



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2017 – 11:32 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 : unknown  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

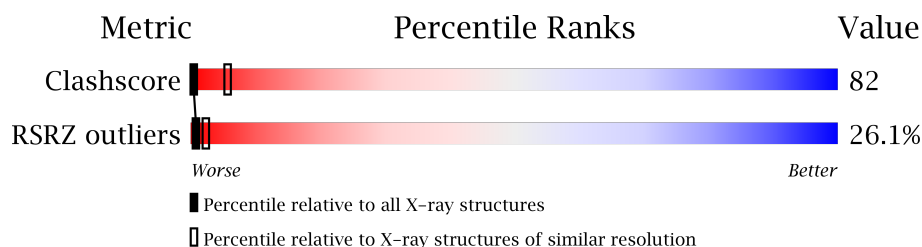
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

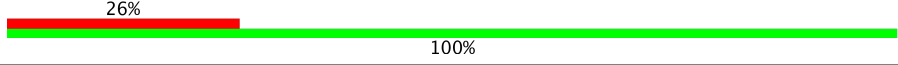
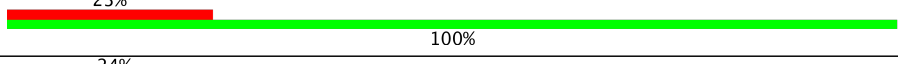
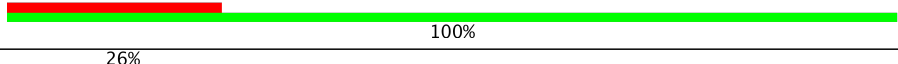
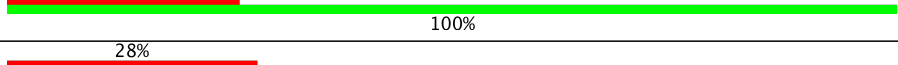
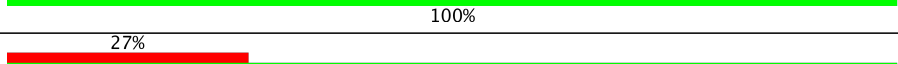
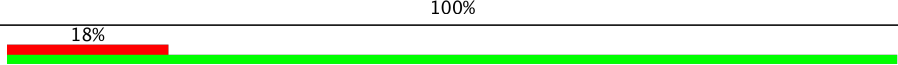
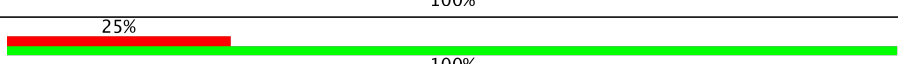


The reported resolution of this entry is 4.33 Å.

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	112137	1025 (5.00-3.68)
RSRZ outliers	101464	1005 (5.04-3.64)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

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Mol	Chain	Length	Quality of chain
1	I	102	27% 
1	J	102	21% 
1	M	102	25% 
1	N	102	24% 
1	R	102	26% 
1	S	102	25% 
1	V	102	27% 
1	W	102	25% 
1	Z	102	25% 
1	c	102	24% 
1	d	102	21% 
1	g	102	22% 
1	h	102	25% 
1	k	102	30% 
1	l	102	20% 
2	2	26	42% 
2	6	26	27% 
2	C	26	19% 
2	G	26	12% 
2	K	26	50% 
2	O	26	46% 
2	T	26	19% 
2	X	26	46% 
2	a	26	23% 
2	e	26	38% 

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Mol	Chain	Length	Quality of chain
2	i	26	<div> <div>23%</div> <div>96%</div> <div>.</div> </div>
2	m	26	<div> <div>23%</div> <div>88%</div> <div>12%</div> </div>
3	3	26	<div> <div>42%</div> <div>92%</div> <div>8%</div> </div>
3	7	26	<div> <div>31%</div> <div>88%</div> <div>12%</div> </div>
3	D	26	<div> <div>23%</div> <div>92%</div> <div>8%</div> </div>
3	H	26	<div> <div>19%</div> <div>88%</div> <div>12%</div> </div>
3	L	26	<div> <div>35%</div> <div>96%</div> <div>.</div> </div>
3	P	26	<div> <div>31%</div> <div>96%</div> <div>.</div> </div>
3	U	26	<div> <div>27%</div> <div>92%</div> <div>8%</div> </div>
3	Y	26	<div> <div>38%</div> <div>96%</div> <div>.</div> </div>
3	b	26	<div> <div>19%</div> <div>81%</div> <div>19%</div> </div>
3	f	26	<div> <div>31%</div> <div>92%</div> <div>8%</div> </div>
3	j	26	<div> <div>31%</div> <div>92%</div> <div>8%</div> </div>
3	n	26	<div> <div>38%</div> <div>85%</div> <div>15%</div> </div>
4	o	99	<div> <div>33%</div> <div>94%</div> <div>6%</div> </div>
4	q	99	<div> <div>25%</div> <div>94%</div> <div>6%</div> </div>

## 2 Entry composition

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
1	8	102	Total 102	C 102	0	0	102
1	9	102	Total 102	C 102	0	0	102
1	c	102	Total 102	C 102	0	0	102
1	d	102	Total 102	C 102	0	0	102
1	g	102	Total 102	C 102	0	0	102
1	h	102	Total 102	C 102	0	0	102
1	k	102	Total 102	C 102	0	0	102
1	l	102	Total 102	C 102	0	0	102

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

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

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

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

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

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

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

There are 14 discrepancies between the modelled and reference sequences:

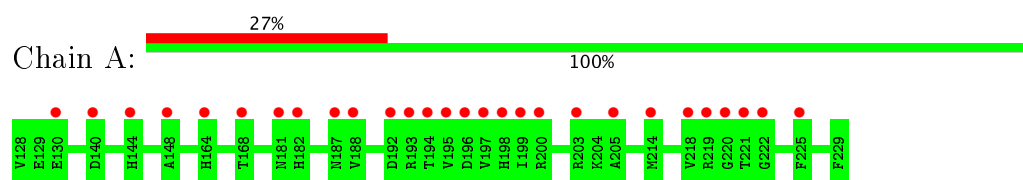
Chain	Residue	Modelled	Actual	Comment	Reference
q	532	MET	-	EXPRESSION TAG	UNP P00579
q	890	GLY	-	LINKER	UNP P00579
q	891	SER	-	LINKER	UNP P00579
q	892	SER	-	LINKER	UNP P00579
q	893	GLY	-	LINKER	UNP P00579
q	894	SER	-	LINKER	UNP P00579
q	895	GLY	-	LINKER	UNP P00579
o	532	MET	-	EXPRESSION TAG	UNP P00579
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



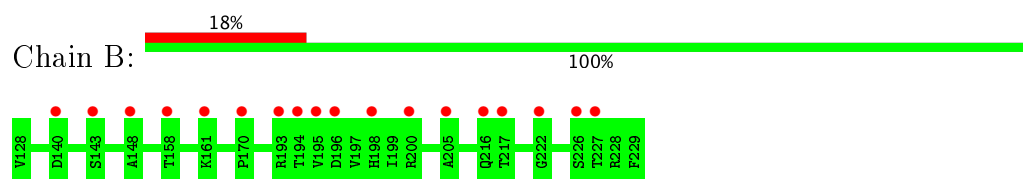
### 3 Residue-property plots [i](#)

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

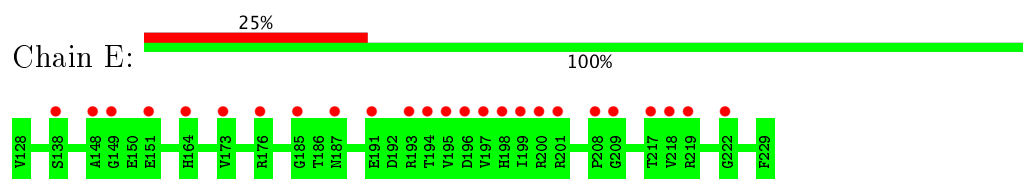
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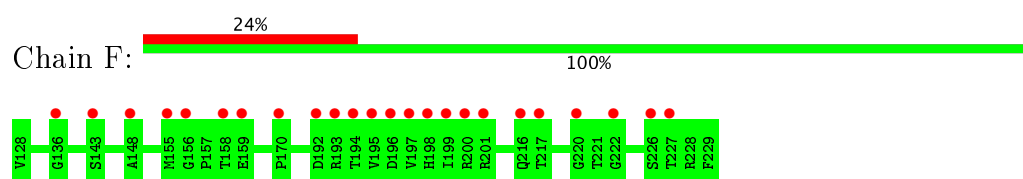
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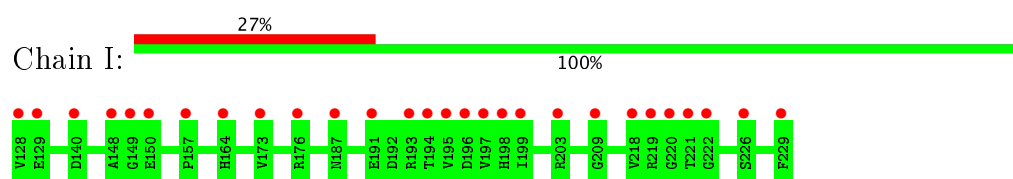
- Molecule 1: Phosphate regulon transcriptional regulatory protein phoB



