



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:57 AM GMT

PDB ID : 4I3H  
Title : A three-gate structure of topoisomerase IV from *Streptococcus pneumoniae*  
Authors : Laponogov, I.; Veselkov, D.A.; Pan, X.-S.; Crevel, I.; Fisher, L.M.; Sanderson, M.R.  
Deposited on : 2012-11-26  
Resolution : 3.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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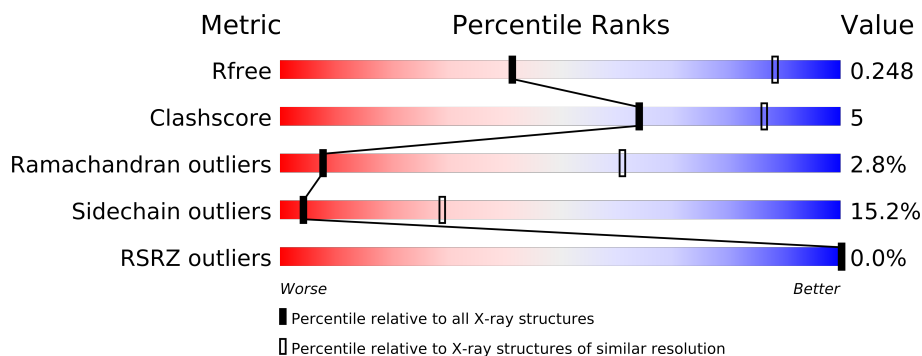
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1098 (4.00-3.40)
Clashscore	79885	1009 (3.94-3.46)
Ramachandran outliers	78287	1016 (3.98-3.42)
Sidechain outliers	78261	1014 (3.98-3.42)
RSRZ outliers	66119	1099 (4.00-3.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	E	34	
1	G	34	
2	F	34	
2	H	34	
3	A	1144	
3	B	1144	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	MG	H	1901	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16228 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	14	Total	C	N	O	P	0	0	0
			282	133	52	83	14			
1	G	20	Total	C	N	O	P	0	0	0
			407	191	77	119	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	14	Total	C	N	O	P	0	0	0
			283	133	51	85	14			
2	H	20	Total	C	N	O	P	0	0	0
			402	189	72	121	20			

- Molecule 3 is a protein called Topoisomerase IV subunit B, DNA topoisomerase 4 subunit A chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1037	Total	C	N	O	S	0	0	0
			7477	4740	1286	1430	21			
3	B	1035	Total	C	N	O	S	0	0	0
			7372	4657	1280	1413	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1000	HIS	-	LINKER	UNP Q3HZ71
B	1000	HIS	-	LINKER	UNP Q3HZ71

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0
4	A	1	Total 1	Mg 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	2	Total 2	O 2	0	0

### 3 Residue-property plots

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

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

Chain E: 



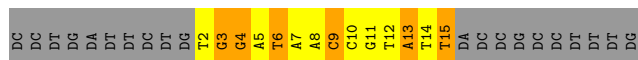
- Molecule 1: DNA (5'-D(\*CP\*AP\*AP\*AP\*GP\*GP\*CP\*GP\*GP\*TP\*AP\*AP\*TP\*AP\*CP\*GP\*GP\*TP\*TP\*AP\*TP\*CP\*CP\*AP\*CP\*AP\*GP\*AP\*AP\*TP\*CP\*AP\*GP\*G)-3')

Chain G: 



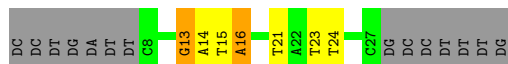
- Molecule 2: DNA (5'-D(\*CP\*CP\*TP\*GP\*AP\*TP\*TP\*CP\*TP\*GP\*TP\*GP\*GP\*AP\*TP\*AP\*AP\*CP\*CP\*GP\*TP\*AP\*TP\*TP\*AP\*CP\*CP\*GP\*CP\*CP\*TP\*TP\*TP\*G)-3')

Chain F: 



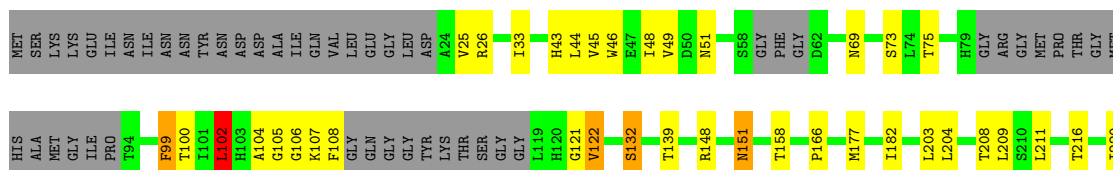
- Molecule 2: DNA (5'-D(\*CP\*CP\*TP\*GP\*AP\*TP\*TP\*CP\*TP\*GP\*TP\*GP\*GP\*AP\*TP\*AP\*AP\*CP\*CP\*GP\*TP\*AP\*TP\*TP\*AP\*CP\*CP\*GP\*CP\*CP\*TP\*TP\*TP\*G)-3')

Chain H: 



- Molecule 3: Topoisomerase IV subunit B, DNA topoisomerase 4 subunit A chimera

Chain A: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.60Å 160.60Å 280.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.82 – 3.70 71.82 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (71.82-3.70) 99.7 (71.82-3.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.10 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.185 , 0.248 0.183 , 0.248	Depositor DCC
$R_{free}$ test set	2007 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	95.5	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 63.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 39830 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	16228	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	E	0.83	1/316 (0.3%)	1.85	12/483 (2.5%)
1	G	0.96	0/457	1.94	12/701 (1.7%)
2	F	0.80	0/317	1.91	10/485 (2.1%)
2	H	0.86	0/450	1.83	13/689 (1.9%)
3	A	0.45	0/7600	0.67	2/10359 (0.0%)
3	B	0.43	0/7491	0.65	2/10214 (0.0%)
All	All	0.50	1/16631 (0.0%)	0.87	51/22931 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	4	DT	C1'-N1	5.18	1.55	1.49

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	20	DA	O4'-C1'-N9	15.76	119.03	108.00
2	H	16	DA	O4'-C4'-C3'	-10.97	99.42	106.00
1	G	24	DA	O4'-C1'-N9	-8.97	101.72	108.00
2	H	21	DT	O4'-C4'-C3'	-8.15	101.11	106.00
2	H	24	DT	O4'-C1'-N1	-8.15	102.30	108.00
2	F	4	DG	N3-C4-C5	7.50	132.35	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	4	DT	N3-C2-O2	-7.35	117.89	122.30
1	G	25	DC	O4'-C1'-C2'	-7.04	100.27	105.90
2	F	15	DT	N3-C4-O4	6.99	124.09	119.90
1	G	20	DA	N9-C1'-C2'	-6.98	99.34	112.60
1	E	4	DT	O4'-C1'-N1	6.83	112.78	108.00
1	G	13	DT	O4'-C1'-C2'	-6.82	100.44	105.90
2	F	6	DT	N3-C4-O4	6.65	123.89	119.90
2	H	13	DG	O4'-C1'-C2'	-6.64	100.59	105.90
2	H	14	DA	O4'-C4'-C3'	-6.58	101.87	104.50
3	A	102	LEU	CA-CB-CG	6.56	130.38	115.30
2	H	21	DT	C4'-C3'-C2'	-6.52	97.23	103.10
1	E	14	DC	C3'-C2'-C1'	-6.39	94.83	102.50
2	F	4	DG	N3-C4-N9	-6.22	122.27	126.00
1	E	9	DT	N3-C4-O4	6.08	123.55	119.90
2	F	6	DT	C5-C4-O4	-6.04	120.67	124.90
1	G	19	DT	N3-C4-O4	6.04	123.52	119.90
1	G	21	DT	O4'-C4'-C3'	-6.00	102.10	104.50
2	F	13	DA	N3-C4-N9	-5.98	122.62	127.40
2	F	13	DA	N1-C2-N3	5.96	132.28	129.30
2	H	21	DT	C5-C4-O4	-5.95	120.73	124.90
1	G	18	DT	N3-C4-O4	5.94	123.47	119.90
1	E	4	DT	N3-C4-O4	5.89	123.44	119.90
1	E	10	DT	N3-C4-O4	5.83	123.40	119.90
2	H	21	DT	N3-C4-O4	5.76	123.36	119.90
1	G	20	DA	O4'-C4'-C3'	5.71	109.42	106.00
1	E	9	DT	C5-C4-O4	-5.66	120.94	124.90
3	B	44	LEU	CA-CB-CG	5.54	128.05	115.30
1	G	25	DC	C3'-C2'-C1'	-5.52	95.88	102.50
2	F	9	DC	N1-C2-O2	5.45	122.17	118.90
3	A	364	LEU	CA-CB-CG	5.42	127.77	115.30
1	G	13	DT	N3-C2-O2	-5.42	119.05	122.30
2	H	13	DG	O4'-C1'-N9	5.36	111.75	108.00
2	H	23	DT	C5-C4-O4	-5.33	121.17	124.90
2	F	13	DA	N9-C4-C5	5.29	107.92	105.80
2	H	15	DT	N3-C4-O4	5.28	123.07	119.90
1	G	9	DG	O4'-C1'-C2'	5.28	110.12	105.90
2	H	14	DA	O4'-C1'-N9	5.24	111.67	108.00
1	E	14	DC	C6-N1-C2	5.20	122.38	120.30
1	E	13	DC	N1-C2-O2	5.14	121.99	118.90
2	H	13	DG	N7-C8-N9	5.14	115.67	113.10
1	E	4	DT	C5-C4-O4	-5.12	121.32	124.90
2	F	3	DG	C3'-C2'-C1'	-5.11	96.37	102.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	196	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	E	4	DT	C6-N1-C2	-5.04	118.78	121.30
1	E	3	DA	O4'-C1'-N9	5.04	111.52	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	102	LEU	Peptide

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	282	0	0	8	1027
1	G	407	0	0	5	0
2	F	283	0	0	8	1027
2	H	402	0	0	2	0
3	A	7477	0	0	42	0
3	B	7372	0	0	38	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	H	1	0	0	0	0
5	E	2	0	0	0	0
All	All	16228	0	0	88	1027

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (88) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:3:DA:N6	2:F:13:DA:N6	2.20	0.89
1:E:3:DA:N1	2:F:13:DA:N1	2.21	0.89
1:E:3:DA:N6	2:F:13:DA:C6	2.47	0.82
3:A:623:GLY:O	3:A:629:ARG:NH2	2.14	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:11:DA:C2	2:F:7:DA:C2	2.72	0.78
3:B:34:GLY:O	3:B:36:THR:N	2.17	0.77
3:B:623:GLY:O	3:B:629:ARG:NH2	2.20	0.75
3:A:304:LYS:O	3:A:306:GLY:N	2.21	0.74
3:B:318:SER:O	3:B:320:TYR:N	2.22	0.73
3:B:99:PHE:O	3:B:101:ILE:N	2.23	0.72
3:A:1397:ASN:O	3:A:1399:ALA:N	2.23	0.72
3:A:51:ASN:ND2	3:A:99:PHE:O	2.22	0.72
1:E:3:DA:C6	2:F:13:DA:N1	2.58	0.71
3:A:132:SER:O	3:A:151:ASN:N	2.25	0.70
3:B:1118:TYR:OH	2:H:16:DA:OP1	2.12	0.68
3:B:227:GLY:O	3:B:230:ASP:N	2.29	0.66
3:A:1006:ASN:N	3:A:1006:ASN:OD1	2.29	0.65
1:E:3:DA:C6	2:F:13:DA:N6	2.65	0.65
3:A:104:ALA:O	3:A:106:GLY:N	2.31	0.64
1:E:3:DA:C6	2:F:13:DA:C6	2.86	0.63
3:A:1171:SER:OG	3:A:1172:ALA:N	2.32	0.62
3:A:1211:PRO:O	3:A:1478:ARG:NH2	2.33	0.62
3:A:1038:LYS:NZ	2:H:13:DG:OP1	2.33	0.61
3:B:1171:SER:OG	3:B:1172:ALA:N	2.31	0.61
3:A:1118:TYR:OH	1:G:16:DG:OP1	2.20	0.60
3:B:488:GLY:N	3:B:525:TYR:O	2.33	0.60
3:A:1107:SER:OG	3:A:1111:ASP:OD1	2.19	0.60
3:B:247:TYR:OH	3:B:258:GLU:OE2	2.20	0.59
3:A:515:GLN:OE1	3:A:1016:ARG:NE	2.37	0.58
3:B:533:GLY:O	3:B:605:ARG:NH1	2.36	0.57
3:B:147:GLN:NE2	3:B:157:THR:O	2.36	0.57
3:B:150:GLU:O	3:B:152:GLY:N	2.37	0.57
3:A:1175:ALA:O	3:A:1328:ASN:ND2	2.39	0.56
3:A:1117:ARG:NH1	1:G:16:DG:OP2	2.38	0.56
3:B:1135:GLU:OE1	3:B:1135:GLU:N	2.39	0.55
3:A:253:ASN:O	3:A:253:ASN:ND2	2.38	0.55
3:B:1406:LYS:O	3:B:1408:SER:N	2.39	0.55
3:B:298:MET:O	3:B:302:ALA:N	2.39	0.55
3:B:1292:ASP:O	3:B:1294:ASP:N	2.40	0.55
3:B:354:PRO:O	3:B:358:GLY:N	2.40	0.54
3:A:1086:VAL:O	3:A:1089:SER:OG	2.26	0.54
3:A:69:ASN:ND2	3:A:73:SER:OG	2.40	0.54
3:A:373:GLU:O	3:A:375:ALA:N	2.42	0.53
3:B:1062:SER:OG	3:B:1119:THR:O	2.27	0.53
3:B:1224:GLU:OE1	3:B:1235:ARG:N	2.41	0.53
3:B:1217:ALA:N	3:B:1258:GLU:OE1	2.41	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:1245:GLU:OE2	3:A:1297:ARG:NH2	2.42	0.53
3:A:132:SER:N	3:A:177:MET:O	2.43	0.52
3:A:341:GLY:O	3:A:343:THR:N	2.43	0.52
3:A:443:GLN:NE2	3:B:1111:ASP:OD2	2.43	0.52
3:B:366:PHE:O	3:B:369:MET:N	2.43	0.51
3:B:151:ASN:OD1	3:B:152:GLY:N	2.44	0.50
3:A:1240:SER:OG	3:A:1321:LEU:O	2.29	0.50
3:B:107:LYS:O	3:B:109:GLY:N	2.45	0.50
3:B:305:THR:O	3:B:307:LEU:N	2.46	0.49
1:E:3:DA:N1	2:F:13:DA:C2	2.80	0.48
3:A:1217:ALA:N	3:A:1258:GLU:OE1	2.48	0.47
3:A:1188:ASP:OD1	3:A:1471:LYS:NZ	2.48	0.47
3:A:629:ARG:NH1	1:G:24:DA:OP1	2.48	0.46
3:A:1177:ASP:N	3:A:1328:ASN:O	2.49	0.46
3:A:361:ALA:O	3:A:365:THR:OG1	2.33	0.46
3:B:216:THR:O	3:B:218:GLU:N	2.48	0.45
3:A:1111:ASP:N	3:A:1111:ASP:OD1	2.48	0.45
3:A:1294:ASP:OD1	3:A:1294:ASP:N	2.50	0.45
3:B:1211:PRO:O	3:B:1478:ARG:NH2	2.50	0.45
3:B:1185:GLU:OE2	3:B:1478:ARG:NH1	2.50	0.44
3:B:366:PHE:O	3:B:368:LEU:N	2.50	0.44
3:B:63:ARG:NH2	3:B:221:GLU:OE1	2.51	0.43
3:B:236:ASN:OD1	3:B:264:ASN:ND2	2.51	0.43
3:A:1428:THR:OG1	3:A:1429:ASN:N	2.51	0.43
3:A:1082:TYR:OH	3:A:1119:THR:OG1	2.37	0.42
3:A:1133:ASP:O	3:A:1138:THR:OG1	2.36	0.42
3:B:1086:VAL:O	3:B:1089:SER:N	2.53	0.42
3:A:1334:ASN:O	3:A:1336:THR:N	2.52	0.42
1:G:8:DG:N2	1:G:9:DG:C4	2.87	0.42
3:B:1082:TYR:OH	3:B:1119:THR:OG1	2.38	0.42
3:A:1135:GLU:N	3:A:1135:GLU:OE1	2.53	0.42
3:A:1102:HIS:N	3:A:1120:GLU:O	2.53	0.42
3:A:510:ASP:OD1	3:A:1028:ARG:NH2	2.53	0.41
3:A:1072:ASN:O	3:A:1144:ASN:ND2	2.54	0.41
3:B:1397:ASN:OD1	3:B:1400:ASP:N	2.54	0.41
3:A:1386:ASP:OD1	3:A:1386:ASP:N	2.54	0.41
3:B:196:ARG:CG	3:B:196:ARG:NH1	2.84	0.40
3:A:373:GLU:C	3:A:375:ALA:N	2.75	0.40
3:A:99:PHE:CD1	3:A:99:PHE:C	2.94	0.40
3:B:1395:SER:O	3:B:1397:ASN:N	2.54	0.40
3:B:1038:LYS:NZ	1:G:13:DT:OP1	2.54	0.40
3:B:336:HIS:O	3:B:349:SER:OG	2.40	0.40

