.16	118.02
3	C	215	0DG	N9-C8-N7	-2.59	108.59	113.40
1	A	122	0DA	C4A-C5A-N7A	-2.59	107.62	110.58
1	A	108	0DG	C8-N7-C5	2.59	108.87	104.26
1	A	121	0DG	C5-C6-N1	2.58	119.83	113.25
1	A	123	0DT	C5-C6-N1	-2.58	120.51	123.31
4	D	103	0DG	C5-C6-N1	2.57	119.79	113.25
3	C	215	0DG	O6-C6-C5	-2.57	119.75	126.53
2	B	121	0DG	O6-C6-C5	-2.56	119.76	126.53
4	D	107	0DT	C1'-N1-C2	2.56	122.66	117.66
1	A	116	0DG	O6-C6-C5	-2.56	119.78	126.53
3	C	212	0DA	C6A-C5A-C4A	2.55	120.66	117.18
1	A	110	0DC	C1'-N1-C2	2.54	122.19	117.83
1	A	118	0DA	C4A-C5A-N7A	-2.53	107.68	110.58
4	D	105	0DT	O4'-C1'-C2'	-2.53	101.52	106.25
2	B	121	0DG	C6-C5-N7	2.51	134.86	130.29
1	A	119	0DC	C4'-O4'-C1'	-2.50	103.58	109.51
2	B	123	0DA	C4A-C5A-N7A	-2.48	107.75	110.58
1	A	121	0DG	C8-N7-C5	2.47	108.67	104.26
3	C	214	0DC	O2-C2-N1	2.44	123.67	118.90
1	A	110	0DC	C2'-C1'-N1	-2.44	107.72	113.81
4	D	102	0DT	C2'-C3'-C4'	2.42	107.71	102.80
1	A	123	0DT	C6-C5-C4	2.42	120.02	118.02
3	C	209	0DG	N2-C2-N3	2.41	124.38	119.67
3	C	209	0DG	O6-C6-C5	-2.41	120.17	126.53
4	D	108	0DG	C8-N7-C5	2.40	108.53	104.26
3	C	212	0DA	C4A-C5A-N7A	-2.39	107.84	110.58
1	A	112	0DG	C1'-N9-C8	2.39	133.28	127.91
1	A	112	0DG	C5-C6-N1	2.37	119.29	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	0DC	C1'-N1-C6	-2.36	116.89	121.53
2	B	125	0DA	C6A-C5A-C4A	2.36	120.39	117.18
1	A	106	0DA	C6A-C5A-C4A	2.35	120.39	117.18
1	A	111	0DT	O2-C2-N1	-2.35	119.74	122.80
4	D	102	0DT	C5M-C5-C6	-2.35	119.68	122.85
1	A	113	0DT	C2'-C1'-N1	2.34	119.67	113.81
1	A	123	0DT	O2-C2-N1	-2.34	119.75	122.80
3	C	215	0DG	N2-C2-N3	2.33	124.22	119.67
3	C	210	0DG	O4'-C1'-C2'	-2.33	101.89	106.25
4	D	105	0DT	O4-C4-C5	-2.33	122.25	124.92
1	A	104	0DC	C1'-N1-C6	-2.32	116.97	121.53
1	A	105	0DG	N2-C2-N3	2.32	124.19	119.67
1	A	109	0DC	C1'-N1-C6	-2.31	116.99	121.53
1	A	112	0DG	N9-C8-N7	-2.30	109.14	113.40
4	D	108	0DG	C1'-N9-C8	2.30	133.06	127.91
1	A	123	0DT	C6-N1-C2	-2.29	119.02	121.30
4	D	106	0DC	O2-C2-N3	-2.29	118.72	122.33
3	C	215	0DG	C8-N7-C5	2.29	108.34	104.26
3	C	213	0DT	O4'-C1'-N1	2.28	111.92	107.86
3	C	210	0DG	C8-N7-C5	2.28	108.32	104.26
3	C	210	0DG	O6-C6-C5	-2.26	120.56	126.53
