Full wwPDB NMR Structure Validation Report (i)

Feb 24, 2022 – 08:05 AM EST

PDB ID	:	1ZQ3
Title	:	NMR Solution Structure of the Bicoid Homeodomain Bound to the Consensus DNA Binding Site TAATCC
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Deposited on	:	2005-05-18

This is a Full wwPDB NMR 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/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

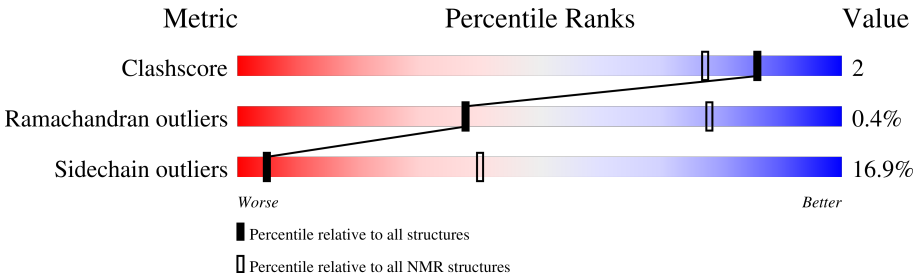
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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%

Mol	Chain	Length	Quality of chain
1	A	13	62% 38%
2	B	13	31% 69%
3	P	68	41% 18% . 38%

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	P:10-P:51 (42)	0.26	3

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 13, 14, 15, 16, 17, 18, 19, 20
2	11, 12

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1960 atoms, of which 871 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP *G)-3'.

Mol	Chain	Residues	Atoms						Trace
1	A	13	Total	C	H	N	O	P	0
			405	124	148	44	77	12	

- Molecule 2 is a DNA chain called 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*G P*C)-3'.

Mol	Chain	Residues	Atoms						Trace
2	B	13	Total	C	H	N	O	P	0
			417	128	147	55	75	12	

- Molecule 3 is a protein called Homeotic bicoid protein.

Mol	Chain	Residues	Atoms					Trace
3	P	68	Total	C	H	N	O	0
			1138	348	576	115	99	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	1	GLY	-	cloning artifact	UNP Q9UAM0

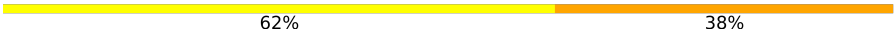
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

Chain A:

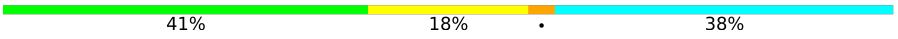


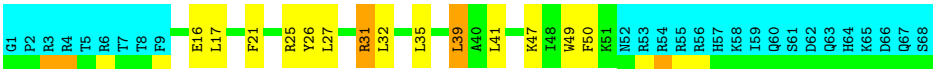
• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B:

• Molecule 3: Homeotic bicoid protein

Chain P:





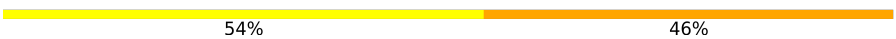
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

Chain A:

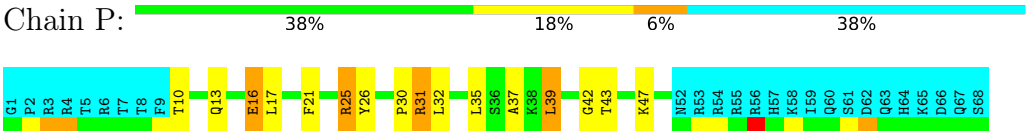


• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B:

• Molecule 3: Homeotic bicoid protein

Chain P:



4.2.2 Score per residue for model 2

• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

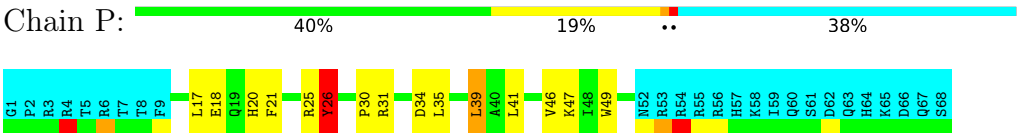
Chain A:

• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B:

• Molecule 3: Homeotic bicoid protein

Chain P:



4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

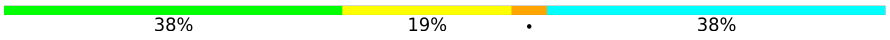
Chain A:

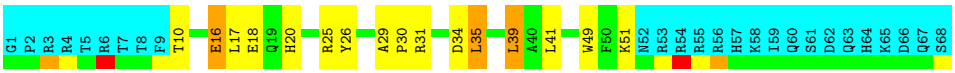
• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B:

• Molecule 3: Homeotic bicoid protein

Chain P:

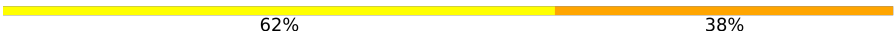




4.2.4 Score per residue for model 4

• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

Chain A:

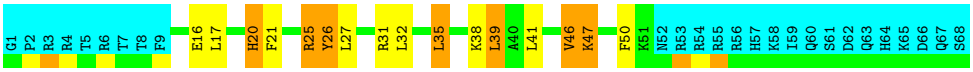


• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B:

• Molecule 3: Homeotic bicoid protein

Chain P:



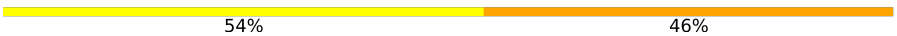
4.2.5 Score per residue for model 5

• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

Chain A:

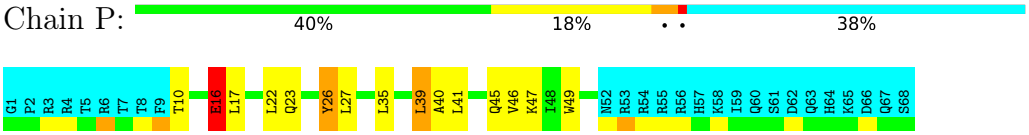
• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B:



• Molecule 3: Homeotic bicoid protein

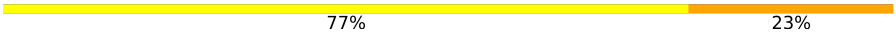
Chain P:

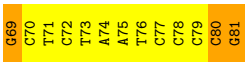


4.2.6 Score per residue for model 6

• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

Chain A:



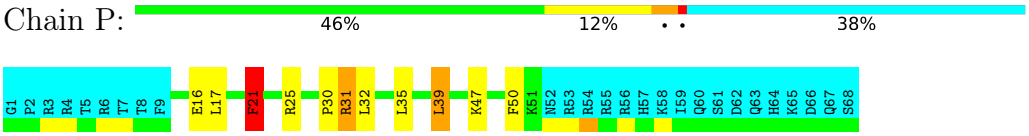


• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B:

• Molecule 3: Homeotic bicoid protein

Chain P:



4.2.7 Score per residue for model 7

• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

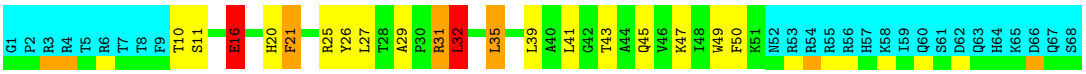
Chain A:

• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B:

• Molecule 3: Homeotic bicoid protein

Chain P:



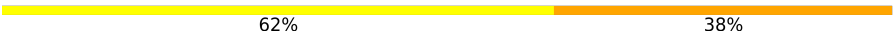
4.2.8 Score per residue for model 8

• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

Chain A:

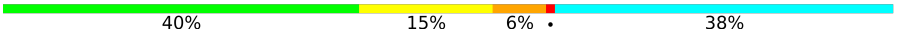
• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B:



• Molecule 3: Homeotic bicoid protein

Chain P:



4.2.9 Score per residue for model 9

• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

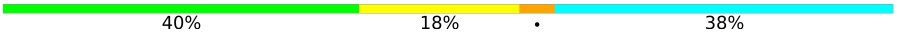
Chain A:

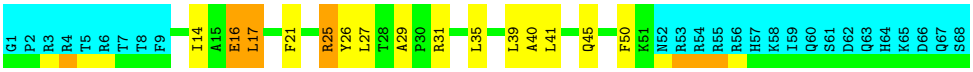
• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B:

• Molecule 3: Homeotic bicoid protein

Chain P:





4.2.10 Score per residue for model 10

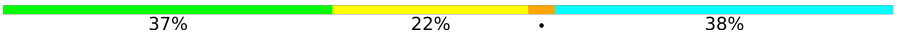
• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

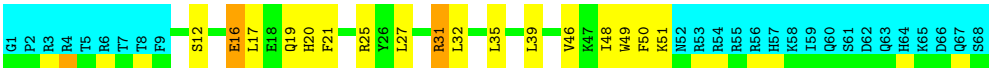
Chain A: 

• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B: 

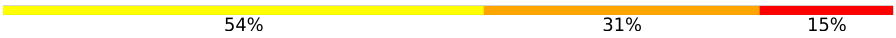
• Molecule 3: Homeotic bicoid protein

Chain P: 



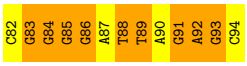
4.2.11 Score per residue for model 11

• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

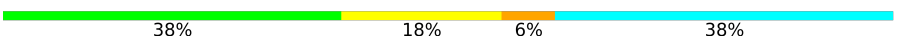
Chain A: 

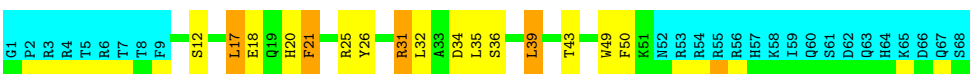
• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B: 



• Molecule 3: Homeotic bicoid protein

Chain P: 



4.2.12 Score per residue for model 12

• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

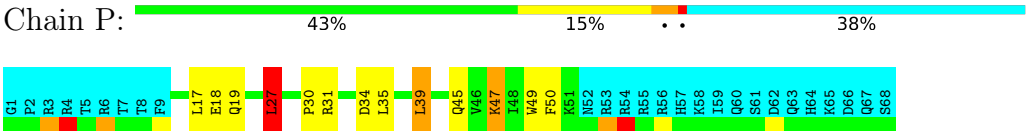
Chain A:

• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B:

• Molecule 3: Homeotic bicoid protein

Chain P:



4.2.13 Score per residue for model 13

• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

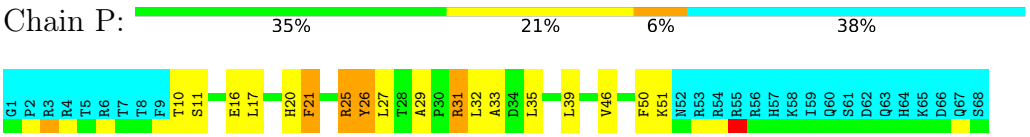
Chain A:

• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B:

• Molecule 3: Homeotic bicoid protein

Chain P:



4.2.14 Score per residue for model 14

• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

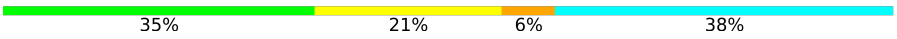
Chain A:

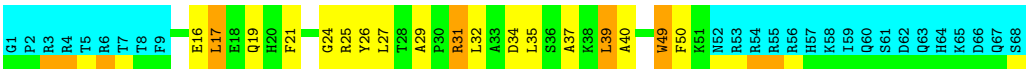
• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B:

• Molecule 3: Homeotic bicoid protein

Chain P:





4.2.15 Score per residue for model 15

• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

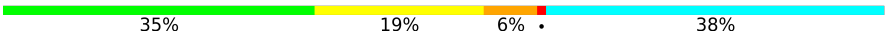
Chain A:

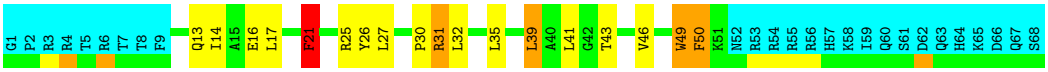
• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B:

• Molecule 3: Homeotic bicoid protein

Chain P:

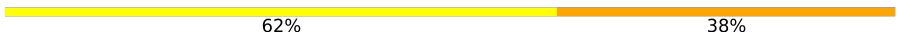




4.2.16 Score per residue for model 16

• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

Chain A:

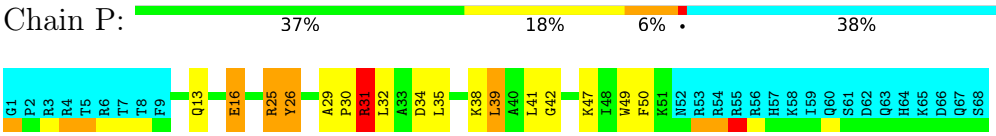


• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B:

• Molecule 3: Homeotic bicoid protein

Chain P:



4.2.17 Score per residue for model 17

• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

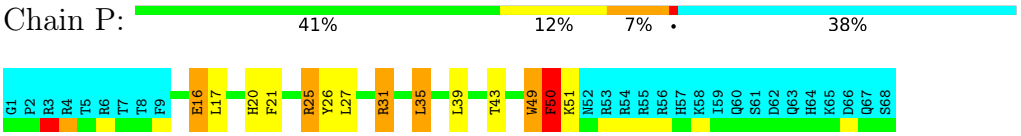
Chain A:

• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B:

• Molecule 3: Homeotic bicoid protein

Chain P:



4.2.18 Score per residue for model 18

• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

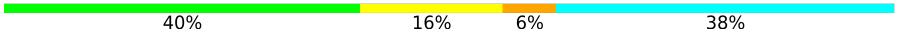
Chain A:

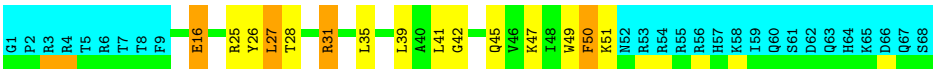
• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B:

• Molecule 3: Homeotic bicoid protein

Chain P:

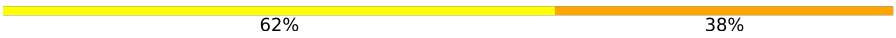




4.2.19 Score per residue for model 19

• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

Chain A:

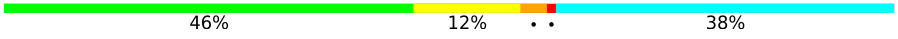


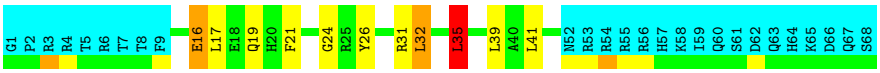
• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B:

• Molecule 3: Homeotic bicoid protein

Chain P:

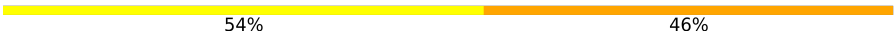




4.2.20 Score per residue for model 20

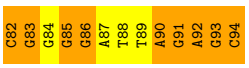
• Molecule 1: 5'-D(*GP*CP*TP*CP*TP*AP*AP*TP*CP*CP*CP*CP*G)-3'

Chain A:



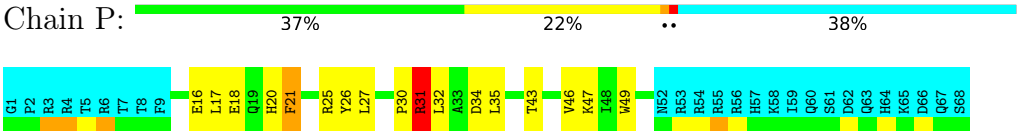
• Molecule 2: 5'-D(*CP*GP*GP*GP*GP*AP*TP*TP*AP*GP*AP*GP*C)-3'

Chain B:



• Molecule 3: Homeotic bicoid protein

Chain P:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *protein structure - fast torsion angle dynamics algorithm (CYANA2.0), DNA structure - NUCGEN and simulated annealing with NMR-derived energy restraints (AMBER7.0), protein-DNA complex - simulated annealing with NMR-derived energy restraints (AMBER7.0), protein-DNA complex refinement - explicit solvent MD simulations (AMBER7.0).*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure solution	2.0
Amber	refinement	7.0

No chemical shift data was provided.

