



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:19 PM GMT

PDB ID : 3T72
Title : PhoB(E)-Sigma70(4)-(RNAP-Betha-flap-tip-helix)-DNA Transcription
Activation Sub-Complex
Authors : Blanco, A.G.; Canals, A.; Bernues, J.; Sola, M.; Coll, M.
Deposited on : 2011-07-29
Resolution : 4.33 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

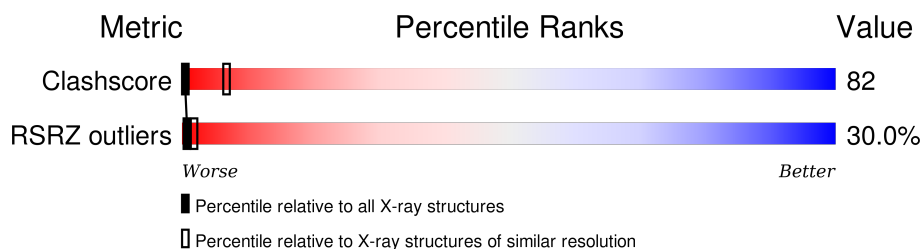
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

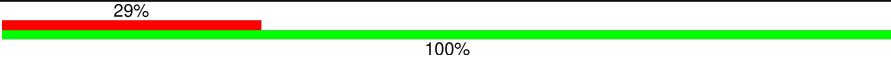
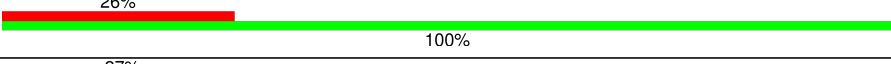
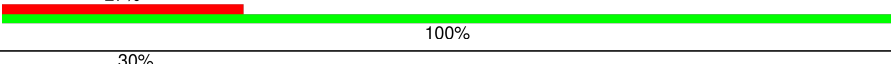
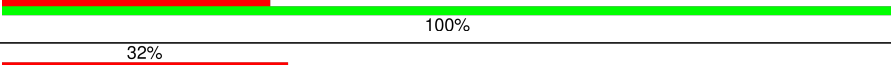
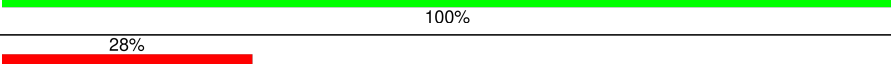

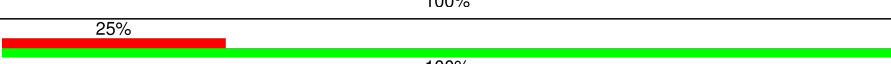
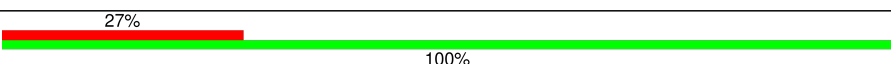

The reported resolution of this entry is 4.33 Å.

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	102246	1171 (5.08-3.60)
RSRZ outliers	91569	1067 (5.08-3.60)

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 ≥ 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	29%
1	J	102	24%
1	M	102	29%
1	N	102	25%
1	R	102	29%
1	S	102	29%
1	V	102	30%
1	W	102	27%
1	Z	102	28%
1	c	102	31%
1	d	102	22%
1	g	102	25%
1	h	102	29%
1	k	102	30%
1	l	102	24%
2	2	26	50%
2	6	26	27%
2	C	26	35%
2	G	26	19%
2	K	26	50%
2	O	26	50%
2	T	26	23%
2	X	26	42%
2	a	26	35%
2	e	26	38%

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Mol	Chain	Length	Quality of chain
2	i	26	<div> <div>35%</div> <div>96%</div> <div>.</div> </div>
2	m	26	<div> <div>31%</div> <div>88%</div> <div>12%</div> </div>
3	3	26	<div> <div>50%</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>35%</div> <div>92%</div> <div>8%</div> </div>
3	H	26	<div> <div>38%</div> <div>88%</div> <div>12%</div> </div>
3	L	26	<div> <div>46%</div> <div>96%</div> <div>.</div> </div>
3	P	26	<div> <div>50%</div> <div>96%</div> <div>.</div> </div>
3	U	26	<div> <div>31%</div> <div>92%</div> <div>8%</div> </div>
3	Y	26	<div> <div>42%</div> <div>96%</div> <div>.</div> </div>
3	b	26	<div> <div>27%</div> <div>81%</div> <div>19%</div> </div>
3	f	26	<div> <div>38%</div> <div>92%</div> <div>8%</div> </div>
3	j	26	<div> <div>42%</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>35%</div> <div>94%</div> <div>6%</div> </div>
4	q	99	<div> <div>28%</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			

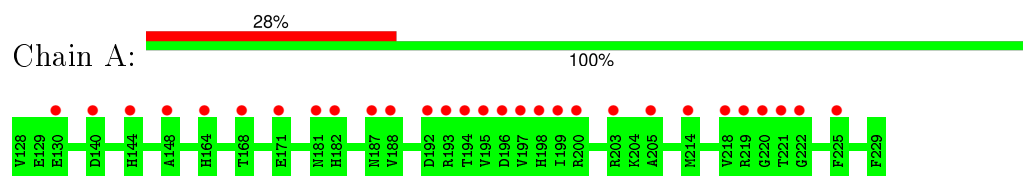
There are 14 discrepancies between the modelled and reference sequences:

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

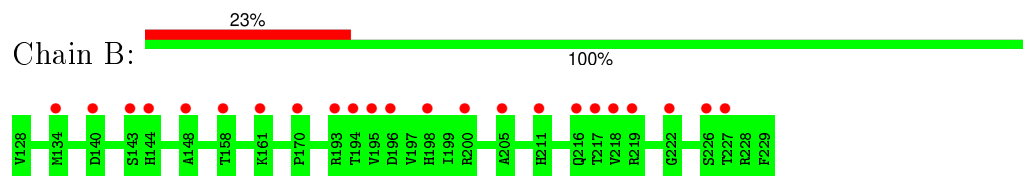
3 Residue-property plots [i](#)

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

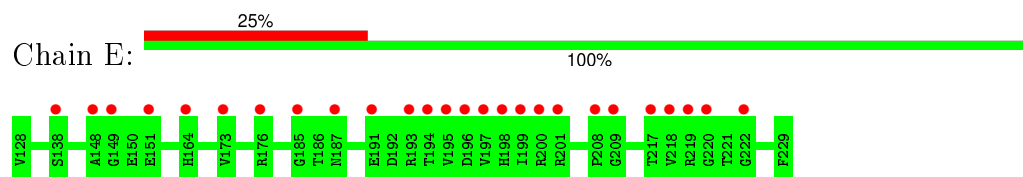
- Molecule 1: Phosphate regulon transcriptional regulatory protein phoB



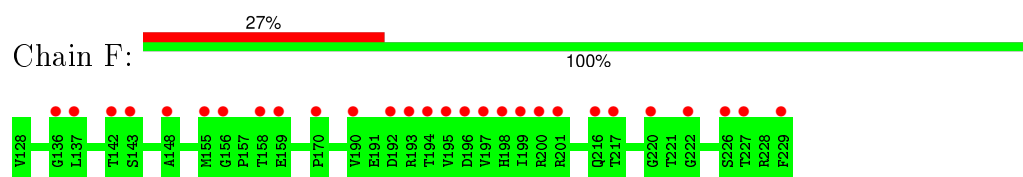
- Molecule 1: Phosphate regulon transcriptional regulatory protein phoB



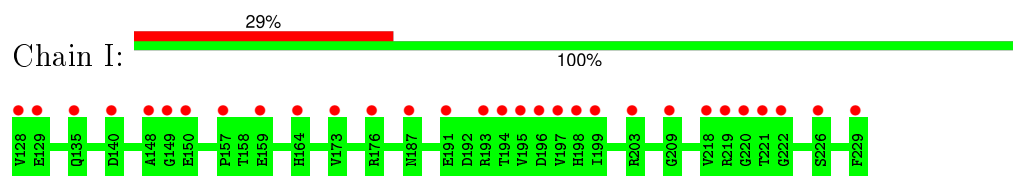
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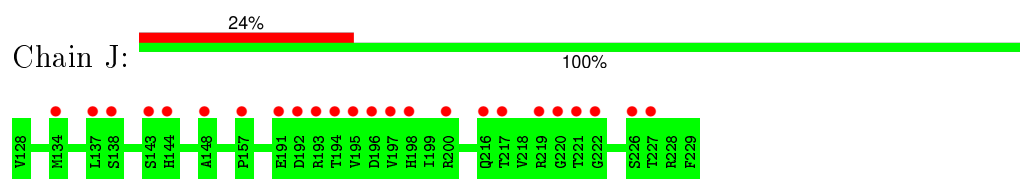
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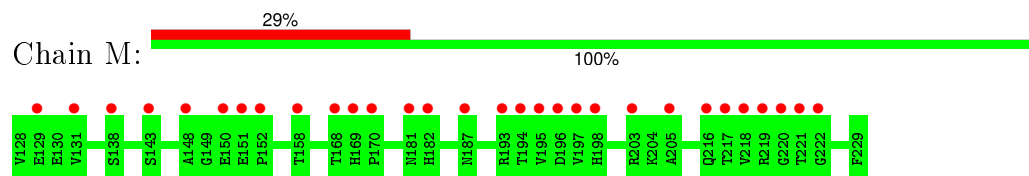
- Molecule 1: Phosphate regulon transcriptional regulatory protein phoB