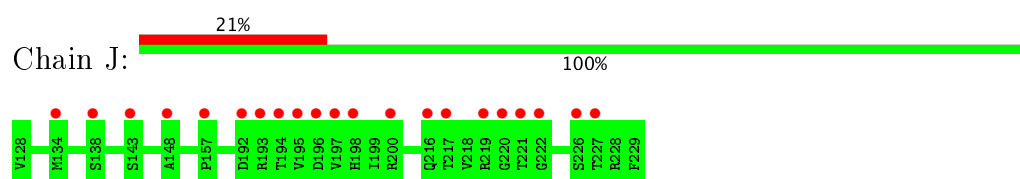
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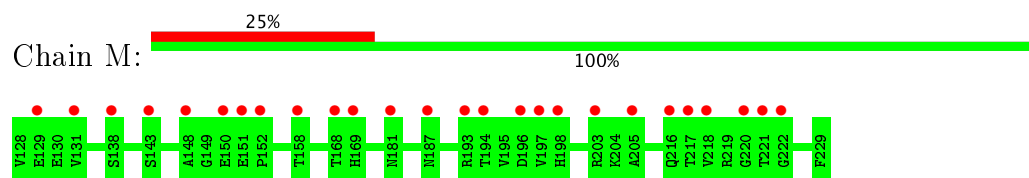
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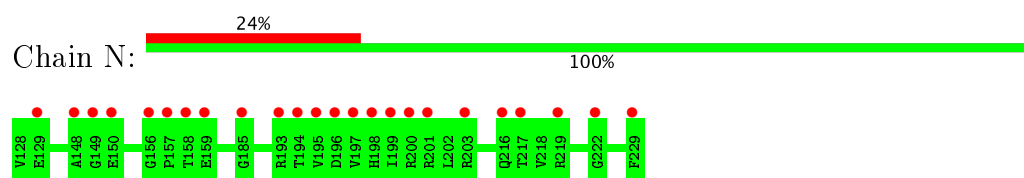
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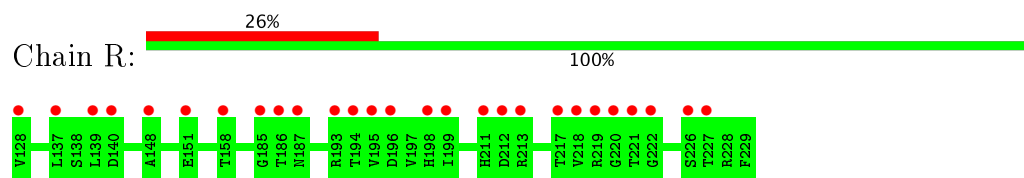
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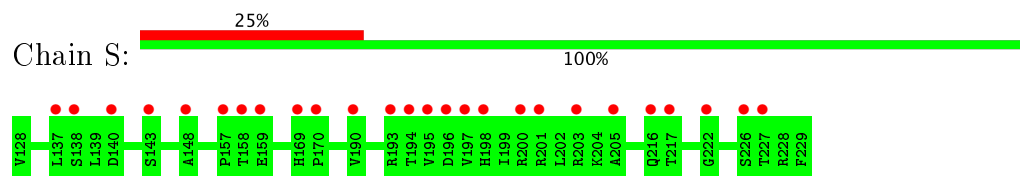
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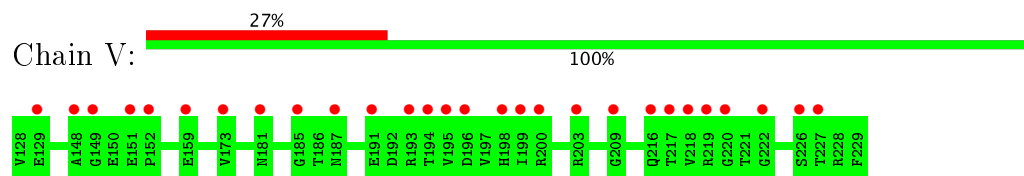
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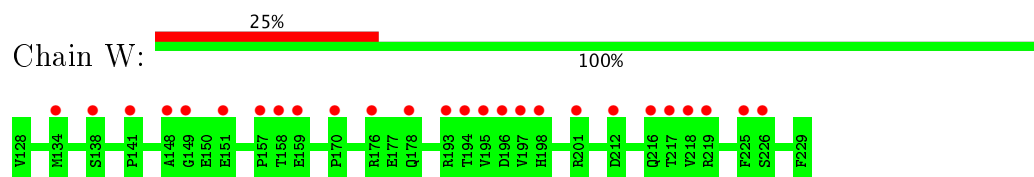
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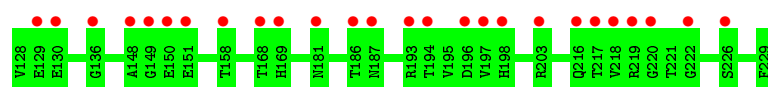
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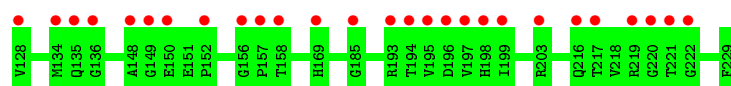
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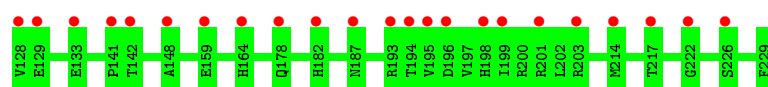
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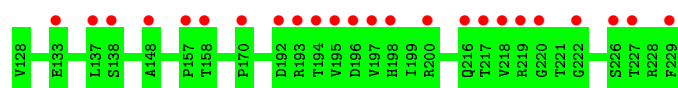
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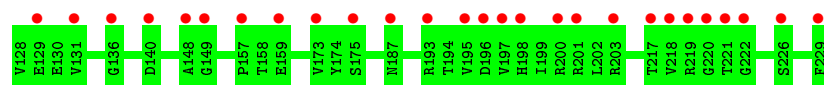
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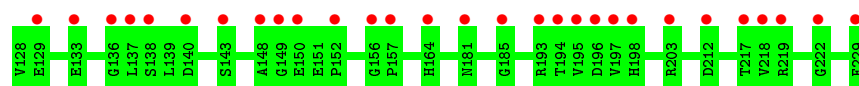
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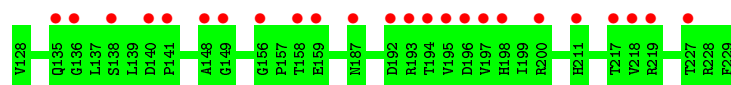
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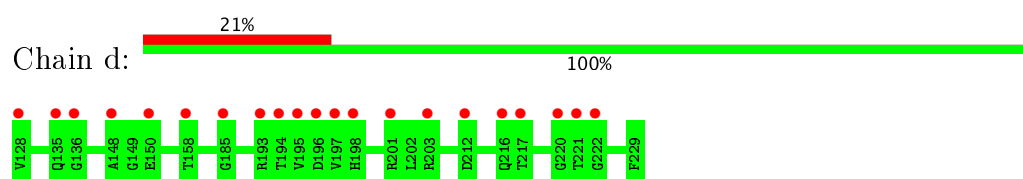
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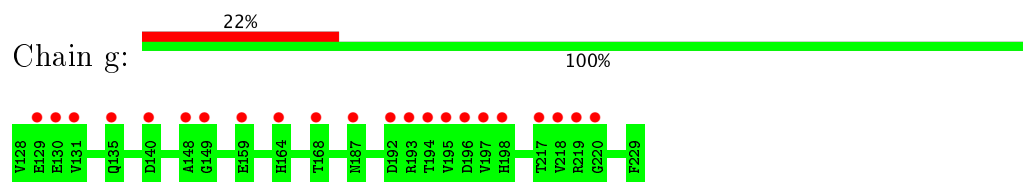
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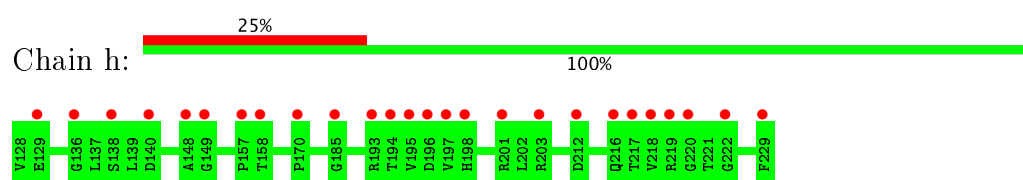
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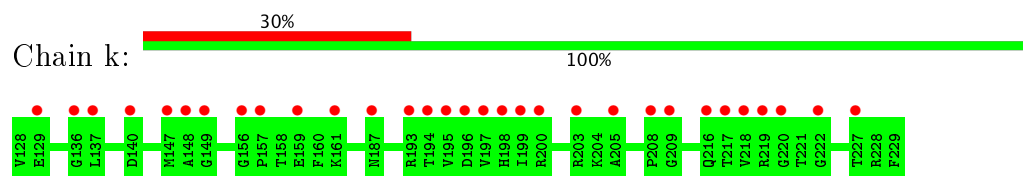
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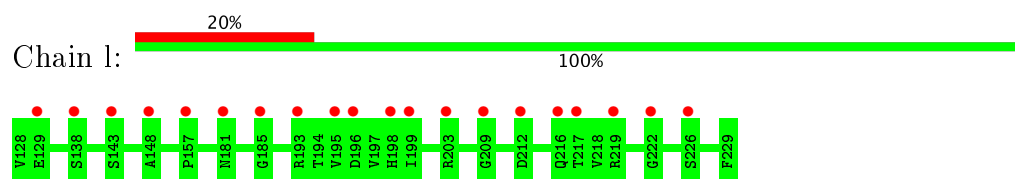
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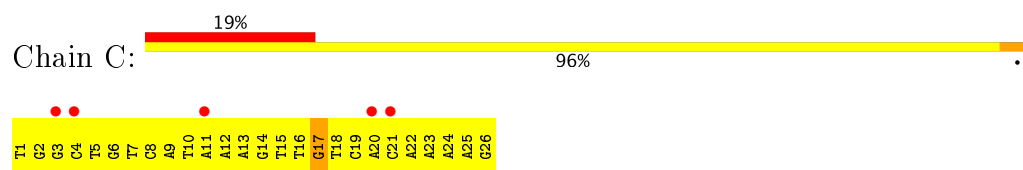
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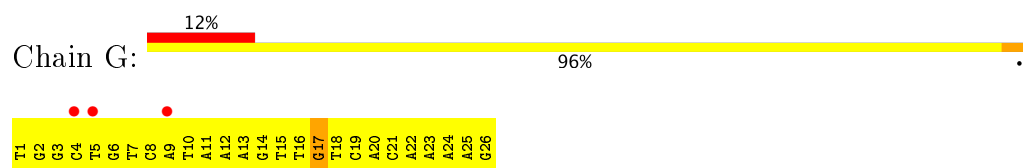
- Molecule 1: Phosphate regulon transcriptional regulatory protein phoB



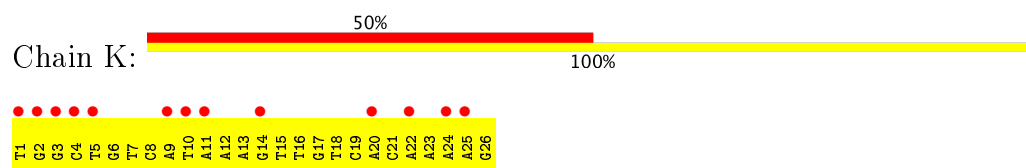
- Molecule 2: PHO BOX DNA (STRAND 1)



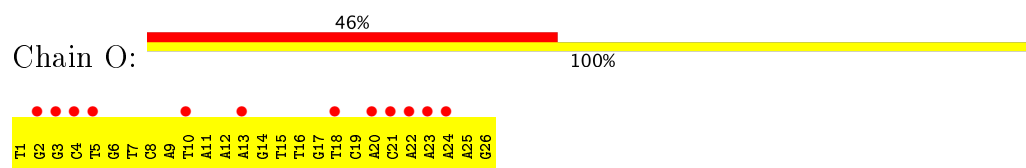
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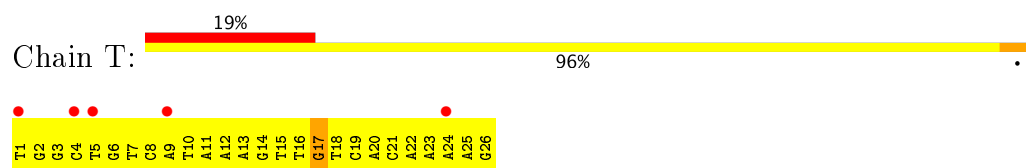
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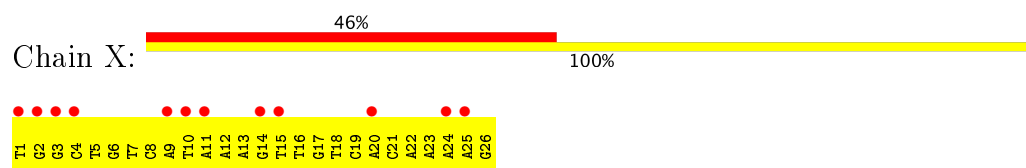
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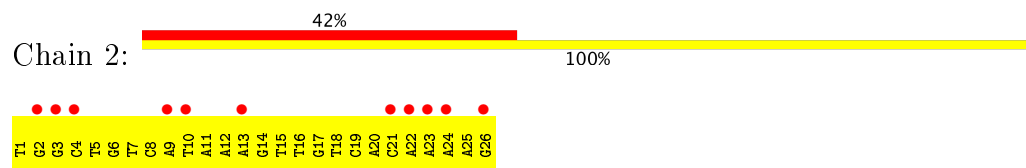
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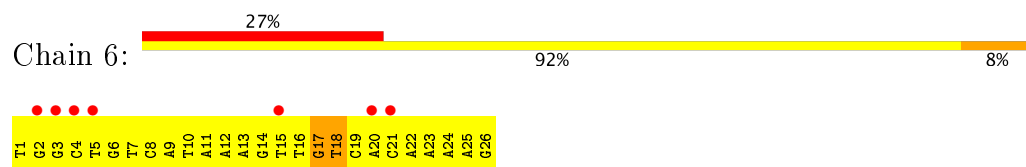
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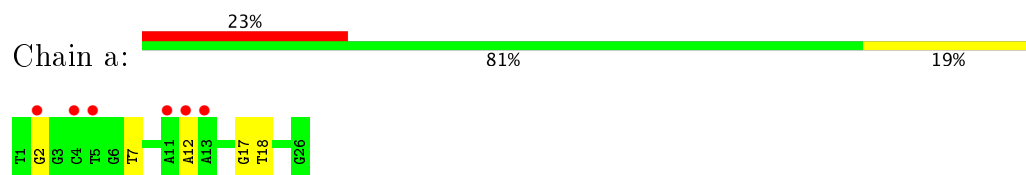
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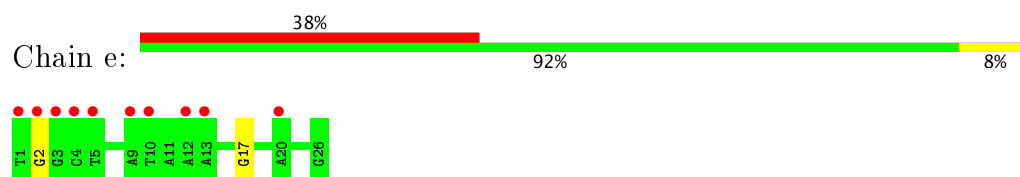
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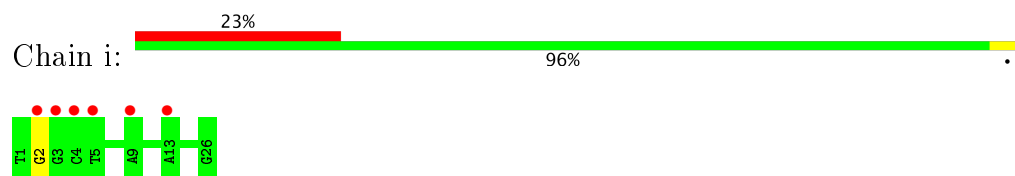
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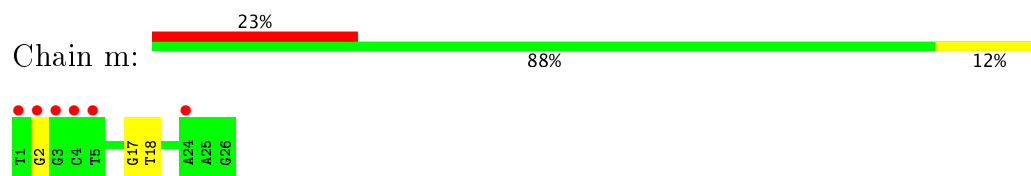
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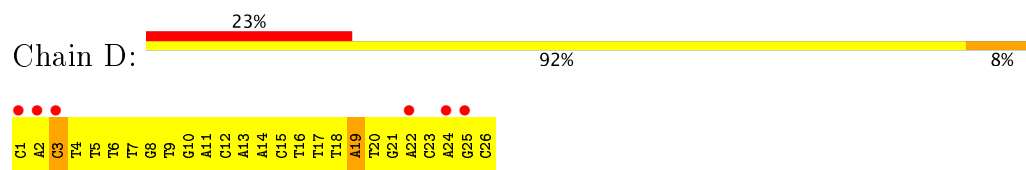
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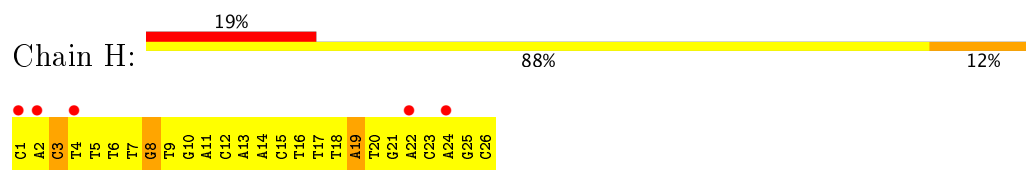
- Molecule 2: PHO BOX DNA (STRAND 1)