All (1027) 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	Distance(Å)	Clash(Å)
1:E:11:DA:O4'	2:F:11:DG:O4'[2_645]	0.02	2.18
1:E:5:DA:N9	2:F:5:DA:N9[2_645]	0.03	2.17
1:E:8:DG:C8	2:F:8:DA:C8[2_645]	0.03	2.17
1:E:12:DT:C4'	2:F:12:DT:C4'[2_645]	0.03	2.17
1:E:7:DG:C3'	2:F:7:DA:C3'[2_645]	0.04	2.16
1:E:7:DG:O3'	2:F:7:DA:O3'[2_645]	0.04	2.16
1:E:11:DA:C4'	2:F:11:DG:C4'[2_645]	0.04	2.16
1:E:2:DA:O5'	2:F:2:DT:O5'[2_645]	0.05	2.15
1:E:7:DG:C4'	2:F:7:DA:C4'[2_645]	0.05	2.15
1:E:7:DG:O4'	2:F:7:DA:O4'[2_645]	0.05	2.15
1:E:7:DG:C2'	2:F:7:DA:C2'[2_645]	0.05	2.15
1:E:8:DG:P	2:F:8:DA:P[2_645]	0.05	2.15
1:E:8:DG:O5'	2:F:8:DA:O5'[2_645]	0.05	2.15
1:E:11:DA:O5'	2:F:11:DG:O5'[2_645]	0.05	2.15
1:E:11:DA:C5'	2:F:11:DG:C5'[2_645]	0.05	2.15
1:E:11:DA:C3'	2:F:11:DG:C3'[2_645]	0.05	2.15
1:E:11:DA:C2'	2:F:11:DG:C2'[2_645]	0.05	2.15
1:E:11:DA:C1'	2:F:11:DG:C1'[2_645]	0.05	2.15
1:E:12:DT:O4'	2:F:12:DT:O4'[2_645]	0.05	2.15
1:E:5:DA:C8	2:F:5:DA:C8[2_645]	0.06	2.14
1:E:6:DC:C4'	2:F:6:DT:C4'[2_645]	0.06	2.14
1:E:7:DG:O5'	2:F:7:DA:O5'[2_645]	0.06	2.14
1:E:7:DG:C5'	2:F:7:DA:C5'[2_645]	0.06	2.14
1:E:8:DG:C5'	2:F:8:DA:C5'[2_645]	0.06	2.14
1:E:8:DG:C3'	2:F:8:DA:C3'[2_645]	0.06	2.14
1:E:12:DT:C5'	2:F:12:DT:C5'[2_645]	0.06	2.14
1:E:12:DT:C3'	2:F:12:DT:C3'[2_645]	0.06	2.14
1:E:12:DT:C6	2:F:12:DT:C6[2_645]	0.06	2.14
1:E:5:DA:C2'	2:F:5:DA:C2'[2_645]	0.07	2.13
1:E:6:DC:C5'	2:F:6:DT:C5'[2_645]	0.07	2.13
1:E:8:DG:C4'	2:F:8:DA:C4'[2_645]	0.07	2.13
1:E:8:DG:N7	2:F:8:DA:N7[2_645]	0.07	2.13
1:E:12:DT:O5'	2:F:12:DT:O5'[2_645]	0.07	2.13
1:E:12:DT:O3'	2:F:12:DT:O3'[2_645]	0.07	2.13
1:E:13:DC:P	2:F:13:DA:P[2_645]	0.07	2.13
1:E:2:DA:C5'	2:F:2:DT:C5'[2_645]	0.08	2.12
1:E:5:DA:C1'	2:F:5:DA:C1'[2_645]	0.08	2.12
1:E:6:DC:O4'	2:F:6:DT:O4'[2_645]	0.08	2.12
1:E:8:DG:OP2	2:F:8:DA:OP2[2_645]	0.08	2.12
1:E:8:DG:C2'	2:F:8:DA:C2'[2_645]	0.08	2.12
1:E:9:DT:C2'	2:F:9:DC:C2'[2_645]	0.08	2.12

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:11:DA:P	2:F:11:DG:P[2_645]	0.08	2.12
1:E:11:DA:OP2	2:F:11:DG:OP2[2_645]	0.08	2.12
1:E:11:DA:O3'	2:F:11:DG:O3'[2_645]	0.08	2.12
1:E:11:DA:N9	2:F:11:DG:N9[2_645]	0.08	2.12
1:E:12:DT:C1'	2:F:12:DT:C1'[2_645]	0.08	2.12
1:E:2:DA:C4'	2:F:2:DT:C4'[2_645]	0.09	2.11
1:E:2:DA:O4'	2:F:2:DT:O4'[2_645]	0.09	2.11
1:E:2:DA:O3'	2:F:2:DT:O3'[2_645]	0.09	2.11
1:E:3:DA:P	2:F:3:DG:P[2_645]	0.09	2.11
1:E:5:DA:C3'	2:F:5:DA:C3'[2_645]	0.09	2.11
1:E:6:DC:O5'	2:F:6:DT:O5'[2_645]	0.09	2.11
1:E:6:DC:C3'	2:F:6:DT:C3'[2_645]	0.09	2.11
1:E:6:DC:O3'	2:F:6:DT:O3'[2_645]	0.09	2.11
1:E:8:DG:O4'	2:F:8:DA:O4'[2_645]	0.09	2.11
1:E:8:DG:O3'	2:F:8:DA:O3'[2_645]	0.09	2.11
1:E:10:DT:O3'	2:F:10:DC:O3'[2_645]	0.09	2.11
1:E:10:DT:C2'	2:F:10:DC:C2'[2_645]	0.09	2.11
1:E:12:DT:C2'	2:F:12:DT:C2'[2_645]	0.09	2.11
1:E:6:DC:C2'	2:F:6:DT:C2'[2_645]	0.10	2.10
1:E:7:DG:C1'	2:F:7:DA:C1'[2_645]	0.10	2.10
1:E:8:DG:C1'	2:F:8:DA:C1'[2_645]	0.10	2.10
1:E:9:DT:O5'	2:F:9:DC:O5'[2_645]	0.10	2.10
1:E:9:DT:C5'	2:F:9:DC:C5'[2_645]	0.10	2.10
1:E:3:DA:O5'	2:F:3:DG:O5'[2_645]	0.11	2.09
1:E:6:DC:C1'	2:F:6:DT:C1'[2_645]	0.11	2.09
1:E:7:DG:P	2:F:7:DA:P[2_645]	0.11	2.09
1:E:9:DT:P	2:F:9:DC:P[2_645]	0.11	2.09
1:E:9:DT:OP2	2:F:9:DC:OP2[2_645]	0.11	2.09
1:E:10:DT:C3'	2:F:10:DC:C3'[2_645]	0.11	2.09
1:E:11:DA:OP1	2:F:11:DG:OP1[2_645]	0.11	2.09
1:E:12:DT:P	2:F:12:DT:P[2_645]	0.11	2.09
1:E:2:DA:C3'	2:F:2:DT:C3'[2_645]	0.12	2.08
1:E:4:DT:P	2:F:4:DG:P[2_645]	0.12	2.08
1:E:8:DG:OP1	2:F:8:DA:OP1[2_645]	0.12	2.08
1:E:12:DT:C5	2:F:12:DT:C5[2_645]	0.12	2.08
1:E:13:DC:O3'	2:F:13:DA:O3'[2_645]	0.12	2.08
1:E:14:DC:O4'	2:F:14:DT:O4'[2_645]	0.12	2.08
1:E:5:DA:O3'	2:F:5:DA:O3'[2_645]	0.13	2.07
1:E:5:DA:N7	2:F:5:DA:N7[2_645]	0.13	2.07
1:E:6:DC:C6	2:F:6:DT:C6[2_645]	0.13	2.07
1:E:8:DG:N9	2:F:8:DA:N9[2_645]	0.13	2.07
1:E:9:DT:C4'	2:F:9:DC:C4'[2_645]	0.13	2.07

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:3:DA:O3'	2:F:3:DG:O3'[2.645]	0.14	2.06
1:E:5:DA:C4'	2:F:5:DA:C4'[2.645]	0.14	2.06
1:E:5:DA:C4	2:F:5:DA:C4[2.645]	0.14	2.06
1:E:6:DC:P	2:F:6:DT:P[2.645]	0.14	2.06
1:E:11:DA:N7	2:F:11:DG:N7[2.645]	0.14	2.06
1:E:12:DT:OP2	2:F:12:DT:OP2[2.645]	0.14	2.06
1:E:3:DA:C2'	2:F:3:DG:C2'[2.645]	0.15	2.05
1:E:7:DG:OP2	2:F:7:DA:OP2[2.645]	0.15	2.05
1:E:7:DG:N9	2:F:7:DA:N9[2.645]	0.15	2.05
1:E:9:DT:C3'	2:F:9:DC:C3'[2.645]	0.15	2.05
1:E:10:DT:C4'	2:F:10:DC:C4'[2.645]	0.15	2.05
1:E:10:DT:O4'	2:F:10:DC:O4'[2.645]	0.15	2.05
1:E:11:DA:C5	2:F:11:DG:C5[2.645]	0.15	2.05
1:E:3:DA:OP2	2:F:3:DG:OP2[2.645]	0.16	2.04
1:E:3:DA:C3'	2:F:3:DG:C3'[2.645]	0.16	2.04
1:E:6:DC:OP2	2:F:6:DT:OP2[2.645]	0.16	2.04
1:E:7:DG:N7	2:F:7:DA:N7[2.645]	0.16	2.04
1:E:9:DT:OP1	2:F:9:DC:OP1[2.645]	0.16	2.04
1:E:12:DT:OP1	2:F:12:DT:OP1[2.645]	0.16	2.04
1:E:12:DT:N1	2:F:12:DT:N1[2.645]	0.16	2.04
1:E:13:DC:O4'	2:F:13:DA:O4'[2.645]	0.16	2.04
1:E:2:DA:P	2:F:2:DT:P[2.645]	0.17	2.03
1:E:7:DG:OP1	2:F:7:DA:OP1[2.645]	0.17	2.03
1:E:10:DT:C1'	2:F:10:DC:C1'[2.645]	0.17	2.03
1:E:11:DA:C8	2:F:11:DG:C8[2.645]	0.17	2.03
1:E:2:DA:C2'	2:F:2:DT:C2'[2.645]	0.19	2.01
1:E:5:DA:C5	2:F:5:DA:C5[2.645]	0.19	2.01
1:E:5:DA:N3	2:F:5:DA:N3[2.645]	0.19	2.01
1:E:6:DC:N1	2:F:6:DT:N1[2.645]	0.19	2.01
1:E:6:DC:C5	2:F:6:DT:C5[2.645]	0.19	2.01
1:E:7:DG:C8	2:F:7:DA:C8[2.645]	0.19	2.01
1:E:9:DT:O4'	2:F:9:DC:O4'[2.645]	0.19	2.01
1:E:9:DT:C1'	2:F:9:DC:C1'[2.645]	0.19	2.01
1:E:11:DA:C4	2:F:11:DG:C4[2.645]	0.19	2.01
1:E:14:DC:C4'	2:F:14:DT:C4'[2.645]	0.19	2.01
1:E:10:DT:C5'	2:F:10:DC:C5'[2.645]	0.20	2.00
1:E:14:DC:P	2:F:14:DT:P[2.645]	0.20	2.00
1:E:3:DA:OP1	2:F:3:DG:OP1[2.645]	0.21	1.99
1:E:6:DC:OP1	2:F:6:DT:OP1[2.645]	0.21	1.99
1:E:7:DG:C5	2:F:7:DA:C5[2.645]	0.21	1.99
1:E:14:DC:O5'	2:F:14:DT:O5'[2.645]	0.21	1.99
1:E:14:DC:OP1	2:F:14:DT:OP1[2.645]	0.22	1.98