6 Model quality (i)

6.1 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 (average) 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	3.27±0.15	37±6/286 (12.9± 2.1%)	4.16±0.24	84±9/438 (19.3± 2.0%)
2	B	3.32±0.13	41±5/304 (13.5± 1.6%)	4.05±0.18	90±9/469 (19.1± 2.0%)
3	P	1.52±0.07	1±1/339 (0.4± 0.3%)	2.04±0.12	11±4/459 (2.4± 0.8%)
All	All	2.78	1588/18580 (8.5%)	3.55	3704/27320 (13.6%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	6.3±1.5
2	B	0.0±0.0	7.5±1.5
3	P	0.0±0.0	1.1±1.1
All	All	0	298

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	76	DT	C5-C7	21.21	1.62	1.50	3	8
1	A	75	DA	N3-C4	16.18	1.44	1.34	7	10
1	A	78	DC	N1-C6	13.77	1.45	1.37	15	6
2	B	92	DA	C6-N6	-12.85	1.23	1.33	7	4
1	A	75	DA	N7-C5	12.56	1.46	1.39	8	8
2	B	83	DG	C8-N7	-12.55	1.23	1.30	18	4
1	A	80	DC	C5'-C4'	12.48	1.65	1.51	17	5
2	B	87	DA	N9-C4	-12.34	1.30	1.37	9	5
1	A	75	DA	C6-N6	-12.14	1.24	1.33	10	9
2	B	82	DC	N3-C4	-12.11	1.25	1.33	7	8
1	A	73	DT	C5-C7	12.06	1.57	1.50	19	11
2	B	86	DG	N7-C5	11.82	1.46	1.39	17	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	69	DG	N7-C5	11.73	1.46	1.39	20	6
1	A	70	DC	N3-C4	-11.68	1.25	1.33	5	3
1	A	81	DG	N3-C4	11.68	1.43	1.35	7	4
2	B	87	DA	N7-C5	-11.66	1.32	1.39	6	9
2	B	94	DC	C4-N4	-11.41	1.23	1.33	8	10
2	B	84	DG	N3-C4	11.30	1.43	1.35	1	5
1	A	72	DC	N1-C6	11.29	1.44	1.37	8	8
2	B	85	DG	C6-N1	-11.24	1.31	1.39	19	6
2	B	84	DG	C4'-O4'	-11.12	1.33	1.45	16	5
2	B	92	DA	N3-C4	11.09	1.41	1.34	14	9
2	B	83	DG	N9-C8	-11.06	1.30	1.37	17	7
1	A	70	DC	N1-C6	11.04	1.43	1.37	10	7
2	B	92	DA	N7-C5	11.01	1.45	1.39	20	6
2	B	91	DG	N3-C4	11.00	1.43	1.35	2	5
2	B	87	DA	C5-C4	-10.93	1.31	1.38	8	8
2	B	88	DT	C5-C6	10.92	1.42	1.34	17	5
2	B	86	DG	N1-C2	-10.92	1.29	1.37	2	3
2	B	89	DT	C5-C7	10.88	1.56	1.50	19	8
2	B	92	DA	C6-N1	-10.82	1.27	1.35	17	7
1	A	72	DC	C4-N4	-10.81	1.24	1.33	17	9
1	A	71	DT	C5-C7	10.77	1.56	1.50	9	7
2	B	91	DG	C4'-O4'	-10.77	1.34	1.45	11	7
2	B	94	DC	C5'-C4'	10.73	1.63	1.51	11	3
1	A	74	DA	N3-C4	10.62	1.41	1.34	16	8
1	A	73	DT	N1-C2	10.57	1.46	1.38	14	9
2	B	86	DG	C5-C4	10.57	1.45	1.38	19	5
2	B	91	DG	N7-C5	10.53	1.45	1.39	2	5
2	B	87	DA	N3-C4	10.46	1.41	1.34	1	8
2	B	90	DA	N7-C5	10.43	1.45	1.39	6	8
1	A	71	DT	C4-C5	10.40	1.54	1.45	13	4
2	B	93	DG	C4'-O4'	-10.35	1.34	1.45	15	6
2	B	86	DG	C5-C6	10.33	1.52	1.42	14	4
1	A	69	DG	N3-C4	10.33	1.42	1.35	10	7
1	A	76	DT	C4'-O4'	-10.23	1.34	1.45	11	6
1	A	74	DA	N7-C5	10.21	1.45	1.39	14	6
1	A	70	DC	C4-N4	-10.01	1.25	1.33	4	9
1	A	79	DC	N1-C6	9.99	1.43	1.37	16	4
1	A	81	DG	N1-C2	-9.98	1.29	1.37	4	6
2	B	89	DT	N3-C4	-9.96	1.30	1.38	15	3
1	A	77	DC	C4-N4	-9.95	1.25	1.33	9	7
2	B	84	DG	N7-C5	9.92	1.45	1.39	1	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	93	DG	N7-C5	9.91	1.45	1.39	10	7
1	A	77	DC	N1-C6	-9.91	1.31	1.37	15	4
1	A	79	DC	C4-N4	-9.88	1.25	1.33	5	4
2	B	88	DT	C5-C7	9.87	1.55	1.50	16	12
2	B	94	DC	C5-C6	9.86	1.42	1.34	5	3
1	A	69	DG	C2-N2	-9.86	1.24	1.34	18	10
2	B	86	DG	N3-C4	9.86	1.42	1.35	6	4
2	B	85	DG	C2-N2	-9.84	1.24	1.34	2	8
1	A	69	DG	N9-C8	-9.84	1.30	1.37	1	4
2	B	90	DA	C6-N6	-9.79	1.26	1.33	5	4
2	B	90	DA	C6-N1	-9.78	1.28	1.35	15	7
1	A	71	DT	C5-C6	9.77	1.41	1.34	1	6
1	A	73	DT	P-O5'	-9.76	1.50	1.59	16	4
1	A	80	DC	C2'-C1'	9.75	1.62	1.52	18	2
1	A	81	DG	C2-N3	9.73	1.40	1.32	5	3
1	A	72	DC	N1-C2	9.68	1.49	1.40	19	2
2	B	83	DG	N3-C4	9.67	1.42	1.35	13	5
2	B	82	DC	N1-C6	-9.58	1.31	1.37	17	4
1	A	79	DC	N3-C4	-9.54	1.27	1.33	3	6
1	A	74	DA	C2'-C1'	9.42	1.61	1.52	18	7
3	P	25	ARG	CZ-NH2	-9.41	1.20	1.33	17	2
2	B	82	DC	C4-N4	-9.40	1.25	1.33	7	7
1	A	73	DT	C4'-C3'	9.40	1.62	1.53	5	4
1	A	74	DA	C5-C4	-9.37	1.32	1.38	12	4
2	B	91	DG	C4'-C3'	9.36	1.62	1.53	3	2
1	A	80	DC	N3-C4	-9.35	1.27	1.33	5	7
2	B	87	DA	C8-N7	9.34	1.38	1.31	17	3
1	A	72	DC	C3'-C2'	9.30	1.63	1.52	5	3
1	A	77	DC	C4'-C3'	9.30	1.62	1.53	14	3
1	A	69	DG	C8-N7	9.29	1.36	1.30	18	3
2	B	93	DG	C5'-C4'	9.22	1.61	1.51	13	6
2	B	84	DG	C6-N1	-9.19	1.33	1.39	10	5
2	B	82	DC	C4'-O4'	-9.16	1.35	1.45	20	5
1	A	77	DC	C2-O2	-9.14	1.16	1.24	7	3
2	B	85	DG	N7-C5	9.09	1.44	1.39	4	7
2	B	90	DA	N9-C4	-9.08	1.32	1.37	2	7
2	B	83	DG	N1-C2	-9.07	1.30	1.37	7	4
1	A	81	DG	C8-N7	9.04	1.36	1.30	6	4
2	B	87	DA	C6-N6	-9.02	1.26	1.33	14	2
2	B	91	DG	O3'-P	-9.01	1.50	1.61	20	9
2	B	91	DG	N9-C4	-9.01	1.30	1.38	10	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	83	DG	C2-N2	-8.98	1.25	1.34	16	8
2	B	89	DT	P-O5'	-8.97	1.50	1.59	12	8
1	A	72	DC	N3-C4	-8.94	1.27	1.33	15	4
1	A	75	DA	C5-C4	-8.91	1.32	1.38	6	6
1	A	74	DA	C4'-C3'	-8.91	1.43	1.52	2	2
1	A	69	DG	C4'-C3'	-8.91	1.43	1.52	3	5
2	B	90	DA	P-O5'	8.86	1.68	1.59	6	4
1	A	76	DT	C2-O2	8.86	1.29	1.22	4	1
2	B	88	DT	C2'-C1'	8.85	1.61	1.52	16	3
1	A	71	DT	C2'-C1'	8.82	1.61	1.52	13	4
2	B	84	DG	C2-N2	-8.82	1.25	1.34	5	7
2	B	93	DG	C6-N1	-8.82	1.33	1.39	10	6
2	B	87	DA	N9-C8	-8.82	1.30	1.37	19	3
2	B	82	DC	C5-C6	8.81	1.41	1.34	17	5
2	B	85	DG	N3-C4	8.78	1.41	1.35	5	6
2	B	82	DC	C2-N3	-8.75	1.28	1.35	12	4
1	A	75	DA	C4'-O4'	-8.72	1.36	1.45	9	4
2	B	84	DG	O3'-P	-8.68	1.50	1.61	3	2
1	A	75	DA	C6-N1	-8.67	1.29	1.35	15	2
1	A	69	DG	C6-N1	-8.64	1.33	1.39	15	2
1	A	70	DC	C5-C6	8.64	1.41	1.34	10	5
1	A	80	DC	P-O5'	8.64	1.68	1.59	13	4
2	B	89	DT	C5-C6	8.63	1.40	1.34	20	7
1	A	80	DC	N1-C6	8.58	1.42	1.37	17	5
2	B	82	DC	C5'-C4'	8.56	1.60	1.51	15	7
1	A	72	DC	C2-N3	8.56	1.42	1.35	15	2
2	B	91	DG	C8-N7	8.55	1.36	1.30	9	2
2	B	94	DC	P-O5'	-8.54	1.51	1.59	18	5
2	B	93	DG	C8-N7	-8.53	1.25	1.30	13	5
1	A	78	DC	C2-O2	-8.49	1.16	1.24	20	1
2	B	92	DA	N9-C4	-8.48	1.32	1.37	12	6
2	B	87	DA	C6-N1	-8.45	1.29	1.35	4	8
1	A	71	DT	C2-N3	-8.44	1.31	1.37	13	5
2	B	83	DG	C5'-C4'	8.42	1.60	1.51	18	6
1	A	71	DT	N1-C6	-8.40	1.32	1.38	9	6
1	A	77	DC	C4'-O4'	-8.35	1.36	1.45	19	4
1	A	79	DC	O4'-C1'	8.35	1.52	1.42	11	1
2	B	85	DG	C2-N3	8.34	1.39	1.32	5	3
1	A	69	DG	N9-C4	8.32	1.44	1.38	15	2
1	A	81	DG	C2-N2	-8.31	1.26	1.34	3	8
2	B	92	DA	C8-N7	8.30	1.37	1.31	8	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	91	DG	P-O5'	-8.28	1.51	1.59	3	1
1	A	80	DC	C5-C6	8.28	1.41	1.34	3	4
1	A	81	DG	N7-C5	8.28	1.44	1.39	5	5
1	A	78	DC	C5'-C4'	8.27	1.60	1.51	8	5
2	B	94	DC	C3'-O3'	-8.27	1.33	1.44	1	2
1	A	74	DA	C5-C6	8.26	1.48	1.41	1	3
1	A	72	DC	C4'-O4'	-8.22	1.36	1.45	9	8
2	B	93	DG	N1-C2	-8.21	1.31	1.37	16	7
1	A	73	DT	C4'-O4'	-8.18	1.36	1.45	2	5
2	B	93	DG	N9-C8	-8.18	1.32	1.37	18	3
2	B	85	DG	N1-C2	-8.16	1.31	1.37	13	4
1	A	73	DT	C4-C5	8.14	1.52	1.45	5	1
2	B	84	DG	C5'-C4'	8.14	1.60	1.51	16	5
2	B	91	DG	C3'-C2'	8.12	1.61	1.52	17	3
2	B	88	DT	C3'-C2'	8.11	1.61	1.52	7	3
1	A	74	DA	C4'-O4'	-8.09	1.36	1.45	4	3
2	B	84	DG	C3'-C2'	8.09	1.61	1.52	11	2
2	B	86	DG	C4'-O4'	-8.07	1.36	1.45	1	2
1	A	76	DT	N1-C6	8.06	1.43	1.38	5	7
2	B	91	DG	N1-C2	-8.05	1.31	1.37	11	5
1	A	76	DT	C3'-C2'	8.05	1.61	1.52	20	2
1	A	71	DT	O3'-P	-8.04	1.51	1.61	17	2
1	A	78	DC	P-O5'	8.03	1.67	1.59	3	3
2	B	92	DA	N9-C8	-8.03	1.31	1.37	12	5
2	B	84	DG	P-O5'	8.02	1.67	1.59	1	4
2	B	85	DG	N9-C4	8.02	1.44	1.38	14	2
2	B	85	DG	C5'-C4'	8.02	1.60	1.51	14	1
2	B	88	DT	N3-C4	8.01	1.45	1.38	3	4
1	A	72	DC	C2'-C1'	7.99	1.60	1.52	6	5
1	A	74	DA	N1-C2	-7.97	1.27	1.34	16	6
1	A	78	DC	N1-C2	-7.96	1.32	1.40	6	2
2	B	89	DT	N1-C2	7.95	1.44	1.38	3	6
2	B	85	DG	C8-N7	7.95	1.35	1.30	11	2
2	B	87	DA	C5'-C4'	7.95	1.60	1.51	16	2
2	B	92	DA	C4'-C3'	7.94	1.61	1.53	15	2
1	A	81	DG	C5-C6	7.93	1.50	1.42	18	3
2	B	89	DT	O4'-C1'	-7.92	1.32	1.42	9	1
1	A	72	DC	C4-C5	7.91	1.49	1.43	3	3
1	A	76	DT	N1-C2	7.91	1.44	1.38	8	6
2	B	83	DG	N7-C5	-7.90	1.34	1.39	18	5
1	A	69	DG	C2'-C1'	-7.90	1.44	1.52	12	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	73	DT	C5'-C4'	7.87	1.60	1.51	10	6
2	B	93	DG	N9-C4	-7.86	1.31	1.38	13	3
2	B	86	DG	N9-C8	-7.86	1.32	1.37	19	4
2	B	89	DT	N1-C6	7.85	1.43	1.38	13	2
1	A	70	DC	C4'-O4'	-7.84	1.37	1.45	17	2
2	B	89	DT	C4-C5	7.83	1.51	1.45	5	5
1	A	72	DC	C5-C6	7.82	1.40	1.34	10	3
2	B	84	DG	N9-C4	-7.80	1.31	1.38	14	4
2	B	84	DG	C3'-O3'	-7.80	1.33	1.44	5	2
1	A	73	DT	N3-C4	-7.78	1.32	1.38	12	4
2	B	88	DT	N1-C2	7.76	1.44	1.38	8	6
1	A	80	DC	C2-O2	-7.76	1.17	1.24	10	3
2	B	84	DG	C8-N7	-7.76	1.26	1.30	20	6
1	A	79	DC	C5'-C4'	7.76	1.59	1.51	9	6
1	A	75	DA	P-O5'	7.75	1.67	1.59	6	3
1	A	69	DG	C5'-C4'	7.72	1.59	1.51	18	5
2	B	85	DG	P-O5'	-7.70	1.52	1.59	19	4
2	B	90	DA	C8-N7	7.68	1.36	1.31	7	3
2	B	88	DT	C5'-C4'	7.68	1.59	1.51	20	6
2	B	91	DG	C6-N1	7.68	1.45	1.39	17	7
1	A	70	DC	C4'-C3'	7.66	1.61	1.53	18	1
1	A	80	DC	C2-N3	7.63	1.41	1.35	13	1
2	B	83	DG	P-O5'	7.63	1.67	1.59	17	4
2	B	85	DG	C3'-C2'	7.63	1.61	1.52	1	2
2	B	92	DA	C5-C4	-7.62	1.33	1.38	6	4
1	A	70	DC	C2'-C1'	7.62	1.59	1.52	1	4
2	B	83	DG	C3'-C2'	7.61	1.61	1.52	10	3
1	A	81	DG	N9-C8	-7.61	1.32	1.37	14	5
1	A	79	DC	C2'-C1'	-7.60	1.44	1.52	17	4
2	B	82	DC	C4-C5	7.60	1.49	1.43	14	2
2	B	84	DG	C6-O6	-7.60	1.17	1.24	16	3
2	B	83	DG	C4'-C3'	7.59	1.60	1.53	16	3
2	B	86	DG	O3'-P	-7.59	1.52	1.61	19	1
2	B	94	DC	N3-C4	-7.55	1.28	1.33	20	7
1	A	74	DA	P-O5'	7.55	1.67	1.59	18	3
2	B	85	DG	C4'-C3'	7.54	1.60	1.53	5	2
1	A	79	DC	O3'-P	-7.53	1.52	1.61	12	3
2	B	94	DC	C2'-C1'	7.53	1.59	1.52	1	3
1	A	78	DC	C4-N4	-7.52	1.27	1.33	19	7
1	A	75	DA	C8-N7	7.52	1.36	1.31	8	3
1	A	78	DC	C2'-C1'	7.52	1.59	1.52	18	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	69	DG	C2-N3	7.51	1.38	1.32	20	3
1	A	74	DA	C6-N1	-7.50	1.30	1.35	19	6
1	A	74	DA	C8-N7	7.49	1.36	1.31	17	2
1	A	78	DC	C5-C6	7.47	1.40	1.34	7	7
2	B	86	DG	C4'-C3'	7.44	1.60	1.53	5	3
2	B	84	DG	C2'-C1'	7.43	1.59	1.52	20	3
2	B	86	DG	C8-N7	7.41	1.35	1.30	8	2
2	B	93	DG	C5-C6	7.41	1.49	1.42	7	4
1	A	76	DT	C2'-C1'	-7.40	1.44	1.52	9	3
1	A	77	DC	P-O5'	-7.40	1.52	1.59	13	4
1	A	73	DT	O3'-P	-7.39	1.52	1.61	2	3
2	B	86	DG	P-O5'	7.38	1.67	1.59	1	4
2	B	90	DA	C5'-C4'	7.38	1.59	1.51	5	5
2	B	83	DG	C5-C4	7.36	1.43	1.38	16	4
1	A	79	DC	C4'-C3'	7.34	1.60	1.53	6	3
1	A	78	DC	O4'-C1'	7.34	1.51	1.42	14	1
1	A	80	DC	C4-N4	-7.32	1.27	1.33	20	8
1	A	74	DA	O4'-C1'	7.30	1.51	1.42	6	5
1	A	77	DC	C5'-C4'	7.29	1.59	1.51	20	3
1	A	74	DA	N9-C8	7.29	1.43	1.37	16	2
1	A	70	DC	O3'-P	-7.28	1.52	1.61	13	1
2	B	86	DG	C5'-C4'	7.26	1.59	1.51	7	5
1	A	74	DA	C6-N6	-7.26	1.28	1.33	7	3
1	A	78	DC	N3-C4	-7.25	1.28	1.33	5	3
1	A	78	DC	C4'-C3'	7.24	1.60	1.53	3	2
1	A	71	DT	N3-C4	-7.21	1.32	1.38	20	5
1	A	69	DG	C3'-C2'	-7.21	1.43	1.52	17	3
2	B	85	DG	N9-C8	-7.19	1.32	1.37	7	2
2	B	88	DT	C4'-O4'	-7.19	1.37	1.45	15	5
