Full wwPDB X-ray Structure Validation Report (i)

Jul 16, 2023 – 06:04 PM EDT

PDB ID	:	3T72
Title	:	PhoB(E)-Sigma70(4)-(RNAP-Betha-flap-tip-helix)-DNA Transcription Activation Sub-Complex
Authors	:	Blanco, A.G.; Canals, A.; Bernues, J.; Sola, M.; Coll, M.
Deposited on	:	2011-07-29
Resolution	:	4.33 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 (i) 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 (1)) were used in the production of this report:

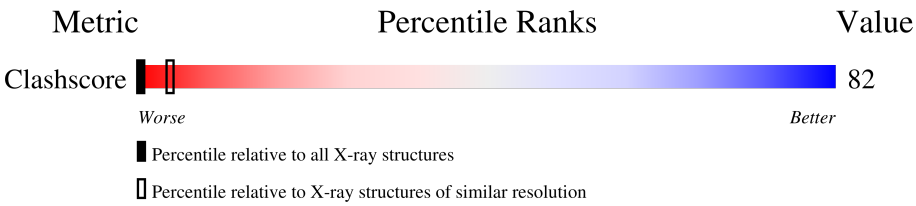
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.33 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))
Clashscore	141614	1081 (4.84-3.80)

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 <=5%

Mol	Chain	Length	Quality of chain
1	1	102	100%
1	4	102	100%
1	5	102	100%
1	8	102	100%
1	9	102	100%
1	A	102	100%
1	B	102	100%
1	E	102	100%
1	F	102	100%
1	I	102	100%
1	J	102	100%

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Mol	Chain	Length	Quality of chain
1	M	102	100%
1	N	102	100%
1	R	102	100%
1	S	102	100%
1	V	102	100%
1	W	102	100%
1	Z	102	100%
1	c	102	100%
1	d	102	100%
1	g	102	100%
1	h	102	100%
1	k	102	100%
1	l	102	100%
2	2	26	100%
2	6	26	92% 8%
2	C	26	96% .
2	G	26	96% .
2	K	26	100%
2	O	26	100%
2	T	26	96% .
2	X	26	100%
2	a	26	81% 19%
2	e	26	92% 8%
2	i	26	96% .
2	m	26	88% 12%

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Mol	Chain	Length	Quality of chain
3	3	26	92% 8%
3	7	26	88% 12%
3	D	26	92% 8%
3	H	26	88% 12%
3	L	26	96% .
3	P	26	96% .
3	U	26	92% 8%
3	Y	26	96% .
3	b	26	81% 19%
3	f	26	92% 8%
3	j	26	92% 8%
3	n	26	85% 15%
4	o	99	94% 6%
4	q	99	94% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15354 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 protein called Phosphate regulon transcriptional regulatory protein phoB.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	102	Total C 102 102	0	0	102
1	B	102	Total C 102 102	0	0	102
1	E	102	Total C 102 102	0	0	102
1	F	102	Total C 102 102	0	0	102
1	I	102	Total C 102 102	0	0	102
1	J	102	Total C 102 102	0	0	102
1	M	102	Total C 102 102	0	0	102
1	N	102	Total C 102 102	0	0	102
1	R	102	Total C 102 102	0	0	102
1	S	102	Total C 102 102	0	0	102
1	V	102	Total C 102 102	0	0	102
1	W	102	Total C 102 102	0	0	102
1	Z	102	Total C 102 102	0	0	102
1	1	102	Total C 102 102	0	0	102
1	4	102	Total C 102 102	0	0	102
1	5	102	Total C 102 102	0	0	102

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
1	8	102	102	102	0	0	102
			Total	C			
1	9	102	102	102	0	0	102
			Total	C			
1	c	102	102	102	0	0	102
			Total	C			
1	d	102	102	102	0	0	102
			Total	C			
1	g	102	102	102	0	0	102
			Total	C			
1	h	102	102	102	0	0	102
			Total	C			
1	k	102	102	102	0	0	102
			Total	C			
1	l	102	102	102	0	0	102

- Molecule 2 is a DNA chain called PHO BOX DNA (STRAND 1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	26	534	256	101	152	25	0	0	0
			Total	C	N	O	P			
2	G	26	534	256	101	152	25	0	0	0
			Total	C	N	O	P			
2	K	26	534	256	101	152	25	0	0	0
			Total	C	N	O	P			
2	O	26	534	256	101	152	25	0	0	0
			Total	C	N	O	P			
2	T	26	534	256	101	152	25	0	0	0
			Total	C	N	O	P			
2	X	26	534	256	101	152	25	0	0	0
			Total	C	N	O	P			
2	2	26	534	256	101	152	25	0	0	0
			Total	C	N	O	P			
2	6	26	534	256	101	152	25	0	0	0
			Total	C	N	O	P			
2	a	26	534	256	101	152	25	0	0	0
			Total	C	N	O	P			
2	e	26	534	256	101	152	25	0	0	0
			Total	C	N	O	P			
2	i	26	534	256	101	152	25	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	m	26	534	256	101	152	25	0	0	0

- Molecule 3 is a DNA chain called PHO BOX DNA (STRAND 2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	26	526	254	91	156	25	0	0	0
3	H	26	526	254	91	156	25	0	0	0
3	L	26	526	254	91	156	25	0	0	0
3	P	26	526	254	91	156	25	0	0	0
3	U	26	526	254	91	156	25	0	0	0
3	Y	26	526	254	91	156	25	0	0	0
3	3	26	526	254	91	156	25	0	0	0
3	7	26	526	254	91	156	25	0	0	0
3	b	26	526	254	91	156	25	0	0	0
3	f	26	526	254	91	156	25	0	0	0
3	j	26	526	254	91	156	25	0	0	0
3	n	26	526	254	91	156	25	0	0	0

- Molecule 4 is a protein called RNA polymerase sigma factor rpoD, DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
4	o	93	93	93	0	0	93
4	q	93	93	93	0	0	93

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	532	MET	-	expression tag	UNP P00579
q	890	GLY	-	linker	UNP P00579
q	891	SER	-	linker	UNP P00579
q	892	SER	-	linker	UNP P00579
q	893	GLY	-	linker	UNP P00579
q	894	SER	-	linker	UNP P00579
q	895	GLY	-	linker	UNP P00579
o	532	MET	-	expression tag	UNP P00579
o	890	GLY	-	linker	UNP P00579
o	891	SER	-	linker	UNP P00579
o	892	SER	-	linker	UNP P00579
o	893	GLY	-	linker	UNP P00579
o	894	SER	-	linker	UNP P00579
o	895	GLY	-	linker	UNP P00579

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Phosphate regulon transcriptional regulatory protein phoB

Chain A: 100%

There are no outlier residues recorded for this chain.

- Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain B: 100%

There are no outlier residues recorded for this chain.

- Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain E: 100%

There are no outlier residues recorded for this chain.

- Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain F: 100%

There are no outlier residues recorded for this chain.

- Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain I: 100%

There are no outlier residues recorded for this chain.

- Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain J: 100%

There are no outlier residues recorded for this chain.

- Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain M: 100%

There are no outlier residues recorded for this chain.

- Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain N: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain R: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain S: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain V: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain W: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain Z: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain 1: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain 4: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain 5: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain 8: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain 9: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain c: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain d: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain g: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain h: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain k: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain l: 100%

There are no outlier residues recorded for this chain.

• Molecule 2: PHO BOX DNA (STRAND 1)

Chain C: 96%

T1 G2 G3 C4 T5 G6 T7 C8 A9 T10 A11 A12 A13 G14 T15 T16 G17 T18 C19 A20 C21 A22 A23 A24 A25 G26

• Molecule 2: PHO BOX DNA (STRAND 1)

Chain G: 96%

T1 G2 G3 C4 T5 G6 T7 C8 A9 T10 A11 A12 A13 G14 T15 T16 G17 T18 C19 A20 C21 A22 A23 A24 A25 G26

• Molecule 2: PHO BOX DNA (STRAND 1)

Chain K: 100%

T1 G2 G3 C4 T5 G6 T7 C8 A9 T10 A11 A12 A13 G14 T15 T16 G17 T18 C19 A20 C21 A22 A23 A24 A25 G26

• Molecule 2: PHO BOX DNA (STRAND 1)

Chain O: 100%

T1 G2 G3 C4 T5 G6 T7 C8 A9 T10 A11 A12 A13 G14 T15 T16 G17 T18 C19 A20 C21 A22 A23 A24 A25 G26

• Molecule 2: PHO BOX DNA (STRAND 1)

Chain T: 96%

T1 G2 G3 C4 T5 G6 T7 C8 A9 T10 A11 A12 A13 G14 T15 T16 G17 T18 C19 A20 C21 A22 A23 A24 A25 G26

• Molecule 2: PHO BOX DNA (STRAND 1)

Chain X: 100%

T1 G2 G3 C4 T5 G6 T7 C8 A9 T10 A11 A12 A13 G14 T15 T16 G17 T18 C19 A20 C21 A22 A23 A24 A25 G26

• Molecule 2: PHO BOX DNA (STRAND 1)

Chain 2: 100%

T1 G2 G3 C4 T5 G6 T7 C8 A9 T10 A11 A12 A13 G14 T15 T16 G17 T18 C19 A20 C21 A22 A23 A24 A25 G26

• Molecule 2: PHO BOX DNA (STRAND 1)

Chain 6: 92% 8%

T1 G2 G3 C4 T5 G6 T7 C8 A9 T10 A11 A12 A13 G14 T15 T16 G17 T18 C19 A20 C21 A22 A23 A24 A25 G26

• Molecule 2: PHO BOX DNA (STRAND 1)

Chain a: 81% 19%

T1 G2 T7 A12 G17 T18 G26

• Molecule 2: PHO BOX DNA (STRAND 1)

Chain e: 92% 8%

T1 G2 G17 G26

• Molecule 2: PHO BOX DNA (STRAND 1)

Chain i: 96% •

T1 G2 G26

• Molecule 2: PHO BOX DNA (STRAND 1)

Chain m: 88% 12%

T1 G2 G17 T18 G26

• Molecule 3: PHO BOX DNA (STRAND 2)

Chain D: 92% 8%

C1 A2 C3 T4 T5 T6 T7 G8 T9 G10 A11 C12 A13 A14 C15 T16 T17 T18 A19 T20 G21 A22 C23 A24 G25 C26

• Molecule 3: PHO BOX DNA (STRAND 2)

Chain H: 88% 12%

C1 A2 C3 T4 T5 T6 T7 G8 T9 G10 A11 C12 A13 A14 C15 T16 T17 T18 A19 T20 G21 A22 C23 A24 G25 C26

• Molecule 3: PHO BOX DNA (STRAND 2)

Chain L: 96% •

C1 A2 C3 T4 T5 T6 T7 G8 T9 G10 A11 C12 A13 A14 C15 T16 T17 T18 A19 T20 G21 A22 C23 A24 G25 C26

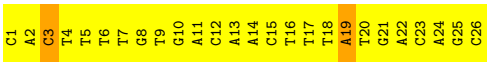
• Molecule 3: PHO BOX DNA (STRAND 2)

Chain P: 96% •

C1 A2 C3 T4 T5 T6 T7 G8 T9 G10 A11 C12 A13 A14 C15 T16 T17 T18 A19 T20 G21 A22 C23 A24 G25 C26

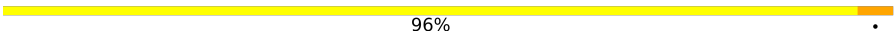
• Molecule 3: PHO BOX DNA (STRAND 2)

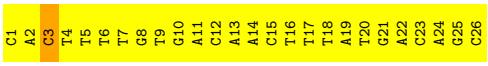
Chain U: 92% 8%



• Molecule 3: PHO BOX DNA (STRAND 2)

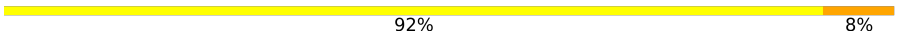
Chain Y:





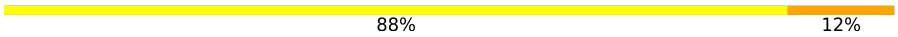
• Molecule 3: PHO BOX DNA (STRAND 2)

Chain 3:



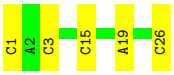
• Molecule 3: PHO BOX DNA (STRAND 2)

Chain 7:



• Molecule 3: PHO BOX DNA (STRAND 2)

Chain b:



• Molecule 3: PHO BOX DNA (STRAND 2)

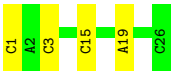
Chain f:

• Molecule 3: PHO BOX DNA (STRAND 2)

Chain j:

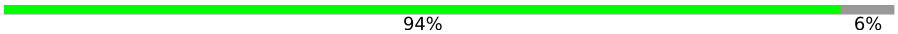
• Molecule 3: PHO BOX DNA (STRAND 2)

Chain n:



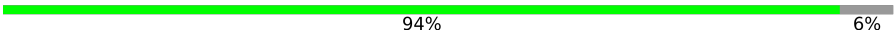
• Molecule 4: RNA polymerase sigma factor rpoD, DNA-directed RNA polymerase subunit beta

Chain o:



• Molecule 4: RNA polymerase sigma factor rpoD, DNA-directed RNA polymerase subunit beta