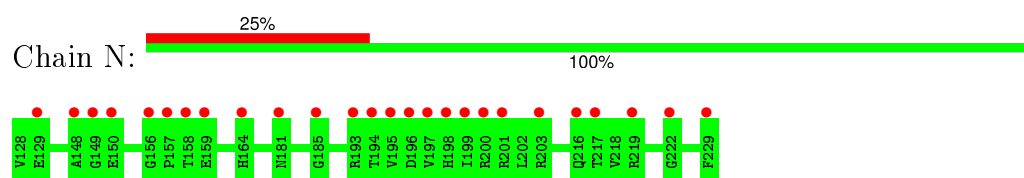
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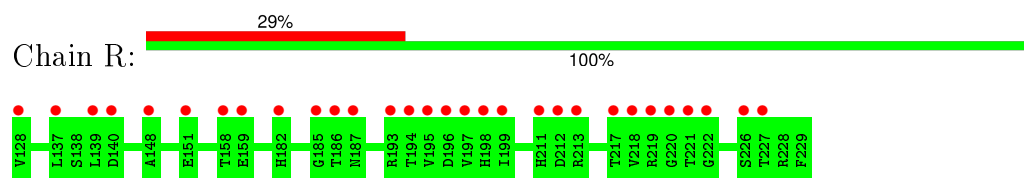
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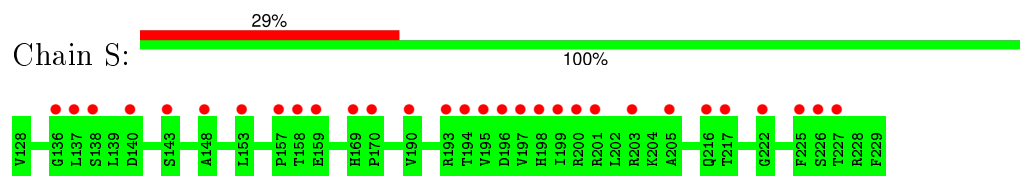
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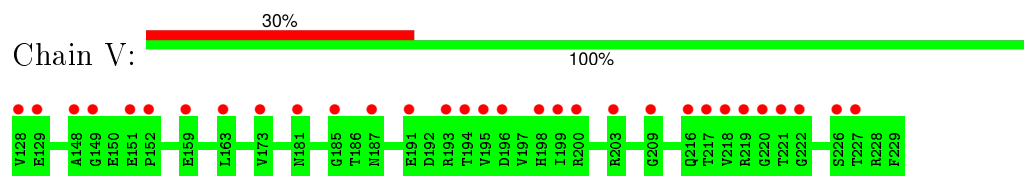
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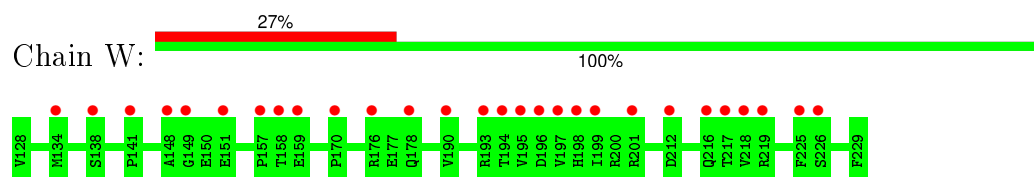
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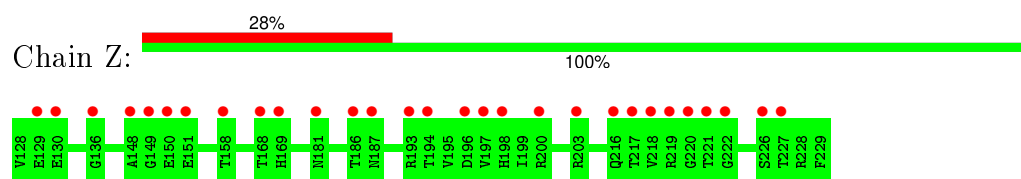
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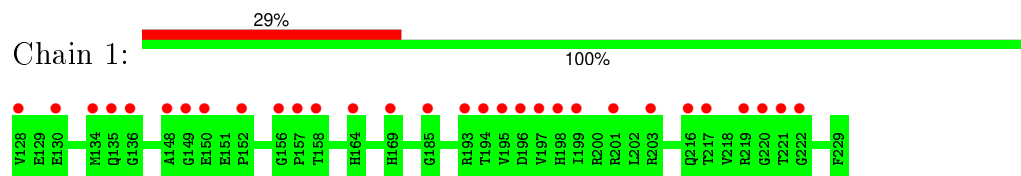
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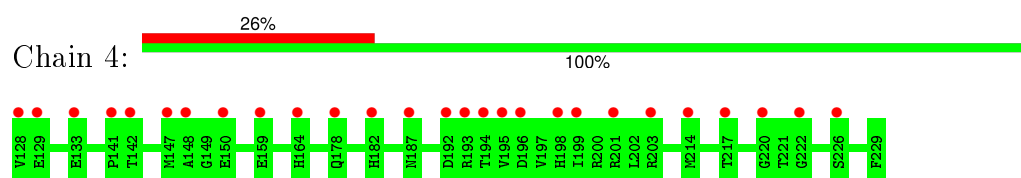
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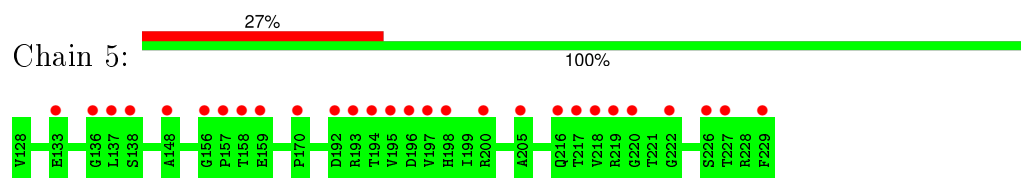
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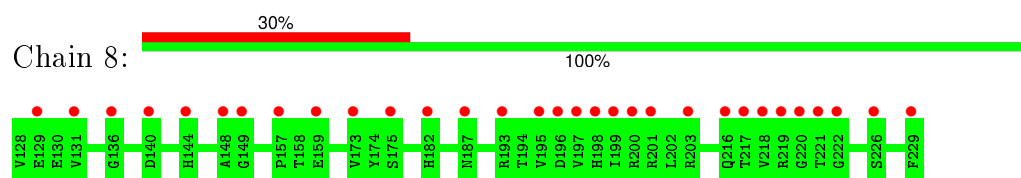
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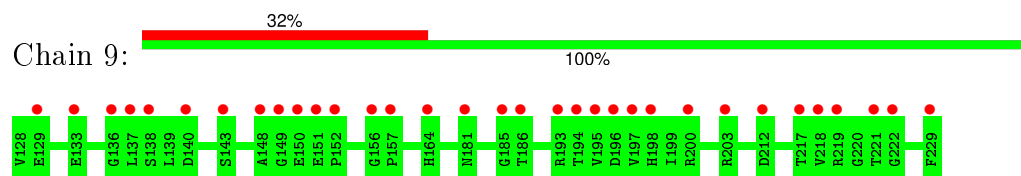
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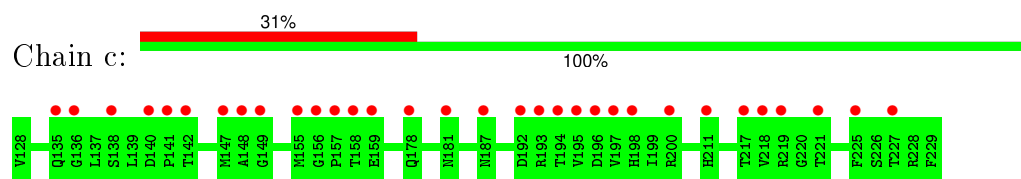
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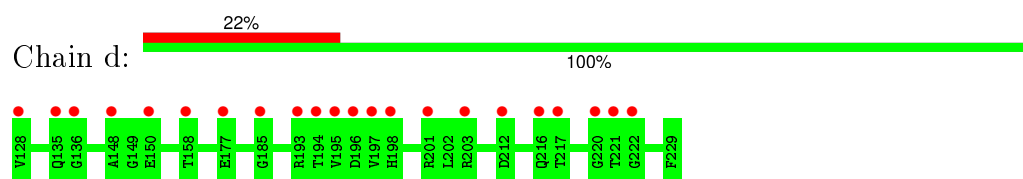
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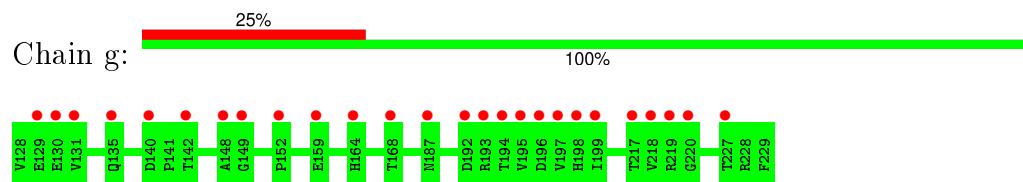
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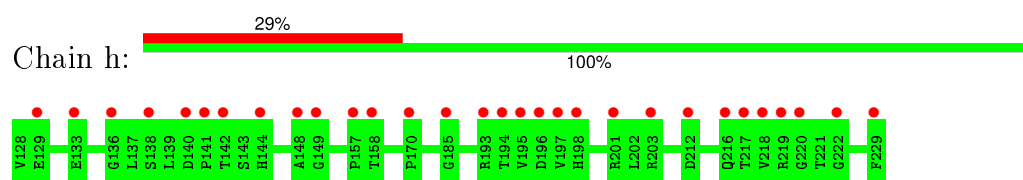
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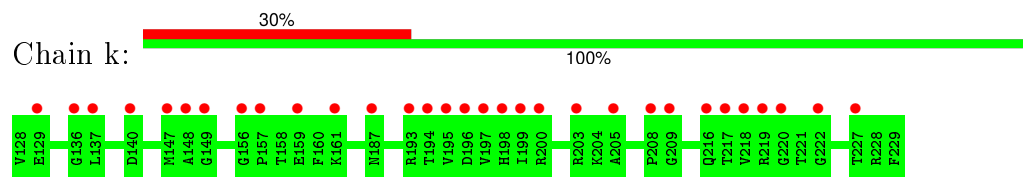
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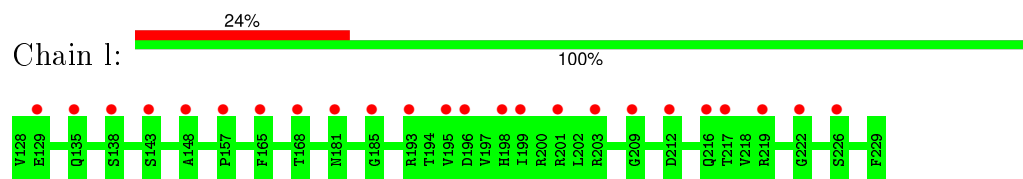
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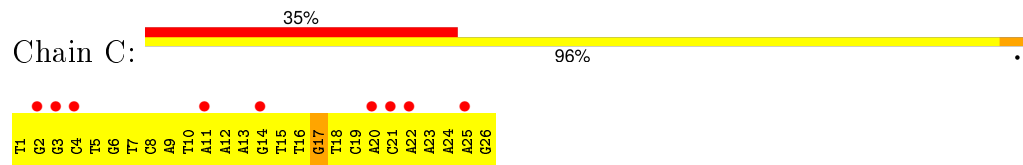
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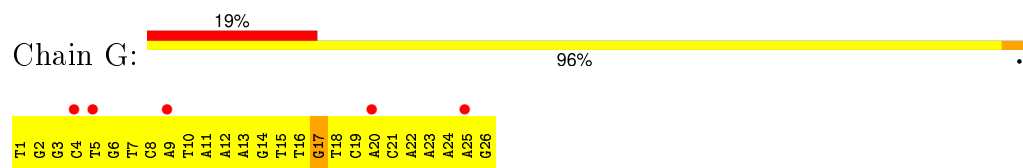
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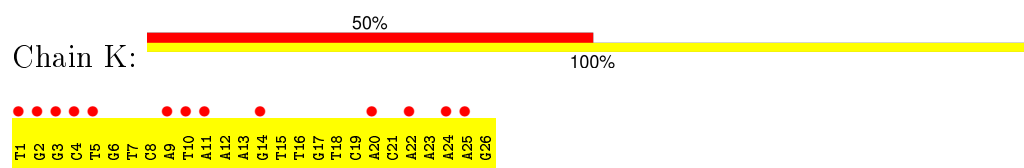
- Molecule 2: PHO BOX DNA (STRAND 1)



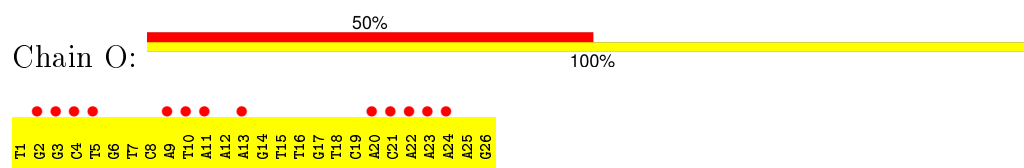
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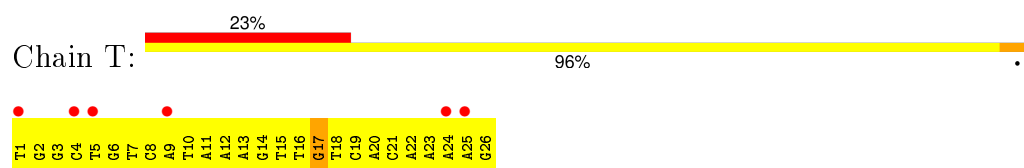
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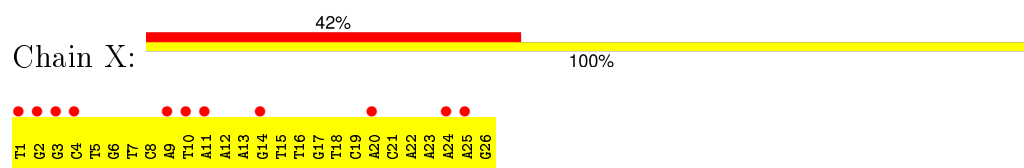
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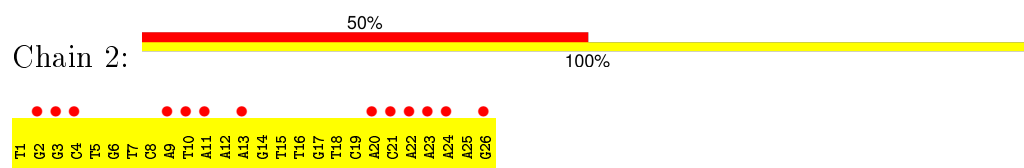
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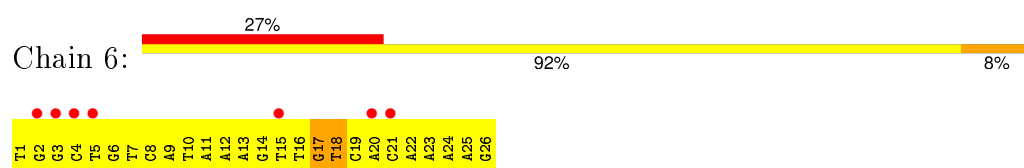
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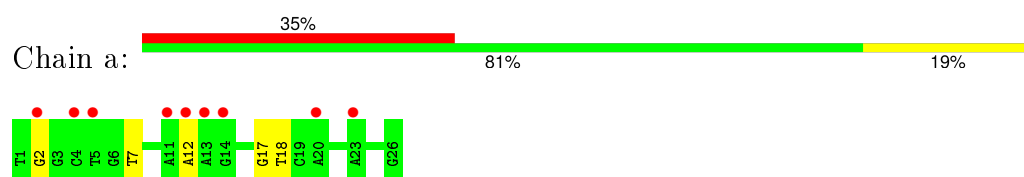
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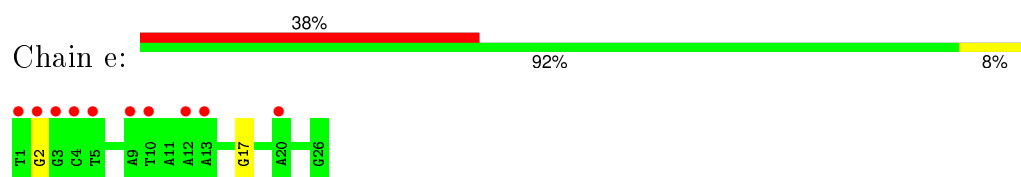
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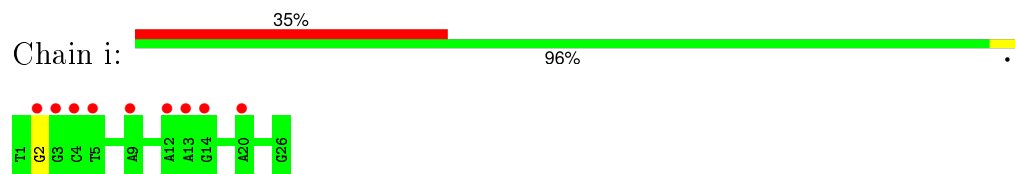
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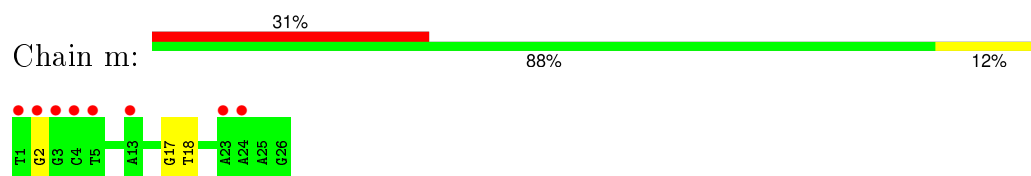
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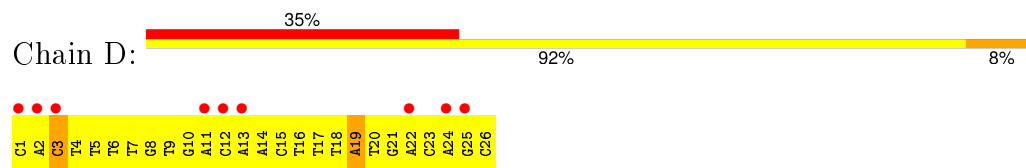
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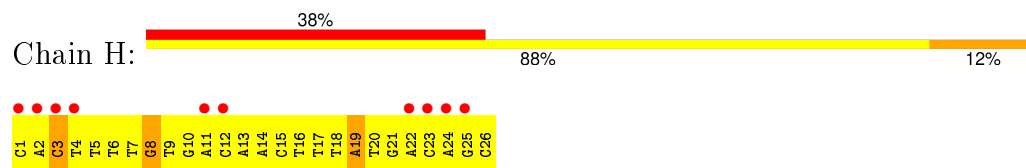
- Molecule 2: PHO BOX DNA (STRAND 1)