1	A	74	DA	N9-C4	-7.18	1.33	1.37	3	4
2	B	85	DG	O4'-C1'	-7.18	1.33	1.42	9	3
1	A	75	DA	N9-C8	7.18	1.43	1.37	17	3
2	B	82	DC	C4'-C3'	7.18	1.60	1.53	11	1
1	A	71	DT	N1-C2	7.17	1.43	1.38	1	7
1	A	74	DA	O3'-P	7.15	1.69	1.61	13	2
2	B	85	DG	C5-C6	7.15	1.49	1.42	12	2
2	B	90	DA	N3-C4	7.14	1.39	1.34	13	10
1	A	80	DC	C4-C5	7.14	1.48	1.43	7	2
1	A	75	DA	C5'-C4'	7.13	1.59	1.51	13	4
2	B	93	DG	C2-N2	-7.12	1.27	1.34	18	5
1	A	80	DC	C4'-C3'	7.12	1.60	1.53	12	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	83	DG	C2'-C1'	7.12	1.59	1.52	4	2
1	A	69	DG	N1-C2	-7.12	1.32	1.37	12	6
1	A	77	DC	C2-N3	7.11	1.41	1.35	3	2
1	A	76	DT	C2-N3	-7.10	1.32	1.37	10	2
2	B	87	DA	C4'-O4'	-7.10	1.38	1.45	11	3
1	A	79	DC	C5-C6	7.10	1.40	1.34	12	2
2	B	86	DG	C6-O6	7.08	1.30	1.24	12	1
2	B	89	DT	C2-O2	7.07	1.28	1.22	13	3
1	A	69	DG	C4'-O4'	-7.07	1.38	1.45	4	3
1	A	81	DG	P-O5'	-7.07	1.52	1.59	9	8
1	A	75	DA	C2'-C1'	7.05	1.59	1.52	9	3
2	B	84	DG	C5-C6	7.05	1.49	1.42	9	3
2	B	84	DG	C4'-C3'	-7.04	1.45	1.52	18	2
2	B	86	DG	C2-N3	7.04	1.38	1.32	2	3
1	A	72	DC	O4'-C1'	7.02	1.50	1.42	2	3
1	A	79	DC	C4'-O4'	-7.00	1.38	1.45	11	4
1	A	76	DT	C5-C6	6.99	1.39	1.34	14	5
1	A	81	DG	N9-C4	-6.99	1.32	1.38	14	2
2	B	90	DA	C4'-O4'	-6.98	1.38	1.45	1	6
1	A	75	DA	N1-C2	-6.98	1.28	1.34	17	3
2	B	86	DG	C2-N2	-6.97	1.27	1.34	20	5
2	B	93	DG	C4'-C3'	6.96	1.60	1.53	6	1
1	A	69	DG	C5-C4	-6.93	1.33	1.38	13	2
2	B	83	DG	C6-N1	-6.93	1.34	1.39	6	1
3	P	24	GLY	CA-C	6.92	1.62	1.51	19	1
1	A	74	DA	C5'-C4'	6.88	1.58	1.51	9	2
2	B	92	DA	C2-N3	6.85	1.39	1.33	6	3
2	B	91	DG	C2-N3	-6.83	1.27	1.32	6	2
2	B	87	DA	P-O5'	-6.81	1.52	1.59	11	1
2	B	93	DG	C2'-C1'	6.80	1.59	1.52	11	2
1	A	79	DC	C4-C5	-6.80	1.37	1.43	12	1
1	A	70	DC	O4'-C1'	-6.78	1.34	1.42	1	2
2	B	89	DT	O3'-P	-6.75	1.53	1.61	17	2
1	A	73	DT	C3'-C2'	6.73	1.60	1.52	13	2
1	A	76	DT	O3'-P	-6.72	1.53	1.61	1	2
1	A	80	DC	O3'-P	-6.72	1.53	1.61	4	2
2	B	89	DT	C4'-C3'	6.71	1.60	1.53	14	4
1	A	79	DC	C3'-C2'	6.71	1.60	1.52	20	1
1	A	72	DC	O3'-P	-6.70	1.53	1.61	18	2
1	A	81	DG	O4'-C1'	-6.70	1.34	1.42	2	2
1	A	78	DC	C4'-O4'	-6.69	1.38	1.45	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	92	DA	O3'-P	-6.68	1.53	1.61	2	3
1	A	70	DC	C2-O2	-6.66	1.18	1.24	19	2
1	A	81	DG	C2'-C1'	-6.65	1.45	1.52	12	2
2	B	91	DG	C5'-C4'	6.64	1.58	1.51	11	4
1	A	78	DC	C3'-C2'	6.63	1.60	1.52	16	2
3	P	11	SER	CB-OG	-6.63	1.33	1.42	7	1
2	B	94	DC	N1-C6	6.60	1.41	1.37	14	3
2	B	87	DA	C2'-C1'	-6.59	1.45	1.52	7	3
1	A	69	DG	C5-C6	6.58	1.49	1.42	20	1
1	A	78	DC	C4-C5	6.58	1.48	1.43	10	6
2	B	82	DC	C2'-C1'	6.58	1.58	1.52	3	5
2	B	83	DG	C5-C6	6.57	1.49	1.42	11	3
1	A	70	DC	P-O5'	-6.56	1.53	1.59	4	2
1	A	71	DT	C5'-C4'	6.56	1.58	1.51	13	3
2	B	93	DG	N3-C4	6.49	1.40	1.35	19	2
2	B	87	DA	C3'-C2'	-6.48	1.44	1.52	8	3
1	A	75	DA	O4'-C1'	-6.47	1.34	1.42	6	2
2	B	87	DA	N1-C2	-6.45	1.28	1.34	14	2
3	P	26	TYR	CE2-CZ	6.44	1.47	1.38	15	1
1	A	77	DC	C3'-O3'	-6.40	1.35	1.44	7	1
2	B	90	DA	C4'-C3'	6.40	1.59	1.53	6	2
2	B	87	DA	C2-N3	-6.37	1.27	1.33	6	3
2	B	94	DC	N1-C2	6.37	1.46	1.40	17	1
2	B	85	DG	C4'-O4'	-6.34	1.38	1.45	5	2
2	B	94	DC	C4'-O4'	6.34	1.51	1.45	11	2
3	P	49	TRP	CD2-CE2	6.34	1.49	1.41	17	1
3	P	26	TYR	CE1-CZ	6.34	1.46	1.38	13	2
1	A	78	DC	O3'-P	-6.31	1.53	1.61	9	1
1	A	80	DC	C3'-C2'	6.31	1.59	1.52	5	1
1	A	73	DT	C2'-C1'	6.31	1.58	1.52	2	2
2	B	84	DG	C5-C4	6.30	1.42	1.38	11	2
2	B	93	DG	O4'-C1'	6.30	1.49	1.42	16	2
2	B	82	DC	O3'-P	-6.30	1.53	1.61	9	2
2	B	90	DA	C3'-C2'	6.30	1.59	1.52	15	2
1	A	76	DT	C4'-C3'	6.28	1.59	1.53	9	2
2	B	92	DA	N1-C2	-6.26	1.28	1.34	1	3
2	B	93	DG	O3'-P	-6.26	1.53	1.61	4	1
1	A	81	DG	C5-C4	-6.24	1.33	1.38	17	2
2	B	93	DG	C2-N3	6.24	1.37	1.32	17	1
2	B	87	DA	C1'-N9	6.21	1.57	1.49	1	1
2	B	91	DG	C2-N2	-6.21	1.28	1.34	8	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	89	DT	C2-N3	6.21	1.42	1.37	9	2
1	A	77	DC	N3-C4	-6.21	1.29	1.33	16	4
1	A	81	DG	C6-N1	-6.20	1.35	1.39	2	4
1	A	72	DC	C3'-O3'	-6.17	1.35	1.44	8	1
3	P	49	TRP	NE1-CE2	6.17	1.45	1.37	16	1
1	A	71	DT	C4'-C3'	6.16	1.59	1.53	15	1
1	A	80	DC	C4'-O4'	-6.16	1.38	1.45	8	3
1	A	75	DA	C4'-C3'	6.16	1.59	1.53	17	3
2	B	88	DT	O3'-P	6.15	1.68	1.61	18	3
1	A	76	DT	C4-C5	6.15	1.50	1.45	12	3
2	B	90	DA	N9-C8	6.14	1.42	1.37	5	2
1	A	80	DC	N1-C2	6.12	1.46	1.40	12	3
1	A	79	DC	C2-N3	-6.12	1.30	1.35	9	1
3	P	26	TYR	CG-CD2	6.11	1.47	1.39	1	1
2	B	83	DG	C2-N3	6.11	1.37	1.32	17	3
3	P	37	ALA	CA-CB	6.08	1.65	1.52	1	1
2	B	87	DA	O3'-P	-6.08	1.53	1.61	4	1
1	A	72	DC	C5'-C4'	6.08	1.58	1.51	18	2
1	A	80	DC	C3'-O3'	-6.07	1.36	1.44	8	1
2	B	92	DA	C5'-C4'	6.05	1.58	1.51	14	2
2	B	91	DG	C2'-C1'	6.03	1.58	1.52	6	3
2	B	92	DA	C5-C6	6.03	1.46	1.41	16	2
2	B	84	DG	N1-C2	-6.02	1.32	1.37	17	5
2	B	86	DG	C2'-C1'	6.01	1.58	1.52	13	5
3	P	36	SER	CB-OG	-6.00	1.34	1.42	11	1
2	B	88	DT	C3'-O3'	-5.99	1.36	1.44	1	1
1	A	76	DT	C4-O4	5.99	1.28	1.23	6	2
2	B	89	DT	C2'-C1'	5.97	1.58	1.52	5	2
1	A	77	DC	O3'-P	-5.96	1.53	1.61	5	3
1	A	72	DC	C2-O2	-5.95	1.19	1.24	19	2
3	P	18	GLU	CG-CD	5.95	1.60	1.51	20	2
1	A	81	DG	C5'-C4'	5.94	1.57	1.51	15	2
1	A	77	DC	C1'-N1	5.93	1.56	1.49	1	1
2	B	86	DG	C3'-O3'	-5.93	1.36	1.44	12	2
2	B	90	DA	C5-C4	-5.89	1.34	1.38	19	3
2	B	93	DG	P-O5'	-5.88	1.53	1.59	19	2
1	A	77	DC	N1-C2	5.88	1.46	1.40	8	3
2	B	88	DT	C4-O4	-5.88	1.18	1.23	5	3
1	A	81	DG	C3'-O3'	-5.87	1.36	1.44	9	1
2	B	88	DT	P-O5'	-5.87	1.53	1.59	10	4
1	A	77	DC	O4'-C1'	-5.85	1.35	1.42	11	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	89	DT	C4'-O4'	-5.84	1.39	1.45	18	2
3	P	50	PHE	CG-CD1	5.84	1.47	1.38	6	1
3	P	21	PHE	CE1-CZ	5.82	1.48	1.37	14	1
2	B	84	DG	N9-C8	-5.81	1.33	1.37	8	1
1	A	79	DC	C2-O2	5.81	1.29	1.24	14	2
1	A	77	DC	C3'-C2'	-5.80	1.45	1.52	15	2
2	B	83	DG	O3'-P	-5.80	1.54	1.61	11	3
2	B	84	DG	C2-N3	5.79	1.37	1.32	14	2
2	B	91	DG	C5-C6	5.78	1.48	1.42	16	2
1	A	74	DA	C3'-O3'	5.77	1.51	1.44	13	1
2	B	83	DG	N9-C4	-5.77	1.33	1.38	20	1
2	B	88	DT	C4-C5	5.77	1.50	1.45	5	2
3	P	31	ARG	CZ-NH1	-5.72	1.25	1.33	13	1
1	A	75	DA	C5-C6	5.72	1.46	1.41	15	2
3	P	12	SER	CB-OG	5.71	1.49	1.42	11	1
2	B	90	DA	C5-C6	-5.69	1.35	1.41	12	1
2	B	88	DT	C2-O2	5.68	1.26	1.22	18	2
1	A	77	DC	C2'-C1'	5.68	1.58	1.52	19	2
1	A	72	DC	C4'-C3'	5.63	1.58	1.53	19	1
1	A	73	DT	C5-C6	5.63	1.38	1.34	14	2
2	B	82	DC	C3'-O3'	5.63	1.51	1.44	8	1
2	B	82	DC	C2-O2	-5.62	1.19	1.24	12	2
3	P	31	ARG	NE-CZ	-5.62	1.25	1.33	7	1
2	B	91	DG	C3'-O3'	-5.62	1.36	1.44	6	1
1	A	74	DA	C1'-N9	5.58	1.56	1.49	9	1
2	B	82	DC	C3'-C2'	-5.57	1.45	1.52	18	2
1	A	69	DG	O4'-C1'	5.55	1.49	1.42	1	1
2	B	84	DG	O4'-C1'	5.54	1.48	1.42	16	2
3	P	42	GLY	N-CA	5.53	1.54	1.46	18	1
1	A	80	DC	C1'-N1	5.52	1.56	1.49	1	1
1	A	69	DG	C6-O6	-5.52	1.19	1.24	18	2
3	P	18	GLU	CD-OE1	5.51	1.31	1.25	11	1
1	A	70	DC	C5'-C4'	5.51	1.57	1.51	7	2
2	B	91	DG	N9-C8	-5.51	1.33	1.37	6	1
2	B	88	DT	N1-C6	-5.50	1.34	1.38	8	1
2	B	87	DA	C5-C6	5.49	1.46	1.41	12	1
2	B	92	DA	C2'-C1'	5.48	1.57	1.52	16	3
2	B	87	DA	C3'-O3'	-5.48	1.36	1.44	14	1
2	B	90	DA	N1-C2	-5.48	1.29	1.34	3	1
1	A	71	DT	C3'-O3'	-5.47	1.36	1.44	1	1
1	A	73	DT	C4-O4	5.47	1.28	1.23	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	74	DA	C3'-C2'	5.46	1.58	1.52	2	2
2	B	93	DG	C6-O6	-5.44	1.19	1.24	14	1
1	A	78	DC	C1'-N1	5.43	1.56	1.49	1	1
2	B	94	DC	C2-O2	-5.43	1.19	1.24	12	1
1	A	81	DG	C4'-C3'	5.42	1.58	1.53	3	1
1	A	79	DC	C3'-O3'	-5.41	1.36	1.44	4	1
1	A	73	DT	C2-O2	5.41	1.26	1.22	5	2
1	A	72	DC	P-O5'	5.41	1.65	1.59	10	1
2	B	91	DG	C5-C4	5.41	1.42	1.38	3	2
1	A	81	DG	C4'-O4'	5.41	1.50	1.45	3	2
2	B	85	DG	O3'-P	-5.40	1.54	1.61	1	2
1	A	71	DT	C4'-O4'	-5.40	1.39	1.45	2	1
1	A	78	DC	C2-N3	5.39	1.40	1.35	19	3
2	B	85	DG	C6-O6	-5.38	1.19	1.24	3	2
1	A	73	DT	C2-N3	5.37	1.42	1.37	9	2
2	B	91	DG	C6-O6	-5.36	1.19	1.24	5	1
3	P	16	GLU	CD-OE1	-5.36	1.19	1.25	5	1
2	B	92	DA	C4'-O4'	-5.35	1.39	1.45	12	1
2	B	88	DT	C1'-N1	5.33	1.56	1.49	16	1
1	A	69	DG	C3'-O3'	-5.32	1.37	1.44	4	1
2	B	88	DT	C4'-C3'	5.32	1.58	1.53	19	2
2	B	90	DA	C2'-C1'	5.32	1.57	1.52	10	1
3	P	21	PHE	CE2-CZ	5.28	1.47	1.37	13	1
3	P	14	ILE	C-O	-5.27	1.13	1.23	9	1
2	B	85	DG	C5-C4	5.26	1.42	1.38	18	2
1	A	76	DT	C5'-C4'	5.24	1.57	1.51	19	2
2	B	83	DG	C4'-O4'	-5.22	1.39	1.45	3	1
2	B	93	DG	C5-C4	-5.22	1.34	1.38	12	1
1	A	76	DT	P-O5'	5.21	1.65	1.59	13	1
2	B	93	DG	C3'-C2'	5.21	1.58	1.52	4	1
3	P	33	ALA	CA-CB	5.20	1.63	1.52	13	1
3	P	28	THR	CB-OG1	-5.20	1.32	1.43	18	1
2	B	86	DG	N9-C4	5.15	1.42	1.38	14	1
1	A	75	DA	C2-N3	-5.15	1.28	1.33	16	1
1	A	81	DG	C1'-N9	5.15	1.55	1.49	15	1
1	A	81	DG	C6-O6	-5.15	1.19	1.24	16	1
2	B	89	DT	C3'-O3'	-5.13	1.37	1.44	9	1
2	B	90	DA	C3'-O3'	-5.11	1.37	1.44	18	1
1	A	71	DT	C2-O2	5.11	1.26	1.22	7	1
2	B	89	DT	C1'-N1	5.11	1.55	1.49	19	1
3	P	25	ARG	CZ-NH1	-5.11	1.26	1.33	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	79	DC	P-O5'	5.10	1.64	1.59	5	1
1	A	73	DT	N1-C6	5.09	1.41	1.38	13	1
1	A	71	DT	P-O5'	-5.08	1.54	1.59	17	1
2	B	83	DG	O4'-C1'	5.07	1.48	1.42	10	1
1	A	75	DA	N9-C4	5.07	1.40	1.37	16	1
2	B	92	DA	C3'-C2'	5.04	1.58	1.52	9	1
3	P	24	GLY	N-CA	5.03	1.53	1.46	8	1
3	P	31	ARG	N-CA	5.03	1.56	1.46	19	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	73	DT	O4'-C1'-N1	24.97	125.48	108.00	9	13
1	A	70	DC	N3-C4-C5	21.75	130.60	121.90	8	12
1	A	81	DG	O4'-C1'-N9	20.25	122.18	108.00	17	11
1	A	75	DA	N1-C6-N6	-20.04	106.58	118.60	19	14
2	B	87	DA	C5-C6-N1	19.90	127.65	117.70	18	10
1	A	70	DC	N1-C2-O2	19.53	130.62	118.90	12	11
2	B	90	DA	O4'-C1'-N9	18.91	121.24	108.00	18	10
1	A	80	DC	N3-C4-C5	18.07	129.13	121.90	3	10
1	A	70	DC	C4-C5-C6	-18.04	108.38	117.40	8	10
1	A	79	DC	N3-C4-C5	17.74	129.00	121.90	19	11
2	B	86	DG	C8-N9-C4	-17.61	99.36	106.40	12	11
2	B	91	DG	N3-C2-N2	-17.54	107.62	119.90	7	11
3	P	25	ARG	NE-CZ-NH1	17.51	129.06	120.30	13	9
2	B	93	DG	N1-C6-O6	-17.48	109.41	119.90	10	10
1	A	74	DA	N1-C6-N6	-17.27	108.24	118.60	3	17
2	B	85	DG	O4'-C1'-N9	17.04	119.93	108.00	20	14
2	B	91	DG	N1-C6-O6	-16.82	109.81	119.90	18	11
1	A	71	DT	C6-C5-C7	-16.81	112.82	122.90	9	17
3	P	31	ARG	NE-CZ-NH2	16.77	128.69	120.30	20	9
1	A	80	DC	N1-C2-O2	16.70	128.92	118.90	20	11
2	B	89	DT	C6-C5-C7	-16.63	112.92	122.90	16	12
1	A	81	DG	C5-N7-C8	-16.63	95.99	104.30	10	10
1	A	73	DT	C6-C5-C7	-16.57	112.95	122.90	19	15
2	B	87	DA	N1-C6-N6	-16.51	108.69	118.60	18	13
3	P	31	ARG	NE-CZ-NH1	16.38	128.49	120.30	2	11
1	A	70	DC	O4'-C4'-C3'	16.34	115.80	106.00	20	8
1	A	81	DG	N7-C8-N9	16.31	121.25	113.10	10	10