Chain q:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	277.30Å 161.40Å 260.10Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	50.00 – 4.33 20.00 – 4.33	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.33) 96.4 (20.00-4.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 4.36Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	(Not available) , (Not available) 0.439 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	189.2	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.012 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.013 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.046 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.028 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.019 for -h,-k,l	Xtriage
F_o,F_c correlation	0.75	EDS
Total number of atoms	15354	wwPDB-VP
Average B, all atoms (Å^2)	77.0	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 36.19 % 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 5.1959e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
2	2	1.87	0/600	0.94	0/925
2	6	1.85	2/600 (0.3%)	0.96	0/925
2	C	1.85	1/600 (0.2%)	0.96	0/925
2	G	1.97	1/600 (0.2%)	0.90	0/925
2	K	1.83	0/600	0.92	0/925
2	O	1.88	0/600	0.94	0/925
2	T	1.97	1/600 (0.2%)	0.89	0/925
2	X	1.82	0/600	0.93	0/925
2	a	1.99	4/600 (0.7%)	0.91	0/925
2	e	1.78	1/600 (0.2%)	0.89	0/925
2	i	1.79	0/600	0.89	0/925
2	m	1.96	2/600 (0.3%)	0.90	0/925
3	3	1.84	1/588 (0.2%)	0.95	1/905 (0.1%)
3	7	1.85	2/588 (0.3%)	0.96	1/905 (0.1%)
3	D	1.85	1/588 (0.2%)	0.96	1/905 (0.1%)
3	H	1.97	2/588 (0.3%)	0.92	1/905 (0.1%)
3	L	1.79	0/588	0.93	1/905 (0.1%)
3	P	1.83	0/588	0.94	1/905 (0.1%)
3	U	1.96	1/588 (0.2%)	0.92	1/905 (0.1%)
3	Y	1.79	0/588	0.93	1/905 (0.1%)
3	b	1.99	3/588 (0.5%)	0.92	1/905 (0.1%)
3	f	1.74	0/588	0.90	1/905 (0.1%)
3	j	1.75	0/588	0.89	1/905 (0.1%)
3	n	1.99	3/588 (0.5%)	0.92	1/905 (0.1%)
All	All	1.87	25/14256 (0.2%)	0.92	12/21960 (0.1%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6	17	DG	N7-C5	-5.82	1.35	1.39
2	m	17	DG	N7-C5	-5.67	1.35	1.39
2	C	17	DG	N7-C5	-5.46	1.35	1.39
2	a	17	DG	N7-C5	-5.41	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	n	15	DC	N3-C4	-5.35	1.30	1.33
3	D	19	DA	N3-C4	-5.29	1.31	1.34
2	6	18	DT	N1-C6	-5.24	1.34	1.38
2	T	17	DG	C5-C6	-5.23	1.37	1.42
3	U	19	DA	N3-C4	-5.23	1.31	1.34
2	a	12	DA	N7-C5	-5.20	1.36	1.39
3	b	19	DA	N3-C4	-5.20	1.31	1.34
2	e	17	DG	N7-C5	-5.19	1.36	1.39
3	b	15	DC	N3-C4	-5.16	1.30	1.33
3	7	15	DC	N1-C6	-5.14	1.34	1.37
3	n	19	DA	N3-C4	-5.13	1.31	1.34
2	G	17	DG	C5-C6	-5.12	1.37	1.42
2	m	18	DT	N1-C6	-5.09	1.34	1.38
3	n	15	DC	N1-C6	-5.07	1.34	1.37
3	H	19	DA	N3-C4	-5.06	1.31	1.34
3	7	19	DA	N3-C4	-5.05	1.31	1.34
3	3	16	DT	C5-C7	-5.05	1.47	1.50
2	a	7	DT	C5-C7	-5.05	1.47	1.50
3	b	15	DC	N1-C6	-5.03	1.34	1.37
2	a	18	DT	N1-C6	-5.03	1.34	1.38
3	H	8	DG	N3-C4	-5.02	1.31	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	3	DC	N1-C1'-C2'	5.88	123.76	112.60
3	H	3	DC	N1-C1'-C2'	5.83	123.68	112.60
3	Y	3	DC	N1-C1'-C2'	5.72	123.47	112.60
3	L	3	DC	N1-C1'-C2'	5.71	123.45	112.60
3	j	3	DC	N1-C1'-C2'	5.71	123.45	112.60
3	D	3	DC	N1-C1'-C2'	5.67	123.38	112.60
3	f	3	DC	N1-C1'-C2'	5.66	123.36	112.60
3	7	3	DC	N1-C1'-C2'	5.64	123.31	112.60
3	b	3	DC	N1-C1'-C2'	5.60	123.24	112.60
3	n	3	DC	N1-C1'-C2'	5.58	123.19	112.60
3	P	3	DC	N1-C1'-C2'	5.46	122.97	112.60
3	3	3	DC	N1-C1'-C2'	5.40	122.86	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	102	0	0	0	0
1	4	102	0	0	0	0
1	5	102	0	0	0	0
1	8	102	0	0	0	0
1	9	102	0	0	0	0
1	A	102	0	0	0	0
1	B	102	0	0	0	0
1	E	102	0	0	0	0
1	F	102	0	0	0	0
1	I	102	0	0	0	0
1	J	102	0	0	0	0
1	M	102	0	0	0	0
1	N	102	0	0	0	0
1	R	102	0	0	0	0
1	S	102	0	0	0	0
1	V	102	0	0	0	0
1	W	102	0	0	0	0
1	Z	102	0	0	0	0
1	c	102	0	0	0	0
1	d	102	0	0	0	0
1	g	102	0	0	0	0
1	h	102	0	0	0	0
1	k	102	0	0	0	0
1	l	102	0	0	0	0
2	2	534	0	295	77	0
2	6	534	0	295	80	0
2	C	534	0	295	80	0
2	G	534	0	295	83	11
2	K	534	0	295	81	8
2	O	534	0	295	85	0
2	T	534	0	295	83	8
2	X	534	0	295	83	8
2	a	534	0	295	0	2
2	e	534	0	295	0	5
2	i	534	0	295	0	1
2	m	534	0	295	0	2
3	3	526	0	297	70	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	7	526	0	297	69	0
3	D	526	0	297	69	0
3	H	526	0	297	71	8
3	L	526	0	297	69	8
3	P	526	0	297	75	3
3	U	526	0	297	70	8
3	Y	526	0	297	70	11
3	b	526	0	297	0	7
3	f	526	0	297	0	4
3	j	526	0	297	0	2
3	n	526	0	297	0	1
4	o	93	0	0	0	0
4	q	93	0	0	0	0
All	All	15354	0	7104	1201	50

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 82.