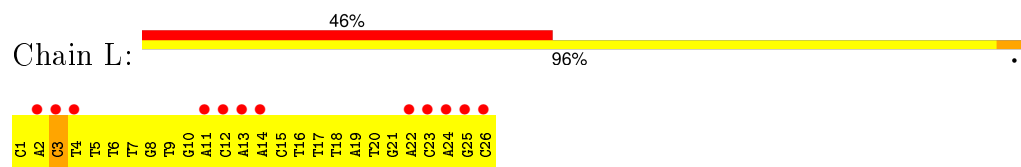
- Molecule 3: PHO BOX DNA (STRAND 2)



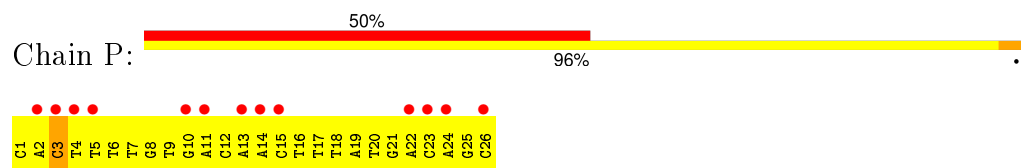
- Molecule 3: PHO BOX DNA (STRAND 2)



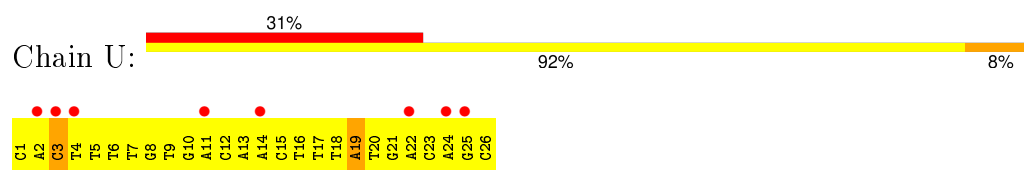
- Molecule 3: PHO BOX DNA (STRAND 2)



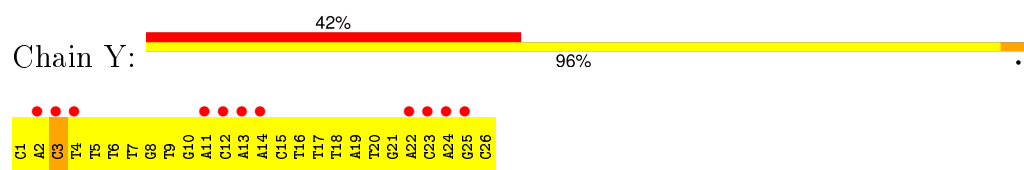
- Molecule 3: PHO BOX DNA (STRAND 2)



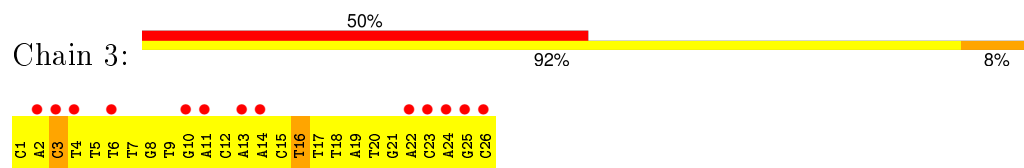
- Molecule 3: PHO BOX DNA (STRAND 2)



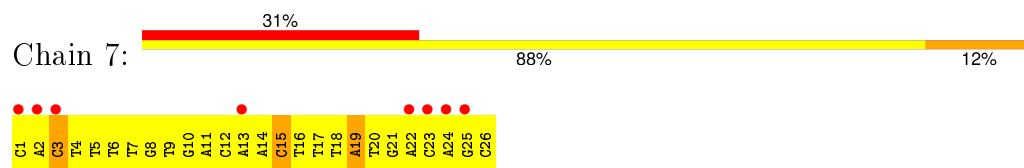
- Molecule 3: PHO BOX DNA (STRAND 2)



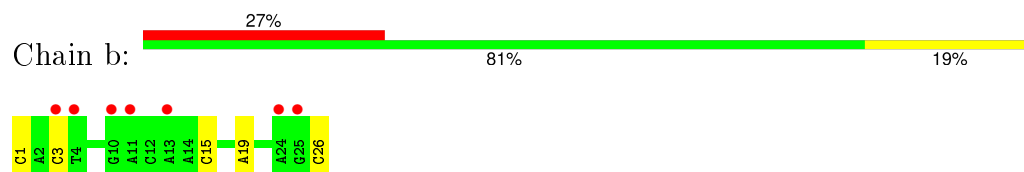
- Molecule 3: PHO BOX DNA (STRAND 2)



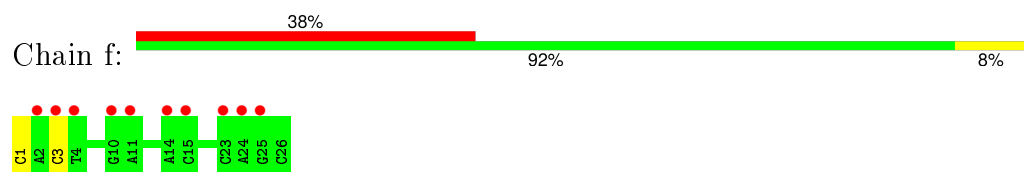
- Molecule 3: PHO BOX DNA (STRAND 2)



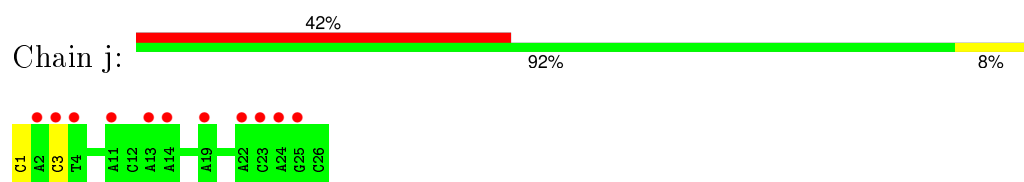
- Molecule 3: PHO BOX DNA (STRAND 2)



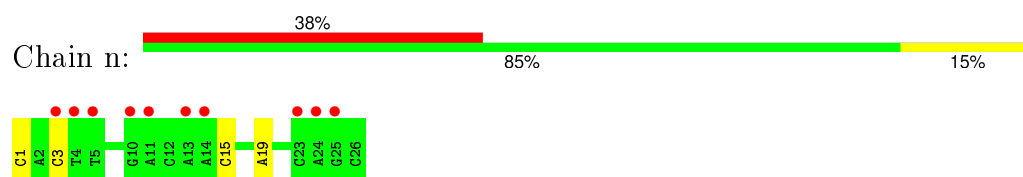
- Molecule 3: PHO BOX DNA (STRAND 2)



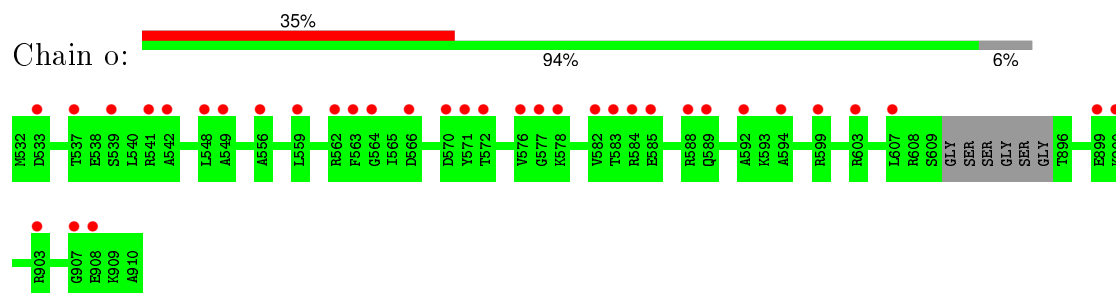
- Molecule 3: PHO BOX DNA (STRAND 2)



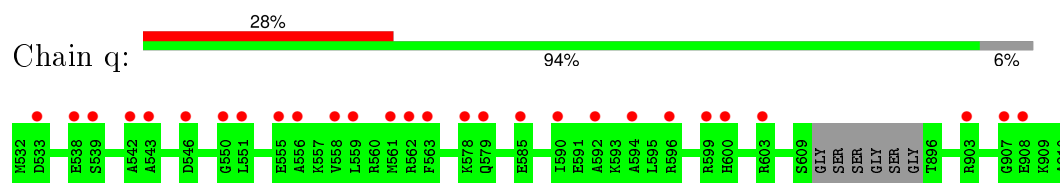
- Molecule 3: PHO BOX DNA (STRAND 2)



- 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, α , β , γ	277.30Å 161.40Å 260.10Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	50.00 – 4.33 20.00 – 4.33	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.33) 96.4 (20.00-4.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	189.2	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	-2.34 , 331.6	EDS
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
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 72977 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	15354	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.19 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.1959e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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
3:L:9:DT:H2''	3:L:10:DG:H5''	1.45	0.97
2:6:24:DA:H4'	2:6:25:DA:OP1	1.61	0.97
2:2:24:DA:H4'	2:2:25:DA:OP1	1.62	0.97
3:D:9:DT:H2''	3:D:10:DG:H5''	1.47	0.97
3:7:9:DT:H2''	3:7:10:DG:H5''	1.47	0.97
2:G:23:DA:H4'	2:G:24:DA:OP1	1.65	0.97
3:H:9:DT:H2''	3:H:10:DG:H5''	1.44	0.96
2:T:24:DA:H4'	2:T:25:DA:OP1	1.62	0.96
2:O:23:DA:H4'	2:O:24:DA:OP1	1.64	0.96
2:C:24:DA:H4'	2:C:25:DA:OP1	1.61	0.96
3:P:9:DT:H2''	3:P:10:DG:H5''	1.46	0.96
3:3:9:DT:H2''	3:3:10:DG:H5''	1.47	0.95
2:O:24:DA:H4'	2:O:25:DA:OP1	1.63	0.95
2:6:23:DA:H4'	2:6:24:DA:OP1	1.64	0.94
2:X:24:DA:H4'	2:X:25:DA:OP1	1.63	0.94
2:K:23:DA:H4'	2:K:24:DA:OP1	1.66	0.94
2:O:11:DA:H2''	2:O:12:DA:H5''	1.50	0.94
2:C:23:DA:H4'	2:C:24:DA:OP1	1.64	0.93
2:O:7:DT:H2''	2:O:8:DC:H5'	1.51	0.93
2:2:23:DA:H4'	2:2:24:DA:OP1	1.64	0.93
2:T:11:DA:H2''	2:T:12:DA:H5''	1.51	0.92
3:L:14:DA:H2''	3:L:15:DC:C5'	1.99	0.92
2:X:11:DA:H2''	2:X:12:DA:H5''	1.51	0.92
2:K:11:DA:H2''	2:K:12:DA:H5''	1.51	0.92
2:X:23:DA:H4'	2:X:24:DA:OP1	1.66	0.92
2:O:6:DG:H2''	2:O:7:DT:H5''	1.51	0.92
2:T:23:DA:H4'	2:T:24:DA:OP1	1.65	0.92
2:2:7:DT:H2''	2:2:8:DC:H5'	1.51	0.92
3:H:14:DA:H2''	3:H:15:DC:C5'	2.00	0.92
2:6:7:DT:H2''	2:6:8:DC:H5'	1.51	0.92
2:G:25:DA:H1'	2:G:26:DG:O4'	1.70	0.91
2:2:6:DG:H2''	2:2:7:DT:H5''	1.50	0.91
2:G:11:DA:H2''	2:G:12:DA:H5''	1.51	0.91

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:8:DG:C2'	3:3:9:DT:H5''	2.08	0.83
2:2:6:DG:H2''	2:2:7:DT:C5'	2.09	0.82
2:C:5:DT:H5'	2:C:5:DT:H6	1.45	0.82
2:6:5:DT:H6	2:6:5:DT:H5'	1.44	0.82
2:O:6:DG:H2''	2:O:7:DT:C5'	2.09	0.82
2:6:12:DA:H2''	2:6:13:DA:H5'	1.62	0.82
2:C:12:DA:H2''	2:C:13:DA:H5'	1.62	0.81
3:P:4:DT:H2''	3:P:5:DT:H72	1.63	0.81
2:O:8:DC:N3	3:P:21:DG:N1	2.26	0.81
2:K:6:DG:H2''	2:K:7:DT:C5'	2.11	0.81
3:U:4:DT:H2''	3:U:5:DT:H72	1.63	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
2:G:12:DA:H2''	2:G:13:DA:H5'	1.63	0.81
2:O:12:DA:H2''	2:O:13:DA:H5'	1.62	0.81
2:G:3:DG:H2''	2:G:4:DC:H5'	1.61	0.80
3:3:13:DA:H2''	3:3:14:DA:OP2	1.81	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:O:7:DT:H2''	2:O:8:DC:C5'	2.11	0.80
2:6:7:DT:H2''	2:6:8:DC:C5'	2.12	0.80
2:T:5:DT:H5'	2:T:5:DT:H6	1.47	0.80
2:C:7:DT:H2''	2:C:8:DC:C5'	2.12	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: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
2:C:6:DG:H2''	2:C:7:DT:C5'	2.12	0.80
3:7:4:DT:H2''	3:7:5:DT:H72	1.64	0.80
3:H:13:DA:H2''	3:H:14:DA:OP2	1.82	0.79
2:X:6:DG:H2''	2:X:7:DT:C5'	2.11	0.79
2:G:6:DG:H2''	2:G:7:DT:C5'	2.11	0.79
3:D:13:DA:H2''	3:D:14:DA:OP2	1.82	0.79
2:G:5:DT:H5'	2:G:5:DT:H6	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)
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:D:4:DT:H2''	3:D:5:DT:H72	1.64	0.79
2:K:3:DG:H2''	2:K:4:DC:H5'	1.64	0.79
3:3:11:DA:H2''	3:3:12:DC:C5'	2.12	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:T:7:DT:H2''	2:T:8:DC:C5'	2.13	0.79
2:O:7:DT:O4	3:P:22:DA:N6	2.14	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
3:U:16:DT:H2'	3:U:17:DT:H72	1.66	0.78
2:O:12:DA:H2''	2:O:13:DA:C5'	2.13	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
3:L:13:DA:H2''	3:L:14:DA:OP2	1.82	0.77
2:G:7:DT:H2''	2:G:8:DC:C5'	2.13	0.77
2:X:7:DT:H2''	2:X:8:DC:C5'	2.14	0.77
2:X:12:DA:H2''	2:X:13:DA:H5'	1.65	0.77
2:O:2:DG:H4'	2:O:2:DG:OP1	1.85	0.77
3:L:11:DA:H2''	3:L:12:DC:C5'	2.15	0.77
3:H:16:DT:H2'	3:H:17:DT:H72	1.66	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
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
3:L:2:DA:H1'	3:L:3:DC:H5'	1.68	0.76
2:K:6:DG:H2'	2:K:7:DT:H71	1.67	0.76
2:G:2:DG:H4'	2:G:2:DG:OP1	1.85	0.76
2:T:2:DG:H4'	2:T:2:DG:OP1	1.85	0.76
3:3:2:DA:H1'	3:3:3:DC:H5'	1.67	0.76
2:K:12:DA:H2''	2:K:13:DA:C5'	2.16	0.76