1	A	75	DA	C5-C6-N1	16.11	125.76	117.70	7	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	71	DT	N3-C2-O2	-16.09	112.65	122.30	3	14
1	A	79	DC	N3-C4-N4	-16.06	106.76	118.00	19	9
1	A	81	DG	N1-C6-O6	-16.02	110.29	119.90	19	7
2	B	84	DG	C5-C6-N1	15.91	119.46	111.50	19	7
2	B	90	DA	C4-C5-C6	-15.90	109.05	117.00	10	13
2	B	92	DA	C4-C5-C6	-15.85	109.07	117.00	1	16
2	B	92	DA	N1-C6-N6	-15.75	109.15	118.60	19	15
1	A	78	DC	C2-N3-C4	-15.72	112.04	119.90	6	8
1	A	71	DT	O4'-C1'-N1	15.65	118.96	108.00	20	11
1	A	78	DC	O4'-C1'-N1	-15.56	97.11	108.00	18	7
2	B	87	DA	C4-C5-C6	-15.52	109.24	117.00	9	12
2	B	89	DT	O4'-C1'-N1	-15.48	97.16	108.00	6	7
2	B	84	DG	N3-C4-C5	-15.47	120.87	128.60	8	11
1	A	78	DC	N3-C4-C5	15.43	128.07	121.90	15	12
2	B	93	DG	O4'-C1'-N9	15.40	118.78	108.00	13	11
2	B	82	DC	N3-C2-O2	-15.38	111.14	121.90	9	18
2	B	85	DG	N1-C6-O6	-15.34	110.70	119.90	5	11
1	A	76	DT	O4'-C4'-C3'	15.31	115.18	106.00	18	8
1	A	69	DG	O4'-C1'-N9	15.30	118.71	108.00	20	10
1	A	70	DC	N3-C4-N4	-15.27	107.31	118.00	7	10
1	A	78	DC	N3-C4-N4	-15.20	107.36	118.00	15	8
2	B	85	DG	C4-C5-N7	-15.20	104.72	110.80	5	7
2	B	85	DG	N3-C4-N9	15.16	135.09	126.00	2	3
2	B	82	DC	N3-C4-N4	-15.15	107.40	118.00	9	11
2	B	88	DT	N3-C2-O2	-15.01	113.29	122.30	14	7
2	B	94	DC	N1-C2-O2	14.98	127.89	118.90	4	11
1	A	80	DC	N3-C2-O2	-14.97	111.42	121.90	20	16
2	B	86	DG	O4'-C1'-N9	14.96	118.47	108.00	10	9
1	A	79	DC	N3-C2-O2	-14.93	111.45	121.90	11	15
1	A	70	DC	N3-C2-O2	-14.91	111.46	121.90	12	12
1	A	73	DT	N3-C2-O2	-14.90	113.36	122.30	10	9
1	A	77	DC	O4'-C1'-N1	14.90	118.43	108.00	8	7
1	A	77	DC	C5-C6-N1	-14.89	113.56	121.00	13	9
2	B	84	DG	N1-C6-O6	-14.85	110.99	119.90	6	10
2	B	82	DC	N1-C2-O2	14.83	127.80	118.90	9	12
2	B	82	DC	C2-N3-C4	-14.81	112.49	119.90	16	9
2	B	83	DG	C4-C5-N7	-14.79	104.89	110.80	10	7
1	A	72	DC	N1-C2-O2	14.78	127.77	118.90	18	10
1	A	75	DA	C4-C5-C6	-14.67	109.66	117.00	11	12
1	A	81	DG	C8-N9-C4	-14.63	100.55	106.40	19	9
1	A	81	DG	C5-C6-N1	14.62	118.81	111.50	10	14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	79	DC	N1-C2-O2	14.60	127.66	118.90	8	12
2	B	90	DA	C5-C6-N1	14.58	124.99	117.70	12	16
3	P	26	TYR	CB-CG-CD2	-14.52	112.29	121.00	8	7
1	A	76	DT	N3-C2-O2	-14.42	113.65	122.30	7	13
2	B	82	DC	N3-C4-C5	14.39	127.66	121.90	5	11
2	B	92	DA	C5-C6-N1	14.37	124.89	117.70	7	14
2	B	93	DG	N3-C4-C5	-14.37	121.41	128.60	14	7
2	B	86	DG	N3-C2-N2	-14.34	109.86	119.90	12	8
2	B	88	DT	C6-C5-C7	-14.28	114.33	122.90	13	17
1	A	79	DC	C2-N3-C4	-14.26	112.77	119.90	19	10
2	B	94	DC	N3-C2-O2	-14.26	111.92	121.90	13	12
2	B	94	DC	N3-C4-C5	14.21	127.58	121.90	17	9
2	B	86	DG	C4-C5-N7	-14.14	105.14	110.80	12	5
1	A	74	DA	N1-C2-N3	-14.04	122.28	129.30	15	10
2	B	86	DG	N3-C4-C5	-14.02	121.59	128.60	12	6
1	A	78	DC	C6-N1-C2	-14.00	114.70	120.30	14	10
2	B	90	DA	N1-C6-N6	-13.94	110.23	118.60	7	20
2	B	91	DG	C5-C6-N1	13.88	118.44	111.50	9	12
1	A	69	DG	N1-C6-O6	-13.81	111.61	119.90	19	10
2	B	93	DG	C5-N7-C8	-13.71	97.44	104.30	3	5
1	A	77	DC	C2-N3-C4	-13.67	113.06	119.90	13	12
2	B	83	DG	C8-N9-C4	13.65	111.86	106.40	2	9
2	B	94	DC	N3-C4-N4	-13.65	108.45	118.00	7	11
2	B	86	DG	N9-C4-C5	13.65	110.86	105.40	12	12
2	B	84	DG	C2-N3-C4	13.64	118.72	111.90	3	6
2	B	91	DG	O4'-C1'-N9	13.63	117.54	108.00	12	4
1	A	81	DG	C4-C5-C6	-13.63	110.62	118.80	11	5
1	A	70	DC	O4'-C1'-N1	-13.54	98.52	108.00	10	6
2	B	83	DG	C2-N3-C4	13.52	118.66	111.90	20	5
1	A	72	DC	C6-N1-C2	-13.51	114.90	120.30	1	9
1	A	72	DC	O4'-C4'-C3'	13.50	114.10	106.00	12	10
2	B	85	DG	N9-C4-C5	-13.48	100.01	105.40	2	5
2	B	87	DA	N9-C4-C5	13.43	111.17	105.80	16	10
2	B	83	DG	N9-C4-C5	13.39	110.76	105.40	10	9
1	A	80	DC	C4'-C3'-C2'	-13.33	91.10	103.10	12	7
1	A	72	DC	N3-C4-C5	13.30	127.22	121.90	12	8
1	A	69	DG	C4-C5-N7	-13.29	105.48	110.80	6	7
1	A	81	DG	O4'-C1'-C2'	-13.27	95.28	105.90	18	6
1	A	73	DT	C4-C5-C6	13.25	125.95	118.00	13	11
1	A	78	DC	O4'-C4'-C3'	13.22	113.93	106.00	9	12
2	B	88	DT	N3-C4-O4	-13.22	111.97	119.90	2	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	81	DG	C6-C5-N7	13.15	138.29	130.40	11	6
2	B	85	DG	C8-N9-C4	-13.14	101.14	106.40	13	7
2	B	87	DA	C4-C5-N7	-13.12	104.14	110.70	16	4
2	B	86	DG	N1-C6-O6	-13.09	112.05	119.90	5	11
2	B	94	DC	O4'-C4'-C3'	13.02	113.81	106.00	10	8
2	B	90	DA	C8-N9-C4	-13.02	100.59	105.80	5	5
1	A	80	DC	O4'-C4'-C3'	12.92	113.75	106.00	16	11
1	A	77	DC	N1-C2-O2	12.91	126.65	118.90	19	13
1	A	77	DC	N3-C2-O2	-12.86	112.90	121.90	19	15
2	B	91	DG	N1-C2-N3	12.80	131.58	123.90	11	6
2	B	93	DG	C4-C5-N7	12.78	115.91	110.80	3	6
2	B	85	DG	N3-C2-N2	-12.77	110.96	119.90	5	9
2	B	92	DA	C8-N9-C4	-12.76	100.70	105.80	7	8
1	A	75	DA	C5-N7-C8	-12.73	97.54	103.90	8	6
2	B	89	DT	N1-C2-N3	12.72	122.23	114.60	6	9
1	A	76	DT	O4'-C1'-N1	12.71	116.89	108.00	15	12
1	A	77	DC	O4'-C4'-C3'	12.69	113.61	106.00	19	10
1	A	76	DT	C5-C6-N1	-12.66	116.10	123.70	2	12
2	B	89	DT	C6-N1-C2	-12.64	114.98	121.30	6	7
1	A	73	DT	O4'-C4'-C3'	12.63	113.58	106.00	13	13
2	B	93	DG	O4'-C1'-C2'	-12.62	95.81	105.90	1	8
2	B	93	DG	C5-C6-N1	12.59	117.79	111.50	7	12
1	A	69	DG	N7-C8-N9	12.54	119.37	113.10	1	7
3	P	26	TYR	CB-CG-CD1	12.53	128.52	121.00	8	6
2	B	89	DT	N3-C4-O4	-12.52	112.39	119.90	15	7
1	A	69	DG	C2-N3-C4	-12.50	105.65	111.90	10	4
2	B	88	DT	C4-C5-C7	12.50	126.50	119.00	3	11
2	B	82	DC	O4'-C1'-C2'	12.48	115.89	105.90	10	3
2	B	85	DG	C2-N3-C4	12.44	118.12	111.90	2	6
1	A	71	DT	C5-C6-N1	-12.44	116.24	123.70	4	11
2	B	93	DG	N3-C2-N2	-12.31	111.28	119.90	19	6
1	A	75	DA	C2-N3-C4	12.29	116.75	110.60	7	7
2	B	94	DC	C5-C6-N1	-12.29	114.86	121.00	20	9
2	B	91	DG	C8-N9-C4	-12.26	101.50	106.40	18	8
1	A	73	DT	C5-C6-N1	-12.22	116.37	123.70	16	8
2	B	85	DG	C5-C6-O6	12.18	135.91	128.60	3	7
1	A	72	DC	O4'-C1'-N1	12.18	116.52	108.00	3	8
1	A	69	DG	C6-N1-C2	-12.13	117.82	125.10	14	6
1	A	73	DT	C2-N3-C4	-12.13	119.92	127.20	5	7
1	A	78	DC	N1-C2-O2	12.11	126.16	118.90	8	10
1	A	77	DC	C5-C4-N4	12.11	128.67	120.20	4	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	77	DC	C6-N1-C2	-12.09	115.47	120.30	9	7
2	B	85	DG	C5-N7-C8	-12.01	98.30	104.30	11	6
2	B	86	DG	N7-C8-N9	11.99	119.09	113.10	12	6
1	A	78	DC	O4'-C1'-C2'	11.99	115.49	105.90	16	4
1	A	76	DT	C6-C5-C7	-11.98	115.71	122.90	18	13
1	A	81	DG	N3-C4-C5	-11.95	122.62	128.60	3	7
1	A	71	DT	O4'-C1'-C2'	-11.95	96.34	105.90	10	6
2	B	91	DG	C6-N1-C2	-11.89	117.97	125.10	9	6
1	A	69	DG	C5-C6-N1	11.83	117.42	111.50	20	12
1	A	81	DG	C5-C6-O6	-11.82	121.51	128.60	15	7
2	B	83	DG	N1-C6-O6	-11.81	112.81	119.90	20	12
1	A	74	DA	C4-C5-C6	-11.80	111.10	117.00	1	14
1	A	76	DT	C1'-O4'-C4'	-11.79	98.31	110.10	18	2
1	A	78	DC	N3-C2-O2	-11.74	113.69	121.90	12	15
2	B	83	DG	C5-C6-N1	11.72	117.36	111.50	20	11
2	B	89	DT	C4-C5-C6	11.69	125.01	118.00	3	9
1	A	74	DA	C5-C6-N1	11.68	123.54	117.70	4	12
1	A	79	DC	C5-C6-N1	-11.68	115.16	121.00	4	11
1	A	69	DG	C4'-C3'-C2'	-11.64	92.63	103.10	2	3
1	A	75	DA	N1-C2-N3	-11.62	123.49	129.30	2	8
1	A	79	DC	C6-N1-C2	-11.58	115.67	120.30	20	7
1	A	80	DC	C2-N3-C4	-11.55	114.13	119.90	15	6
1	A	76	DT	C6-N1-C2	-11.54	115.53	121.30	19	9
1	A	72	DC	N3-C2-O2	-11.53	113.83	121.90	14	14
1	A	71	DT	C4-C5-C6	11.52	124.91	118.00	4	8
2	B	92	DA	O4'-C1'-N9	11.50	116.05	108.00	1	9
1	A	77	DC	N3-C4-N4	-11.49	109.95	118.00	4	11
1	A	73	DT	C4-C5-C7	11.48	125.89	119.00	6	10
2	B	87	DA	C8-N9-C4	-11.47	101.21	105.80	6	8
2	B	91	DG	O4'-C4'-C3'	11.40	112.84	106.00	17	8
1	A	75	DA	C5-C6-N6	11.39	132.81	123.70	19	3
2	B	82	DC	C5-C6-N1	-11.37	115.31	121.00	16	4
1	A	77	DC	N3-C4-C5	11.36	126.44	121.90	1	9
2	B	85	DG	C5-C6-N1	11.36	117.18	111.50	6	8
2	B	85	DG	C6-C5-N7	11.35	137.21	130.40	5	2
2	B	88	DT	O4'-C4'-C3'	11.35	112.81	106.00	19	5
1	A	75	DA	O4'-C1'-N9	11.34	115.94	108.00	8	10
1	A	70	DC	C2-N3-C4	-11.33	114.23	119.90	7	10
1	A	73	DT	O4'-C1'-C2'	-11.33	96.84	105.90	9	9
1	A	71	DT	N3-C4-O4	-11.31	113.11	119.90	15	6
1	A	79	DC	O4'-C1'-N1	11.29	115.91	108.00	5	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	91	DG	N7-C8-N9	11.29	118.74	113.10	18	8
2	B	82	DC	C6-N1-C2	-11.24	115.80	120.30	7	10
1	A	75	DA	C6-C5-N7	11.23	140.16	132.30	15	5
1	A	74	DA	C5-N7-C8	-11.21	98.29	103.90	1	4
1	A	71	DT	N1-C2-N3	11.19	121.31	114.60	13	5
1	A	70	DC	O4'-C1'-C2'	11.18	114.84	105.90	16	6
2	B	88	DT	C2-N3-C4	-11.07	120.56	127.20	11	6
1	A	71	DT	O4'-C4'-C3'	11.06	112.64	106.00	19	8
2	B	84	DG	C8-N9-C4	-11.05	101.98	106.40	4	9
2	B	93	DG	O4'-C4'-C3'	11.05	112.63	106.00	17	9
1	A	76	DT	N1-C2-N3	11.04	121.22	114.60	19	11
1	A	74	DA	O4'-C1'-N9	-10.93	100.35	108.00	5	10
2	B	83	DG	N3-C4-C5	-10.84	123.18	128.60	10	8
1	A	71	DT	C5-C4-O4	10.80	132.46	124.90	12	7
2	B	92	DA	O4'-C4'-C3'	10.80	112.48	106.00	14	4
1	A	76	DT	N3-C4-O4	-10.78	113.43	119.90	10	3
1	A	74	DA	C6-C5-N7	10.76	139.83	132.30	4	5
1	A	69	DG	N9-C4-C5	10.75	109.70	105.40	8	9
2	B	90	DA	C1'-O4'-C4'	-10.75	99.35	110.10	9	3
2	B	88	DT	O4'-C1'-N1	10.71	115.50	108.00	13	9
2	B	90	DA	C5-N7-C8	-10.71	98.55	103.90	4	11
2	B	84	DG	N7-C8-N9	10.69	118.44	113.10	3	7
2	B	88	DT	C5-C6-N1	-10.67	117.30	123.70	19	9
1	A	76	DT	O4'-C1'-C2'	10.64	114.41	105.90	18	5
1	A	74	DA	N9-C4-C5	10.62	110.05	105.80	17	7
2	B	89	DT	O4'-C4'-C3'	10.57	112.34	106.00	15	6
1	A	77	DC	O4'-C1'-C2'	-10.56	97.45	105.90	13	4
1	A	73	DT	N3-C4-O4	-10.56	113.57	119.90	20	4
2	B	89	DT	O4'-C1'-C2'	10.51	114.31	105.90	2	3
2	B	92	DA	N1-C2-N3	-10.46	124.07	129.30	17	7
1	A	74	DA	C5-C6-N6	10.45	132.06	123.70	20	5
2	B	84	DG	N3-C2-N2	-10.45	112.59	119.90	12	7
1	A	78	DC	C4-C5-C6	10.42	122.61	117.40	4	6
2	B	89	DT	C5-C4-O4	10.42	132.19	124.90	16	6
3	P	25	ARG	NE-CZ-NH2	10.39	125.50	120.30	3	10
1	A	81	DG	C4-C5-N7	-10.37	106.65	110.80	18	4
2	B	83	DG	C5-N7-C8	-10.30	99.15	104.30	9	6
1	A	75	DA	N9-C4-C5	10.28	109.91	105.80	6	4
1	A	74	DA	C2-N3-C4	10.28	115.74	110.60	15	6
2	B	88	DT	C4'-C3'-C2'	-10.27	93.86	103.10	19	1
2	B	87	DA	N7-C8-N9	10.25	118.92	113.80	19	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	78	DC	N1-C2-N3	10.23	126.36	119.20	6	3
1	A	71	DT	C2-N3-C4	-10.21	121.07	127.20	15	3
1	A	69	DG	C6-C5-N7	10.20	136.52	130.40	18	6
1	A	80	DC	C6-N1-C2	-10.19	116.22	120.30	4	6
1	A	69	DG	O4'-C4'-C3'	-10.19	99.89	106.00	17	7
2	B	89	DT	N3-C2-O2	-10.18	116.19	122.30	6	13
1	A	81	DG	N3-C2-N2	-10.18	112.78	119.90	7	7