All (1201) 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)
2:T:25:DA:H2"	2:T:26:DG:H5"	1.19	1.18
2:K:25:DA:H2"	2:K:26:DG:H5"	1.21	1.17
2:G:25:DA:H2"	2:G:26:DG:H5"	1.19	1.17
3:U:14:DA:H2"	3:U:15:DC:H5"	1.27	1.16
2:6:25:DA:H2"	2:6:26:DG:H5"	1.22	1.15
3:Y:14:DA:H2"	3:Y:15:DC:H5"	1.27	1.14
2:C:25:DA:H2"	2:C:26:DG:H5"	1.21	1.14
2:X:25:DA:H2"	2:X:26:DG:H5"	1.21	1.14
3:P:14:DA:H2"	3:P:15:DC:H5"	1.29	1.11
3:3:14:DA:H2"	3:3:15:DC:H5"	1.29	1.11
3:L:14:DA:H2"	3:L:15:DC:H5"	1.27	1.11
3:H:14:DA:H2"	3:H:15:DC:H5"	1.27	1.10
2:O:25:DA:H2"	2:O:26:DG:H5"	1.22	1.09
2:2:25:DA:H2"	2:2:26:DG:H5"	1.22	1.08
3:D:14:DA:H2"	3:D:15:DC:H5"	1.27	1.06
3:D:14:DA:C2'	3:D:15:DC:H5"	1.85	1.06
3:7:14:DA:H2"	3:7:15:DC:H5"	1.27	1.06
3:7:14:DA:C2'	3:7:15:DC:H5"	1.85	1.06
3:Y:14:DA:C2'	3:Y:15:DC:H5"	1.85	1.06
3:L:14:DA:C2'	3:L:15:DC:H5"	1.85	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:14:DA:C2'	3:U:15:DC:H5"	1.86	1.04
3:3:14:DA:C2'	3:3:15:DC:H5"	1.88	1.04
3:H:14:DA:C2'	3:H:15:DC:H5"	1.87	1.03
3:P:14:DA:C2'	3:P:15:DC:H5"	1.88	1.02
3:U:9:DT:H2"	3:U:10:DG:H5"	1.44	1.00
2:G:24:DA:H4'	2:G:25:DA:OP1	1.62	0.99
2:K:24:DA:H4'	2:K:25:DA:OP1	1.63	0.98
3:Y:9:DT:H2"	3:Y:10:DG:H5"	1.45	0.98
3:L:9:DT:H2"	3:L:10:DG:H5"	1.45	0.97
2:6:24:DA:H4'	2:6:25:DA:OP1	1.61	0.97
2:2:24:DA:H4'	2:2:25:DA:OP1	1.62	0.97
3:D:9:DT:H2"	3:D:10:DG:H5"	1.47	0.97
3:7:9:DT:H2"	3:7:10:DG:H5"	1.47	0.97
2:G:23:DA:H4'	2:G:24:DA:OP1	1.65	0.97
3:H:9:DT:H2"	3:H:10:DG:H5"	1.44	0.96
2:O:23:DA:H4'	2:O:24:DA:OP1	1.64	0.96
2:T:24:DA:H4'	2:T:25:DA:OP1	1.62	0.96
2:C:24:DA:H4'	2:C:25:DA:OP1	1.61	0.96
3:P:9:DT:H2"	3:P:10:DG:H5"	1.46	0.96
3:3:9:DT:H2"	3:3:10:DG:H5"	1.47	0.95
2:O:24:DA:H4'	2:O:25:DA:OP1	1.63	0.95
2:6:23:DA:H4'	2:6:24:DA:OP1	1.64	0.94
2:X:24:DA:H4'	2:X:25:DA:OP1	1.63	0.94
2:K:23:DA:H4'	2:K:24:DA:OP1	1.66	0.94
2:O:11:DA:H2"	2:O:12:DA:H5"	1.50	0.94
2:C:23:DA:H4'	2:C:24:DA:OP1	1.64	0.93
2:O:7:DT:H2"	2:O:8:DC:H5'	1.51	0.93
2:2:23:DA:H4'	2:2:24:DA:OP1	1.64	0.93
2:T:11:DA:H2"	2:T:12:DA:H5"	1.51	0.92
3:L:14:DA:H2"	3:L:15:DC:C5'	1.99	0.92
2:X:11:DA:H2"	2:X:12:DA:H5"	1.51	0.92
2:K:11:DA:H2"	2:K:12:DA:H5"	1.51	0.92
2:X:23:DA:H4'	2:X:24:DA:OP1	1.66	0.92
2:O:6:DG:H2"	2:O:7:DT:H5"	1.51	0.92
2:T:23:DA:H4'	2:T:24:DA:OP1	1.65	0.92
2:2:7:DT:H2"	2:2:8:DC:H5'	1.51	0.92
3:H:14:DA:H2"	3:H:15:DC:C5'	2.00	0.92
2:6:7:DT:H2"	2:6:8:DC:H5'	1.51	0.92
2:G:25:DA:H1'	2:G:26:DG:O4'	1.70	0.91
2:2:6:DG:H2"	2:2:7:DT:H5"	1.50	0.91
2:G:11:DA:H2"	2:G:12:DA:H5"	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:7:DT:H2"	2:G:8:DC:H5'	1.52	0.91
3:U:14:DA:H2"	3:U:15:DC:C5'	2.00	0.91
3:D:14:DA:H2"	3:D:15:DC:C5'	2.00	0.91
2:C:7:DT:H2"	2:C:8:DC:H5'	1.51	0.91
3:U:8:DG:H2"	3:U:9:DT:C5'	2.00	0.91
3:Y:14:DA:H2"	3:Y:15:DC:C5'	2.00	0.91
3:7:14:DA:H2"	3:7:15:DC:C5'	2.00	0.91
3:L:5:DT:H1'	3:L:6:DT:H5"	1.52	0.90
2:T:25:DA:H1'	2:T:26:DG:O4'	1.71	0.90
2:C:11:DA:H2"	2:C:12:DA:H5"	1.52	0.90
2:X:6:DG:H2"	2:X:7:DT:H5"	1.52	0.90
3:H:8:DG:H2"	3:H:9:DT:C5'	2.01	0.90
2:K:25:DA:H1'	2:K:26:DG:O4'	1.72	0.90
2:O:25:DA:H1'	2:O:26:DG:O4'	1.72	0.90
2:T:7:DT:H2"	2:T:8:DC:H5'	1.52	0.90
2:2:11:DA:H2"	2:2:12:DA:H5"	1.50	0.90
2:G:6:DG:H2"	2:G:7:DT:H5"	1.53	0.90
2:X:7:DT:H2"	2:X:8:DC:H5'	1.53	0.90
2:X:25:DA:H1'	2:X:26:DG:O4'	1.72	0.90
3:3:14:DA:H2"	3:3:15:DC:C5'	2.02	0.90
2:6:11:DA:H2"	2:6:12:DA:H5"	1.53	0.90
2:T:6:DG:H2"	2:T:7:DT:H5"	1.53	0.89
2:C:6:DG:H2"	2:C:7:DT:H5"	1.53	0.89
3:Y:8:DG:H2"	3:Y:9:DT:C5'	2.02	0.89
2:2:25:DA:H1'	2:2:26:DG:O4'	1.72	0.89
2:K:6:DG:H2"	2:K:7:DT:H5"	1.52	0.89
3:Y:5:DT:H1'	3:Y:6:DT:H5"	1.52	0.89
2:6:6:DG:H2"	2:6:7:DT:H5"	1.53	0.89
2:2:13:DA:H1'	2:2:14:DG:H5'	1.55	0.89
2:G:13:DA:H1'	2:G:14:DG:H5'	1.55	0.89
3:H:5:DT:H1'	3:H:6:DT:H5"	1.54	0.89
3:U:8:DG:H2"	3:U:9:DT:H5"	1.52	0.89
3:H:8:DG:H2"	3:H:9:DT:H5"	1.53	0.89
3:P:14:DA:H2"	3:P:15:DC:C5'	2.02	0.89
2:G:25:DA:C2'	2:G:26:DG:H5"	2.03	0.89
3:3:5:DT:H1'	3:3:6:DT:H5"	1.54	0.89
2:6:13:DA:H1'	2:6:14:DG:H5'	1.54	0.89
2:C:13:DA:H1'	2:C:14:DG:H5'	1.54	0.89
3:D:5:DT:H1'	3:D:6:DT:H5"	1.52	0.89
3:7:5:DT:H1'	3:7:6:DT:H5"	1.52	0.88
2:C:25:DA:H1'	2:C:26:DG:O4'	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:11:DA:H1'	3:D:12:DC:H5"	1.56	0.88
3:3:8:DG:H2"	3:3:9:DT:C5'	2.04	0.88
3:7:11:DA:H1'	3:7:12:DC:H5"	1.56	0.88
2:K:7:DT:H2"	2:K:8:DC:H5'	1.53	0.88
3:P:8:DG:H2"	3:P:9:DT:C5'	2.04	0.88
2:6:25:DA:H1'	2:6:26:DG:O4'	1.72	0.88
3:L:8:DG:H2"	3:L:9:DT:C5'	2.02	0.88
3:L:8:DG:H2"	3:L:9:DT:H5"	1.54	0.88
3:U:8:DG:C2'	3:U:9:DT:H5"	2.04	0.88
2:O:13:DA:H1'	2:O:14:DG:H5'	1.54	0.88
3:D:8:DG:H2"	3:D:9:DT:H5"	1.55	0.87
3:7:8:DG:H2"	3:7:9:DT:H5"	1.55	0.87
3:P:8:DG:H2"	3:P:9:DT:H5"	1.56	0.87
3:7:8:DG:H2"	3:7:9:DT:C5'	2.03	0.87
3:D:8:DG:H2"	3:D:9:DT:C5'	2.03	0.87
3:3:8:DG:H2"	3:3:9:DT:H5"	1.56	0.87
3:H:8:DG:C2'	3:H:9:DT:H5"	2.05	0.87
3:P:11:DA:H1'	3:P:12:DC:H5"	1.56	0.87
2:T:13:DA:H1'	2:T:14:DG:H5'	1.55	0.87
3:Y:8:DG:H2"	3:Y:9:DT:H5"	1.55	0.86
3:P:5:DT:H1'	3:P:6:DT:H5"	1.55	0.86
2:X:25:DA:C2'	2:X:26:DG:H5"	2.05	0.86
3:H:11:DA:H1'	3:H:12:DC:H5"	1.56	0.86
3:U:5:DT:H1'	3:U:6:DT:H5"	1.54	0.86
2:T:25:DA:C2'	2:T:26:DG:H5"	2.03	0.86
2:K:25:DA:C2'	2:K:26:DG:H5"	2.05	0.85
3:U:11:DA:H1'	3:U:12:DC:H5"	1.56	0.85
2:K:13:DA:H1'	2:K:14:DG:H5'	1.57	0.85
3:L:8:DG:C2'	3:L:9:DT:H5"	2.07	0.85
2:C:25:DA:C2'	2:C:26:DG:H5"	2.05	0.85
2:2:25:DA:C2'	2:2:26:DG:H5"	2.06	0.84
3:3:11:DA:H1'	3:3:12:DC:H5"	1.56	0.84
3:Y:8:DG:C2'	3:Y:9:DT:H5"	2.07	0.84
2:6:25:DA:C2'	2:6:26:DG:H5"	2.05	0.84
3:L:11:DA:H1'	3:L:12:DC:H5"	1.57	0.84
2:X:13:DA:H1'	2:X:14:DG:H5'	1.57	0.84
3:P:8:DG:C2'	3:P:9:DT:H5"	2.08	0.84
2:O:25:DA:C2'	2:O:26:DG:H5"	2.06	0.83
3:D:8:DG:C2'	3:D:9:DT:H5"	2.07	0.83
3:7:8:DG:C2'	3:7:9:DT:H5"	2.07	0.83
3:Y:11:DA:H1'	3:Y:12:DC:H5"	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:8:DG:C2'	3:3:9:DT:H5"	2.08	0.83
2:2:6:DG:H2"	2:2:7:DT:C5'	2.09	0.82
2:C:5:DT:H5'	2:C:5:DT:H6	1.45	0.82
2:6:5:DT:H5'	2:6:5:DT:H6	1.44	0.82
2:O:6:DG:H2"	2:O:7:DT:C5'	2.09	0.82
2:6:12:DA:H2"	2:6:13:DA:H5'	1.62	0.82
2:C:12:DA:H2"	2:C:13:DA:H5'	1.62	0.81
3:P:4:DT:H2"	3:P:5:DT:H72	1.63	0.81
2:O:8:DC:N3	3:P:21:DG:N1	2.26	0.81
2:K:6:DG:H2"	2:K:7:DT:C5'	2.11	0.81
2:O:5:DT:H6	2:O:5:DT:H5'	1.46	0.81
3:U:4:DT:H2"	3:U:5:DT:H72	1.63	0.81
2:2:5:DT:H6	2:2:5:DT:H5'	1.46	0.81
3:3:4:DT:H2"	3:3:5:DT:H72	1.63	0.81
2:G:12:DA:H2"	2:G:13:DA:H5'	1.63	0.81
2:O:12:DA:H2"	2:O:13:DA:H5'	1.62	0.81
2:G:3:DG:H2"	2:G:4:DC:H5'	1.61	0.80
2:O:8:DC:N4	3:P:21:DG:O6	2.12	0.80
3:3:13:DA:H2"	3:3:14:DA:OP2	1.81	0.80
2:T:6:DG:H2"	2:T:7:DT:C5'	2.11	0.80
2:C:3:DG:H2"	2:C:4:DC:H5'	1.64	0.80
2:2:7:DT:H2"	2:2:8:DC:C5'	2.11	0.80
2:2:12:DA:H2"	2:2:13:DA:H5'	1.62	0.80
2:T:3:DG:H2"	2:T:4:DC:H5'	1.62	0.80
2:O:7:DT:H2"	2:O:8:DC:C5'	2.11	0.80
2:6:7:DT:H2"	2:6:8:DC:C5'	2.12	0.80
2:C:7:DT:H2"	2:C:8:DC:C5'	2.12	0.80
2:T:5:DT:H6	2:T:5:DT:H5'	1.47	0.80
2:6:3:DG:H2"	2:6:4:DC:H5'	1.64	0.80
3:7:13:DA:H2"	3:7:14:DA:OP2	1.82	0.80
3:H:4:DT:H2"	3:H:5:DT:H72	1.63	0.80
2:C:6:DG:H2"	2:C:7:DT:C5'	2.12	0.80
3:U:13:DA:H2"	3:U:14:DA:OP2	1.81	0.80
3:Y:4:DT:H2"	3:Y:5:DT:H72	1.64	0.80
3:7:4:DT:H2"	3:7:5:DT:H72	1.64	0.80
3:H:13:DA:H2"	3:H:14:DA:OP2	1.82	0.79
2:X:6:DG:H2"	2:X:7:DT:C5'	2.11	0.79
3:D:13:DA:H2"	3:D:14:DA:OP2	1.82	0.79
2:G:6:DG:H2"	2:G:7:DT:C5'	2.11	0.79
2:G:5:DT:H6	2:G:5:DT:H5'	1.46	0.79
2:6:6:DG:H2"	2:6:7:DT:C5'	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4:DT:H2"	3:D:5:DT:H72	1.64	0.79
2:K:5:DT:H5'	2:K:5:DT:H6	1.47	0.79
3:L:4:DT:H2"	3:L:5:DT:H72	1.64	0.79
3:P:13:DA:H2"	3:P:14:DA:OP2	1.81	0.79
2:K:3:DG:H2"	2:K:4:DC:H5'	1.64	0.79
3:P:11:DA:H2"	3:P:12:DC:C5'	2.13	0.79
3:3:11:DA:H2"	3:3:12:DC:C5'	2.12	0.79
3:Y:13:DA:H2"	3:Y:14:DA:OP2	1.82	0.79
2:O:7:DT:O4	3:P:22:DA:N6	2.14	0.79
2:T:7:DT:H2"	2:T:8:DC:C5'	2.13	0.79
2:X:3:DG:H2"	2:X:4:DC:H5'	1.64	0.78
2:T:12:DA:H2"	2:T:13:DA:H5'	1.63	0.78
2:K:12:DA:H2"	2:K:13:DA:H5'	1.65	0.78
2:O:12:DA:H2"	2:O:13:DA:C5'	2.13	0.78
3:U:16:DT:H2'	3:U:17:DT:H72	1.66	0.78
2:6:12:DA:H2"	2:6:13:DA:C5'	2.13	0.78
2:X:5:DT:H6	2:X:5:DT:H5'	1.48	0.78
2:C:12:DA:H2"	2:C:13:DA:C5'	2.14	0.77
3:D:11:DA:H2"	3:D:12:DC:C5'	2.14	0.77
2:2:12:DA:H2"	2:2:13:DA:C5'	2.13	0.77
3:7:11:DA:H2"	3:7:12:DC:C5'	2.15	0.77
2:G:7:DT:H2"	2:G:8:DC:C5'	2.13	0.77
3:L:13:DA:H2"	3:L:14:DA:OP2	1.82	0.77
2:X:7:DT:H2"	2:X:8:DC:C5'	2.14	0.77
2:O:2:DG:H4'	2:O:2:DG:OP1	1.85	0.77
2:X:12:DA:H2"	2:X:13:DA:H5'	1.65	0.77
3:H:16:DT:H2'	3:H:17:DT:H72	1.66	0.77
3:L:11:DA:H2"	3:L:12:DC:C5'	2.15	0.77
3:H:11:DA:H2"	3:H:12:DC:C5'	2.15	0.77
2:O:3:DG:H2"	2:O:4:DC:H5'	1.65	0.77
2:2:3:DG:H2"	2:2:4:DC:H5'	1.65	0.76
2:G:12:DA:H2"	2:G:13:DA:C5'	2.15	0.76
2:X:2:DG:H4'	2:X:2:DG:OP1	1.86	0.76
3:L:2:DA:H1'	3:L:3:DC:H5'	1.68	0.76
2:T:12:DA:H2"	2:T:13:DA:C5'	2.15	0.76
3:U:11:DA:H2"	3:U:12:DC:C5'	2.15	0.76
2:G:2:DG:H4'	2:G:2:DG:OP1	1.85	0.76
2:K:6:DG:H2'	2:K:7:DT:H71	1.67	0.76
2:T:2:DG:OP1	2:T:2:DG:H4'	1.85	0.76
3:3:2:DA:H1'	3:3:3:DC:H5'	1.67	0.76
3:H:9:DT:C2'	3:H:10:DG:H5"	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2:DG:OP1	2:K:2:DG:H4'	1.86	0.76
2:K:12:DA:H2"	2:K:13:DA:C5'	2.16	0.76
2:K:7:DT:H2"	2:K:8:DC:C5'	2.14	0.76
3:P:2:DA:H1'	3:P:3:DC:H5'	1.67	0.75
3:D:16:DT:H2'	3:D:17:DT:H72	1.68	0.75
3:P:16:DT:H2'	3:P:17:DT:H72	1.68	0.75
3:7:16:DT:H2'	3:7:17:DT:H72	1.68	0.75
3:Y:11:DA:H2"	3:Y:12:DC:C5'	2.15	0.75
2:2:2:DG:H4'	2:2:2:DG:OP1	1.85	0.75
2:T:1:DT:H2'	2:T:2:DG:C8	2.22	0.75
3:L:9:DT:C2'	3:L:10:DG:H5"	2.17	0.75
3:U:9:DT:C2'	3:U:10:DG:H5"	2.15	0.75