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:11:DA:C2'	2:G:12:DA:H5''	2.19	0.72
3:3:8:DG:H1'	3:3:9:DT:H5''	1.72	0.72
3:U:8:DG:H1'	3:U:9:DT:H5''	1.72	0.72
2:C:11:DA:C2'	2:C:12:DA:H5''	2.19	0.72
2:6:11:DA:C2'	2:6:12:DA:H5''	2.19	0.72
2:T:11:DA:C2'	2:T:12:DA:H5''	2.19	0.72
2:2:19:DC:H2''	2:2:20:DA:C8	2.25	0.72
2:C:15:DT:H1'	2:C:16:DT:H5'	1.71	0.72
3:Y:8:DG:H1'	3:Y:9:DT:H5''	1.72	0.72
2:O:19:DC:H6	2:O:19:DC:H5'	1.55	0.72
3:P:9:DT:C2'	3:P:10:DG:H5''	2.18	0.71
2:O:19:DC:H2''	2:O:20:DA:C8	2.25	0.71
2:O:6:DG:H2'	2:O:7:DT:H71	1.72	0.71
3:P:8:DG:H1'	3:P:9:DT:H5''	1.71	0.71
2:2:19:DC:H6	2:2:19:DC:H5'	1.55	0.71
2:6:15:DT:H1'	2:6:16:DT:H5'	1.71	0.71
3:H:8:DG:H1'	3:H:9:DT:H5''	1.72	0.71
3:D:2:DA:H1'	3:D:3:DC:H5'	1.69	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:L:8:DG:H1'	3:L:9:DT:H5''	1.72	0.71
3:7:8:DG:H1'	3:7:9:DT:H5''	1.73	0.71
3:7:2:DA:H1'	3:7:3:DC:H5'	1.70	0.71
2:G:19:DC:H2''	2:G:20:DA:C8	2.25	0.71
2:2:15:DT:H1'	2:2:16:DT:H5'	1.72	0.71
2:T:2:DG:H2''	2:T:3:DG:C8	2.26	0.70
2:T:19:DC:H2''	2:T:20:DA:C8	2.25	0.70
2:O:6:DG:C2'	2:O:7:DT:H5''	2.20	0.70
3:D:8:DG:H1'	3:D:9:DT:H5''	1.73	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
3:U:4:DT:H4'	3:U:5:DT:OP1	1.92	0.69
2:K:2:DG:H2''	2:K:3:DG:C8	2.28	0.69
2:C:2:DG:H2''	2:C:3:DG:C8	2.28	0.69
2:6:6:DG:C2'	2:6:7:DT:H5''	2.23	0.69
2:G:6:DG:C2'	2:G:7:DT:H5''	2.23	0.68
2:G:19:DC:H5'	2:G:19:DC:H6	1.57	0.68
2:2:2:DG:H2''	2:2:3:DG:C8	2.29	0.68
2:O:2:DG:H2''	2:O:3:DG:C8	2.28	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:X:6:DG:C2'	2:X:7:DT:H5''	2.23	0.68
2:C:15:DT:H6	2:C:15:DT:H5'	1.58	0.68
2:6:15:DT:H5'	2:6:15:DT:H6	1.58	0.68
2:C:6:DG:C2'	2:C:7:DT:H5''	2.23	0.68
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
3:H:19:DA:H1'	3:H:20:DT:H5''	1.77	0.67
3:P:4:DT:H4'	3:P:5:DT:OP1	1.94	0.67
3:P:1:DC:H2''	3:P:2:DA:C8	2.29	0.67
2:6:19:DC:H6	2:6:19:DC:H5'	1.58	0.67
3:U:7:DT:H2''	3:U:8:DG:H8	1.59	0.67
2:C:19:DC: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
3:7:4: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
3:7:1:DC:H2''	3:7:2: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
3:P:11:DA:C1'	3:P:12:DC:H5''	2.25	0.66
2:2:15:DT:H6	2:2:15:DT:H5'	1.59	0.66
3:U:19:DA:H1'	3:U:20:DT:H5''	1.77	0.66
3:H:7:DT:H2''	3:H:8:DG:H8	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:2:DA:H1'	3:3:3:DC:C5'	2.25	0.66
3:3:1:DC:H2''	3:3:2:DA:C8	2.29	0.66
3:H:11:DA:C1'	3:H:12:DC:H5''	2.25	0.66
3:U:1:DC:H2''	3:U:2:DA:C8	2.30	0.66
3:L:19:DA:H1'	3:L:20:DT:H5''	1.78	0.66
3:D:11:DA:C1'	3:D:12:DC:H5''	2.26	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:L:2:DA:H1'	3:L:3:DC:C5'	2.25	0.65
3:H:2:DA:H1'	3:H:3:DC:C5'	2.26	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:L:7:DT:H2''	3:L:8:DG:H8	1.62	0.64
2:C:1:DT:H3'	2:C:2:DG:H5''	1.80	0.64
3:7:2:DA:H1'	3:7:3:DC:C5'	2.27	0.64
3:Y:19:DA:H1'	3:Y:20:DT:H5''	1.78	0.64
3:3:22:DA:H1'	3:3:23:DC:H5''	1.79	0.64
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
2:6:1:DT:H3'	2:6:2:DG:H5''	1.80	0.64
3:H:22:DA:H1'	3:H:23:DC:H5''	1.79	0.64
3:7:22:DA:H1'	3:7:23:DC:H5''	1.79	0.64
3:P:7:DT:H2''	3:P:8:DG:H8	1.62	0.64
3:P:19:DA:H1'	3:P:20:DT:H5''	1.78	0.64
3:D:22:DA:H1'	3:D:23:DC:H5''	1.79	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:U:11:DA:H2''	3:U:12:DC:H5'	1.80	0.63
3:H:11:DA:H2''	3:H:12:DC:H5'	1.80	0.63
2:X:8:DC:H5'	2:X:8:DC:H6	1.64	0.63
2:O:2:DG:OP1	2:O:2:DG:C4'	2.46	0.63
2:G:2:DG:C4'	2:G:2:DG:OP1	2.46	0.63
2:2:2:DG:OP1	2:2:2:DG:C4'	2.46	0.63
3:7:19:DA:H1'	3:7:20:DT:H5''	1.80	0.63
3:Y:22:DA:H1'	3:Y:23:DC:H5''	1.80	0.63
3:L:11:DA:C1'	3:L:12:DC:H5''	2.27	0.63
3:H:16:DT:H5'	3:H:16:DT:H6	1.63	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
3:H:8:DG:C1'	3:H:9:DT:H5''	2.28	0.63
2:2:24:DA:C4'	2:2:25:DA:OP1	2.45	0.63
2:C:2:DG:OP1	2:C:2:DG:C4'	2.46	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
2:2:5: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
3:U:16:DT:H6	3:U:16:DT:H5'	1.63	0.62
2:K:8:DC:H6	2:K:8:DC:H5'	1.64	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
2:6:2:DG:C4'	2:6:2:DG:OP1	2.46	0.62
3:U:10:DG:H1'	3:U:11:DA:H5'	1.80	0.62
3:L:11:DA:H2''	3:L:12:DC:H5'	1.80	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:P:17:DT:H1'	3:P:18:DT:H5''	1.81	0.62
3:L:24:DA:H2''	3:L:25:DG:OP2	1.99	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
2:G:8:DC:H6	2:G:8:DC:H5'	1.65	0.62
3:D:10:DG:H1'	3:D:11:DA:H5'	1.80	0.62
2:G:9:DA:H1'	2:G:10:DT:H5'	1.82	0.62

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:4:DC:H1'	2:2:5:DT:H5''	1.86	0.58
3:P:11:DA:C2'	3:P:12:DC:C5'	2.81	0.58
3:D:14:DA:C3'	3:D:15:DC:H5''	2.28	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
3:Y:17:DT:H1'	3:Y:18:DT:H5''	1.84	0.58
2:O:4:DC:H1'	2:O:5:DT:H5''	1.86	0.58
2:C:7:DT:H2''	2:C:8:DC:H6	1.67	0.58
2:6:4:DC:H1'	2:6:5:DT:H5''	1.86	0.58
2:O:13:DA:C1'	2:O:14:DG:H5'	2.32	0.58
3:D:11:DA:C2'	3:D:12:DC:C5'	2.82	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:L:24:DA:H1'	3:L:25:DG:O5'	2.03	0.58
2:C:12:DA:H1'	2:C:13:DA:H5''	1.86	0.57
3:D:7:DT:H2''	3:D:8:DG:C8	2.37	0.57
2:6:12:DA:H1'	2:6:13:DA:H5''	1.86	0.57
2:K:23:DA:C4'	2:K:24:DA:OP1	2.48	0.57
2:C:4:DC:H1'	2:C:5:DT:H5''	1.86	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
3:3:7:DT:H2''	3:3:8:DG:C8	2.39	0.57
2:2:17:DG:H2''	2:2:18:DT:C5'	2.35	0.57
3:D:5:DT:H1'	3:D:6:DT:C5'	2.30	0.57
2:K:4:DC:H1'	2:K:5:DT:H5''	1.87	0.57
3:Y:11:DA:C2'	3:Y:12:DC:C5'	2.82	0.57
3:7:7:DT:H2''	3:7:8:DG:C8	2.38	0.57
2:T:18:DT:H2''	2:T:19:DC:H5'	1.87	0.57
3:Y:24:DA:H1'	3:Y:25:DG:O5'	2.04	0.57
2:T:13:DA:C1'	2:T:14:DG:H5'	2.31	0.57
2:G:12:DA:H1'	2:G:13:DA:H5''	1.86	0.57
2:X:12:DA:H1'	2:X:13:DA:H5''	1.86	0.57
2:2:9:DA:H1'	2:2:10:DT:H5'	1.85	0.57
3:7:5:DT:H1'	3:7:6:DT:C5'	2.31	0.57
2:T:19:DC:C6	2:T:19:DC:H5'	2.37	0.57
2:2:18:DT:H2''	2:2:19:DC:H5'	1.86	0.57
2:O:18:DT:H2''	2:O:19:DC: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)
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:C:17:DG:H2''	2:C:18:DT:C5'	2.35	0.57
2:6:17:DG:H2''	2:6:18:DT:C5'	2.35	0.57
2:K:24:DA:C4'	2:K:25:DA:OP1	2.46	0.57
2:G:19:DC:C6	2:G:19:DC:H5'	2.38	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:G:18:DT:H2''	2:G:19:DC:H5'	1.86	0.57
2:6:19:DC:C6	2:6:19:DC:H5'	2.38	0.57
2:X:2:DG:H8	2:X:2:DG:H5''	1.70	0.56
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:5:DT:H5'	2:X:5:DT:C6	2.36	0.56
3:Y:4:DT:C2'	3:Y:5:DT:H72	2.35	0.56
3:3:4:DT:C2'	3:3:5:DT:H72	2.34	0.56
2:X:18:DT:H2''	2:X:19:DC:H5'	1.87	0.56
2:C:19:DC:C6	2:C:19:DC:H5'	2.38	0.56
2:T:2:DG:H5''	2:T:2:DG:H8	1.71	0.56
3:P:7:DT:H2''	3:P:8:DG:C8	2.39	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: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:D:24:DA:H1'	3:D:25:DG:O5'	2.05	0.56
3:L:11:DA:C2'	3:L:12:DC:C5'	2.82	0.56
3:H:24:DA:H1'	3:H:25:DG:O5'	2.06	0.56
3:7:24:DA:H1'	3:7:25:DG:O5'	2.06	0.56
3:U:10:DG:H2''	3:U:11:DA:O5'	2.05	0.56
2:K:2:DG:H5''	2:K:2:DG:H8	1.70	0.56
3:3:24:DA:H1'	3:3:25:DG:O5'	2.06	0.56
3:P:6:DT:H2''	3:P:7:DT:O5'	2.06	0.56
3:D:10:DG:H2''	3:D:11:DA:O5'	2.04	0.56
3:7:10:DG:H2''	3:7:11:DA:O5'	2.04	0.55
2:G:11:DA:C2	3:H:19:DA:C2	2.94	0.55
2:G:24:DA:C4'	2:G:25:DA:OP1	2.45	0.55
2:X:4:DC:H1'	2:X:5:DT:H5''	1.87	0.55
3:3:14:DA:C3'	3:3:15:DC:H5''	2.29	0.55
2:G:2:DG:H8	2:G:2:DG:H5''	1.71	0.55