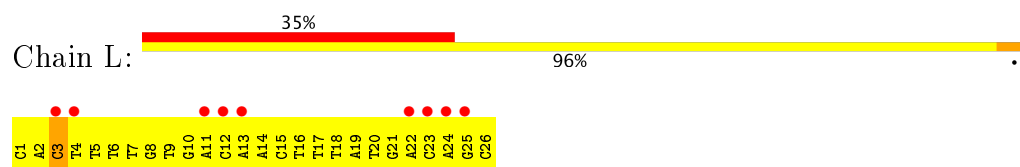
- Molecule 3: PHO BOX DNA (STRAND 2)



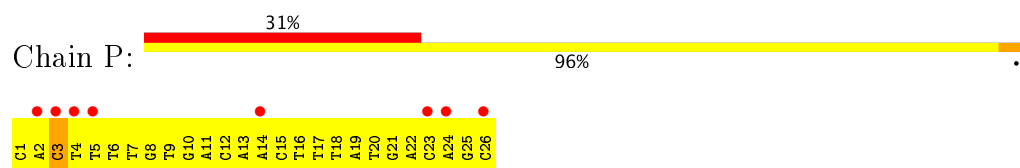
- Molecule 3: PHO BOX DNA (STRAND 2)



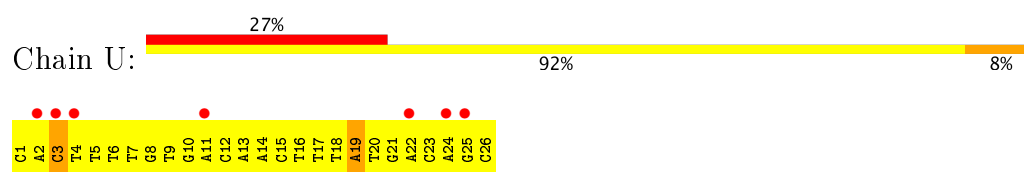
- Molecule 3: PHO BOX DNA (STRAND 2)



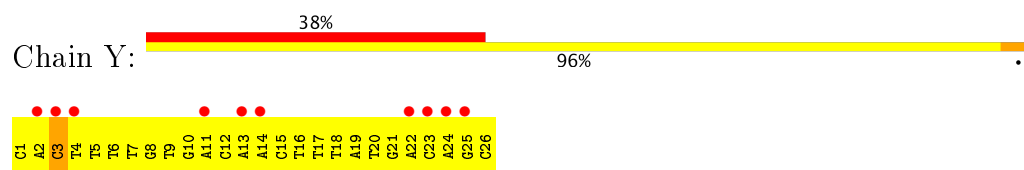
- Molecule 3: PHO BOX DNA (STRAND 2)



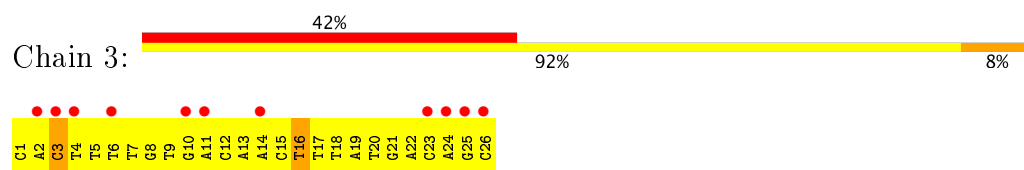
- Molecule 3: PHO BOX DNA (STRAND 2)



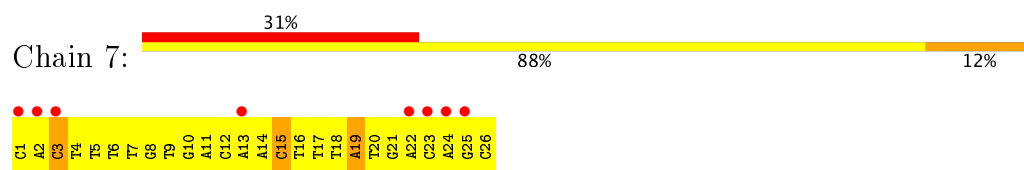
- Molecule 3: PHO BOX DNA (STRAND 2)



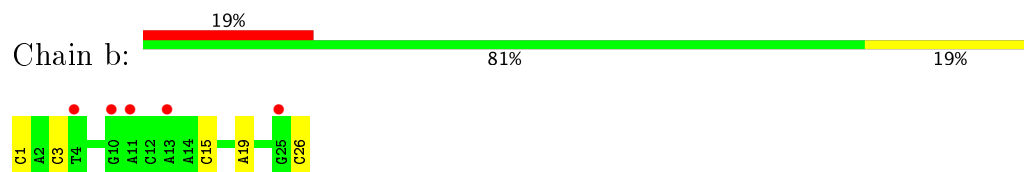
- Molecule 3: PHO BOX DNA (STRAND 2)



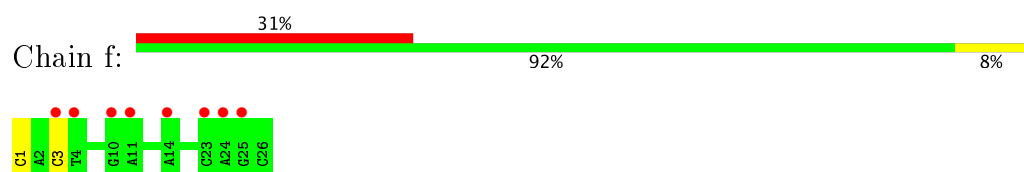
- Molecule 3: PHO BOX DNA (STRAND 2)



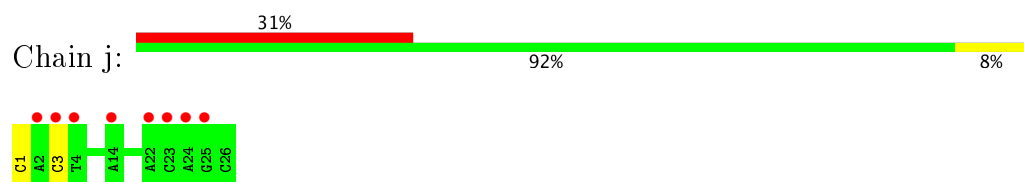
- Molecule 3: PHO BOX DNA (STRAND 2)



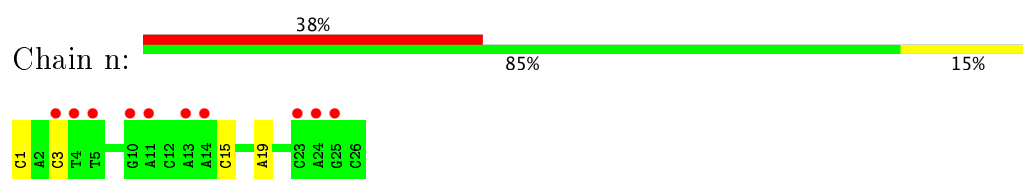
- Molecule 3: PHO BOX DNA (STRAND 2)



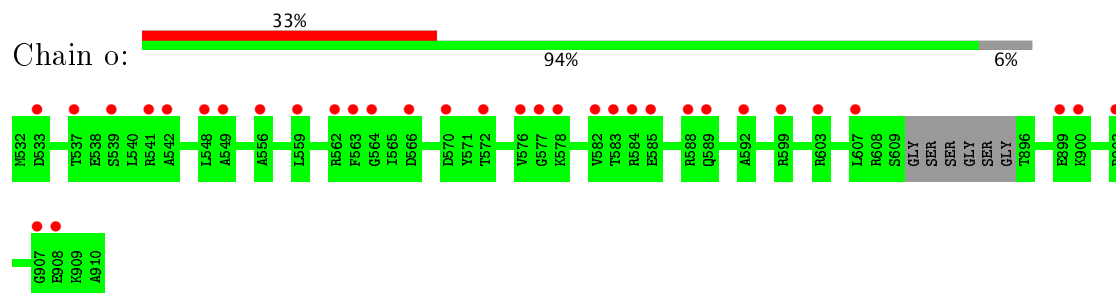
- Molecule 3: PHO BOX DNA (STRAND 2)



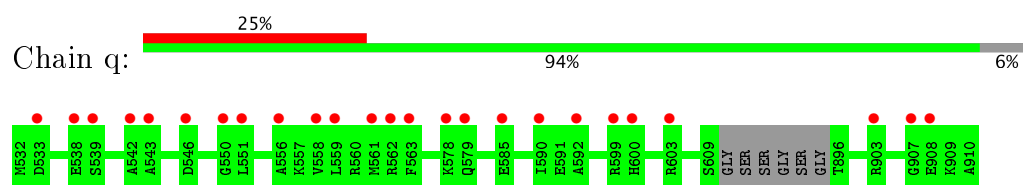
- Molecule 3: PHO BOX DNA (STRAND 2)



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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 4.36Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	(Not available) , (Not available) 0.485 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	189.2	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	-2.34 , 331.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	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	0.84	EDS
Total number of atoms	15354	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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(°)	Ideal(°)
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 ⓘ