3	C	213	0DT	O2-C2-N1	-2.25	119.86	122.80
4	D	103	0DG	O6-C6-C5	-2.25	120.60	126.53
1	A	121	0DG	O4'-C1'-N9	2.24	111.85	107.86
1	A	116	0DG	O4'-C1'-C2'	-2.22	102.10	106.25
1	A	112	0DG	C8-N7-C5	2.21	108.20	104.26
3	C	209	0DG	N1-C2-N3	-2.21	119.28	123.32
4	D	105	0DT	C2'-C1'-N1	2.20	119.31	113.81
1	A	108	0DG	C4-C5-N7	-2.19	107.19	110.67
1	A	110	0DC	C4'-O4'-C1'	-2.19	104.30	109.51
4	D	103	0DG	C8-N7-C5	2.19	108.16	104.26
1	A	112	0DG	O4'-C1'-C2'	-2.19	102.16	106.25
3	C	209	0DG	C8-N7-C5	2.18	108.15	104.26
3	C	211	0DC	C2'-C3'-C4'	-2.18	98.38	102.80
1	A	107	0DT	C2'-C1'-N1	2.18	119.26	113.81
1	A	117	0DG	N9-C4-N3	2.17	130.30	125.95
1	A	112	0DG	C1'-N9-C4	-2.16	119.66	125.50
3	C	211	0DC	C1'-N1-C2	2.16	121.53	117.83
1	A	116	0DG	N9-C8-N7	-2.14	109.43	113.40
1	A	125	0DA	N3A-C4A-N9A	2.14	130.80	127.17
1	A	110	0DC	O4'-C4'-C5'	2.14	116.18	109.33
1	A	117	0DG	N1-C2-N3	-2.14	119.41	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	119	0DC	C4'-O4'-C1'	-2.11	104.50	109.51
1	A	105	0DG	N9-C8-N7	-2.11	109.50	113.40
2	B	122	0DT	C6-N1-C2	-2.10	119.22	121.30
2	B	122	0DT	C5-C6-N1	-2.09	121.04	123.31
3	C	214	0DC	N4-C4-N3	2.09	121.65	117.91
1	A	117	0DG	O6-C6-C5	-2.09	121.02	126.53
1	A	104	0DC	O2-C2-N3	-2.09	119.04	122.33
1	A	125	0DA	C5A-C4A-N9A	2.08	108.08	105.81
4	D	104	0DA	C6A-C5A-C4A	2.07	120.00	117.18
1	A	117	0DG	C3'-C2'-C1'	-2.07	97.54	102.60
1	A	123	0DT	C5M-C5-C6	-2.07	120.05	122.85
4	D	103	0DG	N9-C4-N3	2.06	130.08	125.95
1	A	113	0DT	C5-C6-N1	-2.06	121.07	123.31
4	D	105	0DT	C5M-C5-C6	-2.06	120.06	122.85
3	C	211	0DC	C6-C5-C4	2.06	120.90	117.53
4	D	103	0DG	C3'-C2'-C1'	-2.05	97.58	102.60
3	C	210	0DG	O4'-C1'-N9	2.05	111.50	107.86
4	D	109	0DT	C6-C5-C4	2.04	119.70	118.02
1	A	112	0DG	C6-C5-C4	2.04	121.89	118.83
1	A	106	0DA	O4'-C4'-C3'	-2.04	101.01	105.65
1	A	115	0DC	C6-C5-C4	2.02	120.85	117.53
1	A	117	0DG	O4'-C1'-C2'	-2.02	102.48	106.25
2	B	121	0DG	N9-C4-N3	2.02	129.99	125.95
1	A	117	0DG	C6-C5-N7	2.01	133.96	130.29
1	A	117	0DG	C8-N7-C5	2.01	107.84	104.26
1	A	104	0DC	O2-C2-N1	2.01	122.83	118.90
1	A	111	0DT	O4'-C1'-C2'	-2.01	102.50	106.25

There are no chirality outliers.