2:C:1:DT:H2'	2:C:2:DG:C8	2.22	0.75
2:6:1:DT:H2'	2:6:2:DG:C8	2.22	0.75
2:O:1:DT:H2'	2:O:2:DG:C8	2.22	0.74
3:Y:2:DA:H1'	3:Y:3:DC:H5'	1.68	0.74
2:G:1:DT:H2'	2:G:2:DG:C8	2.22	0.74
2:G:6:DG:H2'	2:G:7:DT:H71	1.70	0.74
3:L:16:DT:H2'	3:L:17:DT:H72	1.69	0.74
2:X:12:DA:H2"	2:X:13:DA:C5'	2.16	0.74
2:K:19:DC:H2"	2:K:20:DA:C8	2.23	0.74
2:O:11:DA:C2'	2:O:12:DA:H5"	2.17	0.74
2:X:6:DG:H2'	2:X:7:DT:H71	1.68	0.74
2:2:1:DT:H2'	2:2:2:DG:C8	2.22	0.74
2:X:19:DC:H2"	2:X:20:DA:C8	2.23	0.74
3:Y:16:DT:H2'	3:Y:17:DT:H72	1.69	0.74
2:X:1:DT:H2'	2:X:2:DG:C8	2.23	0.74
2:2:11:DA:C2'	2:2:12:DA:H5"	2.17	0.74
3:H:2:DA:H1'	3:H:3:DC:H5'	1.69	0.73
3:Y:9:DT:C2'	3:Y:10:DG:H5"	2.18	0.73
2:K:1:DT:H2'	2:K:2:DG:C8	2.23	0.73
2:C:2:DG:OP1	2:C:2:DG:H4'	1.85	0.73
2:6:2:DG:OP1	2:6:2:DG:H4'	1.85	0.73
3:3:16:DT:H2'	3:3:17:DT:H72	1.69	0.73
2:T:6:DG:H2'	2:T:7:DT:H71	1.70	0.73
3:U:2:DA:H1'	3:U:3:DC:H5'	1.68	0.73
2:6:6:DG:H2'	2:6:7:DT:H71	1.70	0.73
3:D:9:DT:C2'	3:D:10:DG:H5"	2.18	0.73
2:C:6:DG:H2'	2:C:7:DT:H71	1.70	0.73
2:X:11:DA:C2'	2:X:12:DA:H5"	2.18	0.73
3:7:9:DT:C2'	3:7:10:DG:H5"	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:15:DT:H1'	2:G:16:DT:H5'	1.69	0.73
3:3:9:DT:C2'	3:3:10:DG:H5"	2.18	0.73
2:K:11:DA:C2'	2:K:12:DA:H5"	2.18	0.72
2:T:15:DT:H1'	2:T:16:DT:H5'	1.69	0.72
2:G:11:DA:C2'	2:G:12:DA:H5"	2.19	0.72
3:3:8:DG:H1'	3:3:9:DT:H5"	1.72	0.72
2:C:11:DA:C2'	2:C:12:DA:H5"	2.19	0.72
3:U:8:DG:H1'	3:U:9:DT:H5"	1.72	0.72
2:6:11:DA:C2'	2:6:12:DA:H5"	2.19	0.72
2:T:11:DA:C2'	2:T:12:DA:H5"	2.19	0.72
2:2:19:DC:H2"	2:2:20:DA:C8	2.25	0.72
2:C:15:DT:H1'	2:C:16:DT:H5'	1.71	0.72
2:O:19:DC:H5'	2:O:19:DC:H6	1.55	0.72
3:Y:8:DG:H1'	3:Y:9:DT:H5"	1.72	0.72
2:O:19:DC:H2"	2:O:20:DA:C8	2.25	0.71
3:P:9:DT:C2'	3:P:10:DG:H5"	2.18	0.71
2:O:6:DG:H2'	2:O:7:DT:H71	1.72	0.71
3:P:8:DG:H1'	3:P:9:DT:H5"	1.71	0.71
2:2:19:DC:H6	2:2:19:DC:H5'	1.55	0.71
2:6:15:DT:H1'	2:6:16:DT:H5'	1.71	0.71
3:D:2:DA:H1'	3:D:3:DC:H5'	1.69	0.71
3:H:8:DG:H1'	3:H:9:DT:H5"	1.72	0.71
2:X:15:DT:H1'	2:X:16:DT:H5'	1.71	0.71
2:K:15:DT:H1'	2:K:16:DT:H5'	1.71	0.71
2:2:6:DG:C2'	2:2:7:DT:H5"	2.20	0.71
2:G:2:DG:H2"	2:G:3:DG:C8	2.26	0.71
3:L:8:DG:H1'	3:L:9:DT:H5"	1.72	0.71
3:7:2:DA:H1'	3:7:3:DC:H5'	1.70	0.71
3:7:8:DG:H1'	3:7:9:DT:H5"	1.73	0.71
2:G:19:DC:H2"	2:G:20:DA:C8	2.25	0.71
2:2:15:DT:H1'	2:2:16:DT:H5'	1.72	0.71
2:T:2:DG:H2"	2:T:3:DG:C8	2.26	0.70
2:T:19:DC:H2"	2:T:20:DA:C8	2.25	0.70
3:D:8:DG:H1'	3:D:9:DT:H5"	1.73	0.70
2:O:6:DG:C2'	2:O:7:DT:H5"	2.20	0.70
2:2:6:DG:H2'	2:2:7:DT:H71	1.71	0.70
2:X:19:DC:H6	2:X:19:DC:H5'	1.57	0.70
3:L:4:DT:H4'	3:L:5:DT:OP1	1.92	0.70
2:6:19:DC:H2"	2:6:20:DA:C8	2.25	0.69
2:T:19:DC:H6	2:T:19:DC:H5'	1.57	0.69
2:C:19:DC:H2"	2:C:20:DA:C8	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:15:DT:H1'	2:O:16:DT:H5'	1.72	0.69
3:Y:4:DT:H4'	3:Y:5:DT:OP1	1.92	0.69
2:K:2:DG:H2"	2:K:3:DG:C8	2.28	0.69
3:U:4:DT:H4'	3:U:5:DT:OP1	1.92	0.69
2:C:2:DG:H2"	2:C:3:DG:C8	2.28	0.69
2:6:6:DG:C2'	2:6:7:DT:H5"	2.23	0.69
2:G:6:DG:C2'	2:G:7:DT:H5"	2.23	0.68
2:G:19:DC:H5'	2:G:19:DC:H6	1.57	0.68
2:K:19:DC:H6	2:K:19:DC:H5'	1.57	0.68
2:O:2:DG:H2"	2:O:3:DG:C8	2.28	0.68
2:2:2:DG:H2"	2:2:3:DG:C8	2.29	0.68
2:6:2:DG:H2"	2:6:3:DG:C8	2.28	0.68
2:C:15:DT:H6	2:C:15:DT:H5'	1.58	0.68
2:X:6:DG:C2'	2:X:7:DT:H5"	2.23	0.68
2:6:15:DT:H5'	2:6:15:DT:H6	1.58	0.68
2:C:6:DG:C2'	2:C:7:DT:H5"	2.23	0.68
2:O:15:DT:H6	2:O:15:DT:H5'	1.59	0.68
3:3:4:DT:H4'	3:3:5:DT:OP1	1.94	0.68
3:H:4:DT:H4'	3:H:5:DT:OP1	1.93	0.68
2:X:2:DG:H2"	2:X:3:DG:C8	2.28	0.68
2:K:6:DG:C2'	2:K:7:DT:H5"	2.23	0.67
3:L:1:DC:H2"	3:L:2:DA:C8	2.29	0.67
3:H:19:DA:H1'	3:H:20:DT:H5"	1.77	0.67
3:P:1:DC:H2"	3:P:2:DA:C8	2.29	0.67
3:P:4:DT:H4'	3:P:5:DT:OP1	1.94	0.67
2:6:19:DC:H6	2:6:19:DC:H5'	1.58	0.67
3:U:7:DT:H2"	3:U:8:DG:H8	1.59	0.67
2:C:19:DC:H6	2:C:19:DC:H5'	1.58	0.67
2:T:6:DG:C2'	2:T:7:DT:H5"	2.23	0.67
3:H:1:DC:H2"	3:H:2:DA:C8	2.30	0.67
3:D:1:DC:H2"	3:D:2:DA:C8	2.30	0.67
3:7:1:DC:H2"	3:7:2:DA:C8	2.30	0.67
3:7:4:DT:H4'	3:7:5:DT:OP1	1.94	0.67
3:D:4:DT:H4'	3:D:5:DT:OP1	1.94	0.67
3:Y:1:DC:H2"	3:Y:2:DA:C8	2.28	0.67
3:P:2:DA:H1'	3:P:3:DC:C5'	2.25	0.67
3:Y:2:DA:H1'	3:Y:3:DC:C5'	2.25	0.67
3:P:11:DA:C1'	3:P:12:DC:H5"	2.25	0.66
2:2:15:DT:H6	2:2:15:DT:H5'	1.59	0.66
3:U:19:DA:H1'	3:U:20:DT:H5"	1.77	0.66
3:H:7:DT:H2"	3:H:8:DG:H8	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:2:DA:H1'	3:3:3:DC:C5'	2.25	0.66
3:3:1:DC:H2"	3:3:2:DA:C8	2.29	0.66
3:H:11:DA:C1'	3:H:12:DC:H5"	2.25	0.66
3:U:1:DC:H2"	3:U:2:DA:C8	2.30	0.66
3:D:11:DA:C1'	3:D:12:DC:H5"	2.26	0.66
3:L:19:DA:H1'	3:L:20:DT:H5"	1.78	0.66
3:7:11:DA:C1'	3:7:12:DC:H5"	2.26	0.66
3:U:11:DA:C1'	3:U:12:DC:H5"	2.26	0.66
3:U:22:DA:H1'	3:U:23:DC:H5"	1.78	0.66
2:6:11:DA:C2	3:7:19:DA:C2	2.84	0.65
2:G:15:DT:H6	2:G:15:DT:H5'	1.61	0.65
2:T:15:DT:H5'	2:T:15:DT:H6	1.61	0.65
3:H:2:DA:H1'	3:H:3:DC:C5'	2.26	0.65
3:L:2:DA:H1'	3:L:3:DC:C5'	2.25	0.65
3:P:22:DA:H1'	3:P:23:DC:H5"	1.79	0.65
3:U:2:DA:H1'	3:U:3:DC:C5'	2.26	0.65
3:3:11:DA:C1'	3:3:12:DC:H5"	2.25	0.65
3:3:11:DA:H2"	3:3:12:DC:H5'	1.78	0.65
3:D:7:DT:H2"	3:D:8:DG:H8	1.61	0.65
2:X:15:DT:H6	2:X:15:DT:H5'	1.61	0.65
2:2:1:DT:H3'	2:2:2:DG:H5"	1.79	0.65
3:3:19:DA:H1'	3:3:20:DT:H5"	1.78	0.65
2:C:11:DA:C2	3:D:19:DA:C2	2.84	0.65
3:D:2:DA:H1'	3:D:3:DC:C5'	2.27	0.65
2:K:15:DT:H6	2:K:15:DT:H5'	1.61	0.64
3:7:7:DT:H2"	3:7:8:DG:H8	1.61	0.64
2:C:1:DT:H3'	2:C:2:DG:H5"	1.80	0.64
3:L:7:DT:H2"	3:L:8:DG:H8	1.62	0.64
3:7:2:DA:H1'	3:7:3:DC:C5'	2.27	0.64
3:Y:19:DA:H1'	3:Y:20:DT:H5"	1.78	0.64
3:3:22:DA:H1'	3:3:23:DC:H5"	1.79	0.64
3:H:22:DA:H1'	3:H:23:DC:H5"	1.79	0.64
2:T:2:DG:OP1	2:T:2:DG:C4'	2.46	0.64
3:U:8:DG:C1'	3:U:9:DT:H5"	2.28	0.64
3:Y:7:DT:H2"	3:Y:8:DG:H8	1.62	0.64
2:6:1:DT:H3'	2:6:2:DG:H5"	1.80	0.64
3:7:22:DA:H1'	3:7:23:DC:H5"	1.79	0.64
3:P:7:DT:H2"	3:P:8:DG:H8	1.62	0.64
3:D:22:DA:H1'	3:D:23:DC:H5"	1.79	0.64
3:P:19:DA:H1'	3:P:20:DT:H5"	1.78	0.64
3:L:22:DA:H1'	3:L:23:DC:H5"	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:11:DA:H2"	3:P:12:DC:H5'	1.78	0.64
2:O:1:DT:H3'	2:O:2:DG:H5"	1.79	0.63
3:H:11:DA:H2"	3:H:12:DC:H5'	1.80	0.63
3:U:11:DA:H2"	3:U:12:DC:H5'	1.80	0.63
2:O:2:DG:OP1	2:O:2:DG:C4'	2.46	0.63
2:X:8:DC:H5'	2:X:8:DC:H6	1.64	0.63
2:G:2:DG:OP1	2:G:2:DG:C4'	2.46	0.63
3:Y:22:DA:H1'	3:Y:23:DC:H5"	1.80	0.63
2:2:2:DG:OP1	2:2:2:DG:C4'	2.46	0.63
3:7:19:DA:H1'	3:7:20:DT:H5"	1.80	0.63
3:H:16:DT:H6	3:H:16:DT:H5'	1.63	0.63
3:L:11:DA:C1'	3:L:12:DC:H5"	2.27	0.63
3:Y:24:DA:H2"	3:Y:25:DG:OP2	1.99	0.63
3:D:19:DA:H1'	3:D:20:DT:H5"	1.80	0.63
2:K:11:DA:C2	3:L:19:DA:C2	2.87	0.63
2:C:2:DG:OP1	2:C:2:DG:C4'	2.46	0.63
3:H:8:DG:C1'	3:H:9:DT:H5"	2.28	0.63
2:2:24:DA:C4'	2:2:25:DA:OP1	2.45	0.63
2:K:2:DG:OP1	2:K:2:DG:C4'	2.47	0.63
2:X:10:DT:H2"	2:X:11:DA:OP2	1.99	0.63
3:Y:11:DA:C1'	3:Y:12:DC:H5"	2.27	0.63
2:2:5:DT:H2"	2:2:6:DG:C8	2.34	0.63
3:3:7:DT:H2"	3:3:8:DG:H8	1.63	0.63
3:3:17:DT:H1'	3:3:18:DT:H5"	1.81	0.63
2:K:8:DC:H5'	2:K:8:DC:H6	1.64	0.62
3:U:16:DT:H6	3:U:16:DT:H5'	1.63	0.62
3:Y:8:DG:C1'	3:Y:9:DT:H5"	2.29	0.62
3:Y:11:DA:H2"	3:Y:12:DC:H5'	1.80	0.62
2:6:2:DG:OP1	2:6:2:DG:C4'	2.46	0.62
3:L:11:DA:H2"	3:L:12:DC:H5'	1.80	0.62
3:U:10:DG:H1'	3:U:11:DA:H5'	1.80	0.62
3:L:24:DA:H2"	3:L:25:DG:OP2	1.99	0.62
3:P:17:DT:H1'	3:P:18:DT:H5"	1.81	0.62
3:U:9:DT:H2"	3:U:10:DG:C5'	2.27	0.62
2:X:2:DG:OP1	2:X:2:DG:C4'	2.47	0.62
3:H:10:DG:H1'	3:H:11:DA:H5'	1.80	0.62
2:T:9:DA:H1'	2:T:10:DT:H5'	1.82	0.62
2:T:1:DT:H3'	2:T:2:DG:H5"	1.81	0.62
3:D:10:DG:H1'	3:D:11:DA:H5'	1.80	0.62
2:G:8:DC:H5'	2:G:8:DC:H6	1.65	0.62
2:G:9:DA:H1'	2:G:10:DT:H5'	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1:DT:H3'	2:X:2:DG:H5"	1.81	0.62
3:L:16:DT:H5'	3:L:16:DT:H6	1.65	0.62
2:O:5:DT:H2"	2:O:6:DG:C8	2.34	0.62
3:P:8:DG:C1'	3:P:9:DT:H5"	2.29	0.62
3:Y:14:DA:C3'	3:Y:15:DC:H5"	2.29	0.62
3:3:8:DG:C1'	3:3:9:DT:H5"	2.29	0.62
2:K:1:DT:H3'	2:K:2:DG:H5"	1.81	0.61
2:2:5:DT:H5'	2:2:5:DT:C6	2.34	0.61
3:7:10:DG:H1'	3:7:11:DA:H5'	1.81	0.61
3:P:4:DT:H2"	3:P:5:DT:C7	2.30	0.61
3:Y:10:DG:H1'	3:Y:11:DA:H5'	1.82	0.61
2:2:8:DC:H5'	2:2:8:DC:H6	1.64	0.61
3:L:8:DG:C1'	3:L:9:DT:H5"	2.29	0.61
2:T:8:DC:H5'	2:T:8:DC:H6	1.65	0.61
3:Y:16:DT:H6	3:Y:16:DT:H5'	1.65	0.61
2:6:5:DT:H2"	2:6:6:DG:C8	2.35	0.61
2:6:24:DA:C4'	2:6:25:DA:OP1	2.44	0.61
2:G:1:DT:H3'	2:G:2:DG:H5"	1.81	0.61
3:U:24:DA:H2"	3:U:25:DG:OP2	2.01	0.61
3:L:5:DT:C1'	3:L:6:DT:H5"	2.30	0.61
3:3:11:DA:C2'	3:3:12:DC:H5"	2.31	0.61
3:7:11:DA:H2"	3:7:12:DC:H5'	1.80	0.61
3:D:11:DA:H2"	3:D:12:DC:H5'	1.80	0.61
3:L:4:DT:H2"	3:L:5:DT:C7	2.31	0.61
3:3:4:DT:H2"	3:3:5:DT:C7	2.30	0.61
2:K:10:DT:H2"	2:K:11:DA:OP2	1.99	0.61
2:O:8:DC:H5'	2:O:8:DC:H6	1.65	0.61
2:O:19:DC:H5'	2:O:19:DC:C6	2.36	0.61
2:T:10:DT:H2"	2:T:11:DA:OP2	2.00	0.61
2:X:1:DT:H3'	2:X:2:DG:C5'	2.31	0.61
3:7:4:DT:H2"	3:7:5:DT:C7	2.31	0.61
2:C:5:DT:H2"	2:C:6:DG:C8	2.35	0.60
3:H:7:DT:H2"	3:H:8:DG:C8	2.36	0.60
3:L:10:DG:H1'	3:L:11:DA:H5'	1.82	0.60
2:2:19:DC:H5'	2:2:19:DC:C6	2.36	0.60
3:3:24:DA:H2"	3:3:25:DG:OP2	2.01	0.60
3:7:17:DT:H1'	3:7:18:DT:H5"	1.82	0.60
2:C:10:DT:H2"	2:C:11:DA:OP2	1.99	0.60
2:C:24:DA:C4'	2:C:25:DA:OP1	2.44	0.60
2:K:7:DT:H2"	2:K:8:DC:H6	1.66	0.60
3:P:16:DT:H6	3:P:16:DT:H5'	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:9:DA:H1'	2:6:10:DT:H5'	1.83	0.60
2:C:9:DA:H1'	2:C:10:DT:H5'	1.83	0.60
2:T:4:DC:H1'	2:T:5:DT:H5"	1.83	0.60
2:X:5:DT:H2"	2:X:6:DG:C8	2.36	0.60
2:2:1:DT:H3'	2:2:2:DG:C5'	2.30	0.60
3:D:8:DG:C1'	3:D:9:DT:H5"	2.30	0.60
3:D:17:DT:H1'	3:D:18:DT:H5"	1.82	0.60
3:H:4:DT:H2"	3:H:5:DT:C7	2.31	0.60
3:P:9:DT:H2"	3:P:10:DG:C8	2.37	0.60