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
3:3:14:DA:H2''	3:3:15:DC:H5''	1.29	1.11
3:P:14:DA:H2''	3:P: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:C2'	3:D:15:DC:H5''	1.85	1.06
3:D:14:DA:H2''	3:D:15:DC:H5''	1.27	1.06
3:7:14:DA:C2'	3:7:15:DC:H5''	1.85	1.06
3:7:14:DA:H2''	3:7:15:DC:H5''	1.27	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
2:6:24:DA:H4'	2:6:25:DA:OP1	1.61	0.97
3:L:9:DT:H2''	3:L:10:DG:H5''	1.45	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
2:2:7:DT:H2''	2:2:8:DC:H5'	1.51	0.92
2:T:23:DA:H4'	2:T:24:DA:OP1	1.65	0.92
2:6:7:DT:H2''	2:6:8:DC:H5'	1.51	0.92
3:H:14:DA:H2''	3:H:15:DC:C5'	2.00	0.92
2:2:6:DG:H2''	2:2:7:DT:H5''	1.50	0.91
2:G:25:DA:H1'	2:G:26:DG:O4'	1.70	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
2:2:11:DA:H2''	2:2:12:DA:H5''	1.50	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
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:G:6:DG:H2''	2:G:7:DT:H5''	1.53	0.90
2:X:25:DA:H1'	2:X:26:DG:O4'	1.72	0.90
2:X:7:DT:H2''	2:X:8:DC:H5'	1.53	0.90
2:T:6:DG:H2''	2:T:7:DT:H5''	1.53	0.89
2:2:25:DA:H1'	2:2:26:DG:O4'	1.72	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
2:6:6:DG:H2''	2:6:7:DT:H5''	1.53	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
2:2:13: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
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:G:25:DA:C2'	2:G:26:DG:H5''	2.03	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)
3:3:8: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
3:D:11:DA:H1'	3:D:12:DC:H5''	1.56	0.88
2:K:7:DT:H2''	2:K:8:DC:H5'	1.53	0.88
2:6:25:DA:H1'	2:6:26:DG:O4'	1.72	0.88
3:P:8:DG:H2''	3:P:9:DT:C5'	2.04	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
3:7:8:DG:H2''	3:7:9:DT:H5''	1.55	0.87
3:D:8:DG:H2''	3:D:9:DT:H5''	1.55	0.87
3:7:8:DG:H2''	3:7:9:DT:C5'	2.03	0.87
3:P:8:DG:H2''	3:P:9:DT:H5''	1.56	0.87
3:3:8:DG:H2''	3:3:9:DT:H5''	1.56	0.87
3:D:8:DG:H2''	3:D:9:DT:C5'	2.03	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
2:6:5:DT:H5'	2:6:5:DT:H6	1.44	0.82
2:C:5:DT:H5'	2:C:5:DT:H6	1.45	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
2:2:5:DT:H5'	2:2:5:DT:H6	1.46	0.81
3:3:4:DT:H2''	3:3:5:DT:H72	1.63	0.81
2:O:5:DT:H5'	2:O:5:DT:H6	1.46	0.81
3:U:4:DT:H2''	3:U: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
3:3:13:DA:H2''	3:3:14:DA:OP2	1.81	0.80
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
2:T:6:DG:H2''	2:T:7:DT:C5'	2.11	0.80
2:2:12:DA:H2''	2:2:13:DA:H5'	1.62	0.80
2:2:7:DT:H2''	2:2:8:DC:C5'	2.11	0.80
2:C:3:DG:H2''	2:C:4:DC:H5'	1.64	0.80
2:T:3:DG:H2''	2:T:4:DC:H5'	1.62	0.80
2:6:7:DT:H2''	2:6:8:DC:C5'	2.12	0.80
2:O:7:DT:H2''	2:O:8:DC:C5'	2.11	0.80
2:C:7:DT:H2''	2:C:8:DC:C5'	2.12	0.80
2:T:5:DT:H5'	2:T:5:DT:H6	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
3:7:4:DT:H2''	3:7:5:DT:H72	1.64	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: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
3:3:11:DA:H2''	3:3:12:DC:C5'	2.12	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: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:H5'	2:X:5:DT:H6	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:OP1	2:X:2:DG:H4'	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
3:3:2:DA:H1'	3:3:3:DC:H5'	1.67	0.76
2:T:2:DG:H4'	2:T:2:DG:OP1	1.85	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:12:DA:H2''	2:K:13:DA:C5'	2.16	0.76
2:K:2:DG:H4'	2:K:2:DG:OP1	1.86	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
3:7:16:DT:H2'	3:7:17:DT:H72	1.68	0.75
3:P:16:DT:H2'	3:P: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
2:6:1:DT:H2'	2:6:2:DG:C8	2.22	0.75
2:C:1:DT:H2'	2:C: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
2:2:11:DA:C2'	2:2:12:DA:H5''	2.17	0.74
2:X:1:DT:H2'	2:X:2:DG:C8	2.23	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
2:6:2:DG:H4'	2:6:2:DG:OP1	1.85	0.73
2:C:2:DG:H4'	2:C:2:DG:OP1	1.85	0.73
3:3:16:DT:H2'	3:3:17:DT:H72	1.69	0.73
2:6:6:DG:H2'	2:6:7:DT:H71	1.70	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
3:D:9:DT:C2'	3:D:10:DG:H5''	2.18	0.73
3:7:9:DT:C2'	3:7:10: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:9:DT:C2'	3:3:10:DG:H5''	2.18	0.73
2:G:15:DT:H1'	2:G:16:DT:H5'	1.69	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
3:3:8:DG:H1'	3:3:9:DT:H5''	1.72	0.72
2:G:11:DA:C2'	2:G:12:DA:H5''	2.19	0.72
2:6:11:DA:C2'	2:6:12:DA:H5''	2.19	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
2:2:19:DC:H2''	2:2:20:DA:C8	2.25	0.72
2:T:11:DA:C2'	2:T:12:DA:H5''	2.19	0.72
2:C:15:DT:H1'	2:C:16:DT:H5'	1.71	0.72
2:O:19:DC:H6	2:O:19:DC:H5'	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
2:2:19: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
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
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
2:2:6:DG:C2'	2:2:7:DT:H5''	2.20	0.71
2:K:15:DT:H1'	2:K:16:DT:H5'	1.71	0.71
2:G:2:DG:H2''	2:G:3:DG:C8	2.26	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
3:L:8:DG:H1'	3:L:9:DT:H5''	1.72	0.71
2:2:15:DT:H1'	2:2:16:DT:H5'	1.72	0.71
2:G:19:DC:H2''	2:G:20:DA:C8	2.25	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:H5'	2:X:19:DC:H6	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:H5'	2:T:19:DC:H6	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
2:6:6:DG:C2'	2:6:7:DT:H5''	2.23	0.69
2:C:2:DG:H2''	2:C:3:DG:C8	2.28	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
2:2:2: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: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
2:6:15:DT:H5'	2:6:15:DT:H6	1.58	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:C:6:DG:C2'	2:C:7:DT:H5''	2.23	0.68
3:3:4:DT:H4'	3:3:5:DT:OP1	1.94	0.68
2:O:15:DT:H6	2:O:15:DT:H5'	1.59	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
2:6:19:DC:H6	2:6:19:DC:H5'	1.58	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
3:U:7:DT:H2''	3:U:8:DG:H8	1.59	0.67
2:C:19:DC:H5'	2:C:19:DC:H6	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
3:7:1: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:1:DC:H2''	3:D:2:DA:C8	2.30	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
2:2:15:DT:H6	2:2:15:DT:H5'	1.59	0.66
3:P:11:DA:C1'	3:P:12:DC:H5''	2.25	0.66
3:U:19:DA:H1'	3:U:20:DT:H5''	1.77	0.66
3:3:2:DA:H1'	3:3:3:DC:C5'	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:7:DT:H2''	3:H:8:DG:H8	1.59	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:H5'	2:G:15:DT:H6	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
3:3:11:DA:C1'	3:3:12:DC:H5''	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:H2''	3:3:12:DC:H5'	1.78	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
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: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
3:7:7:DT:H2''	3:7:8:DG:H8	1.61	0.64
2:K:15:DT:H5'	2:K:15:DT:H6	1.61	0.64
3:7:2:DA:H1'	3:7:3:DC:C5'	2.27	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
3:3:22:DA:H1'	3:3:23:DC:H5''	1.79	0.64
3:Y:19:DA:H1'	3:Y:20:DT:H5''	1.78	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:H:22:DA:H1'	3:H:23:DC:H5''	1.79	0.64
2:T:2:DG:C4'	2:T:2:DG:OP1	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
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
2:2:2: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
2:G:2:DG:C4'	2:G:2:DG:OP1	2.46	0.63
3:Y:22:DA:H1'	3:Y:23:DC:H5''	1.80	0.63
3:H:16:DT:H5'	3:H:16:DT:H6	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
2:2:24:DA:C4'	2:2:25:DA:OP1	2.45	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
2:2:5:DT:H2''	2:2:6:DG:C8	2.34	0.63
3:3:17:DT:H1'	3:3:18:DT:H5''	1.81	0.63
3:3:7:DT:H2''	3:3:8:DG:H8	1.63	0.63
2:K:2:DG:C4'	2:K:2:DG:OP1	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
2:6:2:DG:C4'	2:6:2:DG:OP1	2.46	0.62
2:K:8:DC:H6	2:K:8:DC:H5'	1.64	0.62
3:U:16:DT:H6	3:U:16:DT:H5'	1.63	0.62
3:Y:11:DA:H2''	3:Y:12:DC:H5'	1.80	0.62
3:Y:8:DG:C1'	3:Y:9:DT:H5''	2.29	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:H6	2:G:8:DC:H5'	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
3:3:8:DG:C1'	3:3:9:DT:H5''	2.29	0.62
3:L:16:DT:H6	3:L:16:DT:H5'	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
2:2:5:DT:C6	2:2:5:DT:H5'	2.34	0.61
3:7:10:DG:H1'	3:7:11:DA:H5'	1.81	0.61
2:K:1:DT:H3'	2:K:2:DG:H5''	1.81	0.61
2:2:8:DC:H5'	2:2:8:DC:H6	1.64	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
2:6:24:DA:C4'	2:6:25:DA:OP1	2.44	0.61
2:6:5:DT:H2''	2:6:6:DG:C8	2.35	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: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
3:7:4:DT:H2''	3:7:5:DT:C7	2.31	0.61
2:K:10:DT:H2''	2:K:11:DA:OP2	1.99	0.61
2:O:19:DC:C6	2:O:19:DC:H5'	2.36	0.61
2:O:8:DC:H5'	2:O:8:DC:H6	1.65	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
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: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
2:6:9:DA:H1'	2:6:10:DT:H5'	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:16:DT:H5'	3:P:16:DT:H6	1.66	0.60
2:2:1:DT:H3'	2:2:2:DG:C5'	2.30	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
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
3:D:17:DT:H1'	3:D:18:DT:H5''	1.82	0.60
3:D:8:DG:C1'	3:D:9:DT:H5''	2.30	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
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
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
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: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
2:6:1:DT:H3'	2:6:2:DG:C5'	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: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:C6	2:X:19:DC:H5'	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
2:2:12:DA:H1'	2:2:13:DA:H5''	1.84	0.59
3:D:16:DT:H5'	3:D:16:DT:H6	1.66	0.59
2:6:18:DT:H2''	2:6:19:DC:H5'	1.84	0.59
2:6:8:DC:H5'	2:6:8:DC:H6	1.67	0.59
3:7:16:DT:H6	3:7:16:DT:H5'	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:10:DT:H2''	2:O:11:DA:OP2	2.02	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
3:3:9: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
3:P:14:DA:C3'	3:P:15:DC:H5''	2.29	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
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
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
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
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:C6	2:K:19:DC:H5'	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
2:6:13: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
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
3:3:11:DA:C2'	3:3:12:DC:C5'	2.80	0.58
3:L:7:DT:H2''	3:L:8:DG:C8	2.39	0.58
2:2:4:DC:H1'	2:2:5:DT:H5''	1.86	0.58
3:D:14:DA:C3'	3:D:15:DC:H5''	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:11:DA:C2'	3:P:12:DC:C5'	2.81	0.58
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: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
2:6:4:DC:H1'	2:6:5:DT:H5''	1.86	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
2:6:7: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
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
2:6:12:DA:H1'	2:6:13:DA:H5''	1.86	0.57
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: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
2:2:17: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
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
3:D:5:DT:H1'	3:D:6:DT:C5'	2.30	0.57
3:7:7:DT:H2''	3:7:8:DG:C8	2.38	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
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
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
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)
2:6:17:DG:H2''	2:6:18:DT:C5'	2.35	0.57
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: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
2:6:19:DC:C6	2:6:19:DC:H5'	2.38	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
2:2:13:DA:C1'	2:2:14:DG:H5'	2.32	0.56
2:O:17:DG:H2''	2:O:18:DT:C5'	2.35	0.56
2:X:2:DG:H8	2:X:2:DG:H5''	1.70	0.56
3:3:4:DT:C2'	3:3:5:DT:H72	2.34	0.56
2:X:5:DT:H5'	2:X:5:DT:C6	2.36	0.56
2:C:19:DC:C6	2:C:19:DC:H5'	2.38	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: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
3:7:24:DA:H1'	3:7:25:DG:O5'	2.06	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
3:3:24:DA:H1'	3:3:25:DG:O5'	2.06	0.56
3:D:10:DG:H2''	3:D:11:DA:O5'	2.04	0.56
2:K:2:DG:H8	2:K:2:DG:H5''	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
3:7:10:DG:H2''	3:7:11:DA:O5'	2.04	0.55
3:3:14:DA:C3'	3:3:15:DC:H5''	2.29	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
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
3:3:10:DG:H2''	3:3:11:DA:O5'	2.06	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
2:2:17:DG:H1'	2:2:18:DT:H5''	1.89	0.55
2:2:7:DT:H2''	2:2:8:DC:H6	1.70	0.55
3:3:6:DT:H2''	3:3:7:DT:O5'	2.06	0.55
2:X:8:DC:H2''	2:X:9:DA:C8	2.42	0.55
2:K:5:DT:C6	2:K:5:DT:H5'	2.36	0.54
2:K:8:DC:H2''	2:K:9:DA:C8	2.42	0.54
2:6:24:DA:H1'	2:6:25:DA:H5'	1.88	0.54
2:K:17:DG:H2''	2:K:18:DT:C5'	2.37	0.54