All (130) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	108	0DG	O4'-C4'-C5'-O5'
1	A	112	0DG	O4'-C4'-C5'-O5'
1	A	118	0DA	O4'-C4'-C5'-O5'
1	A	121	0DG	O4'-C4'-C5'-O5'
2	B	119	0DC	O4'-C4'-C5'-O5'
2	B	121	0DG	O4'-C4'-C5'-O5'
3	C	212	0DA	O4'-C4'-C5'-O5'
3	C	213	0DT	O4'-C4'-C5'-O5'
4	D	104	0DA	C4'-C5'-O5'-P
4	D	106	0DC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	D	108	0DG	O4'-C4'-C5'-O5'
4	D	108	0DG	C3'-C4'-C5'-O5'
1	A	104	0DC	C3'-C4'-C5'-O5'
2	B	119	0DC	C2'-C1'-N1-C2
1	A	104	0DC	O4'-C4'-C5'-O5'
1	A	108	0DG	C3'-C4'-C5'-O5'
1	A	109	0DC	C3'-C4'-C5'-O5'
1	A	112	0DG	C3'-C4'-C5'-O5'
1	A	113	0DT	O4'-C4'-C5'-O5'
1	A	114	0DA	O4'-C4'-C5'-O5'
1	A	117	0DG	C3'-C4'-C5'-O5'
1	A	123	0DT	O4'-C4'-C5'-O5'
1	A	123	0DT	C3'-C4'-C5'-O5'
1	A	124	0DC	O4'-C4'-C5'-O5'
2	B	119	0DC	C3'-C4'-C5'-O5'
2	B	125	0DA	O4'-C4'-C5'-O5'
3	C	213	0DT	C3'-C4'-C5'-O5'
4	D	104	0DA	C3'-C4'-C5'-O5'
4	D	105	0DT	O4'-C4'-C5'-O5'
4	D	109	0DT	C3'-C4'-C5'-O5'
2	B	119	0DC	C2'-C1'-N1-C6
2	B	120	0DC	C2'-C1'-N1-C6
1	A	106	0DA	O4'-C4'-C5'-O5'
1	A	106	0DA	C3'-C4'-C5'-O5'
1	A	109	0DC	O4'-C4'-C5'-O5'
1	A	111	0DT	C3'-C4'-C5'-O5'
1	A	115	0DC	O4'-C4'-C5'-O5'
1	A	115	0DC	C3'-C4'-C5'-O5'
1	A	117	0DG	O4'-C4'-C5'-O5'
1	A	119	0DC	C3'-C4'-C5'-O5'
1	A	124	0DC	C3'-C4'-C5'-O5'
2	B	121	0DG	C3'-C4'-C5'-O5'
2	B	125	0DA	C3'-C4'-C5'-O5'
3	C	211	0DC	O4'-C4'-C5'-O5'
4	D	105	0DT	C3'-C4'-C5'-O5'
4	D	105	0DT	C2'-C1'-N1-C6
2	B	120	0DC	C2'-C1'-N1-C2
1	A	119	0DC	O4'-C1'-N1-C6
4	D	102	0DT	O4'-C1'-N1-C6
1	A	113	0DT	C3'-C4'-C5'-O5'
1	A	118	0DA	C3'-C4'-C5'-O5'
1	A	119	0DC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	121	0DG	C3'-C4'-C5'-O5'
3	C	211	0DC	C3'-C4'-C5'-O5'
4	D	106	0DC	C3'-C4'-C5'-O5'
2	B	122	0DT	C2'-C1'-N1-C6
4	D	102	0DT	C2'-C1'-N1-C6
2	B	122	0DT	C2'-C1'-N1-C2
4	D	102	0DT	C2'-C1'-N1-C2
4	D	102	0DT	O4'-C1'-N1-C2
1	A	111	0DT	O4'-C4'-C5'-O5'
3	C	209	0DG	O4'-C4'-C5'-O5'
3	C	212	0DA	C3'-C4'-C5'-O5'