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:3:DG:H2''	2:T:4:DC:C5'	2.38	0.51
2:X:13:DA:C1'	2:X:14:DG:H5'	2.34	0.51
3:3:15:DC:H2''	3:3:16:DT:H5''	1.92	0.51
3: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:O:24:DA:C4'	2:O:25:DA:OP1	2.45	0.51
3:U:19:DA:H2''	3:U:20:DT:C5'	2.39	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: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: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:C:7:DT:C2	2:C:8:DC:C5	2.99	0.51
2:6:7:DT:C2	2:6:8:DC:C5	2.99	0.51
2:G:2:DG:C2'	2:G:3:DG:C8	2.93	0.51
2:X:7:DT:C2	2:X:8:DC:C5	2.99	0.51
2:C:22:DA:H2''	2:C:23:DA:H5'	1.91	0.51
3:3:9:DT:H2''	3:3:10:DG:C5'	2.29	0.51
2:2:24:DA:H1'	2:2:25: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
2:6:12: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
3:U:21:DG:H2''	3:U:22:DA:OP2	2.10	0.51
2:X:24:DA:C4'	2:X:25:DA:OP1	2.46	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
2:2:15:DT:C1'	2:2:16:DT:H5'	2.40	0.51
3:U:9:DT:C3'	3:U:10:DG:H5''	2.38	0.51
2:K:7:DT:C2'	2:K:8:DC:C5'	2.88	0.51
2:6:22:DA:H2''	2:6:23:DA:H5'	1.91	0.51
3:P:15:DC:H2''	3:P:16:DT:H5''	1.92	0.51
3:7:19:DA:H2''	3:7:20:DT:C5'	2.41	0.51
3:U:9:DT:H6	3:U:9:DT:H5'	1.76	0.51
2:K:7:DT:C2	2:K:8:DC:C5	2.99	0.51
3:7:22:DA:H1'	3:7:23:DC:C5'	2.40	0.51
2:K:6:DG:H2''	2:K:7:DT:H5'	1.93	0.51
3:Y:9:DT:H5'	3:Y:9:DT:H6	1.76	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:D:22:DA:H1'	3:D:23:DC:C5'	2.40	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
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:G:3:DG:H2''	2:G:4:DC:C5'	2.38	0.50
2:X:23:DA:H1'	2:X:24:DA:H5'	1.93	0.50
3:D:12:DC:H2''	3:D:13:DA:C8	2.46	0.50
2:T:15:DT:H2''	2:T:16:DT:O5'	2.10	0.50
3:H:22:DA:H1'	3:H:23:DC:C5'	2.40	0.50
2:T:25:DA:C2	2:T:26:DG:C4	2.99	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
3:7:12:DC:H2''	3:7:13:DA:C8	2.46	0.50
2:G:7:DT:C2'	2:G:8:DC:C5'	2.87	0.50
2:O:8:DC:H2''	2:O:9:DA:C8	2.46	0.50
3:H:5:DT:H1'	3:H:6:DT:C5'	2.32	0.50
2:2:6:DG:H2''	2:2:7:DT:H5'	1.91	0.50
3:3:12:DC:H2''	3:3:13:DA:C8	2.47	0.50
2:O:6:DG:C2	3:P:24:DA:C2	2.99	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
3:7:15:DC:H2''	3:7:16:DT:C5'	2.42	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:U:12:DC:H2''	3:U:13:DA:C8	2.47	0.50
3:Y:19:DA:H2''	3:Y:20:DT:H5'	1.92	0.50
3:3:22:DA:H1'	3:3:23:DC:C5'	2.40	0.50
2:C:15:DT:H2''	2:C:16:DT:O5'	2.12	0.50
2:6:15:DT:H2''	2:6:16:DT:O5'	2.12	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
2:6:25:DA:C2	2:6:26:DG:C4	2.99	0.50
2:X:25:DA:C2	2:X:26:DG:C4	3.00	0.50
3:P:12:DC:H2''	3:P:13:DA:C8	2.47	0.50
3:D:15:DC:H2''	3:D:16:DT:C5'	2.42	0.50
2:T:12:DA:C2'	2:T:13:DA:H5''	2.41	0.50
3:L:19:DA:H2''	3:L:20:DT:H5'	1.92	0.50
3:Y:19:DA:H2''	3:Y:20:DT:C5'	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:25:DA:C2	2:C:26:DG:C4	2.99	0.50
2:O:12:DA:H2''	2:O:13:DA:H5''	1.93	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:K:15:DT:H2''	2:K:16:DT:O5'	2.11	0.50
2:G:22:DA:H2''	2:G:23:DA:H5'	1.94	0.50
2:6:3:DG:H2''	2:6:4:DC:C5'	2.39	0.50
2:6:17:DG:H2''	2:6:18:DT:H5'	1.94	0.50
2:K:23:DA:H1'	2:K:24:DA:H5'	1.93	0.49
2:G:6:DG:C2'	2:G:7:DT:H71	2.41	0.49
2:X:11:DA:H2''	2:X:12:DA:C5'	2.34	0.49
2:2:25:DA:C2	2:2:26:DG:C4	2.99	0.49
3:7:9:DT:H5'	3:7:9:DT:H6	1.77	0.49
2:C:17:DG:H2''	2:C:18:DT:H5'	1.94	0.49
3:H:12:DC:H2''	3:H:13:DA:C8	2.47	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
2:K:15:DT:H2'	2:K:16:DT:H72	1.94	0.49
2:T:7:DT:C2	2:T:8:DC:C5	2.99	0.49
3:3:9:DT:C3'	3:3:10:DG:H5''	2.40	0.49
3:P:19:DA:H2''	3:P:20:DT:H5'	1.94	0.49
2:C:11:DA:H2''	2:C:12:DA:C5'	2.36	0.49
3:7:14:DA:C1'	3:7:15:DC:H5''	2.42	0.49
2:T:22:DA:H2''	2:T:23:DA:H5'	1.94	0.49
2:K:12:DA:C2'	2:K:13:DA:H5''	2.43	0.49
2:G:12:DA:H2''	2:G:13:DA:H5''	1.94	0.49
2:X:6:DG:C2'	2:X:7:DT:H71	2.39	0.49
2:G:7:DT:C2	2:G:8:DC:C5	3.00	0.49
3:P:21:DG:H2''	3:P:22:DA:OP2	2.12	0.49
3:D:18:DT:H1'	3:D:19:DA:H5'	1.93	0.49
2:K:6:DG:C2'	2:K:7:DT:H71	2.39	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
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
2:O:6:DG:C2'	2:O:7:DT:H71	2.42	0.49
2:O:17:DG:H2''	2:O:18:DT:H5'	1.94	0.49
3:7:21: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
3:3:19:DA:H2''	3:3:20:DT:H5'	1.94	0.49
2:C:3:DG:H2''	2:C:4:DC:C5'	2.39	0.49

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:15:DT:H2'	2:X:16:DT:H72	1.94	0.47
2:T:6:DG:C2'	2:T:7:DT:H71	2.41	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:C:2:DG:C2'	2:C:3:DG:C8	2.95	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
3:H:14:DA:C1'	3:H:15:DC:H5''	2.42	0.47
3:H:8:DG:H2''	3:H:9:DT:H5'	1.92	0.47
3:Y:10:DG:H2''	3:Y:11:DA:H8	1.79	0.47
2:C:7:DT:C2'	2:C:8:DC:H5''	2.44	0.47
3:L:24:DA:H1'	3:L:25:DG:C5'	2.44	0.47
2:G:12:DA:C2'	2:G:13:DA:C5'	2.89	0.47
3:3:15:DC:H2''	3:3:16:DT:C5'	2.45	0.47
2:G:17:DG:H2''	2:G:18:DT:H5'	1.96	0.47
2:6:7:DT:C2'	2:6:8:DC:H5''	2.44	0.47
2:T:17:DG:H2''	2:T:18:DT:H5'	1.97	0.47
3:Y:11:DA:H1'	3:Y:12:DC:C5'	2.36	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
3:3:10: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:H:11:DA:H1'	3:H:12:DC:C5'	2.35	0.46
3:D:10:DG:H2''	3:D:11:DA:H8	1.81	0.46
3:7:10:DG:H2''	3:7:11:DA:H8	1.81	0.46
2:X:20:DA:H2''	2:X:21:DC:OP2	2.16	0.46
3:U:14:DA:C1'	3:U:15:DC:H5''	2.42	0.46
3:3:25:DG:C4	3:3:26:DC:C4	3.04	0.46
2:O:2:DG:C2'	2:O:3:DG:C8	2.96	0.46
3:D:8:DG:H2''	3:D:9:DT:H5'	1.94	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:H:24:DA:H1'	3:H:25:DG:C5'	2.45	0.46
3:P:8:DG:H2''	3:P:9:DT:H5'	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:3:DG:H2''	2:O:4:DC:C5'	2.41	0.46
3:P:4:DT:H2'	3:P:4:DT:O5'	2.16	0.46
2:C:3:DG:C2'	2:C:4:DC:H5'	2.42	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
3:H:10:DG:H2''	3:H:11:DA:H8	1.80	0.46
2:X:6:DG:H2''	2:X:7:DT:H5'	1.93	0.46
2:6:4:DC:C2'	2:6:5:DT:H71	2.46	0.46
2:X:17:DG:H2''	2:X:18:DT:H5'	1.96	0.46
2:2:15:DT:H2'	2:2:16:DT:H72	1.98	0.46
3:U:10:DG:H2''	3:U:11:DA:H8	1.81	0.45
2:O:3:DG:C2'	2:O:4:DC:H5'	2.43	0.45
2:T:7:DT:C2'	2:T:8:DC:H5''	2.46	0.45
3:L:14:DA:C3'	3:L:15:DC:H5''	2.29	0.45
3:Y:23:DC:H2''	3:Y:24:DA:C8	2.52	0.45
3:P:25:DG:C4	3:P:26:DC:C4	3.04	0.45
2:O:15:DT:H2'	2:O:16:DT:H72	1.98	0.45
3:H:16:DT:H2'	3:H:17:DT:C7	2.42	0.45
3:Y:4:DT:O5'	3:Y:4:DT:H2'	2.17	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
2:K:15:DT:H2''	2:K:16:DT:C5'	2.46	0.45
3:D:24:DA:H1'	3:D:25:DG:C5'	2.46	0.45
2:K:12:DA:C2'	2:K:13:DA:C5'	2.91	0.45
2:G:7:DT:C2'	2:G:8:DC:H5''	2.46	0.45
2:X:12:DA:H2''	2:X:13:DA:H5''	1.96	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:15:DT:H2''	2:X:16:DT:C5'	2.46	0.45
2:G:15:DT:H2''	2:G:16:DT:C5'	2.47	0.45
2:T:12:DA:C2'	2:T:13:DA:C5'	2.89	0.45
2:T:24:DA:C4'	2:T:25:DA:OP1	2.45	0.45
2:X:2:DG:H2''	2:X:3:DG:H8	1.80	0.45
2:6:17:DG:C2'	2:6:18:DT:H5''	2.47	0.45
3:7:24:DA:H1'	3:7:25:DG:C5'	2.46	0.45
2:K:2:DG:H2''	2:K:3:DG:H8	1.80	0.45
3:3:24:DA:H1'	3:3:25:DG:C5'	2.47	0.45
2:G:24:DA:H1'	2:G:25:DA:C5'	2.47	0.45
2:2:2:DG:H2''	2:2:3:DG:H8	1.80	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:7:DT:C2'	2:X:8:DC:H5''	2.46	0.45
3:3:4:DT:H2'	3:3:4:DT:O5'	2.16	0.45
3:D:4:DT:H2'	3:D:4:DT:O5'	2.16	0.45
3:D:5:DT:H2''	3:D:6:DT:H5'	1.98	0.45
2:T:15:DT:H2'	2:T:16:DT:H72	1.98	0.45
3:L:23:DC:H2''	3:L:24:DA:C8	2.52	0.45
2:X:2:DG:H5''	2:X:2:DG:C8	2.52	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
2:K:20:DA:H2''	2:K:21:DC:OP2	2.16	0.45
2:G:15:DT:H2'	2:G:16:DT:H72	1.98	0.45
2:O:20:DA:H2''	2:O:21:DC:OP2	2.18	0.45
3:7:25:DG:C4	3:7:26:DC:C4	3.05	0.45
3:D:25:DG:C4	3:D:26:DC:C4	3.05	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:O:17:DG:C2'	2:O:18:DT:H5''	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
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
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: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
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
3:L:4:DT:O5'	3:L:4:DT:H2'	2.17	0.44
2:2:6:DG:C2'	2:2:7:DT:H71	2.42	0.44
2:6:6:DG:H2''	2:6:7:DT:H5'	1.93	0.44
2:K:7:DT:H2''	2:K:8:DC:C6	2.50	0.44
2:C:24:DA:H1'	2:C:25:DA:C5'	2.46	0.44
2:X:15:DT:C2'	2:X:16:DT:H5'	2.48	0.44
2:T:15:DT:H2''	2:T:16:DT:C5'	2.47	0.44
3:U:4:DT:O5'	3:U:4:DT:H2'	2.18	0.44
3:H:5:DT:H2''	3:H:6:DT:H5'	2.00	0.44
2:X:4:DC:C2'	2:X:5:DT:H71	2.48	0.44
3:3:8:DG:H2''	3:3:9:DT:H5'	1.95	0.44