3:7:6:DT:H2''	3:7:7:DT:O5'	2.07	0.54
3:Y:9:DT:H2''	3:Y:10:DG:C5'	2.28	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
3:7:5:DT:C1'	3:7:6:DT:H5''	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
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
2:6:16:DT:H2''	2:6:17:DG:C8	2.43	0.54
3:H:4:DT:C2'	3:H:5:DT:H72	2.34	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
3:D:15:DC:H2'	3:D:16:DT:H72	1.90	0.54
2:6:2:DG:H8	2:6:2:DG:H5''	1.73	0.53
2:C:2:DG:H8	2:C:2:DG:H5''	1.73	0.53
2:2:2:DG:H5''	2:2:2:DG:H8	1.73	0.53
2:G:5:DT:C6	2:G:5:DT:H5'	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:9:DT:H5'	3:P:9:DT:H6	1.74	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
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
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: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
2:T:15:DT:C1'	2:T:16:DT:H5'	2.37	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
2:K:16:DT:H2''	2:K:17:DG:C8	2.44	0.53
3:P:18:DT:H1'	3:P:19:DA:H5'	1.90	0.53
3:P:5:DT:H1'	3:P:6:DT:C5'	2.33	0.53
3:3:5:DT:H1'	3:3:6:DT:C5'	2.32	0.53
3:D:15:DC:H2''	3:D:16:DT:H5''	1.90	0.53
3:D:9:DT:H2''	3:D:10:DG:C5'	2.30	0.53
3:L:12:DC:H2''	3:L:13:DA:C8	2.44	0.53
2:O:2:DG:H8	2:O:2:DG:H5''	1.73	0.53
3:Y:5:DT:H1'	3:Y:6:DT:C5'	2.31	0.53
3:7:9:DT:H2''	3:7:10:DG:C5'	2.30	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
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
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:15:DC:H2''	3:U:16:DT:H5''	1.91	0.53
3:U:6:DT:H2''	3:U:7:DT:O5'	2.09	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
2:6:23:DA:C4'	2:6:24:DA:OP1	2.46	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
2:6:8:DC:H2''	2:6:9:DA:C8	2.45	0.52
2:O:23:DA:H1'	2:O:24:DA:H5'	1.90	0.52
2:O:22:DA:H2''	2:O:23:DA:H5'	1.91	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
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
2:2:12:DA:C2'	2:2:13:DA:H5''	2.40	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: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:15:DC:H2''	3:Y:16:DT:H5''	1.92	0.52
3:Y:14:DA:C1'	3:Y:15:DC:H5''	2.39	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
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
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:17:DG:H1'	2:X:18:DT:H5''	1.91	0.52
2:X:7:DT:C2'	2:X:8:DC:C5'	2.88	0.52
3:Y:15:DC:H2'	3:Y:16:DT:H72	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:15:DC:H2''	3:3:16:DT:H5''	1.92	0.51
2:O:24:DA:C4'	2:O:25:DA:OP1	2.45	0.51
3:P:22:DA:H1'	3:P:23:DC:C5'	2.40	0.51
3:P:9:DT:C3'	3:P:10:DG:H5''	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
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
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: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
2:6:7:DT:C2	2:6:8:DC:C5	2.99	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
2:2:24: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: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
2:2:15:DT:C1'	2:2:16:DT:H5'	2.40	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
2:6:22: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'	2.88	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
3:7:22:DA:H1'	3:7:23:DC:C5'	2.40	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: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:15:DT:H2''	2:T:16:DT:O5'	2.10	0.50
2:T:2:DG:C2'	2:T:3:DG:C8	2.93	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
3:7:12:DC:H2''	3:7:13:DA:C8	2.46	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
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
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
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
3:7:15:DC:H2''	3:7:16:DT:C5'	2.42	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
3:3:22: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
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
2:6:25:DA:C2	2:6:26:DG:C4	2.99	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
2:2:23: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:C:25:DA:C2	2:C:26:DG:C4	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:6:17:DG:H2''	2:6:18:DT:H5'	1.94	0.50
2:6:3:DG:H2''	2:6:4:DC:C5'	2.39	0.50
2:G:22:DA:H2''	2:G:23:DA:H5'	1.94	0.50
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
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
3:D:14:DA:C1'	3:D:15:DC:H5''	2.42	0.49
3:D:9:DT:H6	3:D:9:DT:H5'	1.77	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
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: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
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
3:3:19: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
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:17:DG:H2''	2:O:18:DT:H5'	1.94	0.49
2:O:6:DG:C2'	2:O:7:DT:H71	2.42	0.49
3:3:19:DA:H2''	3:3:20:DT:H5'	1.94	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)
2:C:3:DG:H2''	2:C:4:DC:C5'	2.39	0.49
3:Y:21:DG:H2''	3:Y:22:DA:OP2	2.13	0.49
2:2:15:DT:H2''	2:2:16:DT:O5'	2.13	0.49
2:2:11:DA:C2	3:3:19:DA:C2	3.01	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: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
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:U:14:DA:C3'	3:U:15:DC:H5''	2.31	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
3:3:14:DA:C1'	3:3:15:DC:H5''	2.42	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: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
2:6:15:DT:C1'	2:6:16:DT:H5'	2.40	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
2:6:2:DG:C2'	2:6:3:DG:C8	2.95	0.48
3:Y:24:DA:H1'	3:Y:25:DG:C5'	2.44	0.48
2:2:2:DG:C2'	2:2:3:DG:C8	2.96	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
3:H:15:DC:H2''	3:H:16:DT:C5'	2.43	0.48
2:2:12:DA:C2'	2:2:13:DA:C5'	2.89	0.48
2:2:7:DT:C2'	2:2:8:DC:H5''	2.44	0.48
2:6:15:DT:H2'	2:6:16:DT:H72	1.96	0.48
2:K:3:DG:H2''	2:K:4:DC:C5'	2.40	0.48
2:2:11:DA:H2''	2:2:12:DA:C5'	2.33	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
2:2:3:DG:H2''	2:2:4:DC:C5'	2.41	0.47
2:X:15:DT:H2'	2:X:16:DT:H72	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:15:DC:H2''	3:Y:16:DT:C5'	2.44	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
3:3:15:DC:H2''	3:3:16:DT:C5'	2.45	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
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
3:3:5:DT:H2''	3:3:6:DT:H5'	1.98	0.46
2:O:6:DG:N2	3:P:24:DA:C2	2.83	0.46
3:7:10:DG:H2''	3:7:11:DA:H8	1.81	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
3:3:25: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: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: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
2:2:2:DG:H2''	2:2:3:DG:O5'	2.16	0.46
2:C:4:DC:C2'	2:C:5:DT:H71	2.46	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
3:H:10:DG:H2''	3:H:11:DA:H8	1.80	0.46
2:X:17:DG:H2''	2:X:18:DT:H5'	1.96	0.46
2:X:6:DG:H2''	2:X:7:DT:H5'	1.93	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:16:DT:H2'	3:P:17:DT:C7	2.44	0.45
3:P:5:DT:H2''	3:P:6:DT:H5'	1.98	0.45
3:Y:4:DT:O5'	3:Y:4:DT:H2'	2.17	0.45
2:G:15:DT:H2''	2:G:16:DT:C5'	2.47	0.45
2:G:7:DT:C2'	2:G:8:DC:H5''	2.46	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
2:6:17: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: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
3:3:24:DA:H1'	3:3:25:DG:C5'	2.47	0.45
2:K:2:DG:H2''	2:K:3:DG:H8	1.80	0.45
2:2:2:DG:H2''	2:2:3:DG:H8	1.80	0.45
2:G:24:DA:H1'	2:G:25:DA:C5'	2.47	0.45
3:3:4:DT:H2'	3:3:4:DT:O5'	2.16	0.45
3:D:4:DT:H2'	3:D:4:DT:O5'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:5:DT:H2''	3:D:6:DT:H5'	1.98	0.45
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
3:7:25:DG:C4	3:7:26:DC:C4	3.05	0.45
3:7:4:DT:O5'	3:7:4:DT:H2'	2.16	0.45
3:7:5:DT:H2''	3:7:6:DT:H5'	1.98	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:H5''	2:X:2:DG:C8	2.52	0.45
2:2:17:DG:C2'	2:2:18:DT:H5''	2.47	0.44
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
2:2:4: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: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: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:16:DT:H2'	3:U:17:DT:C7	2.42	0.44
3:U:8:DG:H2''	3:U:9:DT:H5'	1.92	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
3:L:4:DT:O5'	3:L:4:DT:H2'	2.17	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:O5'	3:U:4:DT:H2'	2.18	0.44
3:3:8:DG:H2''	3:3:9:DT:H5'	1.95	0.44
2:K:15:DT:C2'	2:K:16:DT:H5'	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:24:DA:H1'	2:O:25:DA:C5'	2.48	0.44
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
2:6:24:DA:H1'	2:6:25:DA:C5'	2.46	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
2:2:24: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
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:23:DA:H1'	2:T:24:DA:C8	2.53	0.43
2:T:2:DG:H2''	2:T:3:DG:O5'	2.18	0.43
2:T:2:DG:C8	2:T:2:DG:H5''	2.53	0.43
2:T:6:DG:H2''	2:T:7:DT:H5'	1.93	0.43
2:2:3:DG:C5	2:2:4:DC:C4	3.06	0.43
3:L:16:DT:H2'	3:L:17:DT:C7	2.44	0.43
2:G:23:DA:H1'	2:G:24:DA:C8	2.53	0.43
2:G:2:DG:H2''	2:G:3:DG:O5'	2.18	0.43
3:P:16:DT:H2''	3:P:17:DT:C6	2.54	0.43
2:6:2:DG:H2''	2:6:3:DG:O5'	2.17	0.43
2:C:2:DG:H2''	2:C:3:DG:O5'	2.18	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
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
2:6:6:DG:C2'	2:6:7:DT:H71	2.42	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
2:6:3:DG:C5	2:6:4:DC:C4	3.07	0.43
2:G:4:DC:C2'	2:G:5:DT:H71	2.49	0.43
3:7:16:DT:H2'	3:7:17:DT:C7	2.44	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
2:2:20:DA:H2''	2:2:21:DC:OP2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:13:DA:C2'	3:3:14:DA:OP2	2.56	0.43
2:T:4:DC:C2'	2:T:5:DT:H71	2.49	0.43
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:C:15:DT:H2''	2:C:16:DT:C5'	2.49	0.43
2:K:2:DG:H5''	2:K:2:DG:C8	2.52	0.43
3:U:19:DA:C1'	3:U:20:DT:H5''	2.46	0.43
2:6:15:DT:H2''	2:6:16:DT:C5'	2.49	0.42
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:23:DC:H2''	3:U:24:DA:C8	2.54	0.42
3:U:5:DT:H2''	3:U: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
3:Y:5:DT:H2''	3:Y:6:DT:H5'	2.00	0.42
2:2:15:DT:H2''	2:2:16:DT:C5'	2.49	0.42
2:6:23:DA:H1'	2:6:24:DA:C8	2.54	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:24:DA:H1'	2:K:25:DA:C5'	2.49	0.42
2:K:2:DG:H2''	2:K:3:DG:O5'	2.19	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: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
3:3:23: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:D:12:DC:H5'	3:D:12:DC:H6	1.84	0.42
3:D:5:DT:H2''	3:D:6:DT:C5'	2.50	0.42
3:U:16:DT:H2''	3:U:17:DT:C6	2.54	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
2:2:23: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: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
3:3:16:DT:H2'	3:3:17:DT:C7	2.44	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:G:3:DG:C5	2:G:4:DC:C4	3.07	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
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:24:DA:H1'	3:Y:25:DG:H5'	2.02	0.42
3:Y:8:DG:H2''	3:Y:9:DT:H5'	1.94	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
2:6:25:DA:C4	2:6:26:DG:C8	3.08	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
2:2:15: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
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
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
2:6:2:DG:H2''	2:6:3:DG:H8	1.80	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: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
2:2:23:DA:C4	2:2:24:DA:N7	2.88	0.41
3:L:24:DA:H1'	3:L:25:DG:H5'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:23:DA:H1'	2:X:24:DA:C8	2.55	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
2:6:8:DC:H2''	2:6:9:DA:O5'	2.21	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:T:23:DA:C4	2:T:24:DA:N7	2.89	0.41
2:X:25:DA:C4	2:X:26:DG:C8	3.09	0.41
2:X:3:DG:H2''	2:X:4:DC:C5'	2.40	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
3:Y:12:DC:H5'	3:Y:12:DC:H6	1.85	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
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
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
2:6:4:DC:H2''	2:6:5:DT:H71	2.04	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
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
3:L:23:DC:H6	3:L:23:DC:H5'	1.86	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
3:H:1:DC:N4	2:X:2:DG:O6[2_456]	1.95	0.25
2:G:1:DT:O4	3:Y:2:DA:N6[4_456]	1.95	0.25
3:L:1:DC:N3	2:T:2:DG:N2[4_446]	1.97	0.23
2:K:2:DG:N2	3:U:1:DC:C2[2_556]	1.97	0.23
3:j:1:DC:N4	2:m:2:DG:O6[4_447]	1.99	0.21
3:L:2:DA:N6	2:T:1:DT:O4[4_446]	1.99	0.21
2:K:2:DG:N1	3:U:1:DC:N3[2_556]	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
3:b:1:DC:C4	2:e:2:DG:N1[4_446]	2.15	0.05
2:a:2:DG:N1	3:f:1:DC:N4[2_456]	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 carbohydrates 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 ⓘ