2	B	86	DG	C5-C6-N1	10.17	116.58	111.50	5	6
2	B	82	DC	C4-C5-C6	-10.17	112.32	117.40	20	6
1	A	72	DC	C2-N3-C4	-10.16	114.82	119.90	14	6
1	A	69	DG	N3-C4-C5	10.12	133.66	128.60	10	7
2	B	93	DG	C4-C5-C6	-10.10	112.74	118.80	7	4
2	B	86	DG	O4'-C4'-C3'	-10.07	99.95	106.00	1	6
2	B	94	DC	C2-N3-C4	-10.07	114.86	119.90	17	7
1	A	74	DA	C8-N9-C4	-10.07	101.77	105.80	1	7
2	B	84	DG	C5-C6-O6	-10.03	122.58	128.60	13	6
2	B	92	DA	C6-N1-C2	-10.03	112.58	118.60	7	3
1	A	71	DT	C4-C5-C7	-10.03	112.98	119.00	10	6
1	A	77	DC	C4-C5-C6	10.02	122.41	117.40	5	6
2	B	82	DC	O4'-C1'-N1	10.02	115.01	108.00	17	8
1	A	80	DC	C1'-O4'-C4'	-10.01	100.09	110.10	16	2
1	A	73	DT	C4'-C3'-C2'	-9.99	94.11	103.10	11	7
2	B	83	DG	C6-N1-C2	-9.98	119.11	125.10	18	7
2	B	87	DA	C5-N7-C8	-9.97	98.91	103.90	1	8
1	A	80	DC	O4'-C1'-C2'	-9.97	97.93	105.90	3	4
2	B	92	DA	N9-C4-C5	9.96	109.79	105.80	7	7
1	A	75	DA	P-O3'-C3'	9.95	131.64	119.70	20	9
1	A	75	DA	C6-N1-C2	-9.90	112.66	118.60	14	6
2	B	93	DG	C6-N1-C2	-9.88	119.17	125.10	5	9
3	P	25	ARG	NH1-CZ-NH2	-9.87	108.54	119.40	13	4
1	A	75	DA	O4'-C1'-C2'	-9.83	98.03	105.90	10	5
2	B	90	DA	N9-C4-C5	-9.82	101.87	105.80	7	5
2	B	91	DG	N9-C4-C5	9.80	109.32	105.40	2	4
2	B	82	DC	C5-C4-N4	9.79	127.06	120.20	9	3
2	B	84	DG	N9-C4-C5	9.79	109.32	105.40	14	6
2	B	93	DG	N3-C4-N9	9.79	131.88	126.00	20	2
2	B	87	DA	O4'-C1'-C2'	-9.78	98.08	105.90	3	4
1	A	78	DC	C5-C4-N4	9.78	127.05	120.20	19	7
2	B	84	DG	N3-C4-N9	9.78	131.87	126.00	13	9
2	B	88	DT	C5-C4-O4	9.76	131.73	124.90	7	4
2	B	93	DG	N9-C4-C5	9.75	109.30	105.40	14	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	85	DG	O4'-C1'-C2'	-9.73	98.11	105.90	2	5
1	A	70	DC	C5-C6-N1	-9.71	116.14	121.00	4	5
2	B	86	DG	N3-C4-N9	9.70	131.82	126.00	13	7
1	A	78	DC	C5-C6-N1	-9.70	116.15	121.00	19	8
2	B	91	DG	C5-N7-C8	-9.69	99.45	104.30	18	10
2	B	94	DC	C4-C5-C6	-9.68	112.56	117.40	1	8
2	B	90	DA	C5-C6-N6	-9.67	115.96	123.70	17	2
2	B	84	DG	O4'-C4'-C3'	-9.63	100.22	106.00	4	7
2	B	88	DT	C4-C5-C6	9.63	123.78	118.00	19	7
2	B	91	DG	O4'-C1'-C2'	9.62	113.60	105.90	3	9
2	B	86	DG	O4'-C1'-C2'	9.62	113.59	105.90	1	4
2	B	86	DG	C4'-C3'-C2'	9.61	111.75	103.10	1	3
2	B	94	DC	C1'-O4'-C4'	-9.59	100.51	110.10	10	5
2	B	90	DA	N1-C2-N3	-9.56	124.52	129.30	10	8
1	A	79	DC	O4'-C4'-C3'	9.55	111.73	106.00	18	3
1	A	75	DA	C8-N9-C4	-9.54	101.98	105.80	17	6
2	B	83	DG	N7-C8-N9	9.51	117.86	113.10	7	13
2	B	91	DG	C5-C6-O6	9.48	134.29	128.60	3	6
1	A	72	DC	N3-C4-N4	-9.47	111.37	118.00	10	5
2	B	90	DA	N7-C8-N9	9.46	118.53	113.80	18	9
2	B	87	DA	C2-N3-C4	-9.45	105.88	110.60	20	7
2	B	91	DG	C4-C5-C6	-9.44	113.14	118.80	1	7
2	B	91	DG	N3-C4-C5	-9.41	123.90	128.60	20	3
1	A	76	DT	C4-C5-C7	-9.37	113.38	119.00	20	4
2	B	86	DG	C6-N1-C2	-9.35	119.49	125.10	8	5
2	B	83	DG	O4'-C4'-C3'	9.35	111.61	106.00	20	5
1	A	69	DG	C4-C5-C6	-9.34	113.19	118.80	5	9
2	B	83	DG	O4'-C1'-N9	-9.32	101.48	108.00	20	10
2	B	82	DC	C1'-O4'-C4'	-9.31	100.79	110.10	10	6
2	B	87	DA	C6-N1-C2	-9.30	113.02	118.60	18	3
2	B	94	DC	C6-N1-C2	-9.30	116.58	120.30	6	7
1	A	80	DC	N3-C4-N4	-9.29	111.50	118.00	11	7
2	B	84	DG	C6-N1-C2	-9.29	119.53	125.10	19	5
1	A	69	DG	C5-N7-C8	-9.28	99.66	104.30	20	5
2	B	82	DC	C3'-C2'-C1'	9.27	113.62	102.50	7	3
1	A	69	DG	C8-N9-C4	9.26	110.11	106.40	5	9
2	B	89	DT	N3-C4-C5	-9.23	109.66	115.20	16	5
1	A	69	DG	N3-C2-N2	-9.23	113.44	119.90	10	6
2	B	87	DA	N1-C2-N3	-9.16	124.72	129.30	9	7
2	B	87	DA	C6-C5-N7	9.15	138.71	132.30	9	8
2	B	82	DC	P-O3'-C3'	9.12	130.64	119.70	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	P	21	PHE	CB-CG-CD1	-9.12	114.42	120.80	6	5
2	B	83	DG	C1'-O4'-C4'	-9.04	101.06	110.10	8	3
1	A	72	DC	C5-C4-N4	-9.03	113.88	120.20	19	5
1	A	69	DG	C5-C6-O6	-9.00	123.20	128.60	10	10
1	A	72	DC	P-O3'-C3'	8.99	130.49	119.70	9	6
2	B	84	DG	O4'-C1'-N9	8.98	114.28	108.00	7	7
2	B	88	DT	N1-C2-N3	8.95	119.97	114.60	4	3
2	B	90	DA	C6-N1-C2	-8.93	113.24	118.60	3	3
1	A	80	DC	C5-C6-N1	-8.92	116.54	121.00	19	4
1	A	75	DA	N3-C4-C5	8.92	133.05	126.80	11	2
2	B	93	DG	C3'-C2'-C1'	8.91	113.19	102.50	1	3
2	B	87	DA	C1'-O4'-C4'	-8.90	101.20	110.10	6	4
1	A	76	DT	C4-C5-C6	8.90	123.34	118.00	2	12
1	A	75	DA	O4'-C4'-C3'	8.89	111.33	106.00	9	7
1	A	76	DT	N1-C2-O2	8.89	130.21	123.10	2	2
3	P	21	PHE	CB-CG-CD2	-8.86	114.60	120.80	1	7
2	B	85	DG	O4'-C4'-C3'	8.84	111.31	106.00	20	7
1	A	69	DG	P-O3'-C3'	8.84	130.31	119.70	3	6
1	A	81	DG	O4'-C4'-C3'	8.84	111.30	106.00	4	4
2	B	86	DG	C3'-C2'-C1'	-8.83	91.90	102.50	1	2
1	A	70	DC	C6-N1-C2	8.82	123.83	120.30	4	7
2	B	86	DG	C6-C5-N7	-8.81	125.11	130.40	9	8
2	B	86	DG	N1-C2-N2	8.81	124.12	116.20	18	3
2	B	82	DC	O4'-C4'-C3'	8.79	111.27	106.00	7	7
2	B	87	DA	O4'-C1'-N9	8.79	114.15	108.00	15	7
1	A	79	DC	C4-C5-C6	-8.76	113.02	117.40	7	7
1	A	81	DG	N1-C2-N3	-8.76	118.65	123.90	11	3
2	B	94	DC	O4'-C1'-N1	8.72	114.11	108.00	13	8
2	B	85	DG	N3-C4-C5	-8.71	124.24	128.60	17	7
2	B	92	DA	C4-C5-N7	8.68	115.04	110.70	10	4
2	B	86	DG	C5-C6-O6	8.67	133.80	128.60	15	6
1	A	74	DA	N7-C8-N9	8.67	118.14	113.80	1	3
1	A	73	DT	N1-C2-N3	8.64	119.78	114.60	6	7
2	B	83	DG	N3-C2-N2	-8.63	113.86	119.90	16	9
2	B	82	DC	N1-C2-N3	8.63	125.24	119.20	16	4
2	B	86	DG	N1-C2-N3	8.62	129.07	123.90	12	5
2	B	90	DA	C6-C5-N7	8.62	138.33	132.30	5	6
3	P	31	ARG	NH1-CZ-NH2	-8.62	109.92	119.40	20	4
1	A	80	DC	O4'-C1'-N1	-8.61	101.97	108.00	17	5
2	B	93	DG	N1-C2-N2	-8.61	108.45	116.20	12	5
2	B	88	DT	O4'-C1'-C2'	-8.59	99.03	105.90	8	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	71	DT	C4'-C3'-C2'	-8.58	95.38	103.10	2	8
2	B	83	DG	C4'-C3'-C2'	-8.57	95.38	103.10	12	6
2	B	84	DG	C4-C5-N7	-8.57	107.37	110.80	3	6
1	A	74	DA	C4-C5-N7	-8.55	106.42	110.70	17	6
2	B	93	DG	N7-C8-N9	8.55	117.38	113.10	3	6
1	A	81	DG	C1'-O4'-C4'	-8.55	101.55	110.10	1	5
1	A	81	DG	C6-N1-C2	-8.53	119.98	125.10	18	10
2	B	91	DG	C6-C5-N7	8.52	135.51	130.40	12	6
2	B	94	DC	C5-C4-N4	8.51	126.16	120.20	20	6
2	B	86	DG	P-O3'-C3'	8.51	129.91	119.70	14	5
2	B	85	DG	N1-C2-N3	8.50	129.00	123.90	15	9
2	B	90	DA	C4-C5-N7	8.49	114.95	110.70	7	5
2	B	85	DG	N7-C8-N9	8.47	117.34	113.10	7	9
1	A	69	DG	N3-C4-N9	-8.47	120.92	126.00	10	4
2	B	92	DA	P-O3'-C3'	8.44	129.83	119.70	7	8
2	B	83	DG	C5-C6-O6	8.41	133.65	128.60	19	5
2	B	89	DT	C2-N3-C4	8.40	132.24	127.20	18	4
1	A	81	DG	C2-N3-C4	8.37	116.08	111.90	12	8
1	A	70	DC	N1-C2-N3	8.36	125.05	119.20	7	7
2	B	83	DG	O4'-C1'-C2'	8.33	112.56	105.90	5	4
2	B	93	DG	C5-C6-O6	8.32	133.59	128.60	10	8
2	B	88	DT	C1'-O4'-C4'	-8.32	101.78	110.10	3	2
1	A	74	DA	C6-N1-C2	-8.28	113.63	118.60	1	6
1	A	72	DC	C1'-O4'-C4'	-8.29	101.81	110.10	18	3
2	B	89	DT	N1-C2-O2	8.28	129.72	123.10	18	1
1	A	74	DA	O4'-C1'-C2'	-8.27	99.28	105.90	10	4
2	B	88	DT	N3-C4-C5	-8.27	110.24	115.20	4	2
1	A	75	DA	C4-C5-N7	8.25	114.82	110.70	18	5
3	P	16	GLU	CA-CB-CG	8.25	131.55	113.40	18	15
1	A	79	DC	O4'-C1'-C2'	8.24	112.50	105.90	7	4
1	A	75	DA	C4'-C3'-C2'	-8.24	95.69	103.10	5	4
1	A	76	DT	P-O3'-C3'	8.23	129.58	119.70	12	3
2	B	92	DA	C5-N7-C8	-8.23	99.79	103.90	1	6
2	B	92	DA	N7-C8-N9	8.22	117.91	113.80	4	3
2	B	90	DA	O4'-C1'-C2'	-8.21	99.33	105.90	15	2
3	P	39	LEU	CB-CG-CD2	-8.20	97.06	111.00	4	3
1	A	78	DC	C3'-C2'-C1'	8.20	112.34	102.50	12	3
1	A	72	DC	O5'-P-OP2	-8.19	98.33	105.70	15	2
2	B	84	DG	N1-C2-N3	-8.15	119.01	123.90	6	4
1	A	72	DC	C4-C5-C6	8.15	121.47	117.40	7	2
1	A	69	DG	O4'-C1'-C2'	-8.13	99.39	105.90	10	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	81	DG	N1-C2-N2	8.05	123.44	116.20	19	2
2	B	93	DG	C4'-C3'-C2'	-8.05	95.86	103.10	1	6
2	B	93	DG	C8-N9-C4	-8.03	103.19	106.40	16	6
2	B	89	DT	C5-C6-N1	-8.02	118.89	123.70	10	8
1	A	70	DC	C5-C4-N4	-8.02	114.59	120.20	10	5
1	A	76	DT	C2-N3-C4	-7.99	122.40	127.20	1	9
2	B	90	DA	O4'-C4'-C3'	7.99	110.80	106.00	19	7
1	A	76	DT	C5-C4-O4	-7.98	119.31	124.90	8	6
2	B	85	DG	C6-N1-C2	-7.98	120.31	125.10	14	9
1	A	75	DA	N7-C8-N9	7.97	117.78	113.80	18	2
2	B	87	DA	P-O3'-C3'	7.97	129.26	119.70	2	5
1	A	70	DC	P-O3'-C3'	7.96	129.25	119.70	10	4
1	A	79	DC	P-O3'-C3'	7.96	129.25	119.70	18	7
2	B	89	DT	C3'-C2'-C1'	-7.94	92.97	102.50	7	2
1	A	79	DC	C5-C4-N4	7.94	125.75	120.20	12	3
1	A	73	DT	C6-N1-C2	-7.91	117.34	121.30	20	4
1	A	74	DA	P-O3'-C3'	7.90	129.18	119.70	3	6
2	B	89	DT	P-O3'-C3'	7.87	129.15	119.70	9	5
2	B	85	DG	N1-C2-N2	-7.87	109.12	116.20	17	4
2	B	83	DG	N3-C4-N9	7.84	130.70	126.00	18	2
3	P	50	PHE	CB-CG-CD1	-7.84	115.31	120.80	15	8
2	B	87	DA	C3'-C2'-C1'	-7.78	93.17	102.50	6	2
3	P	31	ARG	CD-NE-CZ	7.77	134.48	123.60	17	2
2	B	86	DG	C4-C5-C6	-7.77	114.14	118.80	3	5
1	A	72	DC	O4'-C1'-C2'	-7.75	99.70	105.90	10	4
2	B	84	DG	C6-C5-N7	7.72	135.03	130.40	19	3
1	A	72	DC	C5-C6-N1	-7.71	117.15	121.00	5	7
2	B	83	DG	N1-C2-N2	-7.70	109.27	116.20	17	2
2	B	85	DG	C3'-C2'-C1'	-7.70	93.27	102.50	1	3
3	P	49	TRP	CB-CG-CD2	7.67	136.58	126.60	5	3
2	B	83	DG	N1-C2-N3	-7.67	119.30	123.90	20	5
1	A	80	DC	C4-C5-C6	7.67	121.23	117.40	18	6
2	B	90	DA	C4'-C3'-C2'	-7.67	96.20	103.10	19	3
2	B	94	DC	O4'-C1'-C2'	-7.66	99.78	105.90	12	5
2	B	93	DG	C2-N3-C4	7.64	115.72	111.90	14	4
3	P	34	ASP	CB-CG-OD1	7.63	125.17	118.30	14	2
1	A	81	DG	N9-C4-C5	7.62	108.45	105.40	7	6
3	P	10	THR	CA-CB-CG2	7.58	123.02	112.40	3	4
2	B	91	DG	C4-C5-N7	-7.57	107.77	110.80	12	4
2	B	92	DA	C1'-O4'-C4'	-7.56	102.54	110.10	10	1
3	P	17	LEU	CB-CG-CD1	7.55	123.83	111.00	20	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	88	DT	N1-C2-O2	-7.54	117.06	123.10	19	3
1	A	72	DC	C4'-C3'-C2'	-7.48	96.37	103.10	17	1
2	B	93	DG	C6-C5-N7	7.47	134.88	130.40	7	6
2	B	90	DA	C2-N3-C4	-7.47	106.86	110.60	13	4
2	B	89	DT	C4-C5-C7	7.46	123.47	119.00	14	6
2	B	84	DG	C4'-C3'-C2'	-7.44	96.40	103.10	20	4
2	B	87	DA	O3'-P-O5'	-7.43	89.89	104.00	6	2
2	B	90	DA	C3'-C2'-C1'	-7.42	93.59	102.50	11	3
1	A	79	DC	C1'-O4'-C4'	-7.42	102.68	110.10	7	3
2	B	84	DG	P-O3'-C3'	7.42	128.61	119.70	13	2
1	A	78	DC	P-O3'-C3'	7.41	128.59	119.70	20	5
2	B	86	DG	C5-N7-C8	-7.40	100.60	104.30	15	5
1	A	73	DT	N3-C4-C5	-7.36	110.79	115.20	13	2
1	A	71	DT	C3'-C2'-C1'	7.33	111.30	102.50	20	4
2	B	86	DG	C2-N3-C4	7.32	115.56	111.90	13	7
2	B	87	DA	N3-C4-N9	-7.31	121.55	127.40	8	3
1	A	80	DC	N1-C2-N3	7.28	124.30	119.20	7	2
2	B	91	DG	C2-N3-C4	-7.28	108.26	111.90	11	3
3	P	39	LEU	CB-CG-CD1	-7.27	98.64	111.00	8	8
2	B	88	DT	P-O5'-C5'	7.27	132.53	120.90	8	1
2	B	84	DG	O4'-C1'-C2'	-7.25	100.10	105.90	14	2