3:U:4:DT:H2"	3:U:5:DT:C7	2.31	0.60
3:3:10:DG:H1'	3:3:11:DA:H5'	1.83	0.60
3:7:8:DG:C1'	3:7:9:DT:H5"	2.30	0.60
2:C:1:DT:H3'	2:C:2:DG:C5'	2.31	0.60
3:D:4:DT:H2"	3:D:5:DT:C7	2.31	0.60
3:U:7:DT:H2"	3:U:8:DG:C8	2.36	0.60
2:X:7:DT:H2"	2:X:8:DC:H6	1.66	0.60
2:T:7:DT:H2"	2:T:8:DC:H6	1.67	0.60
3:U:9:DT:H2"	3:U:10:DG:C8	2.37	0.60
3:3:16:DT:H6	3:3:16:DT:H5'	1.66	0.60
2:6:10:DT:H2"	2:6:11:DA:OP2	1.99	0.60
3:H:17:DT:H1'	3:H:18:DT:H5"	1.84	0.60
3:P:11:DA:C2'	3:P:12:DC:H5"	2.31	0.60
3:H:9:DT:H2"	3:H:10:DG:C5'	2.27	0.60
2:O:1:DT:H3'	2:O:2:DG:C5'	2.30	0.60
2:6:1:DT:H3'	2:6:2:DG:C5'	2.31	0.60
2:G:10:DT:H2"	2:G:11:DA:OP2	2.00	0.60
3:H:24:DA:H2"	3:H:25:DG:OP2	2.01	0.60
2:O:23:DA:C4'	2:O:24:DA:OP1	2.46	0.60
3:P:10:DG:H1'	3:P:11:DA:H5'	1.83	0.60
2:X:19:DC:H5'	2:X:19:DC:C6	2.37	0.60
2:C:5:DT:H5'	2:C:5:DT:C6	2.33	0.60
2:T:11:DA:C2	3:U:19:DA:C2	2.90	0.60
3:D:16:DT:H5'	3:D:16:DT:H6	1.66	0.59
2:2:12:DA:H1'	2:2:13:DA:H5"	1.84	0.59
2:G:7:DT:H2"	2:G:8:DC:H6	1.67	0.59
3:H:11:DA:C2'	3:H:12:DC:H5"	2.32	0.59
2:K:5:DT:H2"	2:K:6:DG:C8	2.37	0.59
3:L:17:DT:H1'	3:L:18:DT:H5"	1.84	0.59
2:O:10:DT:H2"	2:O:11:DA:OP2	2.02	0.59
2:6:8:DC:H5'	2:6:8:DC:H6	1.67	0.59
2:6:18:DT:H2"	2:6:19:DC:H5'	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7:16:DT:H6	3:7:16:DT:H5'	1.66	0.59
2:G:1:DT:H3'	2:G:2:DG:C5'	2.32	0.59
2:C:18:DT:H2"	2:C:19:DC:H5'	1.84	0.59
2:K:1:DT:H3'	2:K:2:DG:C5'	2.31	0.59
3:P:24:DA:H2"	3:P:25:DG:OP2	2.01	0.59
3:Y:9:DT:H2"	3:Y:10:DG:C8	2.37	0.59
3:P:14:DA:C3'	3:P:15:DC:H5"	2.29	0.59
3:3:9:DT:H2"	3:3:10:DG:C8	2.36	0.59
2:6:5:DT:H5'	2:6:5:DT:C6	2.33	0.59
2:C:8:DC:H5'	2:C:8:DC:H6	1.67	0.59
3:D:11:DA:C2'	3:D:12:DC:H5"	2.32	0.59
3:H:9:DT:H2"	3:H:10:DG:C8	2.37	0.59
3:L:9:DT:H2"	3:L:10:DG:C8	2.38	0.59
2:2:10:DT:H2"	2:2:11:DA:OP2	2.01	0.59
3:7:24:DA:H2"	3:7:25:DG:OP2	2.01	0.59
3:D:9:DT:H2"	3:D:10:DG:C8	2.37	0.59
2:K:9:DA:H1'	2:K:10:DT:H5'	1.84	0.59
3:L:11:DA:C2'	3:L:12:DC:H5"	2.32	0.59
2:O:12:DA:H1'	2:O:13:DA:H5"	1.85	0.59
3:U:17:DT:H1'	3:U:18:DT:H5"	1.84	0.59
3:7:9:DT:H2"	3:7:10:DG:C8	2.37	0.59
3:7:11:DA:C2'	3:7:12:DC:H5"	2.33	0.59
2:C:13:DA:C1'	2:C:14:DG:H5'	2.31	0.59
3:D:24:DA:H2"	3:D:25:DG:OP2	2.01	0.59
3:H:5:DT:C1'	3:H:6:DT:H5"	2.32	0.59
2:K:19:DC:H5'	2:K:19:DC:C6	2.37	0.59
3:L:5:DT:H1'	3:L:6:DT:C5'	2.31	0.59
2:X:9:DA:H1'	2:X:10:DT:H5'	1.84	0.59
2:T:5:DT:H2"	2:T:6:DG:C8	2.38	0.59
3:U:11:DA:C2'	3:U:12:DC:H5"	2.32	0.59
2:G:5:DT:H2"	2:G:6:DG:C8	2.38	0.58
2:G:4:DC:H1'	2:G:5:DT:H5"	1.84	0.58
3:L:9:DT:H2"	3:L:10:DG:C5'	2.28	0.58
2:T:12:DA:H1'	2:T:13:DA:H5"	1.85	0.58
3:Y:11:DA:C2'	3:Y:12:DC:H5"	2.32	0.58
2:6:13:DA:C1'	2:6:14:DG:H5'	2.31	0.58
3:7:14:DA:C3'	3:7:15:DC:H5"	2.28	0.58
3:L:7:DT:H2"	3:L:8:DG:C8	2.39	0.58
3:3:11:DA:C2'	3:3:12:DC:C5'	2.80	0.58
3:D:14:DA:C3'	3:D:15:DC:H5"	2.28	0.58
3:P:11:DA:C2'	3:P:12:DC:C5'	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:4:DT:H2"	3:Y:5:DT:C7	2.31	0.58
3:Y:7:DT:H2"	3:Y:8:DG:C8	2.39	0.58
2:2:4:DC:H1'	2:2:5:DT:H5"	1.86	0.58
2:G:13:DA:C1'	2:G:14:DG:H5'	2.31	0.58
2:O:5:DT:H5'	2:O:5:DT:C6	2.34	0.58
2:G:23:DA:C4'	2:G:24:DA:OP1	2.47	0.58
2:O:9:DA:H1'	2:O:10:DT:H5'	1.85	0.58
2:C:7:DT:H2"	2:C:8:DC:H6	1.67	0.58
2:O:4:DC:H1'	2:O:5:DT:H5"	1.86	0.58
3:Y:17:DT:H1'	3:Y:18:DT:H5"	1.84	0.58
2:6:4:DC:H1'	2:6:5:DT:H5"	1.86	0.58
3:D:11:DA:C2'	3:D:12:DC:C5'	2.82	0.58
3:L:24:DA:H1'	3:L:25:DG:O5'	2.03	0.58
2:O:13:DA:C1'	2:O:14:DG:H5'	2.32	0.58
2:6:7:DT:H2"	2:6:8:DC:H6	1.67	0.58
3:7:11:DA:C2'	3:7:12:DC:C5'	2.82	0.58
2:C:12:DA:H1'	2:C:13:DA:H5"	1.86	0.57
3:D:7:DT:H2"	3:D:8:DG:C8	2.37	0.57
2:6:12:DA:H1'	2:6:13:DA:H5"	1.86	0.57
2:C:4:DC:H1'	2:C:5:DT:H5"	1.86	0.57
2:K:23:DA:C4'	2:K:24:DA:OP1	2.48	0.57
2:T:1:DT:H3'	2:T:2:DG:C5'	2.31	0.57
3:U:11:DA:C2'	3:U:12:DC:C5'	2.82	0.57
2:2:17:DG:H2"	2:2:18:DT:C5'	2.35	0.57
3:3:7:DT:H2"	3:3:8:DG:C8	2.39	0.57
3:D:5:DT:H1'	3:D:6:DT:C5'	2.30	0.57
2:K:4:DC:H1'	2:K:5:DT:H5"	1.87	0.57
2:T:18:DT:H2"	2:T:19:DC:H5'	1.87	0.57
3:Y:11:DA:C2'	3:Y:12:DC:C5'	2.82	0.57
3:Y:24:DA:H1'	3:Y:25:DG:O5'	2.04	0.57
3:7:7:DT:H2"	3:7:8:DG:C8	2.38	0.57
2:G:12:DA:H1'	2:G:13:DA:H5"	1.86	0.57
2:O:18:DT:H2"	2:O:19:DC:H5'	1.86	0.57
2:T:13:DA:C1'	2:T:14:DG:H5'	2.31	0.57
2:T:19:DC:H5'	2:T:19:DC:C6	2.37	0.57
2:X:12:DA:H1'	2:X:13:DA:H5"	1.86	0.57
2:2:9:DA:H1'	2:2:10:DT:H5'	1.85	0.57
2:2:18:DT:H2"	2:2:19:DC:H5'	1.86	0.57
3:7:5:DT:H1'	3:7:6:DT:C5'	2.31	0.57
3:H:11:DA:C2'	3:H:12:DC:C5'	2.82	0.57
3:P:4:DT:C2'	3:P:5:DT:H72	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:17:DG:H2"	2:C:18:DT:C5'	2.35	0.57
3:H:10:DG:H2"	3:H:11:DA:O5'	2.05	0.57
2:O:7:DT:H2"	2:O:8:DC:H6	1.70	0.57
2:6:17:DG:H2"	2:6:18:DT:C5'	2.35	0.57
2:G:19:DC:H5'	2:G:19:DC:C6	2.38	0.57
2:K:24:DA:C4'	2:K:25:DA:OP1	2.46	0.57
2:G:18:DT:H2"	2:G:19:DC:H5'	1.86	0.57
2:T:5:DT:H5'	2:T:5:DT:C6	2.35	0.57
3:Y:5:DT:C1'	3:Y:6:DT:H5"	2.30	0.57
2:6:19:DC:H5'	2:6:19:DC:C6	2.38	0.57
2:O:17:DG:H2"	2:O:18:DT:C5'	2.35	0.56
2:X:2:DG:H5"	2:X:2:DG:H8	1.70	0.56
2:2:13:DA:C1'	2:2:14:DG:H5'	2.32	0.56
2:C:19:DC:H5'	2:C:19:DC:C6	2.38	0.56
2:X:5:DT:H5'	2:X:5:DT:C6	2.36	0.56
2:X:18:DT:H2"	2:X:19:DC:H5'	1.87	0.56
3:Y:4:DT:C2'	3:Y:5:DT:H72	2.35	0.56
3:3:4:DT:C2'	3:3:5:DT:H72	2.34	0.56
3:P:7:DT:H2"	3:P:8:DG:C8	2.39	0.56
2:T:2:DG:H5"	2:T:2:DG:H8	1.71	0.56
3:3:5:DT:C1'	3:3:6:DT:H5"	2.31	0.56
2:K:12:DA:H1'	2:K:13:DA:H5"	1.85	0.56
3:L:4:DT:C2'	3:L:5:DT:H72	2.35	0.56
3:U:24:DA:H1'	3:U:25:DG:O5'	2.06	0.56
3:D:24:DA:H1'	3:D:25:DG:O5'	2.05	0.56
3:H:15:DC:H2'	3:H:16:DT:H72	1.88	0.56
3:P:5:DT:C1'	3:P:6:DT:H5"	2.31	0.56
3:H:24:DA:H1'	3:H:25:DG:O5'	2.06	0.56
3:L:11:DA:C2'	3:L:12:DC:C5'	2.82	0.56
3:7:24:DA:H1'	3:7:25:DG:O5'	2.06	0.56
3:D:10:DG:H2"	3:D:11:DA:O5'	2.04	0.56
2:K:2:DG:H5"	2:K:2:DG:H8	1.70	0.56
3:P:6:DT:H2"	3:P:7:DT:O5'	2.06	0.56
3:U:10:DG:H2"	3:U:11:DA:O5'	2.05	0.56
3:3:24:DA:H1'	3:3:25:DG:O5'	2.06	0.56
3:7:10:DG:H2"	3:7:11:DA:O5'	2.04	0.55
2:G:11:DA:C2	3:H:19:DA:C2	2.94	0.55
2:G:24:DA:C4'	2:G:25:DA:OP1	2.45	0.55
2:X:4:DC:H1'	2:X:5:DT:H5"	1.87	0.55
3:3:14:DA:C3'	3:3:15:DC:H5"	2.29	0.55
2:G:2:DG:H5"	2:G:2:DG:H8	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:18:DT:H2"	2:K:19:DC:H5'	1.87	0.55
3:P:24:DA:H1'	3:P:25:DG:O5'	2.06	0.55
3:P:10:DG:H2"	3:P:11:DA:O5'	2.07	0.55
3:U:15:DC:H2'	3:U:16:DT:H72	1.88	0.55
3:L:10:DG:H2"	3:L:11:DA:O5'	2.06	0.55
2:X:17:DG:H2"	2:X:18:DT:C5'	2.37	0.55
2:T:17:DG:H2"	2:T:18:DT:C5'	2.37	0.55
2:X:11:DA:C2	3:Y:19:DA:C2	2.95	0.55
2:C:24:DA:H1'	2:C:25:DA:H5'	1.88	0.55
3:U:4:DT:C2'	3:U:5:DT:H72	2.34	0.55
3:3:10:DG:H2"	3:3:11:DA:O5'	2.06	0.55
2:X:8:DC:H2"	2:X:9:DA:C8	2.42	0.55
2:2:7:DT:H2"	2:2:8:DC:H6	1.70	0.55
2:2:17:DG:H1'	2:2:18:DT:H5"	1.89	0.55
3:3:6:DT:H2"	3:3:7:DT:O5'	2.06	0.55
2:K:5:DT:H5'	2:K:5:DT:C6	2.36	0.54
2:K:8:DC:H2"	2:K:9:DA:C8	2.42	0.54
2:K:17:DG:H2"	2:K:18:DT:C5'	2.37	0.54
2:6:24:DA:H1'	2:6:25:DA:H5'	1.88	0.54
3:Y:9:DT:H2"	3:Y:10:DG:C5'	2.28	0.54
3:7:6:DT:H2"	3:7:7:DT:O5'	2.07	0.54
3:D:6:DT:H2"	3:D:7:DT:O5'	2.07	0.54
2:O:7:DT:C2'	2:O:8:DC:C5'	2.85	0.54
3:P:9:DT:H2"	3:P:10:DG:C5'	2.29	0.54
2:C:23:DA:H1'	2:C:24:DA:H5'	1.90	0.54
3:D:5:DT:C1'	3:D:6:DT:H5"	2.29	0.54
2:O:17:DG:H1'	2:O:18:DT:H5"	1.90	0.54
2:T:24:DA:H1'	2:T:25:DA:H5'	1.89	0.54
3:7:5:DT:C1'	3:7:6:DT:H5"	2.29	0.54
2:6:23:DA:H1'	2:6:24:DA:H5'	1.90	0.54
2:C:16:DT:H2"	2:C:17:DG:C8	2.43	0.54
2:G:17:DG:H2"	2:G:18:DT:C5'	2.37	0.54
3:H:4:DT:C2'	3:H:5:DT:H72	2.34	0.54
2:6:16:DT:H2"	2:6:17:DG:C8	2.43	0.54
3:D:15:DC:H2'	3:D:16:DT:H72	1.90	0.54
2:2:23:DA:H1'	2:2:24:DA:H5'	1.90	0.54
3:7:4:DT:C2'	3:7:5:DT:H72	2.35	0.54
2:C:2:DG:H5"	2:C:2:DG:H8	1.73	0.53
2:6:2:DG:H5"	2:6:2:DG:H8	1.73	0.53
2:G:5:DT:H5'	2:G:5:DT:C6	2.35	0.53
2:2:2:DG:H5"	2:2:2:DG:H8	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:9:DT:H6	3:P:9:DT:H5'	1.74	0.53
3:D:4:DT:C2'	3:D:5:DT:H72	2.35	0.53
2:G:15:DT:C1'	2:G:16:DT:H5'	2.38	0.53
2:G:24:DA:H1'	2:G:25:DA:H5'	1.90	0.53
2:K:17:DG:H1'	2:K:18:DT:H5"	1.91	0.53
3:L:6:DT:H2"	3:L:7:DT:O5'	2.08	0.53
3:Y:10:DG:H2"	3:Y:11:DA:O5'	2.06	0.53
2:2:16:DT:H2"	2:2:17:DG:C8	2.44	0.53
2:6:7:DT:C2'	2:6:8:DC:C5'	2.86	0.53
3:7:15:DC:H2"	3:7:16:DT:H5"	1.90	0.53
3:7:15:DC:H2'	3:7:16:DT:H72	1.91	0.53
2:C:7:DT:C2'	2:C:8:DC:C5'	2.86	0.53
2:K:13:DA:C1'	2:K:14:DG:H5'	2.33	0.53
2:O:8:DC:O2	3:P:21:DG:N2	2.29	0.53
3:3:9:DT:H6	3:3:9:DT:H5'	1.73	0.53
2:6:17:DG:H1'	2:6:18:DT:H5"	1.91	0.53
2:T:15:DT:C1'	2:T:16:DT:H5'	2.37	0.53
2:K:16:DT:H2"	2:K:17:DG:C8	2.44	0.53
3:P:5:DT:H1'	3:P:6:DT:C5'	2.33	0.53
3:P:18:DT:H1'	3:P:19:DA:H5'	1.90	0.53
3:3:11:DA:H1'	3:3:12:DC:C5'	2.35	0.53
3:3:18:DT:H1'	3:3:19:DA:H5'	1.90	0.53
3:D:9:DT:H2"	3:D:10:DG:C5'	2.30	0.53
3:D:15:DC:H2"	3:D:16:DT:H5"	1.90	0.53
3:L:12:DC:H2"	3:L:13:DA:C8	2.44	0.53
2:O:2:DG:H5"	2:O:2:DG:H8	1.73	0.53
3:Y:5:DT:H1'	3:Y:6:DT:C5'	2.31	0.53
3:3:5:DT:H1'	3:3:6:DT:C5'	2.32	0.53
2:C:17:DG:H1'	2:C:18:DT:H5"	1.91	0.53
3:H:6:DT:H2"	3:H:7:DT:O5'	2.09	0.53
3:L:18:DT:H1'	3:L:19:DA:H5'	1.91	0.53
3:Y:6:DT:H2"	3:Y:7:DT:O5'	2.09	0.53
3:7:9:DT:H2"	3:7:10:DG:C5'	2.30	0.53
2:C:8:DC:H2"	2:C:9:DA:C8	2.44	0.53
2:G:15:DT:H2"	2:G:16:DT:O5'	2.09	0.53
3:H:15:DC:H2"	3:H:16:DT:H5"	1.91	0.53
3:H:19:DA:H2"	3:H:20:DT:C5'	2.39	0.53
3:U:6:DT:H2"	3:U:7:DT:O5'	2.09	0.53
3:U:15:DC:H2"	3:U:16:DT:H5"	1.91	0.53
2:2:7:DT:C2'	2:2:8:DC:C5'	2.85	0.53
3:3:15:DC:H2'	3:3:16:DT:H72	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:11:DA:C2	3:P:19:DA:C2	2.97	0.52
2:G:17:DG:H1'	2:G:18:DT:H5"	1.91	0.52
3:H:9:DT:C3'	3:H:10:DG:H5"	2.38	0.52