3	C	214	0DC	O4'-C4'-C5'-O5'
1	A	119	0DC	C2'-C1'-N1-C6
4	D	102	0DT	C3'-C4'-C5'-O5'
1	A	110	0DC	O4'-C4'-C5'-O5'
1	A	114	0DA	C3'-C4'-C5'-O5'
1	A	116	0DG	O4'-C4'-C5'-O5'
4	D	104	0DA	O4'-C4'-C5'-O5'
3	C	210	0DG	O4'-C4'-C5'-O5'
3	C	215	0DG	O4'-C4'-C5'-O5'
4	D	109	0DT	O4'-C4'-C5'-O5'
1	A	119	0DC	O4'-C1'-N1-C2
2	B	120	0DC	O4'-C1'-N1-C6
2	B	122	0DT	O4'-C1'-N1-C6
4	D	105	0DT	O4'-C1'-N1-C6
1	A	119	0DC	C2'-C1'-N1-C2
4	D	105	0DT	C2'-C1'-N1-C2
1	A	116	0DG	C3'-C4'-C5'-O5'
1	A	119	0DC	C4'-C5'-O5'-P
1	A	111	0DT	C2'-C1'-N1-C6
4	D	104	0DA	C2'-C1'-N9A-C4A
3	C	212	0DA	O4'-C1'-N9A-C4A
4	D	104	0DA	O4'-C1'-N9A-C4A
1	A	110	0DC	C3'-C4'-C5'-O5'
3	C	209	0DG	C3'-C4'-C5'-O5'
2	B	120	0DC	O4'-C1'-N1-C2
2	B	122	0DT	O4'-C1'-N1-C2
1	A	125	0DA	C3'-C4'-C5'-O5'
3	C	210	0DG	C3'-C4'-C5'-O5'
3	C	211	0DC	C2'-C1'-N1-C6
4	D	105	0DT	O4'-C1'-N1-C2
1	A	125	0DA	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	C	214	0DC	C3'-C4'-C5'-O5'
3	C	215	0DG	C3'-C4'-C5'-O5'
4	D	102	0DT	O4'-C4'-C5'-O5'
4	D	109	0DT	C2'-C1'-N1-C6
1	A	111	0DT	O4'-C1'-N1-C6
3	C	211	0DC	C2'-C1'-N1-C2
4	D	109	0DT	C2'-C1'-N1-C2
3	C	211	0DC	O4'-C1'-N1-C6
1	A	107	0DT	C3'-C4'-C5'-O5'
1	A	111	0DT	C2'-C1'-N1-C2
1	A	112	0DG	C4'-C5'-O5'-P
1	A	118	0DA	C2'-C1'-N9A-C4A
1	A	125	0DA	C2'-C1'-N9A-C4A
2	B	123	0DA	C2'-C1'-N9A-C4A
1	A	124	0DC	C2'-C1'-N1-C6
2	B	122	0DT	C4'-C5'-O5'-P
4	D	103	0DG	C4'-C5'-O5'-P
3	C	212	0DA	O4'-C1'-N9A-C8A
3	C	211	0DC	O4'-C1'-N1-C2
1	A	124	0DC	O4'-C1'-N1-C6
4	D	109	0DT	O4'-C1'-N1-C6
1	A	111	0DT	C4'-C5'-O5'-P
1	A	113	0DT	C4'-C5'-O5'-P
1	A	117	0DG	C4'-C5'-O5'-P
1	A	111	0DT	O4'-C1'-N1-C2
3	C	209	0DG	C4'-C5'-O5'-P
4	D	109	0DT	O4'-C1'-N1-C2
1	A	122	0DA	C2'-C1'-N9A-C4A
3	C	212	0DA	C2'-C1'-N9A-C4A
3	C	212	0DA	C4'-C5'-O5'-P
3	C	212	0DA	C2'-C1'-N9A-C8A
1	A	124	0DC	C2'-C1'-N1-C2
1	A	124	0DC	O4'-C1'-N1-C2
1	A	122	0DA	O4'-C1'-N9A-C4A
1	A	107	0DT	O4'-C4'-C5'-O5'
3	C	214	0DC	C2'-C1'-N1-C6

There are no ring outliers.