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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
2:K:15:DT:C2'	2:K:16:DT:H5'	2.48	0.44
3:U:25:DG:C4	3:U:26:DC:C4	3.05	0.44
2:T:24:DA:H1'	2:T:25:DA:C5'	2.47	0.44
2:6:24:DA:H1'	2:6:25:DA:C5'	2.46	0.44
2:O:4:DC:C2'	2:O:5:DT:H71	2.47	0.44
2:C:7:DT:H2''	2:C:8:DC:C6	2.51	0.44
2:X:17:DG:C2'	2:X:18:DT:H5''	2.48	0.44
2:T:20:DA:H2''	2:T:21:DC:OP2	2.18	0.44
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:H5''	2:T:2:DG:C8	2.53	0.43
2:T:6:DG:H2''	2:T:7:DT:H5'	1.93	0.43
3:L:5:DT:H2''	3:L:6:DT:H5'	2.00	0.43
3:3:16:DT:H2''	3:3:17:DT:C6	2.53	0.43
2:2:24:DA:H1'	2:2:25:DA:C5'	2.48	0.43
2:C:6:DG:C2'	2:C:7:DT:H71	2.42	0.43
3:L:16:DT:H2'	3:L:17:DT:C7	2.44	0.43
2:2:3:DG:C5	2:2:4:DC:C4	3.06	0.43
2:G: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:C:2:DG:H2''	2:C:3:DG:O5'	2.18	0.43
2:6:2:DG:H2''	2:6:3:DG:O5'	2.17	0.43
3:L:19:DA:C1'	3:L:20:DT:H5''	2.48	0.43
3:Y:14:DA:H1'	3:Y:15:DC:H5''	2.00	0.43
2:O:3:DG:C5	2:O:4:DC:C4	3.06	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
2:T:2:DG:H2''	2:T:3:DG:H8	1.78	0.43
3:H:4:DT:H2'	3:H:4:DT:O5'	2.18	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
2:G:4:DC:C2'	2:G:5:DT:H71	2.49	0.43
2:6:3:DG:C5	2:6:4:DC:C4	3.07	0.43
2:T:4:DC:H1'	2:T:5:DT:C5'	2.49	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
3:7:16:DT:H2'	3:7:17:DT:C7	2.44	0.43
2:T:4:DC:C2'	2:T:5:DT:H71	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:24:DA:H1'	2:X:25:DA:C5'	2.48	0.43
3:3:13:DA:C2'	3:3:14:DA:OP2	2.56	0.43
2:X:15:DT:H2''	2:X:16:DT:H5'	2.01	0.43
2:2:20:DA:H2''	2:2:21:DC:OP2	2.18	0.43
3:U:19:DA:C1'	3:U:20:DT:H5''	2.46	0.43
2:K:2:DG:H5''	2:K:2:DG:C8	2.52	0.43
2:C:15:DT:H2''	2:C:16:DT:C5'	2.49	0.43
3:U:5:DT:H2''	3:U:6:DT:H5'	2.00	0.42
2:K:3:DG:C5	2:K:4:DC:C4	3.07	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:O:12:DA:C2'	2:O:13:DA:C5'	2.89	0.42
2:6:15:DT:H2''	2:6:16:DT:C5'	2.49	0.42
3:U:23:DC:H2''	3:U:24:DA:C8	2.54	0.42
2:2:15:DT:H2''	2:2:16:DT:C5'	2.49	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
2:6:23:DA:H1'	2:6:24:DA:C8	2.54	0.42
2:O:23:DA:H1'	2:O: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:T:11:DA:H2''	2:T:12:DA:C5'	2.35	0.42
2:K:17:DG:C2'	2:K:18:DT:H5''	2.48	0.42
3:U:16:DT:H2''	3:U:17:DT:C6	2.54	0.42
3:3:23:DC:H2''	3:3:24:DA:C8	2.54	0.42
3: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
3:7:5:DT:H2''	3:7:6:DT:C5'	2.50	0.42
3:L:8:DG:H2''	3:L:9:DT:H5'	1.94	0.42
3:H:16:DT:H2''	3:H:17:DT:C6	2.54	0.42
2:X:2:DG:H2''	2:X:3:DG:O5'	2.19	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
3:3:5:DT:H2''	3:3:6:DT:C5'	2.50	0.42
2:2:23:DA:H1'	2:2:24:DA:C8	2.55	0.42
2:C:2:DG:H2''	2:C:3:DG:H8	1.80	0.42
3:7:12:DC:H5'	3:7:12:DC:H6	1.84	0.42
2:T:25:DA:C4	2:T:26:DG:C8	3.08	0.42

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:24:DA:H1'	3:L:25:DG:H5'	2.02	0.41
2:6:23:DA:C4	2:6:24:DA:N7	2.88	0.41
3:3:19:DA:C1'	3:3:20:DT:H5''	2.48	0.41
3:7:19:DA:C1'	3:7:20:DT:H5''	2.49	0.41
2:T:23:DA:C4	2:T:24:DA:N7	2.89	0.41
3:H:19:DA:C1'	3:H:20:DT:H5''	2.46	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
3:Y:12:DC:H5'	3:Y:12:DC:H6	1.85	0.41
3:P:19:DA:C1'	3:P:20:DT:H5''	2.48	0.41
2:O:25:DA:C4	2:O:26:DG:C8	3.08	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
2:6:8:DC:H2''	2:6:9:DA:O5'	2.21	0.41
2:T:7:DT:H2''	2:T:8:DC:C6	2.51	0.41
2:K:25:DA:C4	2:K:26:DG:C8	3.09	0.41
2:X:23:DA:C4	2:X:24:DA:N7	2.88	0.41
3:Y:16:DT:H2'	3:Y:17:DT:C7	2.44	0.41
3:3:14:DA:H1'	3:3:15:DC:H5''	2.02	0.41
3:D:16:DT:H2''	3:D:17:DT:C6	2.56	0.41
3:7:16:DT:H2''	3:7:17:DT:C6	2.56	0.41
3:H:23:DC:H5'	3:H:23:DC:H6	1.86	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:G:3:DG:C2'	2:G:4:DC:C5'	3.00	0.40
2:X:4:DC:H1'	2:X:5:DT:C5'	2.52	0.40
2:O:4:DC:H1'	2:O:5:DT:C5'	2.51	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
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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	102/102 (100%)	1.52	30 (29%) 1 2	56, 70, 90, 95	0
1	4	102/102 (100%)	1.54	27 (26%) 1 2	60, 73, 89, 91	0
1	5	102/102 (100%)	1.49	28 (27%) 1 2	56, 70, 90, 95	0
1	8	102/102 (100%)	1.70	31 (30%) 1 2	60, 73, 89, 91	0
1	9	102/102 (100%)	1.69	33 (32%) 1 2	56, 70, 90, 95	0
1	A	102/102 (100%)	1.59	29 (28%) 1 2	60, 73, 89, 91	0
1	B	102/102 (100%)	1.43	23 (22%) 1 2	56, 70, 90, 95	0
1	E	102/102 (100%)	1.62	26 (25%) 1 2	60, 73, 89, 91	0
1	F	102/102 (100%)	1.58	28 (27%) 1 2	56, 70, 90, 95	0
1	I	102/102 (100%)	1.53	30 (29%) 1 2	60, 73, 89, 91	0
1	J	102/102 (100%)	1.60	24 (23%) 1 2	56, 70, 90, 95	0
1	M	102/102 (100%)	1.69	30 (29%) 1 2	60, 73, 89, 91	0
1	N	102/102 (100%)	1.63	26 (25%) 1 2	56, 70, 90, 95	0
1	R	102/102 (100%)	1.73	30 (29%) 1 2	60, 73, 89, 91	0
1	S	102/102 (100%)	1.68	30 (29%) 1 2	56, 70, 90, 95	0
1	V	102/102 (100%)	1.68	31 (30%) 1 2	60, 73, 89, 91	0
1	W	102/102 (100%)	1.60	28 (27%) 1 2	56, 70, 90, 95	0
1	Z	102/102 (100%)	1.56	29 (28%) 1 2	60, 73, 89, 91	0
1	c	102/102 (100%)	1.63	32 (31%) 1 2	60, 73, 89, 91	0
1	d	102/102 (100%)	1.50	22 (21%) 1 2	56, 70, 90, 95	0
1	g	102/102 (100%)	1.51	26 (25%) 1 2	60, 73, 89, 91	0
1	h	102/102 (100%)	1.65	30 (29%) 1 2	56, 70, 90, 95	0
1	k	102/102 (100%)	1.83	31 (30%) 1 2	60, 73, 89, 91	0
1	l	102/102 (100%)	1.50	24 (23%) 1 2	56, 70, 90, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	2	26/26 (100%)	1.99	13 (50%) 0 1	62, 79, 87, 88	0
2	6	26/26 (100%)	1.74	7 (26%) 1 2	62, 79, 87, 88	0
2	C	26/26 (100%)	1.76	9 (34%) 0 1	62, 79, 87, 88	0
2	G	26/26 (100%)	1.37	5 (19%) 2 3	62, 79, 87, 88	0
2	K	26/26 (100%)	1.90	13 (50%) 0 1	62, 79, 87, 88	0
2	O	26/26 (100%)	2.07	13 (50%) 0 1	62, 79, 87, 88	0
2	T	26/26 (100%)	1.45	6 (23%) 1 2	62, 79, 87, 88	0
2	X	26/26 (100%)	1.79	11 (42%) 0 1	62, 79, 87, 88	0
2	a	26/26 (100%)	1.72	9 (34%) 0 1	62, 79, 87, 88	0
2	e	26/26 (100%)	1.86	10 (38%) 0 1	62, 79, 87, 88	0
2	i	26/26 (100%)	1.78	9 (34%) 0 1	62, 79, 87, 88	0
2	m	26/26 (100%)	1.66	8 (30%) 1 2	62, 79, 87, 88	0
3	3	26/26 (100%)	2.03	13 (50%) 0 1	61, 79, 93, 94	0
3	7	26/26 (100%)	1.60	8 (30%) 1 2	61, 79, 93, 94	0
3	D	26/26 (100%)	1.51	9 (34%) 0 1	61, 79, 93, 94	0
3	H	26/26 (100%)	1.45	10 (38%) 0 1	61, 79, 93, 94	0
3	L	26/26 (100%)	1.71	12 (46%) 0 1	61, 79, 93, 94	0
3	P	26/26 (100%)	1.87	13 (50%) 0 1	61, 79, 93, 94	0
3	U	26/26 (100%)	1.65	8 (30%) 1 2	61, 79, 93, 94	0
3	Y	26/26 (100%)	1.72	11 (42%) 0 1	61, 79, 93, 94	0
3	b	26/26 (100%)	1.65	7 (26%) 1 2	61, 79, 93, 94	0
3	f	26/26 (100%)	1.76	10 (38%) 0 1	61, 79, 93, 94	0
3	j	26/26 (100%)	1.81	11 (42%) 0 1	61, 79, 93, 94	0
3	n	26/26 (100%)	1.79	10 (38%) 0 1	61, 79, 93, 94	0
4	o	93/99 (93%)	1.86	35 (37%) 0 1	19, 23, 79, 88	0
4	q	93/99 (93%)	1.78	28 (30%) 1 2	19, 23, 79, 88	0
All	All	3258/3270 (99%)	1.64	976 (29%) 1 2	19, 73, 90, 95	0

All (976) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	185	GLY	12.4
1	R	187	ASN	11.9