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	1	102/102 (100%)	1.41	27 (26%) 1 2	56, 70, 90, 95	0
1	4	102/102 (100%)	1.43	23 (22%) 1 2	60, 73, 89, 91	0
1	5	102/102 (100%)	1.38	24 (23%) 1 2	56, 70, 90, 95	0
1	8	102/102 (100%)	1.59	27 (26%) 1 2	60, 73, 89, 91	0
1	9	102/102 (100%)	1.58	29 (28%) 1 2	56, 70, 90, 95	0
1	A	102/102 (100%)	1.48	28 (27%) 1 2	60, 73, 89, 91	0
1	B	102/102 (100%)	1.32	18 (17%) 2 4	56, 70, 90, 95	0
1	E	102/102 (100%)	1.51	25 (24%) 1 2	60, 73, 89, 91	0
1	F	102/102 (100%)	1.46	24 (23%) 1 2	56, 70, 90, 95	0
1	I	102/102 (100%)	1.42	28 (27%) 1 2	60, 73, 89, 91	0
1	J	102/102 (100%)	1.49	21 (20%) 1 3	56, 70, 90, 95	0
1	M	102/102 (100%)	1.58	26 (25%) 1 2	60, 73, 89, 91	0
1	N	102/102 (100%)	1.51	24 (23%) 1 2	56, 70, 90, 95	0
1	R	102/102 (100%)	1.62	27 (26%) 1 2	60, 73, 89, 91	0
1	S	102/102 (100%)	1.57	26 (25%) 1 2	56, 70, 90, 95	0
1	V	102/102 (100%)	1.56	28 (27%) 1 2	60, 73, 89, 91	0
1	W	102/102 (100%)	1.49	26 (25%) 1 2	56, 70, 90, 95	0
1	Z	102/102 (100%)	1.45	26 (25%) 1 2	60, 73, 89, 91	0
1	c	102/102 (100%)	1.52	24 (23%) 1 2	60, 73, 89, 91	0
1	d	102/102 (100%)	1.39	21 (20%) 1 3	56, 70, 90, 95	0
1	g	102/102 (100%)	1.40	22 (21%) 1 3	60, 73, 89, 91	0
1	h	102/102 (100%)	1.54	26 (25%) 1 2	56, 70, 90, 95	0
1	k	102/102 (100%)	1.71	31 (30%) 0 2	60, 73, 89, 91	0
1	l	102/102 (100%)	1.39	20 (19%) 1 3	56, 70, 90, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	2	26/26 (100%)	1.80	11 (42%) 0 2	62, 79, 87, 88	0
2	6	26/26 (100%)	1.58	7 (26%) 1 2	62, 79, 87, 88	0
2	C	26/26 (100%)	1.58	5 (19%) 1 3	62, 79, 87, 88	0
2	G	26/26 (100%)	1.17	3 (11%) 5 7	62, 79, 87, 88	0
2	K	26/26 (100%)	1.72	13 (50%) 0 1	62, 79, 87, 88	0
2	O	26/26 (100%)	1.90	12 (46%) 0 2	62, 79, 87, 88	0
2	T	26/26 (100%)	1.27	5 (19%) 1 3	62, 79, 87, 88	0
2	X	26/26 (100%)	1.61	12 (46%) 0 2	62, 79, 87, 88	0
2	a	26/26 (100%)	1.53	6 (23%) 1 2	62, 79, 87, 88	0
2	e	26/26 (100%)	1.68	10 (38%) 0 2	62, 79, 87, 88	0
2	i	26/26 (100%)	1.59	6 (23%) 1 2	62, 79, 87, 88	0
2	m	26/26 (100%)	1.47	6 (23%) 1 2	62, 79, 87, 88	0
3	3	26/26 (100%)	1.87	11 (42%) 0 2	61, 79, 93, 94	0
3	7	26/26 (100%)	1.39	8 (30%) 0 2	61, 79, 93, 94	0
3	D	26/26 (100%)	1.30	6 (23%) 1 2	61, 79, 93, 94	0
3	H	26/26 (100%)	1.25	5 (19%) 1 3	61, 79, 93, 94	0
3	L	26/26 (100%)	1.51	9 (34%) 0 2	61, 79, 93, 94	0
3	P	26/26 (100%)	1.70	8 (30%) 0 2	61, 79, 93, 94	0
3	U	26/26 (100%)	1.46	7 (26%) 1 2	61, 79, 93, 94	0
3	Y	26/26 (100%)	1.53	10 (38%) 0 2	61, 79, 93, 94	0
3	b	26/26 (100%)	1.47	5 (19%) 1 3	61, 79, 93, 94	0
3	f	26/26 (100%)	1.57	8 (30%) 0 2	61, 79, 93, 94	0
3	j	26/26 (100%)	1.63	8 (30%) 0 2	61, 79, 93, 94	0
3	n	26/26 (100%)	1.61	10 (38%) 0 2	61, 79, 93, 94	0
4	o	93/99 (93%)	1.73	33 (35%) 0 2	19, 23, 79, 88	0
4	q	93/99 (93%)	1.66	25 (26%) 1 2	19, 23, 79, 88	0
All	All	3258/3270 (99%)	1.51	850 (26%) 1 2	19, 73, 90, 95	0