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:10:DT:N1	2:F:10:DC:N1[2.645]	0.23	1.97
1:E:3:DA:C5'	2:F:3:DG:C5'[2.645]	0.24	1.96
1:E:9:DT:O3'	2:F:9:DC:O3'[2.645]	0.24	1.96
1:E:10:DT:O5'	2:F:10:DC:O5'[2.645]	0.24	1.96
1:E:11:DA:C6	2:F:11:DG:C6[2.645]	0.24	1.96
1:E:14:DC:C5'	2:F:14:DT:C5'[2.645]	0.24	1.96
1:E:10:DT:C2	2:F:10:DC:C2[2.645]	0.25	1.95
1:E:3:DA:C4'	2:F:3:DG:C4'[2.645]	0.26	1.94
1:E:5:DA:O4'	2:F:5:DA:O4'[2.645]	0.26	1.94
1:E:8:DG:C5	2:F:8:DA:C5[2.645]	0.26	1.94
1:E:10:DT:O2	2:F:10:DC:O2[2.645]	0.26	1.94
1:E:2:DA:C1'	2:F:2:DT:C1'[2.645]	0.27	1.93
1:E:4:DT:C5'	2:F:4:DG:C5'[2.645]	0.27	1.93
1:E:10:DT:P	2:F:10:DC:P[2.645]	0.27	1.93
1:E:10:DT:C6	2:F:10:DC:C6[2.645]	0.27	1.93
1:E:4:DT:OP2	2:F:4:DG:OP2[2.645]	0.28	1.92
1:E:11:DA:N6	2:F:11:DG:O6[2.645]	0.28	1.92
1:E:14:DC:OP2	2:F:14:DT:OP2[2.645]	0.28	1.92
1:E:3:DA:O4'	2:F:3:DG:O4'[2.645]	0.29	1.91
1:E:5:DA:C6	2:F:5:DA:C6[2.645]	0.29	1.91
1:E:5:DA:C2	2:F:5:DA:C2[2.645]	0.29	1.91
1:E:7:DG:C4	2:F:7:DA:C4[2.645]	0.29	1.91
1:E:9:DT:N1	2:F:9:DC:N1[2.645]	0.29	1.91
1:E:10:DT:OP2	2:F:10:DC:OP2[2.645]	0.29	1.91
1:E:3:DA:C1'	2:F:3:DG:C1'[2.645]	0.31	1.89
1:E:7:DG:O6	2:F:7:DA:N6[2.645]	0.31	1.89
1:E:8:DG:C4	2:F:8:DA:C4[2.645]	0.31	1.89
1:E:7:DG:C6	2:F:7:DA:C6[2.645]	0.32	1.88
1:E:4:DT:OP1	2:F:4:DG:OP1[2.645]	0.33	1.87
1:E:9:DT:C6	2:F:9:DC:C6[2.645]	0.33	1.87
1:E:10:DT:C5	2:F:10:DC:C5[2.645]	0.33	1.87
1:E:12:DT:C4	2:F:12:DT:C4[2.645]	0.33	1.87
1:E:5:DA:N1	2:F:5:DA:N1[2.645]	0.34	1.86
1:E:6:DC:C2	2:F:6:DT:C2[2.645]	0.34	1.86
1:E:10:DT:OP1	2:F:10:DC:OP1[2.645]	0.34	1.86
1:E:10:DT:N3	2:F:10:DC:N3[2.645]	0.34	1.86
1:E:5:DA:N6	2:F:5:DA:N6[2.645]	0.35	1.85
1:E:11:DA:N3	2:F:11:DG:N3[2.645]	0.35	1.85
1:E:13:DC:C3'	2:F:13:DA:C3'[2.645]	0.35	1.85
1:E:8:DG:O6	2:F:8:DA:N6[2.645]	0.36	1.84
1:E:9:DT:O2	2:F:9:DC:O2[2.645]	0.37	1.83
1:E:6:DC:C4	2:F:6:DT:C4[2.645]	0.38	1.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:9:DT:C2	2:F:9:DC:C2[2_645]	0.38	1.82
1:E:14:DC:C3'	2:F:14:DT:C3'[2_645]	0.38	1.82
1:E:12:DT:C2	2:F:12:DT:C2[2_645]	0.39	1.81
1:E:12:DT:O4	2:F:12:DT:O4[2_645]	0.41	1.79
1:E:14:DC:C2'	2:F:14:DT:C2'[2_645]	0.41	1.79
1:E:6:DC:N3	2:F:6:DT:N3[2_645]	0.42	1.78
1:E:8:DG:C6	2:F:8:DA:C6[2_645]	0.42	1.78
1:E:13:DC:C4'	2:F:13:DA:C4'[2_645]	0.42	1.78
1:E:15:DA:O4'	2:F:15:DT:C4'[2_645]	0.42	1.78
1:E:4:DT:N1	2:F:4:DG:C4[2_645]	0.43	1.77
1:E:6:DC:O2	2:F:6:DT:O2[2_645]	0.43	1.77
1:E:9:DT:C5	2:F:9:DC:C5[2_645]	0.43	1.77
1:E:10:DT:C4	2:F:10:DC:C4[2_645]	0.43	1.77
1:E:11:DA:N1	2:F:11:DG:N1[2_645]	0.43	1.77
1:E:15:DA:N7	2:F:15:DT:C6[2_645]	0.43	1.77
1:E:4:DT:O5'	2:F:4:DG:O5'[2_645]	0.44	1.76
1:E:4:DT:O2	2:F:4:DG:C2[2_645]	0.44	1.76
1:E:6:DC:N4	2:F:6:DT:O4[2_645]	0.44	1.76
1:E:14:DC:C1'	2:F:14:DT:C1'[2_645]	0.44	1.76
1:E:12:DT:N3	2:F:12:DT:N3[2_645]	0.45	1.75
1:E:10:DT:O4	2:F:10:DC:N4[2_645]	0.46	1.74
1:E:4:DT:N3	2:F:4:DG:C6[2_645]	0.47	1.73
1:E:3:DA:N9	2:F:3:DG:N9[2_645]	0.48	1.72
1:E:8:DG:N3	2:F:8:DA:N3[2_645]	0.48	1.72
1:E:7:DG:N3	2:F:7:DA:N3[2_645]	0.50	1.70
1:E:11:DA:C2	2:F:11:DG:C2[2_645]	0.50	1.70
1:E:14:DC:O3'	2:F:14:DT:O3'[2_645]	0.50	1.70
1:E:15:DA:C6	2:F:15:DT:N3[2_645]	0.50	1.70
1:E:5:DA:P	2:F:5:DA:P[2_645]	0.51	1.69
1:E:9:DT:N3	2:F:9:DC:N3[2_645]	0.51	1.69
1:E:12:DT:O2	2:F:12:DT:O2[2_645]	0.51	1.69
1:E:15:DA:N9	2:F:15:DT:C1'[2_645]	0.51	1.69
1:E:4:DT:C4'	2:F:4:DG:C4'[2_645]	0.52	1.68
1:E:3:DA:C8	2:F:3:DG:C8[2_645]	0.53	1.67
1:E:7:DG:N1	2:F:7:DA:N1[2_645]	0.56	1.64
1:E:5:DA:C5'	2:F:5:DA:C5'[2_645]	0.57	1.63
1:E:9:DT:C4	2:F:9:DC:C4[2_645]	0.57	1.63
1:E:8:DG:N1	2:F:8:DA:N1[2_645]	0.58	1.62
1:E:4:DT:O4'	2:F:4:DG:O4'[2_645]	0.59	1.61
1:E:13:DC:C1'	2:F:13:DA:C1'[2_645]	0.59	1.61
1:E:8:DG:C2	2:F:8:DA:C2[2_645]	0.61	1.59
1:E:2:DA:N9	2:F:2:DT:N1[2_645]	0.63	1.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:4:DT:C6	2:F:4:DG:N7[2_645]	0.64	1.56
1:E:7:DG:C2	2:F:7:DA:C2[2_645]	0.65	1.55
1:E:13:DC:C2'	2:F:13:DA:C2'[2_645]	0.65	1.55
1:E:13:DC:C5	2:F:13:DA:N7[2_645]	0.65	1.55
1:E:9:DT:O4	2:F:9:DC:N4[2_645]	0.66	1.54
1:E:2:DA:N7	2:F:2:DT:C5[2_645]	0.69	1.51
1:E:15:DA:C5'	2:F:15:DT:O5'[2_645]	0.69	1.51
1:E:13:DC:C2	2:F:13:DA:N3[2_645]	0.70	1.50
1:E:15:DA:C2	2:F:15:DT:O2[2_645]	0.70	1.50
1:E:2:DA:C6	2:F:2:DT:C4[2_645]	0.72	1.48
1:E:2:DA:N6	2:F:2:DT:O4[2_645]	0.73	1.47
1:E:3:DA:C4	2:F:3:DG:C4[2_645]	0.73	1.47
1:E:13:DC:OP1	2:F:13:DA:OP1[2_645]	0.73	1.47
1:E:13:DC:OP2	2:F:13:DA:OP2[2_645]	0.73	1.47
1:E:14:DC:N1	2:F:14:DT:N1[2_645]	0.73	1.47
1:E:2:DA:C5	2:F:2:DT:C5[2_645]	0.74	1.46
1:E:15:DA:P	2:F:15:DT:P[2_645]	0.74	1.46
1:E:14:DC:C2	2:F:14:DT:O2[2_645]	0.76	1.44
1:E:15:DA:OP2	2:F:15:DT:OP2[2_645]	0.76	1.44
1:E:13:DC:C6	2:F:13:DA:N9[2_645]	0.77	1.43
1:E:2:DA:C8	2:F:2:DT:C6[2_645]	0.78	1.42
1:E:3:DA:N7	2:F:3:DG:N7[2_645]	0.78	1.42
1:E:4:DT:C1'	2:F:4:DG:C1'[2_645]	0.78	1.42
1:E:4:DT:C3'	2:F:4:DG:C3'[2_645]	0.80	1.40
1:E:13:DC:N4	2:F:13:DA:N6[2_645]	0.81	1.39
1:E:2:DA:OP2	2:F:2:DT:OP2[2_645]	0.82	1.38
1:E:13:DC:C5	2:F:13:DA:C5[2_645]	0.82	1.38
1:E:14:DC:C6	2:F:14:DT:C6[2_645]	0.82	1.38
1:E:15:DA:C5'	2:F:15:DT:C5'[2_645]	0.82	1.38
1:E:3:DA:C2	2:F:3:DG:N1[2_645]	0.83	1.37
1:E:15:DA:P	2:F:15:DT:OP1[2_645]	0.83	1.37
1:E:15:DA:OP1	2:F:15:DT:OP1[2_645]	0.83	1.37
1:E:3:DA:N3	2:F:3:DG:N3[2_645]	0.85	1.35
1:E:13:DC:O5'	2:F:13:DA:O5'[2_645]	0.85	1.35
1:E:2:DA:C5	2:F:2:DT:C4[2_645]	0.87	1.33
1:E:4:DT:O4	2:F:4:DG:O6[2_645]	0.87	1.33
1:E:2:DA:C6	2:F:2:DT:O4[2_645]	0.88	1.32
1:E:4:DT:C2'	2:F:4:DG:C2'[2_645]	0.88	1.32
1:E:3:DA:C5	2:F:3:DG:C5[2_645]	0.89	1.31
1:E:4:DT:C1'	2:F:4:DG:N9[2_645]	0.89	1.31
1:E:4:DT:O2	2:F:4:DG:N3[2_645]	0.89	1.31
1:E:13:DC:C4	2:F:13:DA:C5[2_645]	0.89	1.31

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:13:DC:C4	2:F:13:DA:C6[2.645]	0.89	1.31
1:E:14:DC:C6	2:F:14:DT:N1[2.645]	0.89	1.31
1:E:15:DA:O5'	2:F:15:DT:O5'[2.645]	0.89	1.31
1:E:2:DA:N3	2:F:2:DT:C2[2.645]	0.90	1.30
1:E:4:DT:C5	2:F:4:DG:N7[2.645]	0.90	1.30
1:E:13:DC:C6	2:F:13:DA:C8[2.645]	0.90	1.30
1:E:14:DC:C4	2:F:14:DT:N3[2.645]	0.91	1.29
1:E:4:DT:C4'	2:F:4:DG:O4'[2.645]	0.93	1.27
1:E:4:DT:C3'	2:F:4:DG:C2'[2.645]	0.95	1.25
1:E:13:DC:N1	2:F:13:DA:C4[2.645]	0.95	1.25
1:E:13:DC:N1	2:F:13:DA:N9[2.645]	0.96	1.24
1:E:15:DA:C5	2:F:15:DT:N1[2.645]	0.96	1.24
1:E:15:DA:C4	2:F:15:DT:N1[2.645]	0.96	1.24
1:E:2:DA:N9	2:F:2:DT:C6[2.645]	0.97	1.23
1:E:4:DT:C6	2:F:4:DG:C8[2.645]	0.97	1.23
1:E:15:DA:N3	2:F:15:DT:O2[2.645]	0.97	1.23
1:E:4:DT:N3	2:F:4:DG:N1[2.645]	0.99	1.21
1:E:4:DT:C4	2:F:4:DG:O6[2.645]	0.99	1.21
1:E:4:DT:C4	2:F:4:DG:C6[2.645]	0.99	1.21
1:E:15:DA:C2'	2:F:15:DT:C3'[2.645]	0.99	1.21
1:E:3:DA:C4	2:F:3:DG:C5[2.645]	1.00	1.20
1:E:5:DA:OP2	2:F:5:DA:OP2[2.645]	1.00	1.20
1:E:2:DA:C4	2:F:2:DT:N1[2.645]	1.02	1.18
1:E:4:DT:N1	2:F:4:DG:N9[2.645]	1.03	1.17
1:E:13:DC:C5'	2:F:13:DA:O5'[2.645]	1.03	1.17
1:E:14:DC:C2	2:F:14:DT:C2[2.645]	1.03	1.17
1:E:3:DA:N1	2:F:3:DG:C6[2.645]	1.04	1.16
1:E:4:DT:C2	2:F:4:DG:C4[2.645]	1.05	1.15
1:E:15:DA:C5	2:F:15:DT:C2[2.645]	1.05	1.15
1:E:3:DA:N3	2:F:3:DG:C4[2.645]	1.06	1.14
1:E:4:DT:C2'	2:F:4:DG:C1'[2.645]	1.07	1.13
1:E:13:DC:O5'	2:F:13:DA:C5'[2.645]	1.07	1.13
1:E:3:DA:N9	2:F:3:DG:C8[2.645]	1.08	1.12
1:E:5:DA:O5'	2:F:5:DA:O5'[2.645]	1.08	1.12
1:E:10:DT:O2	2:F:10:DC:C2[2.645]	1.08	1.12
1:E:3:DA:C5	2:F:3:DG:N7[2.645]	1.09	1.11
1:E:3:DA:C6	2:F:3:DG:C6[2.645]	1.09	1.11
1:E:15:DA:C1'	2:F:15:DT:C3'[2.645]	1.09	1.11
1:E:14:DC:N1	2:F:14:DT:C1'[2.645]	1.10	1.10
1:E:15:DA:N6	2:F:15:DT:C4[2.645]	1.10	1.10
1:E:10:DT:C4	2:F:10:DC:N4[2.645]	1.11	1.09
1:E:2:DA:C4	2:F:2:DT:C2[2.645]	1.12	1.08