3:L:15:DC:H2'	3:L:16:DT:H72	1.90	0.52
2:X:24:DA:H1'	2:X:25:DA:H5'	1.91	0.52
2:6:23:DA:C4'	2:6:24:DA:OP1	2.46	0.52
2:O:22:DA:H2"	2:O:23:DA:H5'	1.91	0.52
2:O:23:DA:H1'	2:O:24:DA:H5'	1.90	0.52
2:T:17:DG:H1'	2:T:18:DT:H5"	1.91	0.52
2:T:23:DA:H1'	2:T:24:DA:H5'	1.91	0.52
2:T:23:DA:C4'	2:T:24:DA:OP1	2.48	0.52
3:U:5:DT:C1'	3:U:6:DT:H5"	2.32	0.52
3:Y:12:DC:H2"	3:Y:13:DA:C8	2.44	0.52
2:6:8:DC:H2"	2:6:9:DA:C8	2.45	0.52
3:H:18:DT:H1'	3:H:19:DA:H5'	1.91	0.52
2:K:15:DT:C1'	2:K:16:DT:H5'	2.39	0.52
2:T:7:DT:C2'	2:T:8:DC:C5'	2.87	0.52
2:O:16:DT:H2"	2:O:17:DG:C8	2.44	0.52
2:X:16:DT:H2"	2:X:17:DG:C8	2.44	0.52
2:2:12:DA:C2'	2:2:13:DA:H5"	2.40	0.52
2:G:8:DC:H2"	2:G:9:DA:C8	2.45	0.52
3:H:19:DA:H2"	3:H:20:DT:H5'	1.90	0.52
3:P:15:DC:H2'	3:P:16:DT:H72	1.90	0.52
3:H:21:DG:H2"	3:H:22:DA:OP2	2.10	0.52
3:L:15:DC:H2"	3:L:16:DT:H5"	1.92	0.52
2:O:24:DA:H1'	2:O:25:DA:H5'	1.90	0.52
2:T:8:DC:H2"	2:T:9:DA:C8	2.45	0.52
3:Y:14:DA:C1'	3:Y:15:DC:H5"	2.39	0.52
3:Y:15:DC:H2"	3:Y:16:DT:H5"	1.92	0.52
3:D:19:DA:H2"	3:D:20:DT:H5'	1.92	0.52
2:G:23:DA:H1'	2:G:24:DA:H5'	1.91	0.52
2:K:24:DA:H1'	2:K:25:DA:H5'	1.91	0.52
3:U:19:DA:H2"	3:U:20:DT:H5'	1.90	0.52
2:2:7:DT:C2	2:2:8:DC:C5	2.98	0.52
3:D:9:DT:C3'	3:D:10:DG:H5"	2.39	0.52
3:U:18:DT:H1'	3:U:19:DA:H5'	1.91	0.52
2:X:7:DT:C2'	2:X:8:DC:C5'	2.88	0.52
2:X:17:DG:H1'	2:X:18:DT:H5"	1.91	0.52
3:Y:15:DC:H2'	3:Y:16:DT:H72	1.90	0.52
2:2:22:DA:H2"	2:2:23:DA:H5'	1.91	0.52
3:7:19:DA:H2"	3:7:20:DT:H5'	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:24:DA:C4'	2:O:25:DA:OP1	2.45	0.51
3:P:9:DT:C3'	3:P:10:DG:H5"	2.40	0.51
3:P:22:DA:H1'	3:P:23:DC:C5'	2.40	0.51
2:T:3:DG:H2"	2:T:4:DC:C5'	2.38	0.51
2:X:13:DA:C1'	2:X:14:DG:H5'	2.34	0.51
3:3:15:DC:H2"	3:3:16:DT:H5"	1.92	0.51
3:U:19:DA:H2"	3:U:20:DT:C5'	2.39	0.51
3:U:22:DA:H1'	3:U:23:DC:C5'	2.40	0.51
2:2:8:DC:H2"	2:2:9:DA:C8	2.46	0.51
3:7:9:DT:C3'	3:7:10:DG:H5"	2.39	0.51
2:G:12:DA:C2'	2:G:13:DA:H5"	2.41	0.51
3:L:22:DA:H1'	3:L:23:DC:C5'	2.41	0.51
2:C:7:DT:C2	2:C:8:DC:C5	2.99	0.51
2:X:23:DA:C4'	2:X:24:DA:OP1	2.48	0.51
3:Y:18:DT:H1'	3:Y:19:DA:H5'	1.91	0.51
2:6:7:DT:C2	2:6:8:DC:C5	2.99	0.51
2:C:22:DA:H2"	2:C:23:DA:H5'	1.91	0.51
3:D:11:DA:H1'	3:D:12:DC:C5'	2.35	0.51
3:D:19:DA:H2"	3:D:20:DT:C5'	2.41	0.51
2:G:2:DG:C2'	2:G:3:DG:C8	2.93	0.51
3:U:21:DG:H2"	3:U:22:DA:OP2	2.10	0.51
2:X:7:DT:C2	2:X:8:DC:C5	2.99	0.51
2:2:24:DA:H1'	2:2:25:DA:H5'	1.91	0.51
3:3:9:DT:H2"	3:3:10:DG:C5'	2.29	0.51
2:6:12:DA:C2'	2:6:13:DA:H5"	2.40	0.51
3:7:11:DA:H1'	3:7:12:DC:C5'	2.35	0.51
2:C:23:DA:C4'	2:C:24:DA:OP1	2.46	0.51
2:O:12:DA:C2'	2:O:13:DA:H5"	2.40	0.51
2:X:24:DA:C4'	2:X:25:DA:OP1	2.46	0.51
2:2:15:DT:C1'	2:2:16:DT:H5'	2.40	0.51
2:K:7:DT:C2'	2:K:8:DC:C5'	2.88	0.51
3:P:15:DC:H2"	3:P:16:DT:H5"	1.92	0.51
3:U:9:DT:C3'	3:U:10:DG:H5"	2.38	0.51
2:6:22:DA:H2"	2:6:23:DA:H5'	1.91	0.51
3:7:19:DA:H2"	3:7:20:DT:C5'	2.41	0.51
2:K:7:DT:C2	2:K:8:DC:C5	2.99	0.51
3:U:9:DT:H6	3:U:9:DT:H5'	1.76	0.51
3:7:22:DA:H1'	3:7:23:DC:C5'	2.40	0.51
3:D:22:DA:H1'	3:D:23:DC:C5'	2.40	0.51
2:K:6:DG:H2"	2:K:7:DT:H5'	1.93	0.51
2:O:25:DA:C2	2:O:26:DG:C4	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:9:DT:H6	3:Y:9:DT:H5'	1.76	0.51
2:C:12:DA:C2'	2:C:13:DA:H5"	2.40	0.51
2:G:16:DT:H2"	2:G:17:DG:C8	2.46	0.51
2:T:16:DT:H2"	2:T:17:DG:C8	2.46	0.51
3:D:12:DC:H2"	3:D:13:DA:C8	2.46	0.50
2:G:3:DG:H2"	2:G:4:DC:C5'	2.38	0.50
3:H:22:DA:H1'	3:H:23:DC:C5'	2.40	0.50
2:T:2:DG:C2'	2:T:3:DG:C8	2.93	0.50
2:T:15:DT:H2"	2:T:16:DT:O5'	2.10	0.50
3:U:5:DT:H1'	3:U:6:DT:C5'	2.32	0.50
2:X:23:DA:H1'	2:X:24:DA:H5'	1.93	0.50
2:G:11:DA:H2"	2:G:12:DA:C5'	2.35	0.50
2:O:7:DT:C2	2:O:8:DC:C5	2.99	0.50
2:T:25:DA:C2	2:T:26:DG:C4	2.99	0.50
3:7:12:DC:H2"	3:7:13:DA:C8	2.46	0.50
2:G:7:DT:C2'	2:G:8:DC:C5'	2.87	0.50
2:O:8:DC:H2"	2:O:9:DA:C8	2.46	0.50
3:H:5:DT:H1'	3:H:6:DT:C5'	2.32	0.50
2:O:6:DG:C2	3:P:24:DA:C2	2.99	0.50
2:2:6:DG:H2"	2:2:7:DT:H5'	1.91	0.50
3:3:12:DC:H2"	3:3:13:DA:C8	2.47	0.50
2:K:25:DA:C2	2:K:26:DG:C4	3.00	0.50
3:L:19:DA:H2"	3:L:20:DT:C5'	2.41	0.50
2:O:6:DG:H2"	2:O:7:DT:H5'	1.91	0.50
2:X:15:DT:C1'	2:X:16:DT:H5'	2.39	0.50
3:Y:22:DA:H1'	3:Y:23:DC:C5'	2.41	0.50
3:7:15:DC:H2"	3:7:16:DT:C5'	2.42	0.50
2:C:15:DT:H2"	2:C:16:DT:O5'	2.12	0.50
3:U:12:DC:H2"	3:U:13:DA:C8	2.47	0.50
3:Y:19:DA:H2"	3:Y:20:DT:H5'	1.92	0.50
3:3:22:DA:H1'	3:3:23:DC:C5'	2.40	0.50
2:6:15:DT:H2"	2:6:16:DT:O5'	2.12	0.50
3:D:15:DC:H2"	3:D:16:DT:C5'	2.42	0.50
2:G:25:DA:C2	2:G:26:DG:C4	2.99	0.50
3:H:9:DT:H6	3:H:9:DT:H5'	1.76	0.50
3:P:12:DC:H2"	3:P:13:DA:C8	2.47	0.50
2:X:25:DA:C2	2:X:26:DG:C4	3.00	0.50
2:6:25:DA:C2	2:6:26:DG:C4	2.99	0.50
2:C:25:DA:C2	2:C:26:DG:C4	2.99	0.50
2:K:15:DT:H2"	2:K:16:DT:O5'	2.11	0.50
3:L:19:DA:H2"	3:L:20:DT:H5'	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:12:DA:H2"	2:O:13:DA:H5"	1.93	0.50
2:T:12:DA:C2'	2:T:13:DA:H5"	2.41	0.50
3:Y:19:DA:H2"	3:Y:20:DT:C5'	2.41	0.50
2:2:23:DA:C4'	2:2:24:DA:OP1	2.46	0.50
3:7:18:DT:H1'	3:7:19:DA:H5'	1.93	0.50
2:G:22:DA:H2"	2:G:23:DA:H5'	1.94	0.50
2:6:3:DG:H2"	2:6:4:DC:C5'	2.39	0.50
2:6:17:DG:H2"	2:6:18:DT:H5'	1.94	0.50
2:C:17:DG:H2"	2:C:18:DT:H5'	1.94	0.49
2:G:6:DG:C2'	2:G:7:DT:H71	2.41	0.49
2:K:23:DA:H1'	2:K:24:DA:H5'	1.93	0.49
2:X:11:DA:H2"	2:X:12:DA:C5'	2.34	0.49
2:2:25:DA:C2	2:2:26:DG:C4	2.99	0.49
3:7:9:DT:H5'	3:7:9:DT:H6	1.77	0.49
3:D:9:DT:H5'	3:D:9:DT:H6	1.77	0.49
3:D:14:DA:C1'	3:D:15:DC:H5"	2.42	0.49
3:H:12:DC:H2"	3:H:13:DA:C8	2.47	0.49
2:K:15:DT:H2'	2:K:16:DT:H72	1.94	0.49
2:C:11:DA:H2"	2:C:12:DA:C5'	2.36	0.49
3:P:19:DA:H2"	3:P:20:DT:H5'	1.94	0.49
2:T:7:DT:C2	2:T:8:DC:C5	2.99	0.49
3:3:9:DT:C3'	3:3:10:DG:H5"	2.40	0.49
3:7:14:DA:C1'	3:7:15:DC:H5"	2.42	0.49
2:G:12:DA:H2"	2:G:13:DA:H5"	1.94	0.49
2:K:12:DA:C2'	2:K:13:DA:H5"	2.43	0.49
2:T:22:DA:H2"	2:T:23:DA:H5'	1.94	0.49
2:X:6:DG:C2'	2:X:7:DT:H71	2.39	0.49
3:D:18:DT:H1'	3:D:19:DA:H5'	1.93	0.49
2:G:7:DT:C2	2:G:8:DC:C5	3.00	0.49
3:P:21:DG:H2"	3:P:22:DA:OP2	2.12	0.49
3:D:21:DG:H2"	3:D:22:DA:OP2	2.11	0.49
2:G:6:DG:H2"	2:G:7:DT:H5'	1.94	0.49
3:H:13:DA:C2'	3:H:14:DA:OP2	2.57	0.49
2:K:6:DG:C2'	2:K:7:DT:H71	2.39	0.49
2:O:6:DG:C2'	2:O:7:DT:H71	2.42	0.49
2:O:17:DG:H2"	2:O:18:DT:H5'	1.94	0.49
3:3:19:DA:H2"	3:3:20:DT:C5'	2.43	0.49
3:3:21:DG:H2"	3:3:22:DA:OP2	2.12	0.49
3:7:21:DG:H2"	3:7:22:DA:OP2	2.11	0.49
2:C:3:DG:H2"	2:C:4:DC:C5'	2.39	0.49
2:C:15:DT:C1'	2:C:16:DT:H5'	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:21:DG:H2"	3:Y:22:DA:OP2	2.13	0.49
3:3:19:DA:H2"	3:3:20:DT:H5'	1.94	0.49
3:L:14:DA:C1'	3:L:15:DC:H5"	2.39	0.49
2:O:15:DT:H2"	2:O:16:DT:O5'	2.13	0.49
2:X:15:DT:H2"	2:X:16:DT:O5'	2.11	0.49
2:2:11:DA:C2	3:3:19:DA:C2	3.01	0.49
2:2:15:DT:H2"	2:2:16:DT:O5'	2.13	0.49
2:C:12:DA:C2'	2:C:13:DA:C5'	2.89	0.49
2:K:22:DA:H2"	2:K:23:DA:H5'	1.94	0.49
2:O:11:DA:H2"	2:O:12:DA:C5'	2.33	0.49
3:U:14:DA:C3'	3:U:15:DC:H5"	2.31	0.49
2:2:17:DG:H2"	2:2:18:DT:H5'	1.94	0.49
2:6:12:DA:C2'	2:6:13:DA:C5'	2.89	0.49
3:L:9:DT:H5'	3:L:9:DT:H6	1.76	0.48
2:X:12:DA:C2'	2:X:13:DA:H5"	2.43	0.48
3:Y:9:DT:C3'	3:Y:10:DG:H5"	2.41	0.48
2:C:15:DT:H2'	2:C:16:DT:H72	1.96	0.48
2:X:22:DA:H2"	2:X:23:DA:H5'	1.94	0.48
3:3:14:DA:C1'	3:3:15:DC:H5"	2.42	0.48
3:L:21:DG:H2"	3:L:22:DA:OP2	2.13	0.48
2:O:15:DT:C1'	2:O:16:DT:H5'	2.41	0.48
2:K:2:DG:C2'	2:K:3:DG:C8	2.95	0.48
3:L:9:DT:C3'	3:L:10:DG:H5"	2.41	0.48
3:P:11:DA:H1'	3:P:12:DC:C5'	2.35	0.48
3:U:11:DA:H1'	3:U:12:DC:C5'	2.35	0.48
2:6:15:DT:C1'	2:6:16:DT:H5'	2.40	0.48
3:Y:24:DA:H1'	3:Y:25:DG:C5'	2.44	0.48
2:6:2:DG:C2'	2:6:3:DG:C8	2.95	0.48
2:T:12:DA:H2"	2:T:13:DA:H5"	1.95	0.48
2:X:2:DG:C2'	2:X:3:DG:C8	2.95	0.48
2:2:2:DG:C2'	2:2:3:DG:C8	2.96	0.48
3:H:15:DC:H2"	3:H:16:DT:C5'	2.43	0.48
2:K:3:DG:H2"	2:K:4:DC:C5'	2.40	0.48
2:2:7:DT:C2'	2:2:8:DC:H5"	2.44	0.48
2:2:12:DA:C2'	2:2:13:DA:C5'	2.89	0.48
2:6:15:DT:H2'	2:6:16:DT:H72	1.96	0.48
3:P:15:DC:H2"	3:P:16:DT:C5'	2.44	0.48
3:U:15:DC:H2"	3:U:16:DT:C5'	2.43	0.48
2:2:11:DA:H2"	2:2:12:DA:C5'	2.33	0.48
2:X:15:DT:H2'	2:X:16:DT:H72	1.94	0.47
3:Y:15:DC:H2"	3:Y:16:DT:C5'	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:3:DG:H2”	2:2:4:DC:C5’	2.41	0.47
2:C:2:DG:C2’	2:C:3:DG:C8	2.95	0.47
3:L:11:DA:H1’	3:L:12:DC:C5’	2.36	0.47
3:L:15:DC:H2”	3:L:16:DT:C5’	2.44	0.47
3:P:19:DA:H2”	3:P:20:DT:C5’	2.43	0.47
2:T:6:DG:C2’	2:T:7:DT:H71	2.41	0.47
3:H:14:DA:C1’	3:H:15:DC:H5”	2.42	0.47
2:K:11:DA:H2”	2:K:12:DA:C5’	2.34	0.47
3:L:10:DG:H2”	3:L:11:DA:H8	1.80	0.47
2:C:7:DT:C2’	2:C:8:DC:H5”	2.44	0.47
3:H:8:DG:H2”	3:H:9:DT:H5’	1.92	0.47
3:L:24:DA:H1’	3:L:25:DG:C5’	2.44	0.47
3:Y:10:DG:H2”	3:Y:11:DA:H8	1.79	0.47
2:G:12:DA:C2’	2:G:13:DA:C5’	2.89	0.47
2:G:17:DG:H2”	2:G:18:DT:H5’	1.96	0.47
3:3:15:DC:H2”	3:3:16:DT:C5’	2.45	0.47
2:T:17:DG:H2”	2:T:18:DT:H5’	1.97	0.47
2:6:7:DT:C2’	2:6:8:DC:H5”	2.44	0.47
2:K:17:DG:H2”	2:K:18:DT:H5’	1.96	0.47
3:U:24:DA:H1’	3:U:25:DG:C5’	2.45	0.47
3:Y:11:DA:H1’	3:Y:12:DC:C5’	2.36	0.47
3:3:10:DG:H2”	3:3:11:DA:H8	1.79	0.47
2:G:3:DG:C2’	2:G:4:DC:H5’	2.39	0.46
2:O:7:DT:C2’	2:O:8:DC:H5”	2.44	0.46
3:P:10:DG:H2”	3:P:11:DA:H8	1.79	0.46
2:O:6:DG:N2	3:P:24:DA:C2	2.83	0.46
3:3:5:DT:H2”	3:3:6:DT:H5’	1.98	0.46
3:D:10:DG:H2”	3:D:11:DA:H8	1.81	0.46
3:H:11:DA:H1’	3:H:12:DC:C5’	2.35	0.46
2:X:20:DA:H2”	2:X:21:DC:OP2	2.16	0.46
3:7:10:DG:H2”	3:7:11:DA:H8	1.81	0.46
3:D:8:DG:H2”	3:D:9:DT:H5’	1.94	0.46
3:H:24:DA:H1’	3:H:25:DG:C5’	2.45	0.46
2:O:2:DG:C2’	2:O:3:DG:C8	2.96	0.46
3:U:14:DA:C1’	3:U:15:DC:H5”	2.42	0.46
3:3:25:DG:C4	3:3:26:DC:C4	3.04	0.46
2:6:3:DG:C2’	2:6:4:DC:H5’	2.42	0.46
3:7:8:DG:H2”	3:7:9:DT:H5’	1.94	0.46