All (850) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	185	GLY	11.8
1	R	187	ASN	11.6

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Mol	Chain	Res	Type	RSRZ
4	o	570	ASP	10.9
4	q	907	GLY	10.7
1	M	129	GLU	10.5
1	V	152	PRO	10.0
1	R	185	GLY	9.9
4	q	543	ALA	9.6
1	k	140	ASP	9.3
4	q	578	LYS	8.6
1	Z	222	GLY	8.5
4	q	538	GLU	8.5
1	V	148	ALA	8.3
4	o	907	GLY	7.9
4	q	562	ARG	7.8
1	S	170	PRO	7.7
1	N	222	GLY	7.3
4	o	563	PHE	7.2
1	c	187	ASN	7.1
1	E	209	GLY	7.0
1	V	151	GLU	7.0
1	E	187	ASN	6.8
1	I	187	ASN	6.8
1	9	129	GLU	6.7
1	8	193	ARG	6.7
4	o	542	ALA	6.7
1	h	148	ALA	6.4
4	q	563	PHE	6.4
1	d	197	VAL	6.3
4	q	533	ASP	6.2
1	l	217	THR	6.1
4	o	537	THR	6.1
4	o	577	GLY	6.0
1	l	222	GLY	6.0
1	B	170	PRO	5.9
1	h	185	GLY	5.8
1	d	222	GLY	5.8
1	8	140	ASP	5.8
1	c	193	ARG	5.8
1	k	197	VAL	5.7
4	q	903	ARG	5.7
1	E	193	ARG	5.7
1	8	197	VAL	5.6
1	l	221	THR	5.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	M	222	GLY	5.6
1	V	187	ASN	5.5
1	F	170	PRO	5.5
1	d	185	GLY	5.5
1	W	193	ARG	5.5
1	l	185	GLY	5.5
4	q	561	MET	5.4
1	N	129	GLU	5.4
1	N	197	VAL	5.4
1	5	196	ASP	5.4
1	M	187	ASN	5.3
1	h	219	ARG	5.3
1	4	128	VAL	5.2
1	I	176	ARG	5.2
1	R	140	ASP	5.2
1	Z	187	ASN	5.1
1	k	193	ARG	5.1
1	h	149	GLY	5.1
1	g	187	ASN	5.1
1	l	128	VAL	5.0
1	N	193	ARG	5.0
1	4	214	MET	5.0
1	S	197	VAL	4.9
1	g	196	ASP	4.9
1	J	226	SER	4.9
1	Z	203	ARG	4.9
1	l	222	GLY	4.9
1	4	198	HIS	4.9
1	R	193	ARG	4.8
1	d	196	ASP	4.8
1	5	222	GLY	4.8
1	Z	197	VAL	4.8
4	q	603	ARG	4.8
1	A	193	ARG	4.8
1	V	196	ASP	4.7
1	I	193	ARG	4.7
1	g	129	GLU	4.7
1	S	196	ASP	4.7
1	E	148	ALA	4.7
1	8	148	ALA	4.6
2	i	4	DC	4.6
1	M	148	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	1	197	VAL	4.6
1	B	148	ALA	4.6
1	k	194	THR	4.6
1	h	196	ASP	4.6
1	N	198	HIS	4.6
1	8	196	ASP	4.6
4	o	562	ARG	4.6
1	V	194	THR	4.5
1	I	197	VAL	4.5
1	4	203	ARG	4.5
4	o	592	ALA	4.5
1	J	197	VAL	4.5
4	o	566	ASP	4.5
1	N	217	THR	4.4
1	S	198	HIS	4.4
1	J	193	ARG	4.4
1	E	198	HIS	4.4
2	e	4	DC	4.4
1	W	134	MET	4.4
1	V	209	GLY	4.4
1	F	193	ARG	4.4
1	c	140	ASP	4.4
1	R	194	THR	4.4
4	q	551	LEU	4.4
1	5	193	ARG	4.3
1	5	194	THR	4.3
1	4	159	GLU	4.3
1	g	131	VAL	4.3
1	V	193	ARG	4.3
1	d	198	HIS	4.3
1	8	149	GLY	4.3
1	k	205	ALA	4.2
1	4	222	GLY	4.2
1	5	148	ALA	4.2
4	q	908	GLU	4.2
1	M	203	ARG	4.2
1	J	196	ASP	4.2
3	7	24	DA	4.2
1	k	198	HIS	4.2
1	9	198	HIS	4.2
1	d	217	THR	4.2
1	Z	148	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
2	O	2	DG	4.2
1	S	194	THR	4.1
1	Z	129	GLU	4.1
1	4	193	ARG	4.1
1	k	129	GLU	4.1
1	V	173	VAL	4.1
1	l	219	ARG	4.1
1	9	193	ARG	4.1
1	k	196	ASP	4.1
1	l	196	ASP	4.1
1	A	203	ARG	4.1
1	g	194	THR	4.1
1	l	193	ARG	4.1
1	l	198	HIS	4.0
1	B	193	ARG	4.0
1	E	196	ASP	4.0
1	h	170	PRO	4.0
1	W	197	VAL	4.0
1	9	181	ASN	4.0
1	V	198	HIS	4.0
1	9	194	THR	3.9
1	g	219	ARG	3.9
1	5	219	ARG	3.9
1	k	222	GLY	3.9
3	L	24	DA	3.9
1	I	198	HIS	3.9
1	k	148	ALA	3.9
1	g	198	HIS	3.9
1	c	158	THR	3.9
2	i	2	DG	3.9
3	n	4	DT	3.9
1	A	222	GLY	3.9
2	K	4	DC	3.9
1	I	173	VAL	3.8
1	R	198	HIS	3.8
1	W	196	ASP	3.8
1	W	198	HIS	3.8
1	V	226	SER	3.8
1	S	193	ARG	3.8
1	l	198	HIS	3.8
2	i	3	DG	3.8
1	E	149	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	g	130	GLU	3.8
1	l	129	GLU	3.8
1	F	194	THR	3.7
1	A	196	ASP	3.7
1	h	222	GLY	3.7
1	R	222	GLY	3.7
4	o	576	VAL	3.7
1	9	212	ASP	3.7
2	a	4	DC	3.7
1	N	203	ARG	3.7
1	4	187	ASN	3.7
3	f	3	DC	3.7
1	E	217	THR	3.7
1	g	218	VAL	3.6
4	o	541	ARG	3.6
3	D	2	DA	3.6
1	g	148	ALA	3.6
1	Z	218	VAL	3.6
1	E	222	GLY	3.6
1	9	185	GLY	3.5
1	V	129	GLU	3.5
1	d	194	THR	3.5
1	l	196	ASP	3.5
1	W	219	ARG	3.5
1	9	196	ASP	3.5
3	Y	2	DA	3.5
1	F	198	HIS	3.5
1	4	201	ARG	3.5
3	j	24	DA	3.5
4	o	533	ASP	3.5
4	q	585	GLU	3.5
1	8	195	VAL	3.5
1	B	194	THR	3.5
1	W	226	SER	3.5
1	k	159	GLU	3.5
1	E	197	VAL	3.5
1	M	193	ARG	3.5
1	8	198	HIS	3.5
1	F	196	ASP	3.4
1	l	181	ASN	3.4
1	A	198	HIS	3.4
2	X	4	DC	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	I	209	GLY	3.4
1	N	148	ALA	3.4
1	c	198	HIS	3.4
1	R	220	GLY	3.4
1	A	205	ALA	3.4
1	Z	158	THR	3.4
1	J	198	HIS	3.4
4	q	592	ALA	3.4
1	4	129	GLU	3.4
1	4	196	ASP	3.4
1	A	140	ASP	3.3
1	8	200	ARG	3.3
1	k	208	PRO	3.3
1	M	205	ALA	3.3
1	g	193	ARG	3.3
1	8	187	ASN	3.3
1	W	157	PRO	3.3
1	J	148	ALA	3.3
1	A	197	VAL	3.3
3	U	22	DA	3.3
1	d	193	ARG	3.3
4	q	599	ARG	3.3
1	B	196	ASP	3.3
1	E	194	THR	3.3
1	8	173	VAL	3.3
2	O	21	DC	3.3
4	o	899	GLU	3.3
1	I	196	ASP	3.3
2	2	2	DG	3.3
1	I	219	ARG	3.3
1	N	156	GLY	3.3
1	W	149	GLY	3.3
3	D	3	DC	3.3
1	B	198	HIS	3.3
1	h	157	PRO	3.3
1	Z	130	GLU	3.3
1	R	186	THR	3.2
1	1	203	ARG	3.2
1	c	217	THR	3.2
3	U	2	DA	3.2
1	J	157	PRO	3.2
1	4	148	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	W	148	ALA	3.2
2	2	21	DC	3.2
1	N	216	GLN	3.2
1	Z	149	GLY	3.2
3	j	4	DT	3.2
1	1	156	GLY	3.2
1	W	170	PRO	3.2
1	8	129	GLU	3.2
2	e	2	DG	3.2
2	m	2	DG	3.2
2	m	4	DC	3.2
1	1	169	HIS	3.2
4	o	589	GLN	3.2
1	c	196	ASP	3.2
4	o	599	ARG	3.2
2	O	24	DA	3.2
1	8	131	VAL	3.2
3	Y	3	DC	3.2
1	M	196	ASP	3.1
1	Z	196	ASP	3.1
1	I	222	GLY	3.1
1	d	148	ALA	3.1
1	S	226	SER	3.1
1	h	129	GLU	3.1
1	B	226	SER	3.1
1	l	203	ARG	3.1
3	f	4	DT	3.1
2	X	2	DG	3.1
1	A	219	ARG	3.1
3	f	24	DA	3.1
1	h	197	VAL	3.1
2	a	2	DG	3.1
1	F	159	GLU	3.1
1	h	229	PHE	3.1
1	N	196	ASP	3.1
1	8	203	ARG	3.1
1	c	219	ARG	3.1
1	1	193	ARG	3.1
3	n	13	DA	3.1
2	O	10	DT	3.1
2	e	1	DT	3.1
1	h	158	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	9	138	SER	3.1
1	W	194	THR	3.0
2	6	20	DA	3.0
1	9	217	THR	3.0
2	2	23	DA	3.0
4	q	550	GLY	3.0
1	h	138	SER	3.0
2	C	20	DA	3.0
2	K	9	DA	3.0
1	E	185	GLY	3.0
2	X	20	DA	3.0
1	B	140	ASP	3.0
1	M	217	THR	3.0
1	k	220	GLY	3.0
4	o	607	LEU	3.0
1	9	148	ALA	3.0
1	9	222	GLY	3.0
3	3	3	DC	3.0
1	Z	219	ARG	3.0
1	d	201	ARG	3.0
1	I	128	VAL	3.0
4	o	564	GLY	3.0
1	4	195	VAL	3.0
1	c	197	VAL	3.0
1	S	222	GLY	3.0
1	h	203	ARG	3.0
1	R	148	ALA	3.0
1	A	214	MET	3.0
1	k	217	THR	3.0
1	S	200	ARG	3.0
1	W	217	THR	3.0
1	5	217	THR	3.0
1	h	198	HIS	3.0
1	1	216	GLN	2.9
1	S	157	PRO	2.9
1	W	178	GLN	2.9
4	o	908	GLU	2.9
2	e	9	DA	2.9
1	W	159	GLU	2.9
2	K	2	DG	2.9
1	l	143	SER	2.9
3	U	25	DG	2.9

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Mol	Chain	Res	Type	RSRZ
4	o	584	ARG	2.9
1	V	220	GLY	2.9
1	V	219	ARG	2.9
4	o	603	ARG	2.9
1	c	148	ALA	2.9
1	I	140	ASP	2.9
1	8	219	ARG	2.9
3	P	5	DT	2.9
2	C	3	DG	2.9
1	4	142	THR	2.9
3	7	2	DA	2.9
1	M	220	GLY	2.9
2	a	12	DA	2.9
1	F	155	MET	2.8
1	I	203	ARG	2.8
3	P	4	DT	2.8
1	1	158	THR	2.8
1	A	200	ARG	2.8
1	Z	194	THR	2.8
1	4	194	THR	2.8
1	g	217	THR	2.8
3	n	11	DA	2.8
1	5	170	PRO	2.8
1	Z	220	GLY	2.8
1	W	158	THR	2.8
1	F	143	SER	2.8
1	N	157	PRO	2.8
1	N	229	PHE	2.8
4	o	578	LYS	2.8
1	J	217	THR	2.8
1	d	220	GLY	2.8
3	f	25	DG	2.8
3	L	11	DA	2.8
3	P	26	DC	2.8
3	U	3	DC	2.8
1	M	197	VAL	2.8
1	d	195	VAL	2.8
1	k	149	GLY	2.8
4	o	900	LYS	2.8
1	W	195	VAL	2.8
1	l	209	GLY	2.8
3	Y	23	DC	2.8