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Mol	Chain	Res	Type	RSRZ
4	o	570	ASP	11.4
4	q	907	GLY	11.3
1	M	129	GLU	10.9
4	q	543	ALA	10.5
1	R	185	GLY	10.4
1	V	152	PRO	10.2
1	k	140	ASP	9.7
1	V	148	ALA	9.1
1	Z	222	GLY	9.0
4	q	538	GLU	8.8
4	q	578	LYS	8.8
4	o	907	GLY	8.3
4	q	562	ARG	8.0
1	S	170	PRO	7.9
1	N	222	GLY	7.7
4	o	563	PHE	7.6
1	E	209	GLY	7.4
1	c	187	ASN	7.3
4	o	542	ALA	7.3
1	V	151	GLU	7.3
1	9	129	GLU	7.0
1	E	187	ASN	7.0
1	h	148	ALA	7.0
1	I	187	ASN	7.0
1	8	193	ARG	6.9
4	q	563	PHE	6.7
1	d	197	VAL	6.6
4	q	533	ASP	6.5
1	l	217	THR	6.5
4	o	537	THR	6.4
4	o	577	GLY	6.4
1	l	222	GLY	6.3
1	h	185	GLY	6.1
1	d	222	GLY	6.1
1	8	140	ASP	6.1
1	k	197	VAL	6.1
1	B	170	PRO	6.0
1	c	193	ARG	6.0
1	l	221	THR	6.0
1	8	197	VAL	5.9
4	q	903	ARG	5.9
1	M	222	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
1	E	193	ARG	5.8
1	d	185	GLY	5.8
1	l	185	GLY	5.8
4	q	561	MET	5.7
1	N	197	VAL	5.7
1	V	187	ASN	5.7
1	N	129	GLU	5.7
1	F	170	PRO	5.6
1	W	193	ARG	5.6
1	5	196	ASP	5.6
1	4	128	VAL	5.5
1	M	187	ASN	5.5
1	h	219	ARG	5.4
1	R	140	ASP	5.4
1	h	149	GLY	5.4
1	I	176	ARG	5.4
1	1	128	VAL	5.3
1	k	193	ARG	5.3
1	Z	187	ASN	5.3
1	4	214	MET	5.3
1	S	197	VAL	5.2
1	g	187	ASN	5.2
1	l	222	GLY	5.2
1	g	196	ASP	5.2
1	N	193	ARG	5.2
1	4	198	HIS	5.1
1	J	226	SER	5.1
1	E	148	ALA	5.1
1	Z	203	ARG	5.1
1	8	148	ALA	5.1
1	Z	197	VAL	5.1
1	M	148	ALA	5.1
1	5	222	GLY	5.1
1	B	148	ALA	5.0
1	d	196	ASP	5.0
2	i	4	DC	5.0
1	R	193	ARG	5.0
1	V	196	ASP	5.0
4	q	603	ARG	4.9
1	S	196	ASP	4.9
1	A	193	ARG	4.9
1	g	129	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
4	o	592	ALA	4.9
1	k	194	THR	4.9
1	I	193	ARG	4.9
1	1	197	VAL	4.9
1	N	198	HIS	4.8
1	V	194	THR	4.8
1	h	196	ASP	4.8
1	8	196	ASP	4.8
1	I	197	VAL	4.8
1	J	197	VAL	4.7
2	e	4	DC	4.7
4	o	562	ARG	4.7
1	N	217	THR	4.7
4	q	551	LEU	4.7
4	o	566	ASP	4.7
1	S	198	HIS	4.7
1	k	205	ALA	4.7
1	E	198	HIS	4.7
1	R	194	THR	4.7
1	4	203	ARG	4.6
1	W	134	MET	4.6
1	V	209	GLY	4.6
1	5	148	ALA	4.6
1	5	194	THR	4.6
1	Z	148	ALA	4.6
1	c	140	ASP	4.6
1	J	193	ARG	4.6
1	g	131	VAL	4.6
1	F	193	ARG	4.5
1	d	198	HIS	4.5
1	4	159	GLU	4.5
1	8	149	GLY	4.5
3	7	24	DA	4.5
1	4	222	GLY	4.5
1	5	193	ARG	4.5
1	d	217	THR	4.5
1	V	193	ARG	4.5
1	k	198	HIS	4.4
1	9	198	HIS	4.4
1	J	196	ASP	4.4
1	S	194	THR	4.4
4	q	908	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
1	V	173	VAL	4.4
1	M	203	ARG	4.4
1	g	194	THR	4.3
1	Z	129	GLU	4.3
1	k	129	GLU	4.3
1	k	196	ASP	4.3
1	l	196	ASP	4.3
1	4	193	ARG	4.3
1	k	148	ALA	4.3
1	l	219	ARG	4.3
1	l	198	HIS	4.3
1	9	193	ARG	4.3
1	W	197	VAL	4.2
1	A	203	ARG	4.2
1	l	193	ARG	4.2
1	9	194	THR	4.2
1	E	196	ASP	4.2
3	L	24	DA	4.2
1	V	198	HIS	4.2
2	K	4	DC	4.2
2	O	2	DG	4.2
1	c	158	THR	4.2
1	B	193	ARG	4.2
1	k	222	GLY	4.2
1	I	198	HIS	4.1
1	g	198	HIS	4.1
1	9	181	ASN	4.1
1	h	170	PRO	4.1
1	A	222	GLY	4.1
1	I	173	VAL	4.1
1	g	219	ARG	4.1
1	5	219	ARG	4.1
1	R	198	HIS	4.1
1	W	198	HIS	4.0
1	W	196	ASP	4.0
1	F	194	THR	4.0
1	l	198	HIS	4.0
1	E	149	GLY	4.0
2	a	4	DC	4.0
1	g	148	ALA	4.0
3	f	3	DC	4.0
1	h	222	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	V	226	SER	4.0
1	R	222	GLY	3.9
1	g	130	GLU	3.9
1	A	196	ASP	3.9
4	o	576	VAL	3.9
1	l	129	GLU	3.9
1	S	193	ARG	3.9
3	D	2	DA	3.9
1	E	217	THR	3.9
2	i	2	DG	3.9
1	9	212	ASP	3.9
1	g	218	VAL	3.9
1	N	203	ARG	3.8
3	Y	2	DA	3.8
1	Z	218	VAL	3.8
2	i	3	DG	3.8
1	d	194	THR	3.8
1	4	187	ASN	3.8
3	j	24	DA	3.8
4	o	541	ARG	3.8
1	E	222	GLY	3.8
1	9	185	GLY	3.8
1	N	148	ALA	3.7
1	A	205	ALA	3.7
1	l	196	ASP	3.7
2	X	4	DC	3.7
1	B	194	THR	3.7
1	V	129	GLU	3.7
1	F	198	HIS	3.7
1	9	196	ASP	3.7
4	q	592	ALA	3.7
1	8	195	VAL	3.7
1	M	205	ALA	3.7
1	E	197	VAL	3.7
1	8	198	HIS	3.7
1	W	219	ARG	3.7
1	J	148	ALA	3.7
4	o	533	ASP	3.7
4	q	585	GLU	3.7
1	A	198	HIS	3.6
1	k	159	GLU	3.6
1	4	201	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	196	ASP	3.6
1	W	226	SER	3.6
1	I	209	GLY	3.6
3	U	22	DA	3.6
2	O	21	DC	3.6
1	Z	158	THR	3.6
3	n	4	DT	3.6
1	c	198	HIS	3.6
1	M	193	ARG	3.6
1	R	220	GLY	3.6
3	D	3	DC	3.6
1	J	198	HIS	3.6
1	4	148	ALA	3.6
1	l	181	ASN	3.6
1	E	194	THR	3.5
1	W	148	ALA	3.5
1	A	197	VAL	3.5
1	4	196	ASP	3.5
1	A	140	ASP	3.5
3	U	2	DA	3.5
1	4	129	GLU	3.5
1	8	173	VAL	3.5
2	2	21	DC	3.5
2	m	4	DC	3.5
1	B	196	ASP	3.5
1	R	186	THR	3.5
1	8	200	ARG	3.5
1	c	217	THR	3.5
1	g	193	ARG	3.5
1	I	196	ASP	3.5
1	d	148	ALA	3.5
1	N	156	GLY	3.5
1	W	149	GLY	3.5
4	o	899	GLU	3.5
1	B	198	HIS	3.5
2	O	24	DA	3.4
3	Y	3	DC	3.4
1	d	193	ARG	3.4
1	8	187	ASN	3.4
4	q	599	ARG	3.4
1	k	208	PRO	3.4
1	W	157	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	Z	130	GLU	3.4
1	Z	149	GLY	3.4
1	I	219	ARG	3.4
1	1	156	GLY	3.4
1	1	169	HIS	3.4
3	f	24	DA	3.4
1	1	203	ARG	3.4
1	8	131	VAL	3.4
3	n	13	DA	3.4
1	8	129	GLU	3.4
1	h	157	PRO	3.3
1	N	216	GLN	3.3
1	I	222	GLY	3.3
1	c	196	ASP	3.3
2	6	20	DA	3.3
2	2	23	DA	3.3
4	o	589	GLN	3.3
2	2	2	DG	3.3
1	9	148	ALA	3.3
2	C	20	DA	3.3
2	K	9	DA	3.3
1	J	157	PRO	3.3
1	M	196	ASP	3.3
1	Z	196	ASP	3.3
2	X	20	DA	3.3
3	3	3	DC	3.3
1	h	229	PHE	3.3
1	h	129	GLU	3.3
4	o	599	ARG	3.3
1	W	170	PRO	3.3
1	h	158	THR	3.3
1	h	197	VAL	3.3
1	S	226	SER	3.3
1	R	148	ALA	3.3
1	B	226	SER	3.3
1	W	194	THR	3.3
1	9	217	THR	3.3
4	o	607	LEU	3.3
1	N	196	ASP	3.2
2	e	2	DG	3.2
2	m	2	DG	3.2
1	F	159	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	M	217	THR	3.2
1	l	203	ARG	3.2
4	q	550	GLY	3.2
1	A	219	ARG	3.2
1	E	185	GLY	3.2
2	e	9	DA	3.2
1	8	203	ARG	3.2
1	c	219	ARG	3.2
1	k	220	GLY	3.2
1	9	138	SER	3.2
1	c	148	ALA	3.2
1	9	222	GLY	3.2
1	l	193	ARG	3.2
1	B	140	ASP	3.2
1	I	128	VAL	3.2
1	k	217	THR	3.2
4	o	564	GLY	3.2
1	W	217	THR	3.2
1	5	217	THR	3.2
1	h	138	SER	3.2
1	4	195	VAL	3.2
1	c	197	VAL	3.2
1	S	222	GLY	3.2
2	X	2	DG	3.2
1	A	214	MET	3.2
3	7	2	DA	3.1
1	h	198	HIS	3.1
2	a	2	DG	3.1
2	a	12	DA	3.1
3	n	11	DA	3.1
1	Z	219	ARG	3.1
1	d	201	ARG	3.1
3	L	11	DA	3.1
1	V	220	GLY	3.1
1	h	203	ARG	3.1
3	P	26	DC	3.1
3	U	3	DC	3.1
1	l	216	GLN	3.1
4	o	908	GLU	3.1
1	S	200	ARG	3.1
1	W	178	GLN	3.1
1	4	142	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	W	159	GLU	3.1
3	Y	23	DC	3.1
3	j	3	DC	3.1
3	P	3	DC	3.1
1	1	158	THR	3.1
2	X	9	DA	3.1
2	2	4	DC	3.1
1	l	143	SER	3.0
1	Z	194	THR	3.0
1	4	194	THR	3.0
1	I	140	ASP	3.0
1	g	217	THR	3.0
1	M	220	GLY	3.0
1	F	155	MET	3.0
1	W	158	THR	3.0
4	o	584	ARG	3.0
2	e	20	DA	3.0
3	L	13	DA	3.0
1	S	157	PRO	3.0
4	o	549	ALA	3.0
1	J	217	THR	3.0
1	V	219	ARG	3.0
3	D	1	DC	3.0
4	o	603	ARG	3.0
3	j	4	DT	3.0
1	N	229	PHE	3.0
1	Z	220	GLY	3.0
1	8	219	ARG	3.0
1	d	220	GLY	3.0
2	O	20	DA	3.0
2	K	2	DG	3.0
1	S	217	THR	3.0
3	U	25	DG	3.0
1	M	197	VAL	3.0
1	d	195	VAL	3.0
1	k	149	GLY	3.0
2	6	21	DC	3.0
3	n	24	DA	3.0
2	T	4	DC	3.0
1	I	203	ARG	3.0
1	W	195	VAL	3.0
3	Y	24	DA	3.0

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Mol	Chain	Res	Type	RSRZ
1	l	209	GLY	3.0
1	A	200	ARG	3.0
1	B	222	GLY	3.0
1	F	148	ALA	3.0
1	9	136	GLY	3.0
1	F	143	SER	2.9
3	D	22	DA	2.9
3	f	11	DA	2.9
4	q	542	ALA	2.9
1	N	199	ILE	2.9
1	g	149	GLY	2.9
1	R	128	VAL	2.9
1	5	198	HIS	2.9
2	C	3	DG	2.9
3	f	4	DT	2.9
1	M	194	THR	2.9
1	Z	169	HIS	2.9
3	H	22	DA	2.9
1	5	170	PRO	2.9
1	g	197	VAL	2.9
4	q	546	ASP	2.9
1	l	185	GLY	2.9
1	l	195	VAL	2.9
3	P	2	DA	2.9
1	c	194	THR	2.9
1	N	157	PRO	2.9
2	O	10	DT	2.9
2	e	1	DT	2.9
3	3	11	DA	2.9
1	I	148	ALA	2.9
1	h	217	THR	2.9
3	f	25	DG	2.9
1	I	220	GLY	2.9
1	k	136	GLY	2.9
3	3	24	DA	2.9
4	o	578	LYS	2.9
2	C	21	DC	2.9
3	n	3	DC	2.9
1	A	194	THR	2.9
3	7	3	DC	2.9
1	N	158	THR	2.9
3	b	13	DA	2.9