3:P:8:DG:H2”	3:P:9:DT:H5’	1.95	0.46
2:C:3:DG:C2’	2:C:4:DC:H5’	2.42	0.46
2:O:3:DG:H2”	2:O:4:DC:C5’	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:4:DT:H2'	3:P:4:DT:O5'	2.16	0.46
2:T:3:DG:C2'	2:T:4:DC:H5'	2.39	0.46
2:X:7:DT:H2"	2:X:8:DC:C6	2.50	0.46
2:C:4:DC:C2'	2:C:5:DT:H71	2.46	0.46
2:2:2:DG:H2"	2:2:3:DG:O5'	2.16	0.46
3:H:10:DG:H2"	3:H:11:DA:H8	1.80	0.46
2:X:6:DG:H2"	2:X:7:DT:H5'	1.93	0.46
2:X:17:DG:H2"	2:X:18:DT:H5'	1.96	0.46
2:2:15:DT:H2'	2:2:16:DT:H72	1.98	0.46
2:6:4:DC:C2'	2:6:5:DT:H71	2.46	0.46
2:O:3:DG:C2'	2:O:4:DC:H5'	2.43	0.45
3:U:10:DG:H2"	3:U:11:DA:H8	1.81	0.45
3:L:14:DA:C3'	3:L:15:DC:H5"	2.29	0.45
2:T:7:DT:C2'	2:T:8:DC:H5"	2.46	0.45
3:Y:23:DC:H2"	3:Y:24:DA:C8	2.52	0.45
2:O:15:DT:H2'	2:O:16:DT:H72	1.98	0.45
3:P:25:DG:C4	3:P:26:DC:C4	3.04	0.45
3:D:24:DA:H1'	3:D:25:DG:C5'	2.46	0.45
3:H:16:DT:H2'	3:H:17:DT:C7	2.42	0.45
2:K:15:DT:H2"	2:K:16:DT:C5'	2.46	0.45
3:P:5:DT:H2"	3:P:6:DT:H5'	1.98	0.45
3:P:16:DT:H2'	3:P:17:DT:C7	2.44	0.45
3:Y:4:DT:O5'	3:Y:4:DT:H2'	2.17	0.45
2:G:7:DT:C2'	2:G:8:DC:H5"	2.46	0.45
2:G:15:DT:H2"	2:G:16:DT:C5'	2.47	0.45
2:K:12:DA:C2'	2:K:13:DA:C5'	2.91	0.45
2:O:2:DG:H2"	2:O:3:DG:O5'	2.16	0.45
3:P:14:DA:C1'	3:P:15:DC:H5"	2.42	0.45
2:X:12:DA:H2"	2:X:13:DA:H5"	1.96	0.45
2:X:15:DT:H2"	2:X:16:DT:C5'	2.46	0.45
2:T:12:DA:C2'	2:T:13:DA:C5'	2.89	0.45
2:T:24:DA:C4'	2:T:25:DA:OP1	2.45	0.45
2:X:2:DG:H2"	2:X:3:DG:H8	1.80	0.45
2:6:17:DG:C2'	2:6:18:DT:H5"	2.47	0.45
3:7:24:DA:H1'	3:7:25:DG:C5'	2.46	0.45
2:K:2:DG:H2"	2:K:3:DG:H8	1.80	0.45
3:3:24:DA:H1'	3:3:25:DG:C5'	2.47	0.45
2:G:24:DA:H1'	2:G:25:DA:C5'	2.47	0.45
2:2:2:DG:H2"	2:2:3:DG:H8	1.80	0.45
3:D:4:DT:H2'	3:D:4:DT:O5'	2.16	0.45
3:D:5:DT:H2"	3:D:6:DT:H5'	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:3:DG:C2'	2:K:4:DC:H5'	2.42	0.45
2:K:7:DT:C2'	2:K:8:DC:H5"	2.46	0.45
3:L:23:DC:H2"	3:L:24:DA:C8	2.52	0.45
2:T:15:DT:H2'	2:T:16:DT:H72	1.98	0.45
2:X:7:DT:C2'	2:X:8:DC:H5"	2.46	0.45
3:3:4:DT:H2'	3:3:4:DT:O5'	2.16	0.45
3:D:25:DG:C4	3:D:26:DC:C4	3.05	0.45
2:G:15:DT:H2'	2:G:16:DT:H72	1.98	0.45
2:K:20:DA:H2"	2:K:21:DC:OP2	2.16	0.45
2:O:20:DA:H2"	2:O:21:DC:OP2	2.18	0.45
2:X:2:DG:C8	2:X:2:DG:H5"	2.52	0.45
3:7:4:DT:H2'	3:7:4:DT:O5'	2.16	0.45
3:7:5:DT:H2"	3:7:6:DT:H5'	1.98	0.45
3:7:25:DG:C4	3:7:26:DC:C4	3.05	0.45
3:D:23:DC:H2"	3:D:24:DA:C8	2.52	0.44
3:L:25:DG:C4	3:L:26:DC:C4	3.05	0.44
2:2:17:DG:C2'	2:2:18:DT:H5"	2.47	0.44
2:O:17:DG:C2'	2:O:18:DT:H5"	2.47	0.44
3:Y:25:DG:C4	3:Y:26:DC:C4	3.05	0.44
2:2:4:DC:C2'	2:2:5:DT:H71	2.47	0.44
2:6:20:DA:H2"	2:6:21:DC:OP2	2.16	0.44
3:7:23:DC:H2"	3:7:24:DA:C8	2.52	0.44
2:C:17:DG:C2'	2:C:18:DT:H5"	2.47	0.44
2:C:20:DA:H2"	2:C:21:DC:OP2	2.15	0.44
2:C:6:DG:H2"	2:C:7:DT:H5'	1.93	0.44
3:H:25:DG:C4	3:H:26:DC:C4	3.05	0.44
2:K:4:DC:C2'	2:K:5:DT:H71	2.48	0.44
3:P:24:DA:H1'	3:P:25:DG:C5'	2.47	0.44
3:U:8:DG:H2"	3:U:9:DT:H5'	1.92	0.44
3:U:16:DT:H2'	3:U:17:DT:C7	2.42	0.44
3:L:4:DT:O5'	3:L:4:DT:H2'	2.17	0.44
2:2:6:DG:C2'	2:2:7:DT:H71	2.42	0.44
2:6:6:DG:H2"	2:6:7:DT:H5'	1.93	0.44
2:C:24:DA:H1'	2:C:25:DA:C5'	2.46	0.44
2:K:7:DT:H2"	2:K:8:DC:C6	2.50	0.44
2:T:15:DT:H2"	2:T:16:DT:C5'	2.47	0.44
2:X:15:DT:C2'	2:X:16:DT:H5'	2.48	0.44
3:H:5:DT:H2"	3:H:6:DT:H5'	2.00	0.44
3:U:4:DT:H2'	3:U:4:DT:O5'	2.18	0.44
2:K:15:DT:C2'	2:K:16:DT:H5'	2.48	0.44
2:O:24:DA:H1'	2:O:25:DA:C5'	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:25:DG:C4	3:U:26:DC:C4	3.05	0.44
2:X:4:DC:C2'	2:X:5:DT:H71	2.48	0.44
3:3:8:DG:H2"	3:3:9:DT:H5'	1.95	0.44
2:C:7:DT:H2"	2:C:8:DC:C6	2.51	0.44
2:O:4:DC:C2'	2:O:5:DT:H71	2.47	0.44
2:T:20:DA:H2"	2:T:21:DC:OP2	2.18	0.44
2:T:24:DA:H1'	2:T:25:DA:C5'	2.47	0.44
2:X:17:DG:C2'	2:X:18:DT:H5"	2.48	0.44
2:6:24:DA:H1'	2:6:25:DA:C5'	2.46	0.44
2:C:6:DG:C2'	2:C:7:DT:H71	2.42	0.43
3:L:5:DT:H2"	3:L:6:DT:H5'	2.00	0.43
2:T:2:DG:C8	2:T:2:DG:H5"	2.53	0.43
2:T:2:DG:H2"	2:T:3:DG:O5'	2.18	0.43
2:T:6:DG:H2"	2:T:7:DT:H5'	1.93	0.43
2:T:23:DA:H1'	2:T:24:DA:C8	2.53	0.43
2:2:24:DA:H1'	2:2:25:DA:C5'	2.48	0.43
3:3:16:DT:H2"	3:3:17:DT:C6	2.53	0.43
3:L:16:DT:H2'	3:L:17:DT:C7	2.44	0.43
2:2:3:DG:C5	2:2:4:DC:C4	3.06	0.43
2:G:2:DG:H2"	2:G:3:DG:O5'	2.18	0.43
2:G:23:DA:H1'	2:G:24:DA:C8	2.53	0.43
3:P:16:DT:H2"	3:P:17:DT:C6	2.54	0.43
2:C:2:DG:H2"	2:C:3:DG:O5'	2.18	0.43
2:6:2:DG:H2"	2:6:3:DG:O5'	2.17	0.43
3:D:23:DC:H6	3:D:23:DC:H5'	1.83	0.43
3:L:19:DA:C1'	3:L:20:DT:H5"	2.48	0.43
2:O:3:DG:C5	2:O:4:DC:C4	3.06	0.43
3:Y:14:DA:H1'	3:Y:15:DC:H5"	2.00	0.43
2:6:7:DT:H2"	2:6:8:DC:C6	2.52	0.43
3:7:23:DC:H6	3:7:23:DC:H5'	1.84	0.43
2:G:17:DG:C2'	2:G:18:DT:H5"	2.49	0.43
3:H:4:DT:H2'	3:H:4:DT:O5'	2.18	0.43
2:T:2:DG:H2"	2:T:3:DG:H8	1.78	0.43
2:6:6:DG:C2'	2:6:7:DT:H71	2.42	0.43
2:G:4:DC:C2'	2:G:5:DT:H71	2.49	0.43
2:6:3:DG:C5	2:6:4:DC:C4	3.07	0.43
2:C:3:DG:C5	2:C:4:DC:C4	3.07	0.43
3:D:16:DT:H2'	3:D:17:DT:C7	2.44	0.43
2:T:4:DC:H1'	2:T:5:DT:C5'	2.49	0.43
3:7:16:DT:H2'	3:7:17:DT:C7	2.44	0.43
2:T:4:DC:C2'	2:T:5:DT:H71	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:15:DT:H2"	2:X:16:DT:H5'	2.01	0.43
2:X:24:DA:H1'	2:X:25:DA:C5'	2.48	0.43
2:2:20:DA:H2"	2:2:21:DC:OP2	2.18	0.43
3:3:13:DA:C2'	3:3:14:DA:OP2	2.56	0.43
2:C:15:DT:H2"	2:C:16:DT:C5'	2.49	0.43
2:K:2:DG:C8	2:K:2:DG:H5"	2.52	0.43
3:U:19:DA:C1'	3:U:20:DT:H5"	2.46	0.43
2:K:3:DG:C5	2:K:4:DC:C4	3.07	0.42
2:O:12:DA:C2'	2:O:13:DA:C5'	2.89	0.42
3:U:5:DT:H2"	3:U:6:DT:H5'	2.00	0.42
3:U:23:DC:H2"	3:U:24:DA:C8	2.54	0.42
3:Y:5:DT:H2"	3:Y:6:DT:H5'	2.00	0.42
3:Y:16:DT:H2"	3:Y:17:DT:C6	2.54	0.42
3:Y:19:DA:C1'	3:Y:20:DT:H5"	2.48	0.42
2:6:15:DT:H2"	2:6:16:DT:C5'	2.49	0.42
2:2:15:DT:H2"	2:2:16:DT:C5'	2.49	0.42
2:G:20:DA:H2"	2:G:21:DC:OP2	2.19	0.42
3:H:23:DC:H2"	3:H:24:DA:C8	2.54	0.42
2:K:2:DG:H2"	2:K:3:DG:O5'	2.19	0.42
2:K:24:DA:H1'	2:K:25:DA:C5'	2.49	0.42
3:L:14:DA:H1'	3:L:15:DC:H5"	2.00	0.42
2:O:23:DA:H1'	2:O:24:DA:C8	2.54	0.42
2:6:23:DA:H1'	2:6:24:DA:C8	2.54	0.42
2:K:17:DG:C2'	2:K:18:DT:H5"	2.48	0.42
2:T:11:DA:H2"	2:T:12:DA:C5'	2.35	0.42
3:D:5:DT:H2"	3:D:6:DT:C5'	2.50	0.42
3:D:12:DC:H5'	3:D:12:DC:H6	1.84	0.42
3:U:16:DT:H2"	3:U:17:DT:C6	2.54	0.42
3:3:23:DC:H2"	3:3:24:DA:C8	2.54	0.42
3:7:5:DT:H2"	3:7:6:DT:C5'	2.50	0.42
3:H:16:DT:H2"	3:H:17:DT:C6	2.54	0.42
3:L:8:DG:H2"	3:L:9:DT:H5'	1.94	0.42
2:X:2:DG:H2"	2:X:3:DG:O5'	2.19	0.42
2:C:2:DG:H2"	2:C:3:DG:H8	1.80	0.42
2:T:3:DG:C5	2:T:4:DC:C4	3.07	0.42
3:U:14:DA:H1'	3:U:15:DC:H5"	2.02	0.42
3:Y:13:DA:C2'	3:Y:14:DA:OP2	2.56	0.42
2:2:23:DA:H1'	2:2:24:DA:C8	2.55	0.42
3:3:5:DT:H2"	3:3:6:DT:C5'	2.50	0.42
3:7:12:DC:H5'	3:7:12:DC:H6	1.84	0.42
2:G:3:DG:C5	2:G:4:DC:C4	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:15:DT:C2'	2:G:16:DT:H5'	2.49	0.42
2:T:15:DT:C2'	2:T:16:DT:H5'	2.49	0.42
2:T:25:DA:C4	2:T:26:DG:C8	3.08	0.42
2:X:12:DA:C2'	2:X:13:DA:C5'	2.91	0.42
3:3:16:DT:H2'	3:3:17:DT:C7	2.44	0.42
2:G:25:DA:C4	2:G:26:DG:C8	3.08	0.42
3:P:23:DC:H2"	3:P:24:DA:C8	2.54	0.42
2:T:17:DG:C2'	2:T:18:DT:H5"	2.49	0.42
3:U:13:DA:C2'	3:U:14:DA:OP2	2.57	0.42
2:C:23:DA:H1'	2:C:24:DA:C8	2.55	0.42
2:K:15:DT:H2"	2:K:16:DT:H5'	2.01	0.42
2:O:15:DT:H2"	2:O:16:DT:C5'	2.49	0.42
3:Y:8:DG:H2"	3:Y:9:DT:H5'	1.94	0.42
3:Y:24:DA:H1'	3:Y:25:DG:H5'	2.02	0.42
2:O:15:DT:C2'	2:O:16:DT:H5'	2.50	0.41
2:X:3:DG:C2'	2:X:4:DC:H5'	2.42	0.41
2:G:4:DC:H1'	2:G:5:DT:C5'	2.49	0.41
2:K:23:DA:H1'	2:K:24:DA:C8	2.55	0.41
3:L:16:DT:H2"	3:L:17:DT:C6	2.55	0.41
3:P:5:DT:H2"	3:P:6:DT:C5'	2.50	0.41
2:X:3:DG:C5	2:X:4:DC:C4	3.07	0.41
2:6:25:DA:C4	2:6:26:DG:C8	3.08	0.41
2:G:2:DG:C8	2:G:2:DG:H5"	2.53	0.41
2:G:7:DT:H2"	2:G:8:DC:C6	2.51	0.41
3:U:23:DC:H6	3:U:23:DC:H5'	1.86	0.41
2:2:15:DT:C2'	2:2:16:DT:H5'	2.50	0.41
2:2:25:DA:C4	2:2:26:DG:C8	3.08	0.41
3:H:14:DA:H1'	3:H:15:DC:H5"	2.02	0.41
3:P:14:DA:H1'	3:P:15:DC:H5"	2.02	0.41
2:C:25:DA:C4	2:C:26:DG:C8	3.09	0.41
3:H:15:DC:C2'	3:H:16:DT:H72	2.51	0.41
2:K:23:DA:C4	2:K:24:DA:N7	2.89	0.41
3:U:24:DA:H1'	3:U:25:DG:H5'	2.02	0.41
2:6:2:DG:H2"	2:6:3:DG:H8	1.80	0.41
2:C:23:DA:C4	2:C:24:DA:N7	2.88	0.41
2:G:2:DG:H2"	2:G:3:DG:H8	1.78	0.41
3:H:24:DA:H1'	3:H:25:DG:H5'	2.02	0.41
2:O:23:DA:C4	2:O:24:DA:N7	2.88	0.41
3:P:23:DC:H5'	3:P:23:DC:H6	1.85	0.41
3:L:24:DA:H1'	3:L:25:DG:H5'	2.02	0.41
2:X:23:DA:H1'	2:X:24:DA:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:23:DA:C4	2:2:24:DA:N7	2.88	0.41
3:3:19:DA:C1'	3:3:20:DT:H5"	2.48	0.41
2:6:23:DA:C4	2:6:24:DA:N7	2.88	0.41
3:7:19:DA:C1'	3:7:20:DT:H5"	2.49	0.41
2:C:8:DC:H2"	2:C:9:DA:O5'	2.21	0.41
3:D:19:DA:C1'	3:D:20:DT:H5"	2.49	0.41
3:H:19:DA:C1'	3:H:20:DT:H5"	2.46	0.41
2:O:25:DA:C4	2:O:26:DG:C8	3.08	0.41
3:P:19:DA:C1'	3:P:20:DT:H5"	2.48	0.41
2:T:23:DA:C4	2:T:24:DA:N7	2.89	0.41
2:X:3:DG:H2"	2:X:4:DC:C5'	2.40	0.41
2:X:25:DA:C4	2:X:26:DG:C8	3.09	0.41
3:Y:12:DC:H5'	3:Y:12:DC:H6	1.85	0.41
2:6:8:DC:H2"	2:6:9:DA:O5'	2.21	0.41
3:D:16:DT:H2"	3:D:17:DT:C6	2.56	0.41
3:H:23:DC:H5'	3:H:23:DC:H6	1.86	0.41
2:K:25:DA:C4	2:K:26:DG:C8	3.09	0.41
2:T:7:DT:H2"	2:T:8:DC:C6	2.51	0.41
2:X:23:DA:C4	2:X:24:DA:N7	2.88	0.41
3:Y:16:DT:H2'	3:Y:17:DT:C7	2.44	0.41
3:3:14:DA:H1'	3:3:15:DC:H5"	2.02	0.41
3:7:16:DT:H2"	3:7:17:DT:C6	2.56	0.41
2:T:12:DA:C1'	2:T:13:DA:H5"	2.51	0.40
2:G:23:DA:C4	2:G:24:DA:N7	2.88	0.40
3:H:12:DC:H5'	3:H:12:DC:H6	1.86	0.40
2:C:15:DT:C2'	2:C:16:DT:H5'	2.51	0.40
2:G:3:DG:C2'	2:G:4:DC:C5'	3.00	0.40
2:O:4:DC:H1'	2:O:5:DT:C5'	2.51	0.40
2:X:4:DC:H1'	2:X:5:DT:C5'	2.52	0.40
2:6:4:DC:H2"	2:6:5:DT:H71	2.04	0.40
3:L:23:DC:H5'	3:L:23:DC:H6	1.86	0.40
3:3:23:DC:H5'	3:3:23:DC:H6	1.85	0.40
2:6:15:DT:C2'	2:6:16:DT:H5'	2.51	0.40