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Mol	Chain	Res	Type	RSRZ
3	j	3	DC	2.8
1	B	222	GLY	2.8
1	S	217	THR	2.8
3	P	3	DC	2.8
1	9	136	GLY	2.8
2	2	4	DC	2.8
2	X	9	DA	2.8
1	R	128	VAL	2.8
1	g	149	GLY	2.8
1	5	198	HIS	2.8
4	q	546	ASP	2.8
1	Z	169	HIS	2.7
3	j	25	DG	2.7
2	e	20	DA	2.7
3	L	13	DA	2.7
1	g	197	VAL	2.7
2	K	3	DG	2.7
3	D	1	DC	2.7
4	o	549	ALA	2.7
1	1	185	GLY	2.7
1	8	175	SER	2.7
1	l	195	VAL	2.7
2	a	5	DT	2.7
1	M	194	THR	2.7
3	b	25	DG	2.7
1	g	159	GLU	2.7
1	N	199	ILE	2.7
1	I	220	GLY	2.7
1	c	194	THR	2.7
1	k	136	GLY	2.7
2	O	20	DA	2.7
1	A	192	ASP	2.7
2	6	5	DT	2.7
2	6	21	DC	2.7
1	J	138	SER	2.7
1	h	217	THR	2.7
2	T	4	DC	2.7
3	n	24	DA	2.7
1	4	141	PRO	2.7
1	9	150	GLU	2.7
1	E	219	ARG	2.7
1	k	147	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	197	VAL	2.7
3	Y	24	DA	2.7
1	A	194	THR	2.7
1	F	148	ALA	2.7
1	E	176	ARG	2.7
1	F	195	VAL	2.7
1	g	220	GLY	2.7
1	N	158	THR	2.7
1	M	143	SER	2.7
1	Z	186	THR	2.7
3	D	22	DA	2.7
3	f	11	DA	2.7
4	q	542	ALA	2.7
1	R	211	HIS	2.7
1	S	158	THR	2.7
1	M	158	THR	2.6
3	7	25	DG	2.6
1	R	195	VAL	2.6
1	F	227	THR	2.6
1	J	194	THR	2.6
1	V	159	GLU	2.6
1	4	182	HIS	2.6
2	6	2	DG	2.6
3	H	22	DA	2.6
1	d	135	GLN	2.6
3	3	25	DG	2.6
1	8	201	ARG	2.6
1	N	195	VAL	2.6
3	P	2	DA	2.6
4	o	559	LEU	2.6
1	I	148	ALA	2.6
1	h	193	ARG	2.6
3	3	11	DA	2.6
1	M	152	PRO	2.6
3	L	4	DT	2.6
1	J	219	ARG	2.6
1	c	195	VAL	2.6
1	h	140	ASP	2.6
1	d	221	THR	2.6
2	C	21	DC	2.6
3	n	3	DC	2.6
1	B	216	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
3	7	3	DC	2.6
3	3	24	DA	2.6
1	5	157	PRO	2.6
4	q	600	HIS	2.6
1	R	139	LEU	2.6
1	5	197	VAL	2.6
4	q	579	GLN	2.6
1	I	221	THR	2.6
1	5	158	THR	2.6
2	X	10	DT	2.6
2	m	3	DG	2.6
1	W	201	ARG	2.6
1	S	195	VAL	2.6
3	b	13	DA	2.6
1	A	181	ASN	2.6
1	J	216	GLN	2.6
1	V	195	VAL	2.5
2	2	22	DA	2.6
1	M	218	VAL	2.5
1	9	140	ASP	2.5
1	k	203	ARG	2.5
1	F	199	ILE	2.5
2	X	24	DA	2.5
3	L	12	DC	2.5
1	R	221	THR	2.5
2	6	3	DG	2.5
3	L	25	DG	2.5
3	b	4	DT	2.5
1	E	201	ARG	2.5
1	1	199	ILE	2.5
2	C	11	DA	2.5
1	A	195	VAL	2.5
1	c	138	SER	2.5
3	L	23	DC	2.5
3	3	2	DA	2.5
1	9	219	ARG	2.5
3	H	24	DA	2.5
1	A	182	HIS	2.5
1	1	135	GLN	2.5
1	V	200	ARG	2.5
1	9	203	ARG	2.5
1	1	220	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	O	4	DC	2.5
1	9	157	PRO	2.5
1	1	157	PRO	2.5
1	I	194	THR	2.5
1	J	195	VAL	2.5
2	T	5	DT	2.5
1	5	227	THR	2.5
1	B	205	ALA	2.5
1	N	150	GLU	2.5
1	9	137	LEU	2.5
1	B	158	THR	2.5
1	B	200	ARG	2.5
1	J	220	GLY	2.5
3	Y	13	DA	2.5
1	I	129	GLU	2.5
3	3	26	DC	2.5
1	A	225	PHE	2.5
1	E	195	VAL	2.5
1	9	197	VAL	2.5
1	E	218	VAL	2.5
1	M	198	HIS	2.5
1	9	218	VAL	2.5
2	6	15	DT	2.5
4	q	558	VAL	2.5
1	N	159	GLU	2.5
2	e	13	DA	2.5
3	n	14	DA	2.5
1	F	217	THR	2.5
1	h	212	ASP	2.5
1	l	212	ASP	2.5
1	V	191	GLU	2.4
3	D	25	DG	2.4
1	A	220	GLY	2.4
1	M	169	HIS	2.4
1	k	156	GLY	2.4
2	K	22	DA	2.4
3	L	3	DC	2.4
1	R	219	ARG	2.4
4	o	582	VAL	2.4
1	Z	217	THR	2.4
1	F	222	GLY	2.4
1	S	205	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	5	195	VAL	2.4
2	K	5	DT	2.4
3	P	14	DA	2.4
1	F	156	GLY	2.4
1	I	195	VAL	2.4
2	O	3	DG	2.4
2	2	3	DG	2.4
2	K	20	DA	2.4
2	O	23	DA	2.4
3	U	24	DA	2.4
1	M	131	VAL	2.4
1	4	199	ILE	2.4
1	8	217	THR	2.4
2	a	11	DA	2.4
1	N	194	THR	2.4
4	o	548	LEU	2.4
1	M	138	SER	2.4
1	R	196	ASP	2.4
1	F	220	GLY	2.4
1	M	216	GLN	2.4
1	g	195	VAL	2.4
1	k	195	VAL	2.4
2	G	9	DA	2.4
3	H	2	DA	2.4
1	c	159	GLU	2.4
1	l	148	ALA	2.4
1	c	227	THR	2.4
2	T	1	DT	2.4
3	Y	22	DA	2.4
3	f	14	DA	2.4
4	o	572	THR	2.4
1	R	151	GLU	2.4
4	q	556	ALA	2.4
1	k	161	LYS	2.4
2	O	22	DA	2.4
1	1	150	GLU	2.4
1	W	216	GLN	2.4
1	5	216	GLN	2.4
1	l	226	SER	2.4
1	V	227	THR	2.4
1	d	158	THR	2.4
2	K	10	DT	2.4

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Mol	Chain	Res	Type	RSRZ
1	9	229	PHE	2.4
1	c	192	ASP	2.4
1	l	217	THR	2.4
1	5	133	GLU	2.4
4	o	585	GLU	2.4
1	c	200	ARG	2.4
1	h	218	VAL	2.4
3	Y	25	DG	2.3
1	W	225	PHE	2.3
1	l	136	GLY	2.3
1	A	144	HIS	2.3
1	Z	198	HIS	2.3
1	c	136	GLY	2.3
1	c	218	VAL	2.3
3	P	24	DA	2.3
3	U	4	DT	2.3
3	3	4	DT	2.3
3	n	5	DT	2.3
1	N	219	ARG	2.3
1	l	138	SER	2.3
2	m	1	DT	2.3
3	7	23	DC	2.3
1	B	227	THR	2.3
1	l	195	VAL	2.3
1	M	151	GLU	2.3
1	E	208	PRO	2.3
1	l	134	MET	2.3
1	8	218	VAL	2.3
1	c	149	GLY	2.3
1	g	164	HIS	2.3
1	I	149	GLY	2.3
1	S	143	SER	2.3
1	k	218	VAL	2.3
2	2	24	DA	2.3
1	B	143	SER	2.3
2	6	4	DC	2.3
1	k	199	ILE	2.3
1	Z	216	GLN	2.3
1	g	135	GLN	2.3
1	k	137	LEU	2.3
1	J	200	ARG	2.3
1	l	157	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	V	222	GLY	2.3
1	R	213	ARG	2.3
1	I	199	ILE	2.3
1	J	227	THR	2.3
1	d	216	GLN	2.3
1	k	157	PRO	2.3
2	K	11	DA	2.3
2	i	13	DA	2.3
3	j	14	DA	2.3
1	S	140	ASP	2.3
1	d	128	VAL	2.3
3	3	23	DC	2.3
1	S	137	LEU	2.3
1	1	194	THR	2.3
1	F	200	ARG	2.3
2	K	14	DG	2.2
3	7	22	DA	2.2
1	A	199	ILE	2.2
1	8	157	PRO	2.2
1	4	226	SER	2.2
1	I	157	PRO	2.2
1	R	212	ASP	2.2
1	Z	226	SER	2.2
2	X	3	DG	2.2
1	A	130	GLU	2.2
1	B	195	VAL	2.2
1	E	191	GLU	2.2
1	N	201	ARG	2.2
1	5	200	ARG	2.2
1	8	221	THR	2.2
1	S	148	ALA	2.2
1	5	226	SER	2.2
2	K	24	DA	2.2
1	8	220	GLY	2.2
1	9	149	GLY	2.2
1	Z	168	THR	2.2
1	8	159	GLU	2.2
1	V	149	GLY	2.2
2	X	1	DT	2.2
1	4	164	HIS	2.2
3	j	2	DA	2.2
1	k	187	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	150	GLU	2.2
1	F	226	SER	2.2
1	5	192	ASP	2.2
1	M	221	THR	2.2
1	k	216	GLN	2.2
2	K	1	DT	2.2
2	e	5	DT	2.2
2	K	25	DA	2.2
4	o	583	THR	2.2
1	E	138	SER	2.2
1	I	226	SER	2.2
1	h	195	VAL	2.2
3	Y	11	DA	2.2
1	J	221	THR	2.2
3	n	25	DG	2.2
1	I	164	HIS	2.2
1	9	195	VAL	2.2
1	J	222	GLY	2.2
1	M	168	THR	2.2
2	i	9	DA	2.2
1	A	221	THR	2.2
1	V	185	GLY	2.2
1	l	149	GLY	2.2
1	k	200	ARG	2.2
1	V	216	GLN	2.2
1	4	178	GLN	2.2
2	G	4	DC	2.2
3	n	23	DC	2.2
1	h	201	ARG	2.2
1	F	158	THR	2.2
3	Y	4	DT	2.2
1	k	219	ARG	2.2
1	N	149	GLY	2.2
1	d	212	ASP	2.2
3	b	11	DA	2.2
1	J	143	SER	2.2
1	S	201	ARG	2.1
1	E	151	GLU	2.1
1	W	212	ASP	2.1
2	e	10	DT	2.1
1	8	136	GLY	2.1
1	c	211	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	4	DC	2.1
2	i	5	DT	2.1
3	H	4	DT	2.1
3	n	10	DG	2.1
1	4	133	GLU	2.1
1	h	194	THR	2.1
2	a	13	DA	2.1
3	3	14	DA	2.1
3	7	13	DA	2.1
1	A	168	THR	2.1
1	R	199	ILE	2.1
1	W	138	SER	2.1
4	o	539	SER	2.1
1	M	181	ASN	2.1
1	Z	150	GLU	2.1
2	e	12	DA	2.1
1	R	218	VAL	2.1
1	S	169	HIS	2.1
1	5	138	SER	2.1
1	8	222	GLY	2.1
2	2	10	DT	2.1
1	E	164	HIS	2.1
1	h	220	GLY	2.1
1	E	199	ILE	2.1
1	B	161	LYS	2.1
1	S	227	THR	2.1
3	3	10	DG	2.1
1	A	148	ALA	2.1
1	F	201	ARG	2.1
2	m	5	DT	2.1
3	3	6	DT	2.1
1	I	218	VAL	2.1
1	W	141	PRO	2.1
1	J	134	MET	2.1
3	f	23	DC	2.1
1	5	218	VAL	2.1
1	F	216	GLN	2.1
1	Z	136	GLY	2.1
1	9	156	GLY	2.1
2	G	5	DT	2.1
1	A	218	VAL	2.1
1	J	192	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	203	ARG	2.1
1	Z	193	ARG	2.1
4	o	588	ARG	2.1
2	e	3	DG	2.1
4	q	559	LEU	2.1
1	S	216	GLN	2.1
1	l	148	ALA	2.1
1	8	226	SER	2.1
1	8	229	PHE	2.1
3	j	23	DC	2.1
4	o	903	ARG	2.1
1	I	150	GLU	2.1
1	5	229	PHE	2.1
1	h	136	GLY	2.1
2	O	5	DT	2.1
4	o	556	ALA	2.1
1	R	226	SER	2.1
1	c	141	PRO	2.1
3	P	23	DC	2.1
2	2	26	DG	2.1
2	X	11	DA	2.1
2	m	24	DA	2.1
3	D	24	DA	2.1
3	L	22	DA	2.1
3	Y	14	DA	2.1
1	l	199	ILE	2.1
1	W	218	VAL	2.1
1	9	133	GLU	2.1
3	H	1	DC	2.1
1	B	217	THR	2.1
1	V	203	ARG	2.1
1	g	168	THR	2.1
3	b	10	DG	2.1
1	Z	181	ASN	2.1
2	X	25	DA	2.1
1	F	192	ASP	2.1
1	S	190	VAL	2.1
1	Z	151	GLU	2.1
1	R	137	LEU	2.1
1	R	227	THR	2.1
3	f	10	DG	2.1
1	W	176	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	138	SER	2.1
1	9	143	SER	2.1
1	c	135	GLN	2.1
1	W	151	GLU	2.1
1	A	164	HIS	2.1
1	V	217	THR	2.1
2	X	14	DG	2.1
1	F	136	GLY	2.1
1	5	220	GLY	2.1
1	9	152	PRO	2.1
1	c	156	GLY	2.1
1	l	216	GLN	2.1
3	7	1	DC	2.1
4	q	590	ILE	2.1
1	4	217	THR	2.1
1	R	158	THR	2.0
1	k	209	GLY	2.0
2	O	13	DA	2.0
2	T	9	DA	2.0
2	2	13	DA	2.0
1	E	173	VAL	2.0
1	N	200	ARG	2.0
1	V	181	ASN	2.0
1	1	152	PRO	2.0
1	9	164	HIS	2.0
1	d	136	GLY	2.0
1	g	140	ASP	2.0
1	g	192	ASP	2.0
1	k	227	THR	2.0
1	h	216	GLN	2.0
4	q	539	SER	2.0
1	A	188	VAL	2.0
1	E	200	ARG	2.0
1	R	217	THR	2.0
3	j	22	DA	2.0
1	5	137	LEU	2.0
2	T	24	DA	2.0
1	V	218	VAL	2.0
1	S	159	GLU	2.0
2	2	9	DA	2.0
3	U	11	DA	2.0
2	X	15	DT	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	187	ASN	2.0
1	V	199	ILE	2.0
1	d	203	ARG	2.0
1	I	229	PHE	2.0
1	I	191	GLU	2.0
1	d	150	GLU	2.0
2	O	18	DT	2.0
1	l	219	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.