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Mol	Chain	Res	Type	RSRZ
1	8	175	SER	2.9
1	g	159	GLU	2.9
1	Z	186	THR	2.9
1	k	147	MET	2.9
1	S	158	THR	2.8
4	o	900	LYS	2.8
1	A	192	ASP	2.8
1	F	197	VAL	2.8
1	M	158	THR	2.8
2	2	22	DA	2.8
1	F	195	VAL	2.8
1	g	220	GLY	2.8
1	F	227	THR	2.8
1	J	194	THR	2.8
2	X	24	DA	2.8
4	o	559	LEU	2.8
1	R	211	HIS	2.8
2	C	11	DA	2.8
3	L	12	DC	2.8
1	J	138	SER	2.8
1	9	150	GLU	2.8
3	3	2	DA	2.8
1	R	195	VAL	2.8
3	j	25	DG	2.8
1	4	182	HIS	2.8
3	H	24	DA	2.8
2	K	3	DG	2.8
3	L	23	DC	2.8
1	R	139	LEU	2.8
3	b	25	DG	2.8
1	d	221	THR	2.8
1	E	219	ARG	2.8
1	M	143	SER	2.8
1	N	195	VAL	2.8
2	O	4	DC	2.8
3	Y	13	DA	2.8
1	E	176	ARG	2.8
1	V	159	GLU	2.8
1	I	221	THR	2.8
1	5	158	THR	2.8
1	c	195	VAL	2.8
1	B	205	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	e	13	DA	2.8
3	3	26	DC	2.8
1	F	199	ILE	2.8
1	4	141	PRO	2.8
3	n	14	DA	2.8
4	q	600	HIS	2.8
1	5	197	VAL	2.7
1	1	199	ILE	2.7
1	d	135	GLN	2.7
1	h	140	ASP	2.7
1	S	195	VAL	2.7
2	K	22	DA	2.7
1	R	221	THR	2.7
3	P	5	DT	2.7
3	P	14	DA	2.7
1	8	201	ARG	2.7
3	7	25	DG	2.7
1	h	193	ARG	2.7
2	K	20	DA	2.7
2	O	23	DA	2.7
3	L	3	DC	2.7
3	U	24	DA	2.7
1	B	216	GLN	2.7
1	V	195	VAL	2.7
2	6	2	DG	2.7
1	M	218	VAL	2.7
1	J	219	ARG	2.7
3	P	4	DT	2.7
1	S	205	ALA	2.7
1	9	137	LEU	2.7
2	a	11	DA	2.7
3	3	25	DG	2.7
4	q	579	GLN	2.7
1	A	195	VAL	2.7
1	9	140	ASP	2.7
1	I	194	THR	2.7
1	5	227	THR	2.7
2	G	9	DA	2.7
3	H	2	DA	2.7
1	W	201	ARG	2.7
1	A	182	HIS	2.7
1	B	158	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	216	GLN	2.7
1	M	152	PRO	2.7
3	Y	22	DA	2.7
3	f	14	DA	2.7
1	1	220	GLY	2.7
2	O	22	DA	2.7
1	A	225	PHE	2.7
1	J	195	VAL	2.7
1	5	157	PRO	2.7
1	J	220	GLY	2.7
2	m	3	DG	2.7
1	A	181	ASN	2.7
1	c	138	SER	2.7
1	k	203	ARG	2.7
1	l	148	ALA	2.6
1	E	201	ARG	2.6
1	F	217	THR	2.6
1	E	195	VAL	2.6
1	9	197	VAL	2.6
1	M	198	HIS	2.6
4	q	556	ALA	2.6
1	E	218	VAL	2.6
1	9	218	VAL	2.6
4	q	558	VAL	2.6
1	1	135	GLN	2.6
1	9	219	ARG	2.6
1	4	199	ILE	2.6
1	Z	217	THR	2.6
1	N	150	GLU	2.6
2	6	3	DG	2.6
3	L	25	DG	2.6
3	P	24	DA	2.6
1	I	129	GLU	2.6
1	V	200	ARG	2.6
1	9	203	ARG	2.6
4	o	548	LEU	2.6
1	M	169	HIS	2.6
1	A	220	GLY	2.6
1	k	156	GLY	2.6
4	o	582	VAL	2.6
1	F	222	GLY	2.6
1	N	159	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
2	a	5	DT	2.6
1	5	195	VAL	2.6
1	h	212	ASP	2.6
1	l	212	ASP	2.6
1	B	200	ARG	2.6
1	8	217	THR	2.6
1	F	156	GLY	2.6
1	I	195	VAL	2.6
1	N	194	THR	2.6
1	M	131	VAL	2.6
2	2	24	DA	2.6
3	7	23	DC	2.6
1	V	191	GLU	2.6
1	9	157	PRO	2.6
2	6	5	DT	2.6
1	1	157	PRO	2.6
1	c	227	THR	2.6
4	o	572	THR	2.6
1	F	220	GLY	2.6
2	K	11	DA	2.6
2	i	13	DA	2.6
3	j	14	DA	2.6
2	6	4	DC	2.6
1	R	219	ARG	2.5
1	g	195	VAL	2.5
1	k	195	VAL	2.5
1	V	227	THR	2.5
1	d	158	THR	2.5
1	l	217	THR	2.5
1	R	196	ASP	2.5
1	9	229	PHE	2.5
3	D	25	DG	2.5
3	3	23	DC	2.5
3	7	22	DA	2.5
1	M	138	SER	2.5
2	O	3	DG	2.5
2	2	3	DG	2.5
1	c	159	GLU	2.5
1	W	225	PHE	2.5
1	M	216	GLN	2.5
1	h	218	VAL	2.5
1	R	151	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	K	24	DA	2.5
1	1	136	GLY	2.5
1	1	150	GLU	2.5
1	A	144	HIS	2.5
1	Z	198	HIS	2.5
3	j	2	DA	2.5
1	c	192	ASP	2.5
1	c	136	GLY	2.5
1	B	227	THR	2.5
3	L	4	DT	2.5
1	c	218	VAL	2.5
2	K	25	DA	2.5
1	W	216	GLN	2.5
1	5	216	GLN	2.5
1	5	133	GLU	2.5
4	o	585	GLU	2.5
1	k	137	LEU	2.5
1	l	226	SER	2.5
3	Y	11	DA	2.5
1	k	199	ILE	2.5
2	i	9	DA	2.5
2	X	10	DT	2.5
1	I	199	ILE	2.5
1	S	148	ALA	2.5
1	1	195	VAL	2.5
1	1	134	MET	2.5
1	S	137	LEU	2.5
1	c	149	GLY	2.5
1	g	164	HIS	2.5
1	c	200	ARG	2.5
1	8	218	VAL	2.5
1	I	149	GLY	2.5
1	k	218	VAL	2.4
1	J	227	THR	2.4
3	b	11	DA	2.4
3	b	4	DT	2.4
1	l	138	SER	2.4
3	Y	25	DG	2.4
1	A	199	ILE	2.4
1	1	194	THR	2.4
1	M	151	GLU	2.4
1	k	161	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	G	4	DC	2.4
3	n	23	DC	2.4
1	V	222	GLY	2.4
2	a	13	DA	2.4
3	3	14	DA	2.4
3	7	13	DA	2.4
1	N	219	ARG	2.4
1	d	128	VAL	2.4
2	e	12	DA	2.4
1	S	143	SER	2.4
2	C	4	DC	2.4
1	B	143	SER	2.4
2	T	5	DT	2.4
1	S	140	ASP	2.4
1	Z	216	GLN	2.4
1	8	221	THR	2.4
1	g	135	GLN	2.4
1	Z	168	THR	2.4
1	d	216	GLN	2.4
1	J	200	ARG	2.4
2	6	15	DT	2.4
1	B	195	VAL	2.4
1	R	213	ARG	2.4
2	X	11	DA	2.4
2	m	24	DA	2.4
3	D	24	DA	2.4
3	L	22	DA	2.4
3	Y	14	DA	2.4
1	E	208	PRO	2.4
1	M	221	THR	2.4
4	o	583	THR	2.4
1	R	212	ASP	2.4
3	f	23	DC	2.4
1	8	220	GLY	2.4
1	9	149	GLY	2.4
2	X	25	DA	2.4
1	4	164	HIS	2.4
1	J	221	THR	2.4
1	V	149	GLY	2.4
1	A	130	GLU	2.4
3	j	23	DC	2.4
1	F	200	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	168	THR	2.4
1	4	226	SER	2.4
1	A	148	ALA	2.4
2	K	5	DT	2.3
1	E	191	GLU	2.3
2	K	14	DG	2.3
1	Z	226	SER	2.3
1	l	157	PRO	2.3
3	P	23	DC	2.3
1	A	221	THR	2.3
1	h	195	VAL	2.3
1	I	164	HIS	2.3
2	O	13	DA	2.3
2	T	9	DA	2.3
2	2	13	DA	2.3
3	H	1	DC	2.3
1	F	158	THR	2.3
1	1	148	ALA	2.3
1	k	157	PRO	2.3
1	J	222	GLY	2.3
1	5	192	ASP	2.3
1	9	195	VAL	2.3
2	X	3	DG	2.3
1	8	159	GLU	2.3
1	5	226	SER	2.3
1	M	150	GLU	2.3
4	o	556	ALA	2.3
1	V	185	GLY	2.3
1	1	149	GLY	2.3
3	j	22	DA	2.3
1	N	201	ARG	2.3
1	5	200	ARG	2.3
1	R	199	ILE	2.3
3	7	1	DC	2.3
1	F	226	SER	2.3
2	T	24	DA	2.3
1	E	138	SER	2.3
1	I	226	SER	2.3
1	8	157	PRO	2.3
1	k	216	GLN	2.3
1	N	149	GLY	2.3
1	h	194	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	T	1	DT	2.3
1	E	199	ILE	2.3
2	2	9	DA	2.3
3	U	11	DA	2.3
1	I	157	PRO	2.3
1	A	168	THR	2.3
1	c	211	HIS	2.3
1	8	136	GLY	2.3
1	k	187	ASN	2.3
3	n	25	DG	2.3
4	q	559	LEU	2.3
2	a	20	DA	2.3
1	S	227	THR	2.3
1	d	212	ASP	2.3
2	K	10	DT	2.3
1	V	216	GLN	2.3
1	W	212	ASP	2.3
1	4	178	GLN	2.3
2	G	25	DA	2.3
1	S	169	HIS	2.3
1	8	222	GLY	2.3
1	R	218	VAL	2.3
1	E	164	HIS	2.3
1	k	200	ARG	2.3
1	E	151	GLU	2.3
1	h	220	GLY	2.3
1	h	201	ARG	2.3
1	l	199	ILE	2.3
1	J	143	SER	2.3
1	J	134	MET	2.3
1	R	137	LEU	2.3
1	k	219	ARG	2.3
2	G	20	DA	2.3
1	I	218	VAL	2.3
1	4	133	GLU	2.3
1	8	229	PHE	2.3
1	Z	136	GLY	2.3
1	5	218	VAL	2.3
1	9	156	GLY	2.3
3	U	4	DT	2.3
3	3	4	DT	2.3
3	n	5	DT	2.3

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Mol	Chain	Res	Type	RSRZ
1	5	229	PHE	2.2
1	S	201	ARG	2.2
1	A	218	VAL	2.2
1	Z	150	GLU	2.2
2	m	1	DT	2.2
1	B	217	THR	2.2
1	g	168	THR	2.2
3	L	2	DA	2.2
3	n	10	DG	2.2
1	W	138	SER	2.2
4	o	539	SER	2.2
4	q	590	ILE	2.2
1	R	227	THR	2.2
1	h	136	GLY	2.2
1	5	138	SER	2.2
3	H	11	DA	2.2
3	j	13	DA	2.2
1	J	192	ASP	2.2
1	V	217	THR	2.2
2	T	25	DA	2.2
1	W	218	VAL	2.2
3	3	10	DG	2.2
1	4	217	THR	2.2
1	S	190	VAL	2.2
1	R	158	THR	2.2
1	M	181	ASN	2.2
1	F	201	ARG	2.2
1	F	216	GLN	2.2
1	5	137	LEU	2.2
1	A	164	HIS	2.2
2	C	22	DA	2.2
2	O	11	DA	2.2
3	f	2	DA	2.2
1	I	150	GLU	2.2
2	e	3	DG	2.2
1	F	136	GLY	2.2
1	S	216	GLN	2.2
1	8	226	SER	2.2
1	5	220	GLY	2.2
1	c	156	GLY	2.2
1	k	227	THR	2.2
1	F	192	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	S	203	ARG	2.2
1	Z	193	ARG	2.2
3	D	12	DC	2.2
4	o	588	ARG	2.2
1	R	217	THR	2.2
1	9	133	GLU	2.2
1	R	226	SER	2.2
1	k	209	GLY	2.2
2	2	26	DG	2.2
1	Z	151	GLU	2.2
2	C	25	DA	2.2
1	V	199	ILE	2.2
4	o	903	ARG	2.2
1	E	173	VAL	2.2
1	9	164	HIS	2.2
3	b	10	DG	2.2
1	J	137	LEU	2.2
1	d	136	GLY	2.2
3	3	13	DA	2.2
1	W	151	GLU	2.2
1	8	199	ILE	2.2
1	A	188	VAL	2.2
1	W	141	PRO	2.2
3	H	12	DC	2.2
3	f	10	DG	2.2
1	V	203	ARG	2.2
1	S	138	SER	2.2
1	9	143	SER	2.2
1	B	161	LYS	2.2
1	c	135	GLN	2.2
2	X	14	DG	2.2
1	g	140	ASP	2.2
1	g	192	ASP	2.2
1	l	216	GLN	2.2
2	O	9	DA	2.2
3	P	11	DA	2.2
3	P	22	DA	2.2
1	I	229	PHE	2.2
1	V	218	VAL	2.2
1	W	176	ARG	2.2
1	9	186	THR	2.2
1	Z	181	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	c	141	PRO	2.1
2	X	1	DT	2.1
1	W	199	ILE	2.1
3	P	13	DA	2.1
1	V	221	THR	2.1
4	q	539	SER	2.1
1	h	216	GLN	2.1
2	K	1	DT	2.1
2	e	5	DT	2.1
1	N	200	ARG	2.1
1	S	136	GLY	2.1
2	i	20	DA	2.1
1	B	144	HIS	2.1
1	8	182	HIS	2.1
1	S	159	GLU	2.1
1	E	200	ARG	2.1
1	8	144	HIS	2.1
3	L	26	DC	2.1
2	m	13	DA	2.1
3	D	11	DA	2.1
1	4	147	MET	2.1
1	B	218	VAL	2.1
1	g	227	THR	2.1
1	E	220	GLY	2.1
1	S	225	PHE	2.1
1	V	181	ASN	2.1
1	9	152	PRO	2.1
1	I	191	GLU	2.1
1	d	150	GLU	2.1
3	P	15	DC	2.1
3	Y	12	DC	2.1
3	Y	4	DT	2.1
1	J	191	GLU	2.1
1	W	190	VAL	2.1
1	4	150	GLU	2.1
1	h	133	GLU	2.1
3	3	22	DA	2.1
3	j	11	DA	2.1
4	q	594	ALA	2.1
3	H	25	DG	2.1
1	4	220	GLY	2.1
1	5	136	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	5	205	ALA	2.1
1	d	203	ARG	2.1
1	l	152	PRO	2.1
1	h	144	HIS	2.1
1	B	134	MET	2.1
1	l	219	ARG	2.1
2	e	10	DT	2.1
2	C	14	DG	2.1
2	a	14	DG	2.1
1	I	159	GLU	2.1
2	2	20	DA	2.1
2	a	23	DA	2.1
3	L	14	DA	2.1
3	b	24	DA	2.1
1	A	187	ASN	2.1
1	S	153	LEU	2.1
1	c	155	MET	2.1
1	g	142	THR	2.1
2	i	5	DT	2.1
3	H	4	DT	2.1
4	q	596	ARG	2.1
1	R	159	GLU	2.1
1	c	142	THR	2.1
1	B	219	ARG	2.1
1	F	137	LEU	2.1
1	l	201	ARG	2.1
1	S	199	ILE	2.1
2	i	12	DA	2.1
3	U	14	DA	2.1
2	2	10	DT	2.1
1	B	211	HIS	2.1
2	C	2	DG	2.1
1	V	128	VAL	2.1
1	M	219	ARG	2.1
1	c	221	THR	2.1
1	l	165	PHE	2.1
1	M	182	HIS	2.1
1	8	216	GLN	2.1
1	c	178	GLN	2.1
2	2	11	DA	2.1
2	m	5	DT	2.1
3	H	3	DC	2.1

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Mol	Chain	Res	Type	RSRZ
3	3	6	DT	2.1
1	Z	227	THR	2.1
2	G	5	DT	2.1
1	9	221	THR	2.1
1	4	192	ASP	2.1
1	c	225	PHE	2.1
1	l	168	THR	2.0
1	F	229	PHE	2.0
1	R	197	VAL	2.0
1	d	177	GLU	2.0
1	g	199	ILE	2.0
1	c	157	PRO	2.0
1	g	152	PRO	2.0
2	O	5	DT	2.0
3	H	23	DC	2.0
3	b	3	DC	2.0
1	I	135	GLN	2.0
1	9	200	ARG	2.0
1	A	171	GLU	2.0
1	9	151	GLU	2.0
4	o	594	ALA	2.0
1	N	181	ASN	2.0
1	F	190	VAL	2.0
1	J	144	HIS	2.0
1	5	156	GLY	2.0
2	i	14	DG	2.0
1	5	159	GLU	2.0
1	l	135	GLN	2.0
2	m	23	DA	2.0
1	F	142	THR	2.0
4	o	571	TYR	2.0
1	M	195	VAL	2.0
1	R	182	HIS	2.0
1	Z	221	THR	2.0
1	l	130	GLU	2.0
1	c	147	MET	2.0
3	D	13	DA	2.0
1	c	181	ASN	2.0
3	f	15	DC	2.0
3	j	19	DA	2.0
4	q	555	GLU	2.0
1	N	164	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	1	164	HIS	2.0
1	h	142	THR	2.0
1	1	201	ARG	2.0
1	M	170	PRO	2.0
1	V	163	LEU	2.0
3	P	10	DG	2.0
1	Z	200	ARG	2.0
1	h	141	PRO	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.