1	A	70	DC	C1'-O4'-C4'	7.24	117.34	110.10	5	5
1	A	77	DC	P-O3'-C3'	7.21	128.35	119.70	7	7
2	B	92	DA	C2-N3-C4	7.16	114.18	110.60	1	4
2	B	92	DA	C6-C5-N7	7.15	137.31	132.30	19	7
1	A	79	DC	N1-C2-N3	7.15	124.20	119.20	16	2
3	P	26	TYR	CG-CD2-CE2	-7.13	115.59	121.30	5	3
2	B	91	DG	O3'-P-O5'	-7.12	90.47	104.00	20	1
1	A	69	DG	N1-C2-N3	7.11	128.17	123.90	12	4
3	P	26	TYR	CG-CD1-CE1	-7.09	115.63	121.30	11	2
3	P	46	VAL	CG1-CB-CG2	-7.09	99.56	110.90	4	2
2	B	92	DA	C5-C6-N6	7.08	129.37	123.70	15	6
1	A	71	DT	C1'-O4'-C4'	-7.08	103.02	110.10	5	4
2	B	90	DA	P-O3'-C3'	7.05	128.16	119.70	12	7
2	B	91	DG	C4'-C3'-C2'	-7.05	96.76	103.10	13	3
2	B	91	DG	N3-C4-N9	-7.03	121.78	126.00	2	4
1	A	71	DT	N1-C2-O2	7.01	128.71	123.10	3	1
2	B	84	DG	N1-C2-N2	7.00	122.50	116.20	16	5
3	P	49	TRP	NE1-CE2-CD2	-7.00	100.31	107.30	3	7
1	A	74	DA	N3-C4-N9	6.97	132.97	127.40	7	2
2	B	87	DA	O4'-C4'-C3'	6.96	110.17	106.00	18	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	88	DT	P-O3'-C3'	6.95	128.04	119.70	19	5
1	A	71	DT	P-O3'-C3'	6.94	128.03	119.70	12	3
2	B	85	DG	C4-C5-C6	-6.93	114.64	118.80	13	3
2	B	90	DA	O5'-P-OP2	-6.91	99.48	105.70	11	2
1	A	71	DT	C6-N1-C2	-6.91	117.85	121.30	15	4
1	A	76	DT	C4'-C3'-C2'	-6.90	96.89	103.10	9	1
1	A	73	DT	P-O3'-C3'	6.89	127.97	119.70	4	3
3	P	49	TRP	CB-CG-CD1	-6.88	118.05	127.00	5	2
1	A	77	DC	C3'-C2'-C1'	-6.88	94.24	102.50	16	1
3	P	18	GLU	OE1-CD-OE2	-6.88	115.04	123.30	3	2
3	P	49	TRP	NE1-CE2-CZ2	6.86	137.94	130.40	3	4
1	A	80	DC	C5-C4-N4	-6.84	115.41	120.20	3	4
2	B	92	DA	N3-C4-C5	6.80	131.56	126.80	10	2
2	B	92	DA	C4'-C3'-C2'	-6.80	96.97	103.10	14	2
2	B	89	DT	O5'-P-OP2	-6.80	99.58	105.70	17	1
1	A	72	DC	N1-C2-N3	6.80	123.96	119.20	14	4
2	B	91	DG	P-O3'-C3'	6.79	127.85	119.70	16	8
1	A	77	DC	N1-C2-N3	6.78	123.94	119.20	5	5
2	B	91	DG	C3'-C2'-C1'	-6.77	94.37	102.50	14	3
1	A	80	DC	O5'-P-OP2	6.77	118.82	110.70	9	1
2	B	85	DG	P-O5'-C5'	6.76	131.71	120.90	3	1
3	P	30	PRO	N-CA-CB	6.75	111.40	103.30	12	6
1	A	77	DC	C1'-O4'-C4'	-6.73	103.37	110.10	18	4
1	A	74	DA	O4'-C4'-C3'	6.71	110.03	106.00	12	4
2	B	91	DG	C1'-O4'-C4'	-6.70	103.40	110.10	19	3
1	A	73	DT	C5-C4-O4	6.68	129.57	124.90	8	2
1	A	74	DA	N3-C4-C5	-6.67	122.13	126.80	7	1
1	A	70	DC	C2-N1-C1'	-6.67	111.46	118.80	4	2
3	P	26	TYR	CD1-CG-CD2	6.67	125.23	117.90	11	1
2	B	93	DG	N1-C2-N3	6.63	127.88	123.90	19	6
2	B	83	DG	O3'-P-O5'	-6.63	91.41	104.00	13	4
1	A	78	DC	C5'-C4'-O4'	6.61	121.86	109.30	5	1
2	B	91	DG	C4-N9-C1'	-6.59	117.94	126.50	15	1
3	P	49	TRP	CD1-NE1-CE2	6.58	114.92	109.00	20	1
2	B	92	DA	C3'-C2'-C1'	-6.58	94.61	102.50	10	1
2	B	87	DA	C4'-C3'-C2'	-6.53	97.22	103.10	18	2
1	A	75	DA	C3'-C2'-C1'	6.52	110.32	102.50	10	1
3	P	49	TRP	CD1-CG-CD2	-6.49	101.11	106.30	18	4
3	P	50	PHE	CB-CG-CD2	-6.45	116.29	120.80	7	8
1	A	76	DT	C3'-C2'-C1'	6.44	110.23	102.50	9	1
1	A	71	DT	N3-C4-C5	-6.44	111.34	115.20	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	87	DA	C5-C6-N6	6.43	128.84	123.70	15	2
1	A	73	DT	C1'-O4'-C4'	-6.43	103.67	110.10	3	4
2	B	88	DT	C6-N1-C2	-6.41	118.09	121.30	4	1
1	A	78	DC	C4'-C3'-C2'	-6.41	97.33	103.10	2	2
3	P	34	ASP	CB-CG-OD2	-6.40	112.54	118.30	16	3
3	P	20	HIS	CB-CA-C	6.38	123.17	110.40	13	2
3	P	49	TRP	CE2-CD2-CG	6.38	112.40	107.30	14	2
1	A	79	DC	C3'-C2'-C1'	-6.36	94.87	102.50	10	2
2	B	93	DG	P-O3'-C3'	6.36	127.33	119.70	7	4
3	P	27	LEU	CB-CG-CD1	6.34	121.78	111.00	15	1
1	A	77	DC	O5'-P-OP1	-6.34	99.99	105.70	17	1
1	A	81	DG	C4'-C3'-C2'	-6.33	97.40	103.10	20	1
1	A	70	DC	O5'-P-OP1	6.33	118.29	110.70	4	1
1	A	72	DC	C4'-C3'-O3'	6.33	125.51	109.70	9	1
3	P	50	PHE	CG-CD1-CE1	-6.32	113.84	120.80	15	2
1	A	81	DG	N3-C4-N9	6.32	129.79	126.00	3	2
3	P	30	PRO	N-CD-CG	6.32	112.67	103.20	6	1
1	A	76	DT	O5'-P-OP2	-6.31	100.02	105.70	20	1
1	A	78	DC	C5'-C4'-C3'	6.31	125.45	114.10	12	2
2	B	83	DG	P-O3'-C3'	6.30	127.26	119.70	10	5
1	A	74	DA	C1'-O4'-C4'	-6.30	103.80	110.10	6	2
3	P	49	TRP	CG-CD2-CE3	-6.29	128.24	133.90	15	2
2	B	89	DT	C4'-C3'-C2'	-6.29	97.44	103.10	14	5
2	B	83	DG	C3'-C2'-C1'	-6.28	94.96	102.50	6	1
1	A	80	DC	O3'-P-O5'	-6.28	92.08	104.00	2	1
3	P	50	PHE	CZ-CE2-CD2	-6.26	112.59	120.10	12	1
1	A	81	DG	C3'-C2'-C1'	-6.25	95.00	102.50	4	3
2	B	91	DG	N1-C2-N2	6.20	121.78	116.20	7	2
2	B	82	DC	C2-N1-C1'	6.17	125.59	118.80	2	1
3	P	10	THR	OG1-CB-CG2	-6.17	95.81	110.00	5	1
2	B	90	DA	N3-C4-C5	6.14	131.10	126.80	10	3
2	B	83	DG	C6-C5-N7	6.13	134.08	130.40	11	4
1	A	74	DA	C3'-C2'-C1'	-6.12	95.15	102.50	4	2
2	B	86	DG	C8-N9-C1'	-6.11	119.05	127.00	2	2
1	A	75	DA	N3-C4-N9	-6.06	122.55	127.40	11	1
2	B	85	DG	C1'-O4'-C4'	-6.00	104.10	110.10	20	2
2	B	88	DT	N1-C1'-C2'	5.99	123.99	112.60	8	1
2	B	91	DG	N9-C1'-C2'	5.99	123.98	112.60	6	1
2	B	94	DC	C2-N1-C1'	5.99	125.38	118.80	6	2
1	A	70	DC	C4'-C3'-C2'	-5.97	97.72	103.10	11	5
2	B	89	DT	C1'-O4'-C4'	-5.97	104.13	110.10	2	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	P	45	GLN	CG-CD-OE1	5.95	133.50	121.60	7	1
1	A	77	DC	C4'-C3'-C2'	-5.95	97.75	103.10	2	6
2	B	86	DG	N9-C1'-C2'	5.95	123.90	112.60	9	3
3	P	22	LEU	CB-CG-CD2	5.92	121.07	111.00	5	1
3	P	32	LEU	CA-CB-CG	5.92	128.91	115.30	8	1
1	A	73	DT	C3'-C2'-C1'	-5.92	95.40	102.50	4	1
3	P	26	TYR	CA-CB-CG	5.92	124.64	113.40	5	1
1	A	78	DC	C2-N1-C1'	5.92	125.31	118.80	6	1
3	P	42	GLY	O-C-N	-5.90	113.25	122.70	16	1
1	A	75	DA	C5'-C4'-O4'	5.89	120.49	109.30	8	2
3	P	46	VAL	CA-CB-CG1	5.88	119.73	110.90	15	1
3	P	40	ALA	N-CA-CB	-5.84	101.92	110.10	9	1
3	P	21	PHE	CG-CD1-CE1	-5.83	114.38	120.80	17	2
2	B	82	DC	C4'-C3'-C2'	5.81	108.33	103.10	10	3
3	P	26	TYR	CD1-CE1-CZ	5.81	125.03	119.80	19	1
1	A	77	DC	OP2-P-O3'	5.80	117.97	105.20	15	1
2	B	84	DG	C1'-O4'-C4'	-5.79	104.31	110.10	20	3
3	P	32	LEU	CB-CG-CD1	-5.79	101.16	111.00	19	2
2	B	88	DT	C5'-C4'-O4'	5.79	120.29	109.30	14	1
1	A	75	DA	OP2-P-O3'	5.77	117.89	105.20	12	1
2	B	82	DC	N1-C1'-C2'	5.77	123.56	112.60	6	1
2	B	85	DG	O3'-P-O5'	-5.77	93.04	104.00	4	1
3	P	23	GLN	O-C-N	-5.76	113.41	123.20	5	1
2	B	85	DG	O5'-P-OP2	-5.74	100.54	105.70	10	1
2	B	85	DG	C4'-C3'-C2'	-5.72	97.95	103.10	2	3
2	B	85	DG	P-O3'-C3'	5.71	126.55	119.70	8	1
1	A	79	DC	C5'-C4'-O4'	5.71	120.14	109.30	9	1
3	P	21	PHE	CD1-CG-CD2	5.70	125.71	118.30	7	1
1	A	79	DC	N1-C1'-C2'	5.70	123.43	112.60	11	1
2	B	83	DG	C4-C5-C6	-5.69	115.39	118.80	15	4
1	A	76	DT	N1-C1'-C2'	5.69	123.41	112.60	14	1
2	B	85	DG	OP2-P-O3'	5.68	117.70	105.20	4	1
2	B	94	DC	O5'-P-OP2	5.68	117.52	110.70	9	1
2	B	83	DG	O5'-P-OP1	-5.68	100.59	105.70	18	1
1	A	70	DC	C3'-C2'-C1'	-5.64	95.73	102.50	16	2
2	B	84	DG	OP2-P-O3'	5.64	117.60	105.20	19	1
1	A	69	DG	N1-C2-N2	5.63	121.27	116.20	17	2
2	B	92	DA	N3-C4-N9	5.63	131.91	127.40	5	2
3	P	29	ALA	N-CA-CB	5.60	117.94	110.10	14	4
3	P	29	ALA	CB-CA-C	5.60	118.50	110.10	3	1
2	B	94	DC	C5'-C4'-C3'	-5.60	104.03	114.10	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	88	DT	C3'-C2'-C1'	-5.59	95.79	102.50	10	1
3	P	37	ALA	CB-CA-C	5.57	118.45	110.10	14	1
1	A	80	DC	C3'-C2'-C1'	-5.54	95.85	102.50	20	2
3	P	34	ASP	O-C-N	-5.53	113.86	122.70	20	1
3	P	50	PHE	CG-CD2-CE2	5.52	126.87	120.80	16	1
2	B	84	DG	C3'-C2'-C1'	5.52	109.12	102.50	14	1
1	A	76	DT	N3-C4-C5	-5.51	111.89	115.20	18	2
2	B	88	DT	O5'-P-OP2	-5.51	100.74	105.70	14	1
1	A	69	DG	C4-N9-C1'	-5.51	119.34	126.50	3	1
2	B	87	DA	N9-C1'-C2'	5.49	123.02	112.60	11	1
1	A	69	DG	C3'-C2'-C1'	-5.48	95.92	102.50	18	1
2	B	93	DG	C5'-C4'-O4'	5.47	119.69	109.30	18	1
2	B	83	DG	OP1-P-OP2	-5.45	111.42	119.60	13	1
2	B	90	DA	C8-N9-C1'	5.44	137.49	127.70	16	1
2	B	82	DC	C5'-C4'-C3'	5.43	123.87	114.10	1	1
2	B	93	DG	C4-N9-C1'	5.42	133.54	126.50	3	1
1	A	73	DT	N1-C2-O2	5.41	127.43	123.10	10	1
3	P	21	PHE	CD1-CE1-CZ	5.41	126.59	120.10	17	1
2	B	85	DG	C4-N9-C1'	-5.39	119.50	126.50	2	1
2	B	94	DC	C4'-C3'-C2'	-5.38	98.25	103.10	4	3
2	B	87	DA	N3-C4-C5	5.38	130.56	126.80	8	3
2	B	92	DA	O4'-C1'-C2'	-5.38	101.60	105.90	8	2
1	A	69	DG	C8-N9-C1'	5.37	133.97	127.00	3	1
1	A	77	DC	C2-N1-C1'	5.36	124.69	118.80	9	2
1	A	76	DT	OP2-P-O3'	5.35	116.98	105.20	2	1
1	A	80	DC	P-O3'-C3'	5.35	126.12	119.70	9	1
3	P	49	TRP	CD2-CE3-CZ3	5.34	125.75	118.80	3	1
1	A	80	DC	C2-N1-C1'	-5.34	112.92	118.80	16	1
2	B	86	DG	OP1-P-O3'	5.33	116.92	105.20	7	1
1	A	72	DC	OP2-P-O3'	5.33	116.92	105.20	6	1
3	P	49	TRP	CG-CD1-NE1	-5.32	104.78	110.10	7	4
1	A	77	DC	O3'-P-O5'	-5.32	93.90	104.00	10	1
1	A	79	DC	O3'-P-O5'	-5.31	93.92	104.00	16	1
2	B	90	DA	N3-C4-N9	-5.30	123.16	127.40	13	2
3	P	13	GLN	CA-CB-CG	-5.29	101.75	113.40	16	1
2	B	86	DG	C1'-O4'-C4'	-5.29	104.81	110.10	14	2
2	B	89	DT	N1-C1'-C2'	5.29	122.65	112.60	11	2
1	A	74	DA	C5'-C4'-C3'	5.29	123.62	114.10	7	1
2	B	94	DC	O5'-C5'-C4'	5.28	124.21	111.00	17	1
1	A	76	DT	O5'-P-OP1	-5.27	100.95	105.70	12	1
2	B	89	DT	OP1-P-O3'	5.27	116.79	105.20	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	72	DC	C6-N1-C1'	-5.25	114.50	120.80	4	1
3	P	47	LYS	O-C-N	5.24	131.08	122.70	2	1
3	P	47	LYS	CB-CG-CD	5.24	125.22	111.60	4	1
2	B	93	DG	C1'-O4'-C4'	-5.23	104.87	110.10	5	2
3	P	40	ALA	CB-CA-C	5.23	117.95	110.10	9	2
1	A	72	DC	N1-C1'-C2'	5.23	122.53	112.60	15	1
2	B	90	DA	C5'-C4'-O4'	5.21	119.19	109.30	10	1
2	B	93	DG	C4'-C3'-O3'	5.21	122.71	109.70	13	1
2	B	83	DG	C4-N9-C1'	-5.18	119.77	126.50	2	1
1	A	79	DC	O5'-P-OP2	-5.17	101.05	105.70	12	1
2	B	92	DA	OP1-P-OP2	-5.14	111.89	119.60	16	1
3	P	49	TRP	CZ3-CH2-CZ2	-5.12	115.46	121.60	11	1
1	A	73	DT	N1-C1'-C2'	5.09	122.27	112.60	4	1
1	A	72	DC	O3'-P-O5'	5.09	113.67	104.00	14	1
1	A	80	DC	C6-N1-C1'	-5.09	114.70	120.80	19	1
1	A	69	DG	C5'-C4'-O4'	5.07	118.94	109.30	7	1
1	A	70	DC	O3'-P-O5'	5.07	113.63	104.00	5	1
1	A	80	DC	C5'-C4'-O4'	-5.06	99.69	109.30	11	1
3	P	35	LEU	CB-CG-CD1	5.06	119.60	111.00	19	1
3	P	31	ARG	CA-CB-CG	5.05	124.51	113.40	11	1
1	A	75	DA	O3'-P-O5'	-5.05	94.41	104.00	9	1
2	B	87	DA	OP1-P-OP2	-5.04	112.04	119.60	7	1
1	A	69	DG	C1'-O4'-C4'	-5.03	105.07	110.10	15	1
3	P	16	GLU	CG-CD-OE1	-5.03	108.24	118.30	7	1
2	B	89	DT	O5'-P-OP1	-5.02	101.18	105.70	1	1
1	A	70	DC	C6-N1-C1'	5.02	126.82	120.80	17	1
1	A	72	DC	C5'-C4'-C3'	5.01	123.12	114.10	9	1
2	B	91	DG	C5'-C4'-O4'	5.01	118.82	109.30	15	1
1	A	75	DA	C5'-C4'-C3'	5.01	123.11	114.10	13	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	69	DG	Sidechain	18
1	A	81	DG	Sidechain	18
2	B	91	DG	Sidechain	17
2	B	85	DG	Sidechain	15
2	B	93	DG	Sidechain	15
2	B	84	DG	Sidechain	14