40 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	106	0DA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	213	0DT	2	0
1	A	107	0DT	2	0
1	A	113	0DT	1	0
1	A	118	0DA	3	0
2	B	124	0DC	1	0
1	A	104	0DC	1	0
4	D	103	0DG	3	0
1	A	119	0DC	3	0
2	B	120	0DC	3	0
2	B	122	0DT	4	0
1	A	125	0DA	2	0
1	A	110	0DC	1	0
1	A	122	0DA	2	0
1	A	108	0DG	1	0
4	D	104	0DA	1	0
1	A	123	0DT	1	0
1	A	115	0DC	2	0
1	A	111	0DT	1	0
4	D	105	0DT	1	0
2	B	119	0DC	3	0
1	A	112	0DG	1	0
3	C	210	0DG	5	0
3	C	209	0DG	3	0
1	A	114	0DA	4	0
2	B	121	0DG	2	0
1	A	117	0DG	4	0
2	B	123	0DA	1	0
1	A	105	0DG	4	0
3	C	212	0DA	2	0
3	C	214	0DC	1	0
4	D	108	0DG	1	0
1	A	120	0DA	3	0
4	D	109	0DT	5	0
1	A	124	0DC	1	0
1	A	109	0DC	1	0
4	D	102	0DT	4	0
4	D	107	0DT	3	0
1	A	116	0DG	3	0
3	C	211	0DC	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	0/22	-	-	-	-
2	B	0/7	-	-	-	-
3	C	0/7	-	-	-	-
4	D	0/8	-	-	-	-
All	All	0/44	-	-	-	-

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	ODT	A	113	20/21	0.88	0.18	180,193,215,221	0
4	ODG	D	108	22/23	0.93	0.07	214,229,255,261	0
4	ODT	D	105	20/21	0.94	0.08	409,426,463,468	0
1	ODC	A	124	19/20	0.94	0.07	493,517,534,541	0
1	ODT	A	111	20/21	0.95	0.19	230,253,264,269	0
1	ODA	A	118	21/22	0.96	0.12	251,279,294,296	0
1	ODG	A	112	22/23	0.96	0.21	201,222,237,242	0
2	ODA	B	123	21/22	0.96	0.13	221,242,253,264	0
1	ODC	A	109	19/20	0.96	0.09	349,356,401,408	0
1	ODA	A	114	21/22	0.96	0.28	167,182,197,202	0
1	ODG	A	121	22/23	0.97	0.08	314,326,339,344	0
1	ODT	A	123	20/21	0.97	0.12	376,422,433,434	0
1	ODC	A	104	16/20	0.97	0.09	366,403,413,414	0
1	ODC	A	115	19/20	0.97	0.22	180,198,212,213	0
3	ODG	C	210	22/23	0.97	0.09	323,334,340,349	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	0DA	C	212	21/22	0.97	0.13	533,551,567,578	0
4	0DG	D	103	22/23	0.97	0.07	505,531,578,592	0
1	0DG	A	116	22/23	0.97	0.12	192,218,228,236	0
4	0DT	D	107	20/21	0.97	0.05	243,265,285,294	0
1	0DA	A	106	21/22	0.97	0.13	459,469,487,487	0
4	0DT	D	109	20/21	0.97	0.06	182,194,211,211	0
2	0DT	B	122	20/21	0.98	0.07	209,231,246,255	0
1	0DA	A	120	21/22	0.98	0.07	275,293,327,340	0
2	0DC	B	124	19/20	0.98	0.13	229,242,250,260	0
2	0DA	B	125	21/22	0.98	0.10	252,261,270,280	0
3	0DG	C	209	22/23	0.98	0.09	304,318,351,360	0
1	0DC	A	110	19/20	0.98	0.09	281,299,310,311	0
3	0DC	C	211	19/20	0.98	0.14	405,447,451,452	0
1	0DA	A	122	21/22	0.98	0.11	339,355,371,378	0
1	0DG	A	117	22/23	0.98	0.07	198,226,250,253	0
4	0DA	D	104	21/22	0.98	0.06	477,498,546,569	0
1	0DG	A	108	22/23	0.98	0.07	507,521,547,567	0
4	0DC	D	106	19/20	0.98	0.06	420,435,465,477	0
2	0DC	B	119	19/20	0.98	0.13	180,186,199,202	0
2	0DC	B	120	19/20	0.98	0.06	186,209,219,221	0
2	0DG	B	121	22/23	0.98	0.07	194,220,238,247	0
1	0DA	A	125	21/22	0.99	0.10	561,604,623,626	0
1	0DC	A	119	19/20	0.99	0.20	249,268,285,291	0
1	0DT	A	107	20/21	0.99	0.17	466,483,514,527	0
1	0DG	A	105	22/23	0.99	0.10	446,474,485,493	0
3	0DT	C	213	20/21	0.99	0.09	551,574,596,598	0
3	0DG	C	215	22/23	0.99	0.07	592,613,637,656	0
4	0DT	D	102	17/21	0.99	0.05	527,548,598,607	0
3	0DC	C	214	19/20	1.00	0.07	567,580,600,607	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.