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:3:DA:C2	2:F:3:DG:C2[2_645]	1.12	1.08
1:E:14:DC:O2	2:F:14:DT:O2[2_645]	1.13	1.07
1:E:13:DC:C5'	2:F:13:DA:C5'[2_645]	1.14	1.06
1:E:5:DA:P	2:F:5:DA:O5'[2_645]	1.15	1.05
1:E:9:DT:O2	2:F:9:DC:C2[2_645]	1.15	1.05
1:E:9:DT:C6	2:F:9:DC:C5[2_645]	1.15	1.05
1:E:10:DT:C6	2:F:10:DC:C5[2_645]	1.15	1.05
1:E:14:DC:C2'	2:F:14:DT:C3'[2_645]	1.15	1.05
1:E:15:DA:C4'	2:F:15:DT:C4'[2_645]	1.15	1.05
1:E:5:DA:OP1	2:F:5:DA:P[2_645]	1.16	1.04
1:E:13:DC:N4	2:F:13:DA:C6[2_645]	1.16	1.04
1:E:15:DA:C1'	2:F:15:DT:C2'[2_645]	1.16	1.04
1:E:14:DC:N3	2:F:14:DT:C2[2_645]	1.17	1.03
1:E:10:DT:N3	2:F:10:DC:C4[2_645]	1.18	1.02
1:E:3:DA:C4'	2:F:3:DG:O4'[2_645]	1.20	1.00
1:E:3:DA:C1'	2:F:3:DG:N9[2_645]	1.20	1.00
1:E:3:DA:C6	2:F:3:DG:O6[2_645]	1.20	1.00
1:E:3:DA:N1	2:F:3:DG:N1[2_645]	1.20	1.00
1:E:2:DA:OP1	2:F:2:DT:OP1[2_645]	1.21	0.99
1:E:10:DT:C2	2:F:10:DC:N3[2_645]	1.21	0.99
1:E:14:DC:C5	2:F:14:DT:C5[2_645]	1.21	0.99
1:E:6:DC:N4	2:F:6:DT:C4[2_645]	1.22	0.98
1:E:9:DT:N1	2:F:9:DC:C6[2_645]	1.22	0.98
1:E:10:DT:P	2:F:10:DC:OP2[2_645]	1.22	0.98
1:E:10:DT:N1	2:F:10:DC:C6[2_645]	1.22	0.98
1:E:12:DT:O2	2:F:12:DT:C2[2_645]	1.22	0.98
1:E:3:DA:O4'	2:F:3:DG:C1'[2_645]	1.23	0.97
1:E:4:DT:C6	2:F:4:DG:C5[2_645]	1.23	0.97
1:E:6:DC:C2	2:F:6:DT:O2[2_645]	1.23	0.97
1:E:7:DG:C8	2:F:7:DA:N9[2_645]	1.23	0.97
1:E:7:DG:O6	2:F:7:DA:C6[2_645]	1.23	0.97
1:E:9:DT:C4	2:F:9:DC:N4[2_645]	1.23	0.97
1:E:14:DC:O5'	2:F:14:DT:C5'[2_645]	1.23	0.97
1:E:15:DA:O4'	2:F:15:DT:O4'[2_645]	1.23	0.97
1:E:4:DT:C2	2:F:4:DG:N3[2_645]	1.24	0.96
1:E:7:DG:C4	2:F:7:DA:N3[2_645]	1.24	0.96
1:E:12:DT:C4	2:F:12:DT:O4[2_645]	1.24	0.96
1:E:5:DA:N1	2:F:5:DA:C2[2_645]	1.25	0.95
1:E:6:DC:C5	2:F:6:DT:C6[2_645]	1.25	0.95
1:E:11:DA:C6	2:F:11:DG:O6[2_645]	1.25	0.95
1:E:5:DA:OP1	2:F:4:DG:O3'[2_645]	1.26	0.94
1:E:5:DA:C6	2:F:5:DA:N1[2_645]	1.26	0.94

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:7:DG:N7	2:F:7:DA:C5[2_645]	1.26	0.94
1:E:8:DG:C6	2:F:8:DA:N6[2_645]	1.26	0.94
1:E:10:DT:C5'	2:F:10:DC:O5'[2_645]	1.26	0.94
1:E:11:DA:N3	2:F:11:DG:C4[2_645]	1.26	0.94
1:E:15:DA:OP2	2:F:15:DT:P[2_645]	1.26	0.94
1:E:15:DA:N6	2:F:15:DT:N3[2_645]	1.26	0.94
1:E:15:DA:C4	2:F:15:DT:C2[2_645]	1.26	0.94
1:E:5:DA:C8	2:F:5:DA:N7[2_645]	1.27	0.93
1:E:6:DC:C4	2:F:6:DT:N3[2_645]	1.27	0.93
1:E:7:DG:N7	2:F:7:DA:C8[2_645]	1.27	0.93
1:E:11:DA:C5	2:F:11:DG:N7[2_645]	1.27	0.93
1:E:13:DC:C2	2:F:13:DA:C4[2_645]	1.27	0.93
1:E:15:DA:C8	2:F:15:DT:C6[2_645]	1.27	0.93
1:E:4:DT:N1	2:F:4:DG:C5[2_645]	1.28	0.92
1:E:7:DG:C5	2:F:7:DA:C4[2_645]	1.28	0.92
1:E:11:DA:C2	2:F:11:DG:N1[2_645]	1.28	0.92
1:E:13:DC:O2	2:F:13:DA:N3[2_645]	1.28	0.92
1:E:15:DA:C1'	2:F:15:DT:C1'[2_645]	1.28	0.92
1:E:5:DA:N6	2:F:5:DA:C6[2_645]	1.29	0.91
1:E:8:DG:C8	2:F:8:DA:N7[2_645]	1.29	0.91
1:E:11:DA:N7	2:F:11:DG:C8[2_645]	1.29	0.91
1:E:13:DC:C4'	2:F:13:DA:C3'[2_645]	1.29	0.91
1:E:13:DC:N3	2:F:13:DA:N1[2_645]	1.29	0.91
1:E:15:DA:N9	2:F:15:DT:C2'[2_645]	1.29	0.91
1:E:15:DA:C6	2:F:15:DT:C2[2_645]	1.29	0.91
1:E:5:DA:C2	2:F:5:DA:N3[2_645]	1.30	0.90
1:E:11:DA:N9	2:F:11:DG:C8[2_645]	1.30	0.90
1:E:11:DA:N1	2:F:11:DG:C6[2_645]	1.30	0.90
1:E:13:DC:C6	2:F:13:DA:C4[2_645]	1.30	0.90
1:E:5:DA:N7	2:F:5:DA:C5[2_645]	1.31	0.89
1:E:5:DA:C4	2:F:5:DA:N3[2_645]	1.31	0.89
1:E:8:DG:N7	2:F:8:DA:C8[2_645]	1.31	0.89
1:E:13:DC:O4'	2:F:13:DA:C1'[2_645]	1.31	0.89
1:E:13:DC:C3'	2:F:13:DA:C2'[2_645]	1.31	0.89
1:E:13:DC:N3	2:F:13:DA:C2[2_645]	1.31	0.89
1:E:15:DA:C2'	2:F:15:DT:C2'[2_645]	1.31	0.89
1:E:2:DA:N7	2:F:2:DT:C6[2_645]	1.32	0.88
1:E:3:DA:N6	2:F:3:DG:O6[2_645]	1.32	0.88
1:E:4:DT:C5'	2:F:4:DG:C4'[2_645]	1.32	0.88
1:E:4:DT:C2	2:F:4:DG:C2[2_645]	1.32	0.88
1:E:5:DA:O5'	2:F:5:DA:C5'[2_645]	1.32	0.88
1:E:6:DC:N3	2:F:6:DT:C2[2_645]	1.32	0.88