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	75	DA	Sidechain	13
2	B	82	DC	Sidechain	13
2	B	83	DG	Sidechain	13
1	A	76	DT	Sidechain	12
2	B	86	DG	Sidechain	12
1	A	73	DT	Sidechain	12
2	B	92	DA	Sidechain	11
2	B	88	DT	Sidechain	10
1	A	74	DA	Sidechain	9
2	B	89	DT	Sidechain	9
2	B	87	DA	Sidechain	9
1	A	70	DC	Sidechain	9
1	A	78	DC	Sidechain	7
1	A	72	DC	Sidechain	7
2	B	90	DA	Sidechain	7
1	A	71	DT	Sidechain	6
2	B	94	DC	Sidechain	6
1	A	79	DC	Sidechain	6
1	A	80	DC	Sidechain	5
1	A	77	DC	Sidechain	4
3	P	20	HIS	Sidechain,Mainchain	4
3	P	26	TYR	Sidechain	3
3	P	50	PHE	Sidechain	3
3	P	31	ARG	Sidechain	3
3	P	25	ARG	Sidechain	2
3	P	42	GLY	Mainchain	1
3	P	46	VAL	Mainchain	1
3	P	21	PHE	Sidechain	1
3	P	11	SER	Mainchain	1
3	P	14	ILE	Mainchain	1
3	P	38	LYS	Mainchain	1