All (50) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:1:DC:N4	2:X:2:DG:N1[2_456]	0.94	1.26
2:K:2:DG:N1	3:U:1:DC:N4[2_556]	0.97	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2:DG:N2	3:U:1:DC:N3[2_556]	1.36	0.84
3:H:1:DC:N3	2:X:2:DG:N2[2_456]	1.37	0.83
2:K:2:DG:C6	3:U:1:DC:N4[2_556]	1.43	0.77
2:G:2:DG:O6	3:Y:1:DC:N4[4_456]	1.45	0.75
2:G:2:DG:N1	3:Y:1:DC:N4[4_456]	1.46	0.74
3:b:1:DC:N4	2:e:2:DG:N1[4_446]	1.47	0.73
3:P:1:DC:O5'	3:3:26:DC:O3'[3_555]	1.50	0.70
3:L:1:DC:N4	2:T:2:DG:O6[4_446]	1.51	0.69
2:G:2:DG:C6	3:Y:1:DC:N4[4_456]	1.52	0.68
3:H:1:DC:N4	2:X:2:DG:C6[2_456]	1.60	0.60
2:K:2:DG:N1	3:U:1:DC:C4[2_556]	1.60	0.60
3:P:26:DC:O3'	3:3:1:DC:O5'[3_545]	1.69	0.51
2:G:2:DG:N2	3:Y:1:DC:N3[4_456]	1.73	0.47
2:G:2:DG:N1	3:Y:1:DC:C4[4_456]	1.73	0.47
3:L:1:DC:N4	2:T:2:DG:N1[4_446]	1.74	0.46
2:K:2:DG:O6	3:U:1:DC:N4[2_556]	1.75	0.45
2:G:2:DG:N1	3:Y:1:DC:N3[4_456]	1.76	0.44
3:H:1:DC:C4	2:X:2:DG:N1[2_456]	1.76	0.44
3:b:1:DC:N3	2:e:2:DG:N2[4_446]	1.78	0.42
3:L:1:DC:N4	2:T:2:DG:C6[4_446]	1.80	0.40
3:L:1:DC:N3	2:T:2:DG:N1[4_446]	1.84	0.36
2:a:2:DG:O6	3:f:1:DC:N4[2_456]	1.86	0.34
2:K:2:DG:C2	3:U:1:DC:N3[2_556]	1.87	0.33
2:i:2:DG:N1	3:n:1:DC:N4[2_557]	1.90	0.30
2:G:2:DG:C2	3:Y:1:DC:N3[4_456]	1.94	0.26
2:G:1:DT:O4	3:Y:2:DA:N6[4_456]	1.95	0.25
3:H:1:DC:N4	2:X:2:DG:O6[2_456]	1.95	0.25
2:K:2:DG:N2	3:U:1:DC:C2[2_556]	1.97	0.23
3:L:1:DC:N3	2:T:2:DG:N2[4_446]	1.97	0.23
2:K:2:DG:N1	3:U:1:DC:N3[2_556]	1.99	0.21
3:L:2:DA:N6	2:T:1:DT:O4[4_446]	1.99	0.21
3:j:1:DC:N4	2:m:2:DG:O6[4_447]	1.99	0.21
2:G:2:DG:N2	3:Y:1:DC:C2[4_456]	2.01	0.19
3:j:1:DC:N4	2:m:2:DG:N1[4_447]	2.01	0.19
3:b:1:DC:N4	2:e:2:DG:C6[4_446]	2.02	0.18
2:G:2:DG:N2	3:Y:1:DC:O2[4_456]	2.03	0.17
3:L:1:DC:C4	2:T:2:DG:N1[4_446]	2.03	0.17
3:H:1:DC:N3	2:X:2:DG:C2[2_456]	2.04	0.16
3:b:26:DC:O3'	3:f:1:DC:C5'[2_456]	2.05	0.15
3:P:1:DC:C5'	3:3:26:DC:O3'[3_555]	2.07	0.13
3:b:1:DC:N4	2:e:2:DG:O6[4_446]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1:DC:O2	2:T:2:DG:N2[4_446]	2.11	0.09
2:G:1:DT:N3	3:Y:2:DA:N1[4_456]	2.13	0.07
3:H:1:DC:C2	2:X:2:DG:N2[2_456]	2.14	0.06
2:a:2:DG:N1	3:f:1:DC:N4[2_456]	2.15	0.05
3:b:1:DC:C4	2:e:2:DG:N1[4_446]	2.15	0.05
3:b:26:DC:O3'	3:f:1:DC:O5'[2_456]	2.18	0.02
3:H:1:DC:N3	2:X:2:DG:N1[2_456]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.