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:8:DG:O4'	2:F:8:DA:C1'[2.645]	1.32	0.88
1:E:11:DA:C4	2:F:11:DG:N9[2.645]	1.32	0.88
1:E:11:DA:C4	2:F:11:DG:C5[2.645]	1.32	0.88
1:E:12:DT:N3	2:F:12:DT:C4[2.645]	1.32	0.88
1:E:12:DT:O4	2:F:12:DT:C4[2.645]	1.32	0.88
1:E:13:DC:C3'	2:F:13:DA:O3'[2.645]	1.32	0.88
1:E:13:DC:C2'	2:F:13:DA:C1'[2.645]	1.32	0.88
1:E:15:DA:C3'	2:F:15:DT:C3'[2.645]	1.32	0.88
1:E:3:DA:N3	2:F:3:DG:C2[2.645]	1.33	0.87
1:E:6:DC:C3'	2:F:6:DT:O3'[2.645]	1.33	0.87
1:E:6:DC:C6	2:F:6:DT:N1[2.645]	1.33	0.87
1:E:7:DG:N1	2:F:7:DA:C2[2.645]	1.33	0.87
1:E:9:DT:C5'	2:F:9:DC:O5'[2.645]	1.33	0.87
1:E:9:DT:O3'	2:F:9:DC:C3'[2.645]	1.33	0.87
1:E:9:DT:C2	2:F:9:DC:N3[2.645]	1.33	0.87
1:E:9:DT:N3	2:F:9:DC:C4[2.645]	1.33	0.87
1:E:10:DT:O3'	2:F:10:DC:C3'[2.645]	1.33	0.87
1:E:12:DT:N1	2:F:12:DT:C6[2.645]	1.33	0.87
1:E:12:DT:C6	2:F:12:DT:C5[2.645]	1.33	0.87
1:E:14:DC:P	2:F:14:DT:OP1[2.645]	1.33	0.87
1:E:15:DA:N7	2:F:15:DT:C5[2.645]	1.33	0.87
1:E:5:DA:C1'	2:F:5:DA:O4'[2.645]	1.34	0.86
1:E:5:DA:C5	2:F:5:DA:C4[2.645]	1.34	0.86
1:E:7:DG:N9	2:F:7:DA:C4[2.645]	1.34	0.86
1:E:10:DT:OP1	2:F:10:DC:P[2.645]	1.34	0.86
1:E:10:DT:C1'	2:F:10:DC:N1[2.645]	1.34	0.86
1:E:11:DA:C8	2:F:11:DG:N7[2.645]	1.34	0.86
1:E:14:DC:OP2	2:F:14:DT:P[2.645]	1.34	0.86
1:E:2:DA:P	2:F:2:DT:OP2[2.645]	1.35	0.85
1:E:5:DA:O4'	2:F:5:DA:C4'[2.645]	1.35	0.85
1:E:5:DA:N7	2:F:5:DA:C8[2.645]	1.35	0.85
1:E:6:DC:O2	2:F:6:DT:C2[2.645]	1.35	0.85
1:E:7:DG:C6	2:F:7:DA:N1[2.645]	1.35	0.85
1:E:8:DG:N9	2:F:8:DA:C8[2.645]	1.35	0.85
1:E:8:DG:C5	2:F:8:DA:N7[2.645]	1.35	0.85
1:E:8:DG:C4	2:F:8:DA:C5[2.645]	1.35	0.85
1:E:12:DT:C5	2:F:12:DT:C6[2.645]	1.35	0.85
1:E:14:DC:O4'	2:F:14:DT:C4'[2.645]	1.35	0.85
1:E:15:DA:C4	2:F:15:DT:C1'[2.645]	1.35	0.85
1:E:2:DA:C1'	2:F:2:DT:C2'[2.645]	1.36	0.84
1:E:5:DA:OP1	2:F:5:DA:OP1[2.645]	1.36	0.84
1:E:5:DA:C8	2:F:5:DA:N9[2.645]	1.36	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:7:DG:C8	2:F:7:DA:N7[2_645]	1.36	0.84
1:E:8:DG:N1	2:F:8:DA:C6[2_645]	1.36	0.84
1:E:9:DT:C1'	2:F:9:DC:N1[2_645]	1.36	0.84
1:E:10:DT:C4'	2:F:10:DC:O4'[2_645]	1.36	0.84
1:E:11:DA:C6	2:F:11:DG:C5[2_645]	1.36	0.84
1:E:12:DT:C2	2:F:12:DT:N3[2_645]	1.36	0.84
1:E:14:DC:N3	2:F:14:DT:O2[2_645]	1.36	0.84
1:E:4:DT:O5'	2:F:4:DG:C5'[2_645]	1.37	0.83
1:E:5:DA:C3'	2:F:5:DA:O3'[2_645]	1.37	0.83
1:E:5:DA:N9	2:F:5:DA:C8[2_645]	1.37	0.83
1:E:7:DG:O4'	2:F:7:DA:C1'[2_645]	1.37	0.83
1:E:8:DG:N9	2:F:8:DA:C4[2_645]	1.37	0.83
1:E:9:DT:P	2:F:9:DC:OP2[2_645]	1.37	0.83
1:E:11:DA:N6	2:F:11:DG:C6[2_645]	1.37	0.83
1:E:12:DT:C5'	2:F:12:DT:O5'[2_645]	1.37	0.83
1:E:12:DT:C1'	2:F:12:DT:O4'[2_645]	1.37	0.83
1:E:12:DT:C2	2:F:12:DT:O2[2_645]	1.37	0.83
1:E:14:DC:C1'	2:F:14:DT:C2'[2_645]	1.37	0.83
1:E:15:DA:N9	2:F:15:DT:N1[2_645]	1.37	0.83
1:E:2:DA:C5'	2:F:2:DT:O5'[2_645]	1.38	0.82
1:E:2:DA:O4'	2:F:2:DT:C4'[2_645]	1.38	0.82
1:E:4:DT:OP1	2:F:4:DG:P[2_645]	1.38	0.82
1:E:5:DA:C4	2:F:5:DA:N9[2_645]	1.38	0.82
1:E:6:DC:O4'	2:F:6:DT:C1'[2_645]	1.38	0.82
1:E:6:DC:C2	2:F:6:DT:N1[2_645]	1.38	0.82
1:E:7:DG:O5'	2:F:7:DA:C5'[2_645]	1.38	0.82
1:E:7:DG:C3'	2:F:7:DA:O3'[2_645]	1.38	0.82
1:E:10:DT:O4'	2:F:10:DC:C1'[2_645]	1.38	0.82
1:E:12:DT:P	2:F:12:DT:OP2[2_645]	1.38	0.82
1:E:12:DT:C4	2:F:12:DT:C5[2_645]	1.38	0.82
1:E:15:DA:N6	2:F:15:DT:O4[2_645]	1.38	0.82
1:E:2:DA:C1'	2:F:2:DT:O4'[2_645]	1.39	0.81
1:E:3:DA:C5'	2:F:3:DG:C4'[2_645]	1.39	0.81
1:E:5:DA:N9	2:F:5:DA:C4[2_645]	1.39	0.81
1:E:5:DA:N3	2:F:5:DA:C4[2_645]	1.39	0.81
1:E:6:DC:C5'	2:F:6:DT:O5'[2_645]	1.39	0.81
1:E:7:DG:OP2	2:F:7:DA:P[2_645]	1.39	0.81
1:E:8:DG:C8	2:F:8:DA:N9[2_645]	1.39	0.81
1:E:11:DA:C5'	2:F:11:DG:O5'[2_645]	1.39	0.81
1:E:11:DA:O3'	2:F:11:DG:C3'[2_645]	1.39	0.81
1:E:11:DA:C1'	2:F:11:DG:O4'[2_645]	1.39	0.81
1:E:11:DA:N3	2:F:11:DG:C2[2_645]	1.39	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:12:DT:O3'	2:F:12:DT:C3'[2_645]	1.39	0.81
1:E:12:DT:C2	2:F:12:DT:N1[2_645]	1.39	0.81
1:E:2:DA:C2	2:F:2:DT:N3[2_645]	1.40	0.80
1:E:4:DT:C5	2:F:4:DG:C5[2_645]	1.40	0.80
1:E:5:DA:C5	2:F:5:DA:C6[2_645]	1.40	0.80
1:E:6:DC:P	2:F:6:DT:OP2[2_645]	1.40	0.80
1:E:6:DC:O4'	2:F:6:DT:C4'[2_645]	1.40	0.80
1:E:7:DG:P	2:F:7:DA:OP1[2_645]	1.40	0.80
1:E:8:DG:N3	2:F:8:DA:C4[2_645]	1.40	0.80
1:E:8:DG:N3	2:F:8:DA:C2[2_645]	1.40	0.80
1:E:9:DT:C4'	2:F:9:DC:O4'[2_645]	1.40	0.80
1:E:9:DT:O4'	2:F:9:DC:C1'[2_645]	1.40	0.80
1:E:12:DT:OP1	2:F:12:DT:P[2_645]	1.40	0.80
1:E:14:DC:O4'	2:F:14:DT:C1'[2_645]	1.40	0.80
1:E:14:DC:N3	2:F:14:DT:N3[2_645]	1.40	0.80
1:E:2:DA:N3	2:F:2:DT:O2[2_645]	1.41	0.79
1:E:3:DA:O5'	2:F:3:DG:C5'[2_645]	1.41	0.79
1:E:3:DA:C3'	2:F:3:DG:C2'[2_645]	1.41	0.79
1:E:3:DA:C3'	2:F:3:DG:O3'[2_645]	1.41	0.79
1:E:3:DA:C8	2:F:3:DG:N7[2_645]	1.41	0.79
1:E:5:DA:N3	2:F:5:DA:C2[2_645]	1.41	0.79
1:E:6:DC:N1	2:F:6:DT:C1'[2_645]	1.41	0.79
1:E:7:DG:N9	2:F:7:DA:C1'[2_645]	1.41	0.79
1:E:8:DG:O5'	2:F:8:DA:C5'[2_645]	1.41	0.79
1:E:8:DG:O3'	2:F:8:DA:C3'[2_645]	1.41	0.79
1:E:10:DT:N1	2:F:10:DC:C2[2_645]	1.41	0.79
1:E:11:DA:C2	2:F:11:DG:N3[2_645]	1.41	0.79
1:E:12:DT:N1	2:F:12:DT:C2[2_645]	1.41	0.79
1:E:2:DA:O3'	2:F:2:DT:C3'[2_645]	1.42	0.78
1:E:3:DA:OP1	2:F:3:DG:P[2_645]	1.42	0.78
1:E:6:DC:C6	2:F:6:DT:C5[2_645]	1.42	0.78
1:E:7:DG:C5	2:F:7:DA:C6[2_645]	1.42	0.78
1:E:7:DG:C6	2:F:7:DA:N6[2_645]	1.42	0.78
1:E:8:DG:C4'	2:F:8:DA:O4'[2_645]	1.42	0.78
1:E:8:DG:C4	2:F:8:DA:N3[2_645]	1.42	0.78
1:E:9:DT:C2	2:F:9:DC:N1[2_645]	1.42	0.78
1:E:9:DT:C2	2:F:9:DC:O2[2_645]	1.42	0.78
1:E:10:DT:C2	2:F:10:DC:O2[2_645]	1.42	0.78
1:E:11:DA:P	2:F:11:DG:OP2[2_645]	1.42	0.78
1:E:11:DA:OP1	2:F:11:DG:P[2_645]	1.42	0.78
1:E:13:DC:C4'	2:F:13:DA:O4'[2_645]	1.42	0.78
1:E:15:DA:O5'	2:F:15:DT:P[2_645]	1.42	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:2:DA:C3'	2:F:2:DT:O3'[2.645]	1.43	0.77
1:E:2:DA:C2'	2:F:2:DT:C3'[2.645]	1.43	0.77
1:E:3:DA:P	2:F:3:DG:OP2[2.645]	1.43	0.77
1:E:4:DT:C2	2:F:4:DG:C5[2.645]	1.43	0.77
1:E:5:DA:C4'	2:F:5:DA:C3'[2.645]	1.43	0.77
1:E:6:DC:C1'	2:F:6:DT:C2'[2.645]	1.43	0.77
1:E:6:DC:N1	2:F:6:DT:C6[2.645]	1.43	0.77
1:E:8:DG:OP2	2:F:8:DA:P[2.645]	1.43	0.77
1:E:8:DG:C1'	2:F:8:DA:N9[2.645]	1.43	0.77
1:E:8:DG:N7	2:F:8:DA:C5[2.645]	1.43	0.77
1:E:8:DG:C5	2:F:8:DA:C6[2.645]	1.43	0.77
1:E:8:DG:O6	2:F:8:DA:C6[2.645]	1.43	0.77
1:E:8:DG:C4	2:F:8:DA:N9[2.645]	1.43	0.77
1:E:10:DT:C2	2:F:10:DC:N1[2.645]	1.43	0.77
1:E:11:DA:O4'	2:F:11:DG:C1'[2.645]	1.43	0.77
1:E:11:DA:C8	2:F:11:DG:N9[2.645]	1.43	0.77
1:E:12:DT:C6	2:F:12:DT:N1[2.645]	1.43	0.77
1:E:13:DC:OP2	2:F:13:DA:P[2.645]	1.43	0.77
1:E:14:DC:C5	2:F:14:DT:C6[2.645]	1.43	0.77
1:E:7:DG:C4'	2:F:7:DA:O4'[2.645]	1.44	0.76
1:E:7:DG:C6	2:F:7:DA:C5[2.645]	1.44	0.76
1:E:7:DG:N3	2:F:7:DA:C2[2.645]	1.44	0.76
1:E:8:DG:C5'	2:F:8:DA:O5'[2.645]	1.44	0.76
1:E:9:DT:C5	2:F:9:DC:C4[2.645]	1.44	0.76
1:E:11:DA:O4'	2:F:11:DG:C4'[2.645]	1.44	0.76
1:E:11:DA:C1'	2:F:11:DG:N9[2.645]	1.44	0.76
1:E:11:DA:N9	2:F:11:DG:C4[2.645]	1.44	0.76
1:E:14:DC:C3'	2:F:14:DT:O3'[2.645]	1.44	0.76
1:E:15:DA:O4'	2:F:15:DT:C3'[2.645]	1.44	0.76
1:E:2:DA:C4'	2:F:2:DT:C5'[2.645]	1.45	0.75
1:E:2:DA:O4'	2:F:2:DT:C1'[2.645]	1.45	0.75
1:E:2:DA:C4	2:F:2:DT:C6[2.645]	1.45	0.75
1:E:4:DT:P	2:F:4:DG:OP2[2.645]	1.45	0.75
1:E:5:DA:N9	2:F:5:DA:C1'[2.645]	1.45	0.75
1:E:5:DA:C4	2:F:5:DA:C5[2.645]	1.45	0.75
1:E:6:DC:C1'	2:F:6:DT:O4'[2.645]	1.45	0.75
1:E:6:DC:C4	2:F:6:DT:O4[2.645]	1.45	0.75
1:E:6:DC:C4	2:F:6:DT:C5[2.645]	1.45	0.75
1:E:7:DG:O3'	2:F:7:DA:C3'[2.645]	1.45	0.75
1:E:7:DG:C4	2:F:7:DA:N9[2.645]	1.45	0.75
1:E:8:DG:P	2:F:8:DA:OP1[2.645]	1.45	0.75
1:E:8:DG:C5'	2:F:8:DA:C4'[2.645]	1.45	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:9:DT:C1'	2:F:9:DC:O4'[2.645]	1.45	0.75
1:E:9:DT:N1	2:F:9:DC:C2'[2.645]	1.45	0.75
1:E:11:DA:C5	2:F:11:DG:C4'[2.645]	1.45	0.75
1:E:12:DT:C4'	2:F:12:DT:O4'[2.645]	1.45	0.75
1:E:12:DT:O4'	2:F:12:DT:C4'[2.645]	1.45	0.75
1:E:12:DT:C2'	2:F:12:DT:C1'[2.645]	1.45	0.75
1:E:12:DT:C1'	2:F:12:DT:N1[2.645]	1.45	0.75
1:E:13:DC:C2	2:F:13:DA:C2[2.645]	1.45	0.75
1:E:14:DC:C3'	2:F:14:DT:C4'[2.645]	1.45	0.75
1:E:15:DA:N7	2:F:15:DT:N1[2.645]	1.45	0.75
1:E:3:DA:C5'	2:F:3:DG:O5'[2.645]	1.46	0.74
1:E:3:DA:O3'	2:F:3:DG:C3'[2.645]	1.46	0.74
1:E:5:DA:C6	2:F:5:DA:C5[2.645]	1.46	0.74
1:E:5:DA:C6	2:F:5:DA:N6[2.645]	1.46	0.74
1:E:6:DC:N1	2:F:6:DT:C2[2.645]	1.46	0.74
1:E:6:DC:C5	2:F:6:DT:C4[2.645]	1.46	0.74
1:E:7:DG:O4'	2:F:7:DA:C4'[2.645]	1.46	0.74
1:E:7:DG:C1'	2:F:7:DA:O4'[2.645]	1.46	0.74
1:E:8:DG:C3'	2:F:8:DA:O3'[2.645]	1.46	0.74
1:E:8:DG:C2	2:F:8:DA:N1[2.645]	1.46	0.74
1:E:9:DT:OP1	2:F:9:DC:P[2.645]	1.46	0.74
1:E:10:DT:C3'	2:F:10:DC:C2'[2.645]	1.46	0.74
1:E:10:DT:C1'	2:F:10:DC:O4'[2.645]	1.46	0.74
1:E:10:DT:C5	2:F:10:DC:C4[2.645]	1.46	0.74
1:E:11:DA:N9	2:F:11:DG:C1'[2.645]	1.46	0.74
1:E:12:DT:O4'	2:F:12:DT:C1'[2.645]	1.46	0.74
1:E:14:DC:C1'	2:F:14:DT:O4'[2.645]	1.46	0.74
1:E:2:DA:O5'	2:F:2:DT:C5'[2.645]	1.47	0.73
1:E:5:DA:O3'	2:F:5:DA:C3'[2.645]	1.47	0.73
1:E:5:DA:C1'	2:F:5:DA:N9[2.645]	1.47	0.73
1:E:5:DA:C5	2:F:5:DA:N7[2.645]	1.47	0.73
1:E:6:DC:OP1	2:F:6:DT:P[2.645]	1.47	0.73
1:E:6:DC:O5'	2:F:6:DT:C5'[2.645]	1.47	0.73
1:E:6:DC:C2'	2:F:6:DT:C3'[2.645]	1.47	0.73
1:E:7:DG:C5'	2:F:7:DA:C4'[2.645]	1.47	0.73
1:E:7:DG:C2	2:F:7:DA:N3[2.645]	1.47	0.73
1:E:8:DG:C4'	2:F:8:DA:C3'[2.645]	1.47	0.73
1:E:8:DG:C1'	2:F:8:DA:C2'[2.645]	1.47	0.73
1:E:8:DG:C5	2:F:8:DA:C4[2.645]	1.47	0.73
1:E:8:DG:C6	2:F:8:DA:C5[2.645]	1.47	0.73
1:E:11:DA:C4'	2:F:11:DG:O4'[2.645]	1.47	0.73
1:E:12:DT:C3'	2:F:12:DT:O3'[2.645]	1.47	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:12:DT:C3'	2:F:12:DT:C2'[2.645]	1.47	0.73
1:E:13:DC:P	2:F:13:DA:OP1[2.645]	1.47	0.73
1:E:3:DA:C4	2:F:3:DG:N9[2.645]	1.48	0.72
1:E:4:DT:C2	2:F:4:DG:N1[2.645]	1.48	0.72
1:E:5:DA:OP2	2:F:5:DA:P[2.645]	1.48	0.72
1:E:5:DA:O4'	2:F:5:DA:C1'[2.645]	1.48	0.72
1:E:5:DA:O3'	2:F:6:DT:P[2.645]	1.48	0.72
1:E:6:DC:C4'	2:F:6:DT:C3'[2.645]	1.48	0.72
1:E:7:DG:C5'	2:F:7:DA:O5'[2.645]	1.48	0.72
1:E:8:DG:O4'	2:F:8:DA:C4'[2.645]	1.48	0.72
1:E:11:DA:O5'	2:F:11:DG:C5'[2.645]	1.48	0.72
1:E:11:DA:C3'	2:F:11:DG:O3'[2.645]	1.48	0.72
1:E:11:DA:C5	2:F:11:DG:C6[2.645]	1.48	0.72
1:E:11:DA:C4	2:F:11:DG:N3[2.645]	1.48	0.72
1:E:12:DT:O5'	2:F:12:DT:C5'[2.645]	1.48	0.72
1:E:13:DC:OP1	2:F:13:DA:P[2.645]	1.48	0.72
1:E:14:DC:N1	2:F:14:DT:C2[2.645]	1.48	0.72
1:E:2:DA:C4	2:F:2:DT:N3[2.645]	1.49	0.71
1:E:5:DA:C5'	2:F:5:DA:C4'[2.645]	1.49	0.71
1:E:5:DA:C2	2:F:5:DA:N1[2.645]	1.49	0.71
1:E:8:DG:C2	2:F:8:DA:N3[2.645]	1.49	0.71
1:E:9:DT:C4'	2:F:9:DC:C5'[2.645]	1.49	0.71
1:E:9:DT:C4'	2:F:9:DC:C3'[2.645]	1.49	0.71
1:E:9:DT:C1'	2:F:9:DC:C2'[2.645]	1.49	0.71
1:E:11:DA:C4'	2:F:11:DG:C5'[2.645]	1.49	0.71
1:E:13:DC:O4'	2:F:13:DA:C4'[2.645]	1.49	0.71
1:E:14:DC:C5	2:F:14:DT:C4[2.645]	1.49	0.71
1:E:3:DA:N9	2:F:3:DG:C4[2.645]	1.50	0.70
1:E:4:DT:OP2	2:F:4:DG:P[2.645]	1.50	0.70
1:E:4:DT:N3	2:F:4:DG:C5[2.645]	1.50	0.70
1:E:6:DC:C4'	2:F:6:DT:O4'[2.645]	1.50	0.70
1:E:7:DG:N9	2:F:7:DA:C8[2.645]	1.50	0.70
1:E:7:DG:C5	2:F:7:DA:N7[2.645]	1.50	0.70
1:E:8:DG:C3'	2:F:8:DA:C2'[2.645]	1.50	0.70
1:E:8:DG:C1'	2:F:8:DA:O4'[2.645]	1.50	0.70
1:E:9:DT:C3'	2:F:9:DC:C2'[2.645]	1.50	0.70
1:E:11:DA:C1'	2:F:11:DG:C2'[2.645]	1.50	0.70
1:E:11:DA:N7	2:F:11:DG:C5[2.645]	1.50	0.70
1:E:12:DT:C4'	2:F:12:DT:C5'[2.645]	1.50	0.70
1:E:13:DC:C6	2:F:13:DA:N7[2.645]	1.50	0.70
1:E:2:DA:P	2:F:2:DT:OP1[2.645]	1.51	0.69
1:E:5:DA:C3'	2:F:5:DA:C2'[2.645]	1.51	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:5:DA:C1'	2:F:5:DA:C2'[2.645]	1.51	0.69
1:E:5:DA:N1	2:F:5:DA:C6[2.645]	1.51	0.69
1:E:6:DC:P	2:F:6:DT:OP1[2.645]	1.51	0.69
1:E:6:DC:C5'	2:F:6:DT:C4'[2.645]	1.51	0.69
1:E:6:DC:O3'	2:F:6:DT:C3'[2.645]	1.51	0.69
1:E:6:DC:C2	2:F:6:DT:N3[2.645]	1.51	0.69
1:E:7:DG:C4'	2:F:7:DA:C3'[2.645]	1.51	0.69
1:E:7:DG:C1'	2:F:7:DA:C2'[2.645]	1.51	0.69
1:E:8:DG:OP1	2:F:8:DA:P[2.645]	1.51	0.69
1:E:8:DG:N9	2:F:8:DA:C1'[2.645]	1.51	0.69
1:E:8:DG:N1	2:F:8:DA:C2[2.645]	1.51	0.69
1:E:9:DT:P	2:F:9:DC:OP1[2.645]	1.51	0.69
1:E:9:DT:O4'	2:F:9:DC:C4'[2.645]	1.51	0.69
1:E:10:DT:C4'	2:F:10:DC:C5'[2.645]	1.51	0.69
1:E:10:DT:C4	2:F:10:DC:C5[2.645]	1.51	0.69
1:E:11:DA:C6	2:F:11:DG:N1[2.645]	1.51	0.69
1:E:12:DT:N3	2:F:12:DT:C2[2.645]	1.51	0.69
1:E:15:DA:C5	2:F:15:DT:C6[2.645]	1.51	0.69
1:E:2:DA:C3'	2:F:2:DT:C4'[2.645]	1.52	0.68
1:E:2:DA:C1'	2:F:2:DT:N1[2.645]	1.52	0.68
1:E:3:DA:C3'	2:F:3:DG:C4'[2.645]	1.52	0.68
1:E:3:DA:N7	2:F:3:DG:C8[2.645]	1.52	0.68
1:E:4:DT:P	2:F:3:DG:O3'[2.645]	1.52	0.68
1:E:6:DC:C4'	2:F:6:DT:C5'[2.645]	1.52	0.68
1:E:7:DG:N1	2:F:7:DA:C6[2.645]	1.52	0.68
1:E:7:DG:C4	2:F:7:DA:C5[2.645]	1.52	0.68
1:E:8:DG:P	2:F:8:DA:OP2[2.645]	1.52	0.68
1:E:9:DT:O5'	2:F:9:DC:C5'[2.645]	1.52	0.68
1:E:10:DT:C3'	2:F:10:DC:O3'[2.645]	1.52	0.68
1:E:10:DT:C2'	2:F:10:DC:C1'[2.645]	1.52	0.68
1:E:11:DA:C2'	2:F:11:DG:C3'[2.645]	1.52	0.68
1:E:12:DT:C3'	2:F:12:DT:C4'[2.645]	1.52	0.68
1:E:13:DC:P	2:F:13:DA:OP2[2.645]	1.52	0.68
1:E:13:DC:N1	2:F:13:DA:N3[2.645]	1.52	0.68
1:E:13:DC:N3	2:F:13:DA:C6[2.645]	1.52	0.68
1:E:2:DA:OP2	2:F:2:DT:P[2.645]	1.53	0.67
1:E:2:DA:C4'	2:F:2:DT:O4'[2.645]	1.53	0.67
1:E:3:DA:OP2	2:F:3:DG:P[2.645]	1.53	0.67
1:E:3:DA:C2'	2:F:3:DG:C1'[2.645]	1.53	0.67
1:E:4:DT:O4'	2:F:4:DG:C1'[2.645]	1.53	0.67
1:E:5:DA:C2'	2:F:5:DA:C1'[2.645]	1.53	0.67
1:E:7:DG:C3'	2:F:7:DA:C4'[2.645]	1.53	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:7:DG:C3'	2:F:7:DA:C2'[2_645]	1.53	0.67
1:E:7:DG:C2'	2:F:7:DA:C3'[2_645]	1.53	0.67
1:E:7:DG:C1'	2:F:7:DA:N9[2_645]	1.53	0.67
1:E:10:DT:C4'	2:F:10:DC:C3'[2_645]	1.53	0.67
1:E:10:DT:C3'	2:F:10:DC:C4'[2_645]	1.53	0.67
1:E:11:DA:C4'	2:F:11:DG:C3'[2_645]	1.53	0.67
1:E:11:DA:C3'	2:F:11:DG:C4'[2_645]	1.53	0.67
1:E:11:DA:C3'	2:F:11:DG:C2'[2_645]	1.53	0.67
1:E:12:DT:N1	2:F:12:DT:C1'[2_645]	1.53	0.67
1:E:12:DT:C5	2:F:12:DT:C4[2_645]	1.53	0.67
1:E:13:DC:O3'	2:F:13:DA:C3'[2_645]	1.53	0.67
1:E:13:DC:O3'	2:F:14:DT:P[2_645]	1.53	0.67
1:E:14:DC:C5'	2:F:14:DT:C4'[2_645]	1.53	0.67
1:E:14:DC:C4'	2:F:14:DT:C5'[2_645]	1.53	0.67
1:E:14:DC:C4	2:F:14:DT:C4[2_645]	1.53	0.67
1:E:2:DA:C4'	2:F:2:DT:C3'[2_645]	1.54	0.66
1:E:2:DA:N1	2:F:2:DT:N3[2_645]	1.54	0.66
1:E:2:DA:N3	2:F:2:DT:N3[2_645]	1.54	0.66
1:E:3:DA:C1'	2:F:3:DG:C2'[2_645]	1.54	0.66
1:E:4:DT:C5'	2:F:4:DG:O5'[2_645]	1.54	0.66
1:E:4:DT:O2	2:F:4:DG:N2[2_645]	1.54	0.66
1:E:5:DA:C4'	2:F:5:DA:O4'[2_645]	1.54	0.66
1:E:10:DT:C1'	2:F:10:DC:C2'[2_645]	1.54	0.66
1:E:11:DA:P	2:F:11:DG:OP1[2_645]	1.54	0.66
1:E:11:DA:OP2	2:F:11:DG:P[2_645]	1.54	0.66
1:E:11:DA:C2'	2:F:11:DG:C1'[2_645]	1.54	0.66
1:E:12:DT:C4'	2:F:12:DT:C3'[2_645]	1.54	0.66
1:E:13:DC:P	2:F:12:DT:O3'[2_645]	1.54	0.66
1:E:14:DC:P	2:F:14:DT:O5'[2_645]	1.54	0.66
1:E:14:DC:C4'	2:F:14:DT:O4'[2_645]	1.54	0.66
1:E:14:DC:O3'	2:F:14:DT:C3'[2_645]	1.54	0.66
1:E:15:DA:N1	2:F:15:DT:N3[2_645]	1.54	0.66
1:E:3:DA:P	2:F:3:DG:OP1[2_645]	1.55	0.65
1:E:3:DA:P	2:F:3:DG:O5'[2_645]	1.55	0.65
1:E:5:DA:C2'	2:F:5:DA:C3'[2_645]	1.55	0.65
1:E:6:DC:N3	2:F:6:DT:C4[2_645]	1.55	0.65
1:E:7:DG:C2'	2:F:7:DA:C1'[2_645]	1.55	0.65
1:E:7:DG:N3	2:F:7:DA:C4[2_645]	1.55	0.65
1:E:8:DG:N2	2:F:8:DA:C2[2_645]	1.55	0.65
1:E:9:DT:O5'	2:F:9:DC:P[2_645]	1.55	0.65
1:E:9:DT:C5'	2:F:9:DC:C4'[2_645]	1.55	0.65
1:E:9:DT:N3	2:F:9:DC:C2[2_645]	1.55	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:10:DT:C6	2:F:10:DC:N1[2.645]	1.55	0.65
1:E:12:DT:C5'	2:F:12:DT:C4'[2.645]	1.55	0.65
1:E:12:DT:C4	2:F:12:DT:N3[2.645]	1.55	0.65
1:E:15:DA:C8	2:F:15:DT:N1[2.645]	1.55	0.65
1:E:15:DA:N1	2:F:15:DT:O2[2.645]	1.55	0.65
1:E:2:DA:N9	2:F:2:DT:C1'[2.645]	1.56	0.64
1:E:2:DA:C5	2:F:2:DT:C6[2.645]	1.56	0.64
1:E:3:DA:C4'	2:F:3:DG:C3'[2.645]	1.56	0.64
1:E:6:DC:P	2:F:6:DT:O5'[2.645]	1.56	0.64
1:E:6:DC:C3'	2:F:6:DT:C4'[2.645]	1.56	0.64
1:E:7:DG:P	2:F:7:DA:O5'[2.645]	1.56	0.64
1:E:7:DG:C4'	2:F:7:DA:C5'[2.645]	1.56	0.64
1:E:8:DG:O3'	2:F:9:DC:P[2.645]	1.56	0.64
1:E:8:DG:C6	2:F:8:DA:N1[2.645]	1.56	0.64
1:E:9:DT:C3'	2:F:9:DC:O3'[2.645]	1.56	0.64
1:E:9:DT:O3'	2:F:10:DC:P[2.645]	1.56	0.64
1:E:9:DT:C2'	2:F:9:DC:C3'[2.645]	1.56	0.64
1:E:10:DT:C5'	2:F:10:DC:C4'[2.645]	1.56	0.64
1:E:10:DT:O4'	2:F:10:DC:C4'[2.645]	1.56	0.64
1:E:10:DT:O4	2:F:10:DC:C4[2.645]	1.56	0.64
1:E:10:DT:C5	2:F:10:DC:C6[2.645]	1.56	0.64
1:E:11:DA:C5'	2:F:11:DG:C4'[2.645]	1.56	0.64
1:E:13:DC:C1'	2:F:13:DA:O4'[2.645]	1.56	0.64
1:E:13:DC:C5	2:F:13:DA:C8[2.645]	1.56	0.64
1:E:15:DA:C5	2:F:15:DT:N3[2.645]	1.56	0.64
1:E:2:DA:O3'	2:F:3:DG:P[2.645]	1.57	0.63
1:E:3:DA:N1	2:F:3:DG:O6[2.645]	1.57	0.63
1:E:4:DT:C3'	2:F:4:DG:C4'[2.645]	1.57	0.63
1:E:4:DT:C4	2:F:4:DG:C5[2.645]	1.57	0.63
1:E:6:DC:OP2	2:F:6:DT:P[2.645]	1.57	0.63
1:E:6:DC:O3'	2:F:7:DA:P[2.645]	1.57	0.63
1:E:7:DG:P	2:F:7:DA:OP2[2.645]	1.57	0.63
1:E:7:DG:OP1	2:F:7:DA:P[2.645]	1.57	0.63
1:E:8:DG:P	2:F:8:DA:O5'[2.645]	1.57	0.63
1:E:8:DG:C4'	2:F:8:DA:C5'[2.645]	1.57	0.63
1:E:8:DG:C3'	2:F:8:DA:C4'[2.645]	1.57	0.63
1:E:8:DG:C2'	2:F:8:DA:C3'[2.645]	1.57	0.63
1:E:9:DT:C3'	2:F:9:DC:C4'[2.645]	1.57	0.63
1:E:9:DT:C2'	2:F:9:DC:C1'[2.645]	1.57	0.63
1:E:9:DT:C6	2:F:9:DC:N1[2.645]	1.57	0.63
1:E:10:DT:O5'	2:F:10:DC:P[2.645]	1.57	0.63
1:E:12:DT:P	2:F:12:DT:OP1[2.645]	1.57	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:15:DA:C1'	2:F:15:DT:O3'[2_645]	1.57	0.63
1:E:6:DC:C3'	2:F:6:DT:C2'[2_645]	1.58	0.62
1:E:6:DC:C1'	2:F:6:DT:N1[2_645]	1.58	0.62
1:E:9:DT:C5	2:F:9:DC:C6[2_645]	1.58	0.62
1:E:10:DT:N3	2:F:10:DC:C2[2_645]	1.58	0.62
1:E:11:DA:P	2:F:10:DC:O3'[2_645]	1.58	0.62
1:E:11:DA:O5'	2:F:11:DG:P[2_645]	1.58	0.62
1:E:11:DA:N1	2:F:11:DG:C2[2_645]	1.58	0.62
1:E:12:DT:OP2	2:F:12:DT:P[2_645]	1.58	0.62
1:E:12:DT:C2'	2:F:12:DT:C3'[2_645]	1.58	0.62
1:E:13:DC:C4'	2:F:13:DA:C5'[2_645]	1.58	0.62
1:E:15:DA:C4'	2:F:15:DT:C3'[2_645]	1.58	0.62
1:E:2:DA:OP1	2:F:2:DT:P[2_645]	1.59	0.61
1:E:2:DA:C5'	2:F:2:DT:C4'[2_645]	1.59	0.61
1:E:4:DT:P	2:F:4:DG:OP1[2_645]	1.59	0.61
1:E:5:DA:C4'	2:F:5:DA:C5'[2_645]	1.59	0.61
1:E:8:DG:C2'	2:F:8:DA:C1'[2_645]	1.59	0.61
1:E:9:DT:OP2	2:F:9:DC:P[2_645]	1.59	0.61
1:E:9:DT:C4	2:F:9:DC:C5[2_645]	1.59	0.61
1:E:9:DT:C4	2:F:9:DC:N3[2_645]	1.59	0.61
1:E:9:DT:O4	2:F:9:DC:C4[2_645]	1.59	0.61
1:E:11:DA:O3'	2:F:12:DT:P[2_645]	1.59	0.61
1:E:12:DT:C1'	2:F:12:DT:C2'[2_645]	1.59	0.61
1:E:13:DC:O5'	2:F:13:DA:P[2_645]	1.59	0.61
1:E:15:DA:C4'	2:F:15:DT:C5'[2_645]	1.59	0.61
1:E:2:DA:O5'	2:F:2:DT:P[2_645]	1.60	0.60
1:E:4:DT:P	2:F:4:DG:O5'[2_645]	1.60	0.60
1:E:4:DT:C2'	2:F:4:DG:N9[2_645]	1.60	0.60
1:E:4:DT:C1'	2:F:4:DG:O4'[2_645]	1.60	0.60
1:E:4:DT:N3	2:F:4:DG:O6[2_645]	1.60	0.60
1:E:7:DG:O3'	2:F:8:DA:P[2_645]	1.60	0.60
1:E:12:DT:P	2:F:12:DT:O5'[2_645]	1.60	0.60
1:E:13:DC:N1	2:F:13:DA:C1'[2_645]	1.60	0.60
1:E:2:DA:P	2:F:2:DT:O5'[2_645]	1.61	0.59
1:E:4:DT:C3'	2:F:4:DG:C1'[2_645]	1.61	0.59
1:E:5:DA:P	2:F:4:DG:O3'[2_645]	1.61	0.59
1:E:5:DA:C3'	2:F:5:DA:C4'[2_645]	1.61	0.59
1:E:8:DG:P	2:F:7:DA:O3'[2_645]	1.61	0.59
1:E:10:DT:C2'	2:F:10:DC:C3'[2_645]	1.61	0.59
1:E:12:DT:O5'	2:F:12:DT:P[2_645]	1.61	0.59
1:E:4:DT:O5'	2:F:4:DG:P[2_645]	1.62	0.58
1:E:6:DC:C2'	2:F:6:DT:C1'[2_645]	1.62	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:8:DG:O5'	2:F:8:DA:P[2.645]	1.62	0.58
1:E:10:DT:O5'	2:F:10:DC:C5'[2.645]	1.62	0.58
1:E:10:DT:C4	2:F:10:DC:N3[2.645]	1.62	0.58
1:E:11:DA:C2	2:F:11:DG:N2[2.645]	1.62	0.58
1:E:14:DC:C5'	2:F:14:DT:O5'[2.645]	1.62	0.58
1:E:15:DA:C6	2:F:15:DT:C4[2.645]	1.62	0.58
1:E:15:DA:N1	2:F:15:DT:C2[2.645]	1.62	0.58
1:E:2:DA:C3'	2:F:2:DT:C2'[2.645]	1.63	0.57
1:E:3:DA:C1'	2:F:3:DG:O4'[2.645]	1.63	0.57
1:E:4:DT:O3'	2:F:4:DG:O3'[2.645]	1.63	0.57
1:E:4:DT:C6	2:F:4:DG:N9[2.645]	1.63	0.57
1:E:7:DG:C2	2:F:7:DA:N1[2.645]	1.63	0.57
1:E:11:DA:P	2:F:11:DG:O5'[2.645]	1.63	0.57
1:E:12:DT:P	2:F:11:DG:O3'[2.645]	1.63	0.57
1:E:13:DC:P	2:F:13:DA:O5'[2.645]	1.63	0.57
1:E:13:DC:C6	2:F:13:DA:C5[2.645]	1.63	0.57
1:E:14:DC:C4'	2:F:14:DT:C3'[2.645]	1.63	0.57
1:E:15:DA:C4	2:F:15:DT:O2[2.645]	1.63	0.57
1:E:3:DA:P	2:F:2:DT:O3'[2.645]	1.64	0.56
1:E:7:DG:P	2:F:6:DT:O3'[2.645]	1.64	0.56
1:E:7:DG:O5'	2:F:7:DA:P[2.645]	1.64	0.56
1:E:10:DT:O3'	2:F:11:DG:P[2.645]	1.64	0.56
1:E:14:DC:P	2:F:14:DT:OP2[2.645]	1.64	0.56
1:E:3:DA:O5'	2:F:3:DG:P[2.645]	1.65	0.55
1:E:3:DA:C2'	2:F:3:DG:C3'[2.645]	1.65	0.55
1:E:4:DT:C1'	2:F:4:DG:C4[2.645]	1.65	0.55
1:E:6:DC:O5'	2:F:6:DT:P[2.645]	1.65	0.55
1:E:14:DC:OP1	2:F:14:DT:P[2.645]	1.65	0.55
1:E:14:DC:C4	2:F:14:DT:C2[2.645]	1.65	0.55
1:E:2:DA:C5	2:F:2:DT:N3[2.645]	1.66	0.54
1:E:9:DT:P	2:F:8:DA:O3'[2.645]	1.66	0.54
1:E:9:DT:P	2:F:9:DC:O5'[2.645]	1.66	0.54
1:E:9:DT:N1	2:F:9:DC:C1'[2.645]	1.66	0.54
1:E:10:DT:P	2:F:10:DC:OP1[2.645]	1.67	0.53
1:E:12:DT:O3'	2:F:13:DA:P[2.645]	1.67	0.53
1:E:14:DC:O5'	2:F:14:DT:P[2.645]	1.67	0.53
1:E:3:DA:C4'	2:F:3:DG:C5'[2.645]	1.68	0.52
1:E:3:DA:C2	2:F:3:DG:C6[2.645]	1.68	0.52
1:E:10:DT:P	2:F:10:DC:O5'[2.645]	1.68	0.52
1:E:10:DT:N1	2:F:10:DC:C1'[2.645]	1.68	0.52
1:E:14:DC:O3'	2:F:15:DT:P[2.645]	1.68	0.52
1:E:2:DA:C2'	2:F:2:DT:C1'[2.645]	1.69	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:2:DA:C8	2:F:2:DT:C5[2_645]	1.69	0.51
1:E:2:DA:C6	2:F:2:DT:N3[2_645]	1.69	0.51
1:E:3:DA:C6	2:F:3:DG:C5[2_645]	1.69	0.51
1:E:14:DC:P	2:F:13:DA:O3'[2_645]	1.69	0.51
1:E:3:DA:O3'	2:F:4:DG:P[2_645]	1.70	0.50
1:E:4:DT:C2	2:F:4:DG:C6[2_645]	1.70	0.50
1:E:4:DT:O2	2:F:4:DG:N1[2_645]	1.70	0.50
1:E:10:DT:P	2:F:9:DC:O3'[2_645]	1.70	0.50
1:E:3:DA:O4'	2:F:3:DG:C4'[2_645]	1.71	0.49
1:E:14:DC:N4	2:F:14:DT:N3[2_645]	1.71	0.49
1:E:15:DA:C1'	2:F:15:DT:C4'[2_645]	1.71	0.49
1:E:4:DT:O3'	2:F:5:DA:O5'[2_645]	1.72	0.48
1:E:7:DG:N2	2:F:7:DA:C2[2_645]	1.72	0.48
1:E:13:DC:O2	2:F:13:DA:C2[2_645]	1.72	0.48
1:E:15:DA:C1'	2:F:15:DT:O4'[2_645]	1.72	0.48
1:E:6:DC:P	2:F:5:DA:O3'[2_645]	1.73	0.47
1:E:13:DC:C1'	2:F:13:DA:N9[2_645]	1.73	0.47
1:E:13:DC:N3	2:F:13:DA:N3[2_645]	1.73	0.47
1:E:15:DA:C2	2:F:15:DT:C2[2_645]	1.73	0.47
1:E:4:DT:C4'	2:F:4:DG:C3'[2_645]	1.74	0.46
1:E:5:DA:P	2:F:5:DA:OP2[2_645]	1.74	0.46
1:E:13:DC:N3	2:F:13:DA:C4[2_645]	1.74	0.46
1:E:4:DT:O3'	2:F:4:DG:C3'[2_645]	1.75	0.45
1:E:4:DT:N1	2:F:4:DG:N3[2_645]	1.75	0.45
1:E:10:DT:OP2	2:F:10:DC:P[2_645]	1.75	0.45
1:E:13:DC:C5'	2:F:13:DA:C4'[2_645]	1.75	0.45
1:E:13:DC:N3	2:F:13:DA:C5[2_645]	1.75	0.45
1:E:14:DC:C2'	2:F:14:DT:C1'[2_645]	1.75	0.45
1:E:15:DA:N3	2:F:15:DT:C2[2_645]	1.75	0.45
1:E:2:DA:N1	2:F:2:DT:C4[2_645]	1.76	0.44
1:E:3:DA:N9	2:F:3:DG:C1'[2_645]	1.76	0.44
1:E:3:DA:C8	2:F:3:DG:N9[2_645]	1.76	0.44
1:E:3:DA:C5	2:F:3:DG:C6[2_645]	1.76	0.44
1:E:4:DT:C4'	2:F:4:DG:C5'[2_645]	1.76	0.44
1:E:4:DT:N1	2:F:4:DG:C8[2_645]	1.76	0.44
1:E:4:DT:C6	2:F:4:DG:C4[2_645]	1.76	0.44
1:E:13:DC:C5	2:F:13:DA:C4[2_645]	1.76	0.44
1:E:15:DA:P	2:F:14:DT:O3'[2_645]	1.76	0.44
1:E:14:DC:C2	2:F:14:DT:N1[2_645]	1.77	0.43
1:E:15:DA:C8	2:F:15:DT:C2'[2_645]	1.77	0.43
1:E:13:DC:C3'	2:F:13:DA:C4'[2_645]	1.78	0.42
1:E:14:DC:N4	2:F:14:DT:C4[2_645]	1.78	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:14:DC:C5	2:F:14:DT:N3[2.645]	1.78	0.42
1:E:4:DT:O3'	2:F:4:DG:C2'[2.645]	1.79	0.41
1:E:15:DA:C2'	2:F:15:DT:O3'[2.645]	1.79	0.41
1:E:2:DA:N6	2:F:2:DT:C4[2.645]	1.80	0.40
1:E:3:DA:C4	2:F:3:DG:N7[2.645]	1.80	0.40
1:E:5:DA:P	2:F:5:DA:OP1[2.645]	1.80	0.40
1:E:5:DA:OP2	2:F:5:DA:O5'[2.645]	1.80	0.40
1:E:15:DA:O5'	2:F:15:DT:OP1[2.645]	1.80	0.40
1:E:15:DA:N9	2:F:15:DT:O4'[2.645]	1.80	0.40
1:E:13:DC:C2'	2:F:13:DA:C3'[2.645]	1.81	0.39
1:E:15:DA:C8	2:F:15:DT:C1'[2.645]	1.81	0.39
1:E:15:DA:C4'	2:F:15:DT:O5'[2.645]	1.82	0.38
1:E:2:DA:N3	2:F:2:DT:N1[2.645]	1.84	0.36
1:E:14:DC:C5	2:F:14:DT:N1[2.645]	1.84	0.36
1:E:2:DA:C4	2:F:2:DT:C5[2.645]	1.85	0.35
1:E:14:DC:N4	2:F:14:DT:O4[2.645]	1.85	0.35
1:E:3:DA:N3	2:F:3:DG:C5[2.645]	1.86	0.34
1:E:5:DA:O5'	2:F:5:DA:P[2.645]	1.86	0.34
1:E:5:DA:C5'	2:F:5:DA:O5'[2.645]	1.87	0.33
1:E:13:DC:C4	2:F:13:DA:N6[2.645]	1.88	0.32
1:E:14:DC:C6	2:F:14:DT:C5[2.645]	1.88	0.32
1:E:2:DA:C2	2:F:2:DT:C2[2.645]	1.89	0.31
1:E:4:DT:O2	2:F:4:DG:C4[2.645]	1.89	0.31
1:E:13:DC:C1'	2:F:13:DA:C2'[2.645]	1.89	0.31
1:E:13:DC:C4	2:F:13:DA:N1[2.645]	1.89	0.31
1:E:14:DC:C3'	2:F:14:DT:C2'[2.645]	1.89	0.31
1:E:2:DA:N1	2:F:2:DT:O4[2.645]	1.90	0.30
1:E:3:DA:C2	2:F:3:DG:N3[2.645]	1.90	0.30
1:E:4:DT:C3'	2:F:4:DG:O4'[2.645]	1.90	0.30
1:E:4:DT:C3'	2:F:4:DG:O3'[2.645]	1.90	0.30
1:E:2:DA:C8	2:F:2:DT:N1[2.645]	1.91	0.29
1:E:2:DA:C4	2:F:2:DT:C4[2.645]	1.91	0.29
1:E:3:DA:C4	2:F:3:DG:C8[2.645]	1.91	0.29
1:E:4:DT:C4'	2:F:4:DG:C1'[2.645]	1.91	0.29
1:E:13:DC:C4	2:F:13:DA:C4[2.645]	1.91	0.29
1:E:3:DA:N3	2:F:3:DG:N1[2.645]	1.92	0.28
1:E:3:DA:C4	2:F:3:DG:N3[2.645]	1.92	0.28
1:E:15:DA:O4'	2:F:15:DT:C5'[2.645]	1.92	0.28
1:E:2:DA:C6	2:F:2:DT:C5[2.645]	1.93	0.27
1:E:4:DT:N1	2:F:4:DG:N7[2.645]	1.93	0.27
1:E:4:DT:O4	2:F:4:DG:C6[2.645]	1.93	0.27
1:E:14:DC:C1'	2:F:14:DT:N1[2.645]	1.93	0.27

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:14:DC:C1'	2:F:14:DT:C3'[2_645]	1.93	0.27
1:E:15:DA:OP2	2:F:15:DT:OP1[2_645]	1.95	0.25
1:E:3:DA:N9	2:F:3:DG:N7[2_645]	1.96	0.24
1:E:13:DC:OP2	2:F:13:DA:O5'[2_645]	1.96	0.24
1:E:14:DC:C6	2:F:14:DT:C2[2_645]	1.96	0.24
1:E:2:DA:OP1	2:F:2:DT:OP2[2_645]	1.97	0.23
1:E:4:DT:O4'	2:F:4:DG:C4'[2_645]	1.97	0.23
1:E:13:DC:C4'	2:F:13:DA:C2'[2_645]	1.97	0.23
1:E:15:DA:P	2:F:15:DT:OP2[2_645]	1.98	0.22
1:E:15:DA:C5'	2:F:15:DT:C4'[2_645]	1.98	0.22
1:E:15:DA:C5	2:F:15:DT:C5[2_645]	1.98	0.22
1:E:2:DA:N9	2:F:2:DT:C2[2_645]	1.99	0.21
1:E:4:DT:O4'	2:F:4:DG:N9[2_645]	1.99	0.21
1:E:13:DC:O5'	2:F:13:DA:OP1[2_645]	1.99	0.21
1:E:2:DA:C5	2:F:2:DT:O4[2_645]	2.00	0.20
1:E:5:DA:O5'	2:F:5:DA:OP1[2_645]	2.00	0.20
1:E:3:DA:N7	2:F:3:DG:C5[2_645]	2.01	0.19
1:E:4:DT:O3'	2:F:5:DA:P[2_645]	2.01	0.19
1:E:13:DC:C4	2:F:13:DA:N7[2_645]	2.01	0.19
1:E:3:DA:C5	2:F:3:DG:C4[2_645]	2.02	0.18
1:E:14:DC:N1	2:F:14:DT:O2[2_645]	2.02	0.18
1:E:14:DC:N1	2:F:14:DT:C6[2_645]	2.02	0.18
1:E:3:DA:O4'	2:F:3:DG:N9[2_645]	2.03	0.17
1:E:15:DA:O3'	2:F:15:DT:O3'[2_645]	2.03	0.17
1:E:2:DA:N7	2:F:2:DT:C4[2_645]	2.04	0.16
1:E:11:DA:C5	2:F:11:DG:C8[2_645]	2.04	0.16
1:E:14:DC:C5	2:F:14:DT:C2[2_645]	2.04	0.16
1:E:14:DC:C6	2:F:14:DT:C1'[2_645]	2.04	0.16
1:E:13:DC:N4	2:F:13:DA:C5[2_645]	2.05	0.15
1:E:15:DA:O4'	2:F:15:DT:C1'[2_645]	2.05	0.15
1:E:3:DA:C4'	2:F:3:DG:C1'[2_645]	2.06	0.14
1:E:4:DT:N3	2:F:4:DG:C2[2_645]	2.06	0.14
1:E:7:DG:C8	2:F:7:DA:C4[2_645]	2.06	0.14
1:E:13:DC:C4'	2:F:13:DA:C1'[2_645]	2.06	0.14
1:E:3:DA:N9	2:F:3:DG:C5[2_645]	2.07	0.13
1:E:3:DA:C5	2:F:3:DG:C8[2_645]	2.07	0.13
1:E:4:DT:O3'	2:F:4:DG:C1'[2_645]	2.07	0.13
1:E:7:DG:C8	2:F:7:DA:C5[2_645]	2.07	0.13
1:E:10:DT:O2	2:F:10:DC:N3[2_645]	2.07	0.13
1:E:13:DC:C5	2:F:13:DA:N9[2_645]	2.07	0.13
1:E:15:DA:C5'	2:F:15:DT:P[2_645]	2.07	0.13
1:E:15:DA:C5	2:F:15:DT:C4[2_645]	2.07	0.13

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:4:DT:O3'	2:F:5:DA:C5'[2.645]	2.08	0.12
1:E:4:DT:C5	2:F:4:DG:C6[2.645]	2.08	0.12
1:E:5:DA:C8	2:F:5:DA:C5[2.645]	2.08	0.12
1:E:10:DT:N3	2:F:10:DC:N4[2.645]	2.08	0.12
1:E:15:DA:C3'	2:F:15:DT:O3'[2.645]	2.08	0.12
1:E:13:DC:C5	2:F:13:DA:C6[2.645]	2.09	0.11
1:E:15:DA:P	2:F:15:DT:O5'[2.645]	2.09	0.11
1:E:11:DA:C4	2:F:11:DG:C8[2.645]	2.10	0.10
1:E:8:DG:C8	2:F:8:DA:C5[2.645]	2.11	0.09
1:E:8:DG:C5	2:F:8:DA:C8[2.645]	2.11	0.09
1:E:14:DC:C2'	2:F:14:DT:O3'[2.645]	2.11	0.09
1:E:14:DC:O2	2:F:15:DT:O4'[2.645]	2.11	0.09
1:E:3:DA:C3'	2:F:3:DG:C1'[2.645]	2.12	0.08
1:E:4:DT:O5'	2:F:4:DG:C4'[2.645]	2.13	0.07
1:E:4:DT:C2'	2:F:4:DG:C8[2.645]	2.13	0.07
1:E:4:DT:C1'	2:F:4:DG:N3[2.645]	2.13	0.07
1:E:7:DG:N7	2:F:7:DA:N9[2.645]	2.13	0.07
1:E:7:DG:N7	2:F:7:DA:C4[2.645]	2.13	0.07
1:E:7:DG:C4	2:F:7:DA:C2[2.645]	2.14	0.06
1:E:11:DA:C2	2:F:11:DG:C4[2.645]	2.14	0.06
1:E:14:DC:C1'	2:F:14:DT:C4'[2.645]	2.14	0.06
1:E:14:DC:N1	2:F:14:DT:C2'[2.645]	2.14	0.06
1:E:15:DA:O4'	2:F:15:DT:O3'[2.645]	2.14	0.06
1:E:5:DA:P	2:F:5:DA:C5'[2.645]	2.15	0.05
1:E:15:DA:C6	2:F:15:DT:O2[2.645]	2.15	0.05
1:E:3:DA:C2	2:F:3:DG:C4[2.645]	2.16	0.04
1:E:4:DT:C5'	2:F:4:DG:O4'[2.645]	2.16	0.04
1:E:4:DT:C2'	2:F:4:DG:O4'[2.645]	2.16	0.04
1:E:5:DA:C8	2:F:5:DA:C4[2.645]	2.16	0.04
1:E:7:DG:C5	2:F:7:DA:N9[2.645]	2.16	0.04
1:E:7:DG:C5	2:F:7:DA:C8[2.645]	2.16	0.04
1:E:11:DA:N1	2:F:11:DG:O6[2.645]	2.16	0.04
1:E:13:DC:C3'	2:F:13:DA:C1'[2.645]	2.16	0.04
1:E:14:DC:O2	2:F:14:DT:C2[2.645]	2.16	0.04
1:E:2:DA:C5	2:F:2:DT:N1[2.645]	2.17	0.03
1:E:3:DA:C4	2:F:3:DG:C6[2.645]	2.17	0.03
1:E:4:DT:C5	2:F:4:DG:C8[2.645]	2.17	0.03
1:E:5:DA:C5	2:F:5:DA:C8[2.645]	2.17	0.03
1:E:6:DC:N3	2:F:6:DT:O2[2.645]	2.17	0.03
1:E:8:DG:N9	2:F:8:DA:C5[2.645]	2.17	0.03
1:E:10:DT:N1	2:F:10:DC:C5[2.645]	2.17	0.03
1:E:10:DT:C2	2:F:10:DC:C4[2.645]	2.17	0.03

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:3:DA:N1	2:F:3:DG:C5[2.645]	2.18	0.02
1:E:3:DA:C2	2:F:3:DG:C5[2.645]	2.18	0.02
1:E:4:DT:C4	2:F:4:DG:N7[2.645]	2.18	0.02
1:E:9:DT:O2	2:F:9:DC:N3[2.645]	2.18	0.02
1:E:11:DA:C5	2:F:11:DG:N9[2.645]	2.18	0.02
1:E:11:DA:C4	2:F:11:DG:N7[2.645]	2.18	0.02
1:E:14:DC:C2'	2:F:14:DT:C4'[2.645]	2.18	0.02
1:E:3:DA:N6	2:F:3:DG:C6[2.645]	2.19	0.01
1:E:6:DC:N4	2:F:6:DT:N3[2.645]	2.19	0.01
1:E:7:DG:O6	2:F:7:DA:N1[2.645]	2.19	0.01
1:E:8:DG:C4	2:F:8:DA:C8[2.645]	2.19	0.01
1:E:9:DT:N1	2:F:9:DC:C5[2.645]	2.19	0.01
1:E:11:DA:C8	2:F:11:DG:C5[2.645]	2.19	0.01
1:E:15:DA:C5	2:F:15:DT:O2[2.645]	2.19	0.01
1:E:15:DA:N3	2:F:15:DT:C1'[2.645]	2.19	0.01
1:E:4:DT:C1'	2:F:4:DG:C2'[2.645]	2.20	0.00
1:E:5:DA:C5	2:F:5:DA:N9[2.645]	2.20	0.00
1:E:11:DA:N9	2:F:11:DG:N7[2.645]	2.20	0.00
1:E:11:DA:N9	2:F:11:DG:C5[2.645]	2.20	0.00
1:E:13:DC:N1	2:F:13:DA:C8[2.645]	2.20	0.00

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. 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	A	1017/1144 (89%)	891 (88%)	101 (10%)	25 (2%)	9	63
3	B	1015/1144 (89%)	868 (86%)	115 (11%)	32 (3%)	6	58
All	All	2032/2288 (89%)	1759 (87%)	216 (11%)	57 (3%)	8	61

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	305	THR
3	A	373	GLU
3	A	1398	LYS

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Mol	Chain	Res	Type
3	B	35	SER
3	B	99	PHE
3	B	100	THR
3	B	108	PHE
3	B	151	ASN
3	B	217	ASP
3	B	318	SER
3	B	367	PHE
3	B	1058	SER
3	B	1293	ARG
3	A	105	GLY
3	A	122	VAL
3	A	151	ASN
3	A	304	LYS
3	A	374	LEU
3	A	488	GLY
3	A	516	THR
3	A	1217	ALA
3	B	37	ASP
3	B	228	VAL
3	B	306	GLY
3	B	343	THR
3	B	370	GLU
3	B	488	GLY
3	B	1169	GLY
3	B	1407	VAL
3	B	1408	SER
3	A	107	LYS
3	A	227	GLY
3	A	340	GLU
3	A	567	LEU
3	A	1169	GLY
3	A	1250	GLY
3	B	95	VAL
3	B	305	THR
3	B	315	LEU
3	B	1217	ALA
3	A	132	SER
3	A	418	PRO
3	A	1168	THR
3	A	1279	ASN
3	B	1079	SER

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Mol	Chain	Res	Type
3	A	121	GLY
3	B	156	VAL
3	B	319	ASP
3	B	1184	ALA
3	A	487	VAL
3	A	1384	ILE
3	B	106	GLY
3	A	166	PRO
3	B	444	GLY
3	B	1221	GLY
3	B	152	GLY
3	B	1384	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. 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	A	672/969 (69%)	565 (84%)	107 (16%)	4	27
3	B	640/969 (66%)	548 (86%)	92 (14%)	5	31
All	All	1312/1938 (68%)	1113 (85%)	199 (15%)	4	29

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	25	VAL
3	A	26	ARG
3	A	33	ILE
3	A	43	HIS
3	A	44	LEU
3	A	45	VAL
3	A	46	TRP
3	A	48	ILE
3	A	49	VAL
3	A	75	THR
3	A	99	PHE
3	A	100	THR
3	A	102	LEU

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Mol	Chain	Res	Type
3	A	108	PHE
3	A	122	VAL
3	A	139	THR
3	A	148	ARG
3	A	158	THR
3	A	182	ILE
3	A	203	LEU
3	A	204	LEU
3	A	208	THR
3	A	209	LEU
3	A	211	LEU
3	A	216	THR
3	A	220	ILE
3	A	231	PHE
3	A	233	SER
3	A	235	LEU
3	A	242	LEU
3	A	245	VAL
3	A	253	ASN
3	A	275	VAL
3	A	286	HIS
3	A	288	THR
3	A	298	MET
3	A	299	ASN
3	A	307	LEU
3	A	324	LEU
3	A	328	LEU
3	A	331	LEU
3	A	337	LEU
3	A	340	GLU
3	A	351	LEU
3	A	363	LYS
3	A	364	LEU
3	A	365	THR
3	A	368	LEU
3	A	378	LEU
3	A	429	LEU
3	A	432	VAL
3	A	453	LEU
3	A	462	THR
3	A	478	THR
3	A	501	ILE

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Mol	Chain	Res	Type
3	A	503	ILE
3	A	520	THR
3	A	524	ARG
3	A	536	TYR
3	A	565	GLU
3	A	583	LEU
3	A	591	LEU
3	A	595	THR
3	A	611	LEU
3	A	620	VAL
3	A	627	GLU
3	A	1006	ASN
3	A	1009	LEU
3	A	1024	ILE
3	A	1028	ARG
3	A	1054	THR
3	A	1055	PHE
3	A	1090	GLN
3	A	1111	ASP
3	A	1117	ARG
3	A	1126	ILE
3	A	1138	THR
3	A	1139	VAL
3	A	1148	THR
3	A	1162	LEU
3	A	1168	THR
3	A	1177	ASP
3	A	1183	LEU
3	A	1208	LEU
3	A	1233	LYS
3	A	1236	VAL
3	A	1237	VAL
3	A	1242	THR
3	A	1244	ILE
3	A	1268	LEU
3	A	1279	ASN
3	A	1288	ARG
3	A	1308	THR
3	A	1321	LEU
3	A	1336	THR
3	A	1342	ILE
3	A	1347	SER

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Mol	Chain	Res	Type
3	A	1350	ILE
3	A	1382	ILE
3	A	1385	LEU
3	A	1386	ASP
3	A	1387	GLU
3	A	1430	THR
3	A	1432	VAL
3	A	1457	ARG
3	A	1462	LEU
3	A	1476	THR
3	B	22	LEU
3	B	45	VAL
3	B	46	TRP
3	B	48	ILE
3	B	75	THR
3	B	94	THR
3	B	95	VAL
3	B	99	PHE
3	B	100	THR
3	B	125	SER
3	B	139	THR
3	B	148	ARG
3	B	151	ASN
3	B	156	VAL
3	B	158	THR
3	B	162	ILE
3	B	175	THR
3	B	181	THR
3	B	182	ILE
3	B	196	ARG
3	B	203	LEU
3	B	208	THR
3	B	211	LEU
3	B	212	THR
3	B	229	GLN
3	B	231	PHE
3	B	235	LEU
3	B	241	ILE
3	B	242	LEU
3	B	272	LEU
3	B	280	THR
3	B	286	HIS

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Mol	Chain	Res	Type
3	B	295	THR
3	B	296	LYS
3	B	303	ARG
3	B	308	LEU
3	B	314	ASN
3	B	318	SER
3	B	324	LEU
3	B	328	LEU
3	B	337	LEU
3	B	351	LEU
3	B	417	THR
3	B	445	ARG
3	B	447	ARG
3	B	453	LEU
3	B	462	THR
3	B	478	THR
3	B	494	GLU
3	B	509	THR
3	B	516	THR
3	B	520	THR
3	B	524	ARG
3	B	536	TYR
3	B	591	LEU
3	B	595	THR
3	B	605	ARG
3	B	1009	LEU
3	B	1024	ILE
3	B	1028	ARG
3	B	1041	GLN
3	B	1052	SER
3	B	1060	ARG
3	B	1062	SER
3	B	1111	ASP
3	B	1120	GLU
3	B	1130	LEU
3	B	1139	VAL
3	B	1167	SER
3	B	1168	THR
3	B	1177	ASP
3	B	1183	LEU
3	B	1208	LEU
3	B	1236	VAL

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Mol	Chain	Res	Type
3	B	1268	LEU
3	B	1276	ARG
3	B	1296	LEU
3	B	1297	ARG
3	B	1300	ILE
3	B	1308	THR
3	B	1321	LEU
3	B	1338	ARG
3	B	1355	GLU
3	B	1374	ILE
3	B	1380	ARG
3	B	1400	ASP
3	B	1405	LEU
3	B	1414	GLU
3	B	1422	LEU
3	B	1452	ILE
3	B	1462	LEU
3	B	1478	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	E	14/34 (41%)	-0.63	0 100 100	144, 201, 233, 259	14 (100%)
1	G	20/34 (58%)	-0.39	0 100 100	66, 82, 159, 192	0
2	F	14/34 (41%)	-0.65	0 100 100	138, 196, 225, 254	14 (100%)
2	H	20/34 (58%)	-0.45	0 100 100	60, 85, 168, 199	0
3	A	1037/1144 (90%)	-0.24	0 100 100	35, 83, 129, 225	0
3	B	1035/1144 (90%)	-0.22	1 (0%) 93 88	44, 89, 136, 212	0
All	All	2140/2424 (88%)	-0.23	1 (0%) 100 100	35, 86, 142, 259	28 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	166	PRO	2.2

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	H	1901	1/1	0.18	5.26	72,72,72,72	0
4	MG	A	1700	1/1	0.20	-0.29	94,94,94,94	0
4	MG	B	1700	1/1	0.08	-1.42	109,109,109,109	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.