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	257	148	140	0±0
2	B	270	147	141	0±0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
3	P	332	344	344	3±2
All	All	17180	12780	12492	63

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 2.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:P:16:GLU:HB2	3:P:39:LEU:HD11	0.62	1.71	17	4
3:P:48:ILE:HD13	3:P:51:LYS:HE2	0.58	1.74	10	1
3:P:17:LEU:HD13	3:P:49:TRP:CG	0.56	2.35	14	1
3:P:13:GLN:HE22	3:P:41:LEU:HD21	0.55	1.58	15	2
3:P:17:LEU:CD2	3:P:39:LEU:HD11	0.53	2.33	9	5
3:P:39:LEU:HD13	3:P:41:LEU:HD12	0.52	1.82	16	1
3:P:27:LEU:HD11	3:P:46:VAL:HG12	0.52	1.81	13	3
3:P:27:LEU:HD12	3:P:47:LYS:HA	0.52	1.82	7	2
3:P:20:HIS:CD2	3:P:35:LEU:HD11	0.51	2.40	4	4
3:P:17:LEU:CD2	3:P:39:LEU:HD21	0.51	2.35	3	2
3:P:16:GLU:HB3	3:P:39:LEU:HD12	0.51	1.82	5	1
3:P:27:LEU:CD1	3:P:47:LYS:HA	0.49	2.37	18	1
3:P:29:ALA:N	3:P:30:PRO:HD2	0.48	2.23	16	1
3:P:27:LEU:HD13	3:P:32:LEU:CD1	0.47	2.40	4	1
2:B:85:DG:N7	3:P:51:LYS:HE3	0.47	2.25	3	1
3:P:35:LEU:HD12	3:P:39:LEU:CD2	0.47	2.39	19	1
2:B:93:DG:C5	2:B:94:DC:C4	0.47	3.03	17	1
3:P:17:LEU:HB3	3:P:49:TRP:CZ3	0.47	2.44	17	1
3:P:17:LEU:HD21	3:P:39:LEU:HD11	0.46	1.86	13	3
3:P:16:GLU:HB2	3:P:39:LEU:CD2	0.46	2.41	10	1
3:P:32:LEU:C	3:P:32:LEU:HD23	0.46	2.32	6	1
3:P:16:GLU:HB3	3:P:39:LEU:CD1	0.45	2.42	5	1
3:P:17:LEU:HG	3:P:39:LEU:HD21	0.45	1.89	6	2
2:B:82:DC:H2"	2:B:83:DG:C8	0.44	2.48	10	1
3:P:16:GLU:HB3	3:P:39:LEU:HD21	0.43	1.89	7	1
2:B:93:DG:C2	2:B:94:DC:C2	0.43	3.07	14	1
3:P:27:LEU:HD11	3:P:50:PHE:CE2	0.43	2.49	17	1
3:P:20:HIS:HB2	3:P:35:LEU:HD11	0.43	1.91	17	1
3:P:32:LEU:HD21	3:P:43:THR:CA	0.42	2.44	7	1
3:P:21:PHE:CD2	3:P:25:ARG:HA	0.42	2.49	4	1
3:P:21:PHE:CD1	3:P:21:PHE:C	0.42	2.93	15	2
3:P:28:THR:H	3:P:31:ARG:HB2	0.42	1.75	8	1
1:A:75:DA:C2	1:A:76:DT:C2	0.42	3.08	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:P:27:LEU:HD21	3:P:50:PHE:CD2	0.42	2.50	17	1
3:P:17:LEU:HB3	3:P:49:TRP:CE3	0.41	2.50	17	1
3:P:49:TRP:CE3	3:P:50:PHE:CD2	0.41	3.07	15	1
1:A:76:DT:C4	1:A:77:DC:N4	0.41	2.89	11	1
3:P:32:LEU:HD21	3:P:43:THR:O	0.41	2.16	15	1
3:P:49:TRP:CE3	3:P:50:PHE:CE2	0.41	3.08	15	1
3:P:35:LEU:HG	3:P:39:LEU:HD11	0.41	1.91	3	1
3:P:17:LEU:HD21	3:P:46:VAL:HG13	0.40	1.93	5	1
3:P:17:LEU:HD21	3:P:39:LEU:HD21	0.40	1.93	5	1
3:P:32:LEU:CD2	3:P:43:THR:HB	0.40	2.47	1	1
3:P:13:GLN:HA	3:P:39:LEU:CD1	0.40	2.46	15	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	42/68 (62%)	40±1 (95±3%)	2±1 (5±3%)	0±0 (0±1%)	38	78
All	All	840/1360 (62%)	799 (95%)	38 (5%)	3 (0%)	38	78

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	P	40	ALA	1
3	P	27	LEU	1
3	P	24	GLY	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	P	34/59 (58%)	28±1 (83±3%)	6±1 (17±3%)	5 40
All	All	680/1180 (58%)	565 (83%)	115 (17%)	5 40

All 19 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	P	35	LEU	20
3	P	31	ARG	15
3	P	21	PHE	10
3	P	32	LEU	9
3	P	41	LEU	8
3	P	16	GLU	7
3	P	47	LYS	7
3	P	26	TYR	6
3	P	27	LEU	6
3	P	25	ARG	4
3	P	39	LEU	4
3	P	45	GLN	4
3	P	19	GLN	4
3	P	43	THR	3
3	P	51	LYS	3
3	P	34	ASP	2
3	P	13	GLN	1
3	P	38	LYS	1
3	P	12	SER	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided