Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:27 PM UTC

PDB ID	:	3T72 / pdb_00003t72
Title	:	PhoB(E)-Sigma70(4)-(RNAP-Betha-flap-tip-helix)-DNA Transcription Activation Sub-Complex
Authors	:	Blanco, A.G.; Canals, A.; Bernues, J.; Sola, M.; Coll, M.
Deposited on	:	2011-07-29
Resolution	:	4.33 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

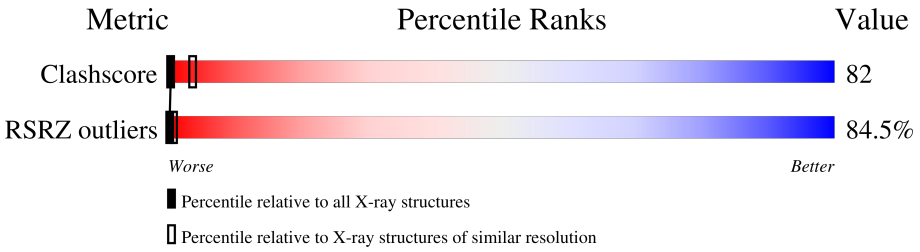
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.33 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1105 (4.76-3.90)
RSRZ outliers	180081	1056 (4.76-3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	90% 100%
1	4	102	87% 100%
1	5	102	89% 100%
1	8	102	90% 100%
1	9	102	93% 100%
1	A	102	90% 100%
1	B	102	88% 100%
1	E	102	87% 100%
1	F	102	88% 100%

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Mol	Chain	Length	Quality of chain
1	I	102	87% 100%
1	J	102	92% 100%
1	M	102	94% 100%
1	N	102	91% 100%
1	R	102	86% 100%
1	S	102	89% 100%
1	V	102	87% 100%
1	W	102	95% 100%
1	Z	102	91% 100%
1	c	102	90% 100%
1	d	102	91% 100%
1	g	102	86% 99%
1	h	102	89% 100%
1	k	102	92% 100%
1	l	102	88% 100%
2	2	26	58% 85% 15%
2	6	26	73% 85% 15%
2	C	26	73% 88% 12%
2	G	26	50% 88% 12%
2	K	26	58% 88% 12%
2	O	26	69% 85% 15%
2	T	26	54% 88% 12%
2	X	26	58% 88% 12%
2	a	26	62% 88% 12%
2	e	26	69% 88% 12%

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Mol	Chain	Length	Quality of chain
2	i	26	62% 88% 12%
2	m	26	62% 88% 12%
3	3	26	69% 96%
3	7	26	58% 96%
3	D	26	65% 96%
3	H	26	73% 96%
3	L	26	62% 96%
3	P	26	62% 96%
3	U	26	58% 96%
3	Y	26	50% 96%
3	b	26	69% 96%
3	f	26	65% 96%
3	j	26	73% 96%
3	n	26	73% 96%
4	o	99	82% 92% 6%
4	q	99	79% 92% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15354 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Phosphate regulon transcriptional regulatory protein phoB.

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	8	102	Total C 102 102	0	0	102
1	9	102	Total C 102 102	0	0	102
1	c	102	Total C 102 102	0	0	102
1	d	102	Total C 102 102	0	0	102
1	g	102	Total C 102 102	0	0	102
1	h	102	Total C 102 102	0	0	102
1	k	102	Total C 102 102	0	0	102
1	l	102	Total C 102 102	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 C N O P 534 256 101 152 25	0	0	0
2	G	26	Total C N O P 534 256 101 152 25	0	0	0
2	K	26	Total C N O P 534 256 101 152 25	0	0	0
2	O	26	Total C N O P 534 256 101 152 25	0	0	0
2	T	26	Total C N O P 534 256 101 152 25	0	0	0
2	X	26	Total C N O P 534 256 101 152 25	0	0	0
2	2	26	Total C N O P 534 256 101 152 25	0	0	0
2	6	26	Total C N O P 534 256 101 152 25	0	0	0
2	a	26	Total C N O P 534 256 101 152 25	0	0	0
2	e	26	Total C N O P 534 256 101 152 25	0	0	0
2	i	26	Total C N O P 534 256 101 152 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:

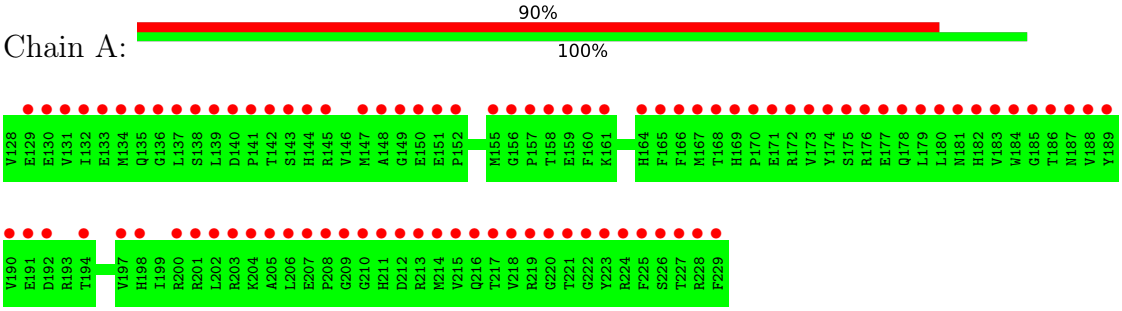
Chain	Residue	Modelled	Actual	Comment	Reference
q	532	MET	-	expression tag	UNP P00579
q	890	GLY	-	linker	UNP P00579
q	891	SER	-	linker	UNP P00579
q	892	SER	-	linker	UNP P00579
q	893	GLY	-	linker	UNP P00579
q	894	SER	-	linker	UNP P00579
q	895	GLY	-	linker	UNP P00579
o	532	MET	-	expression tag	UNP P00579
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, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

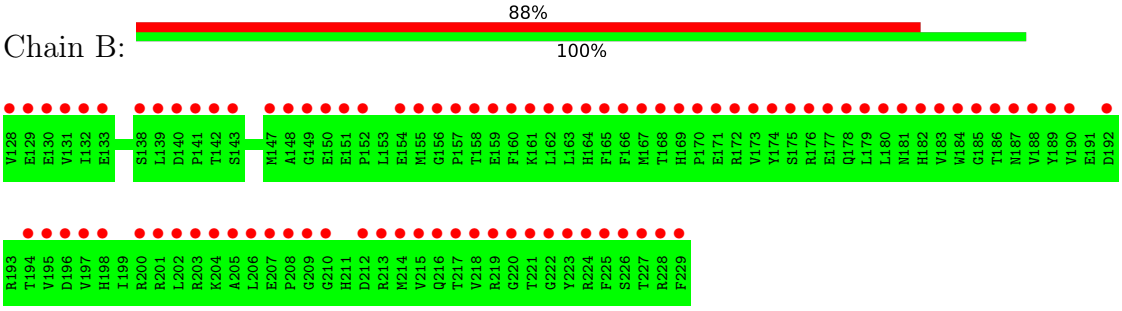
• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain A:



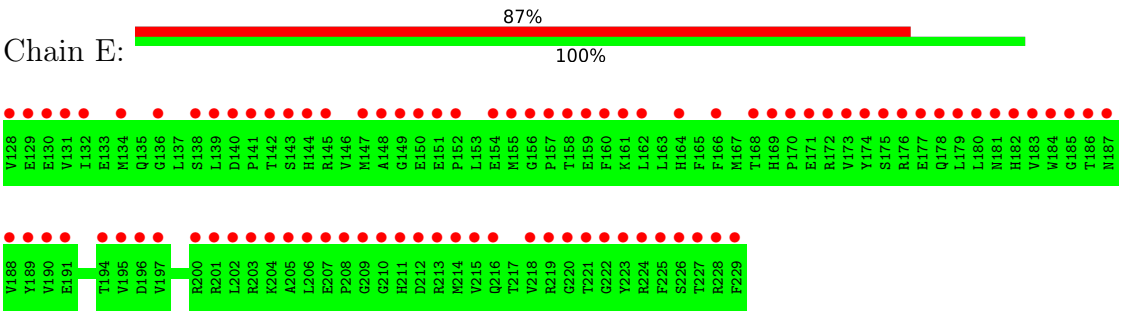
• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain B:



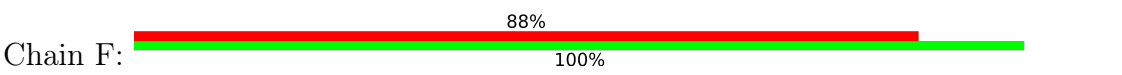
• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

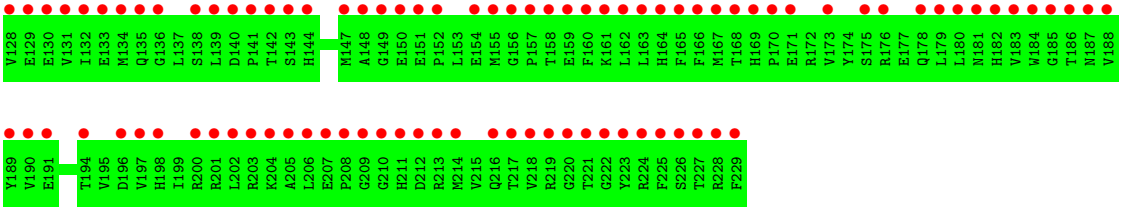
Chain E:



• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain F:

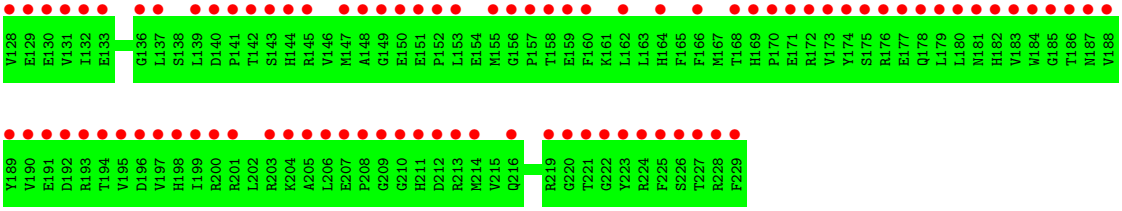




• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

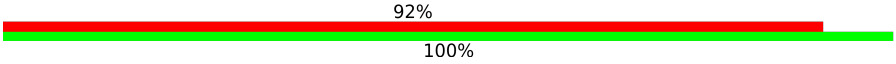
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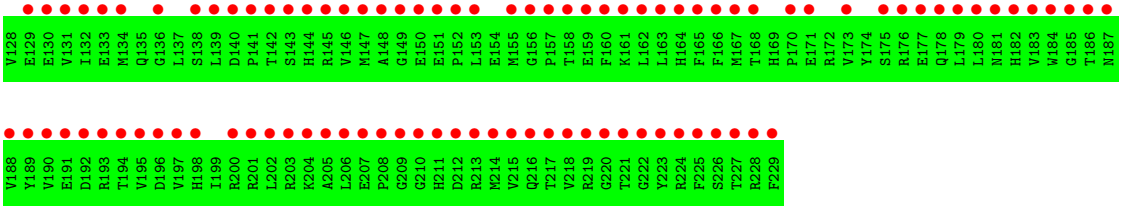




• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

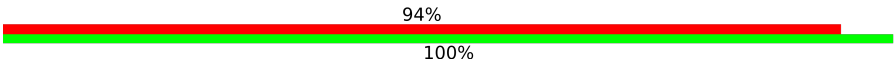
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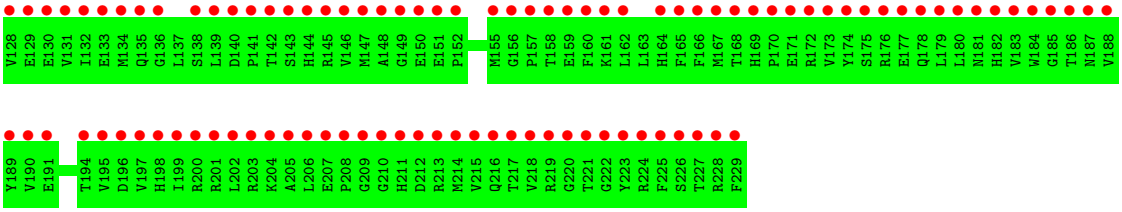




• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

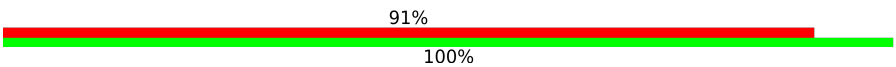
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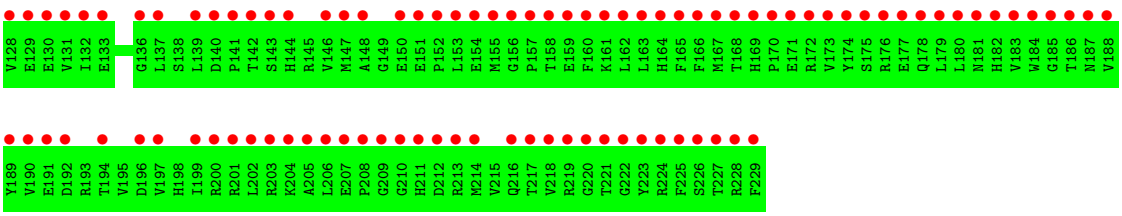




• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain N:

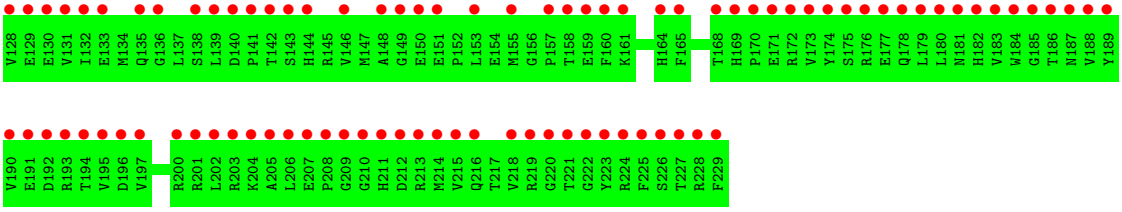




• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain R:

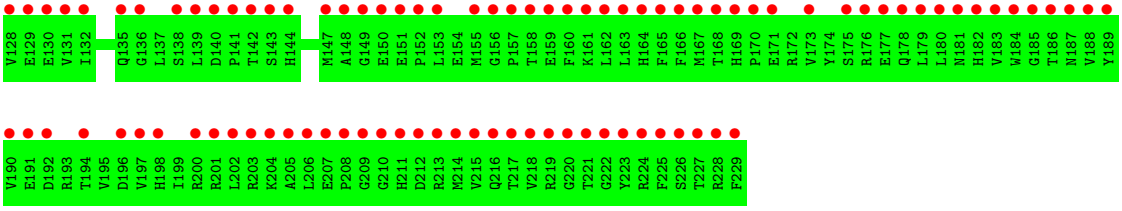




• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain S:

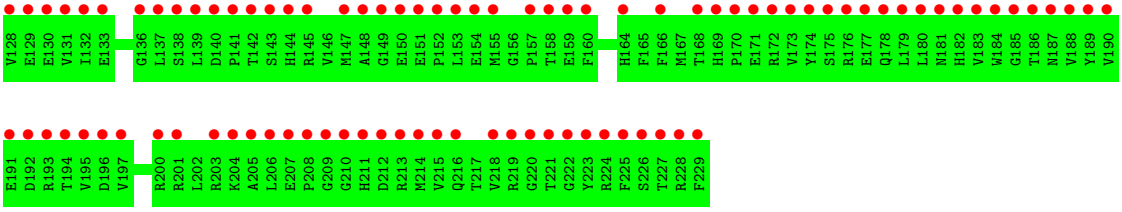




• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

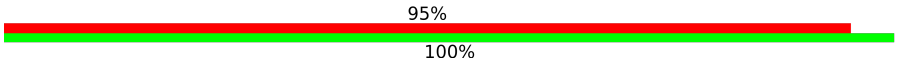
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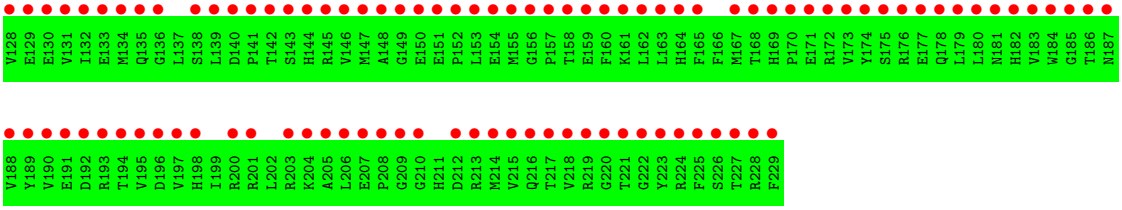




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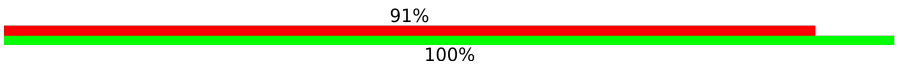
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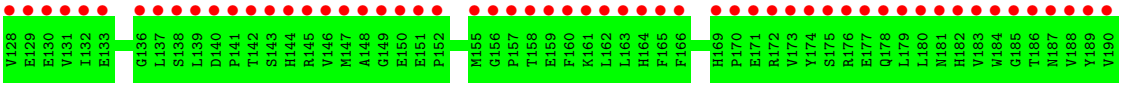


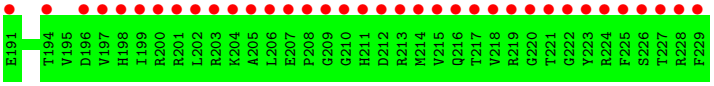


• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

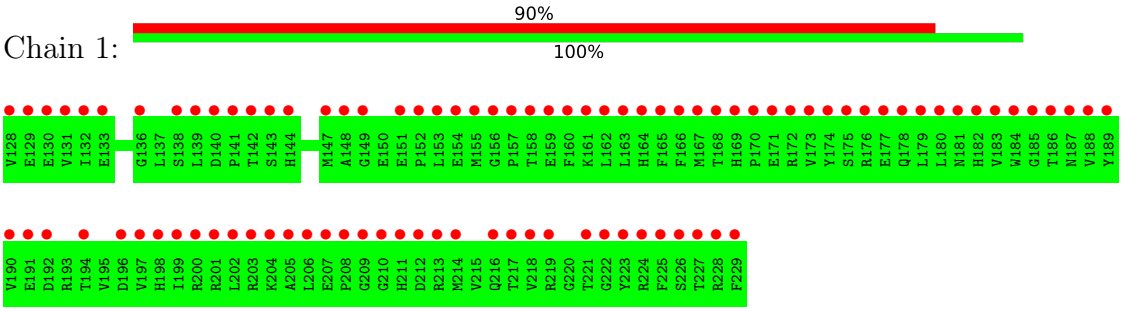
Chain Z:



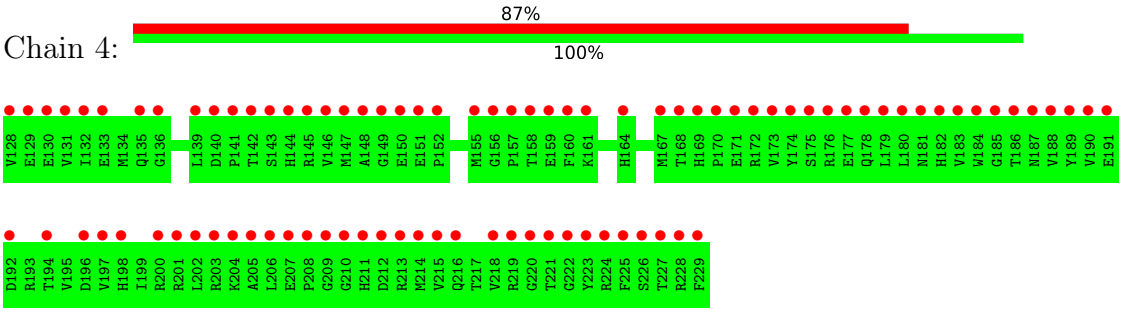




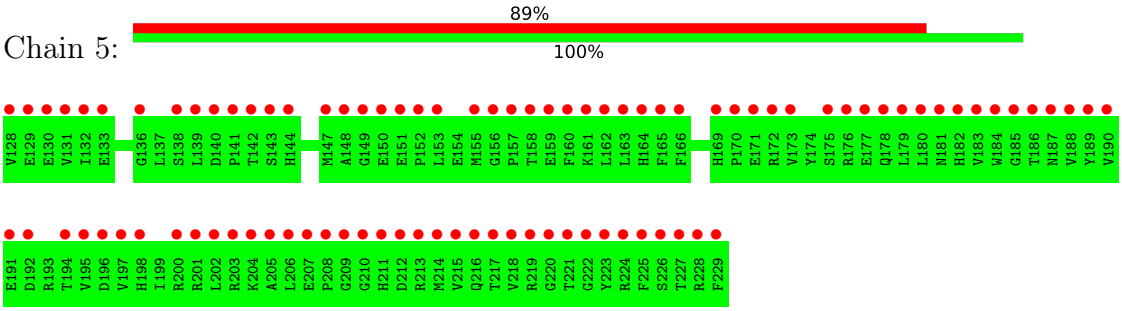
• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB



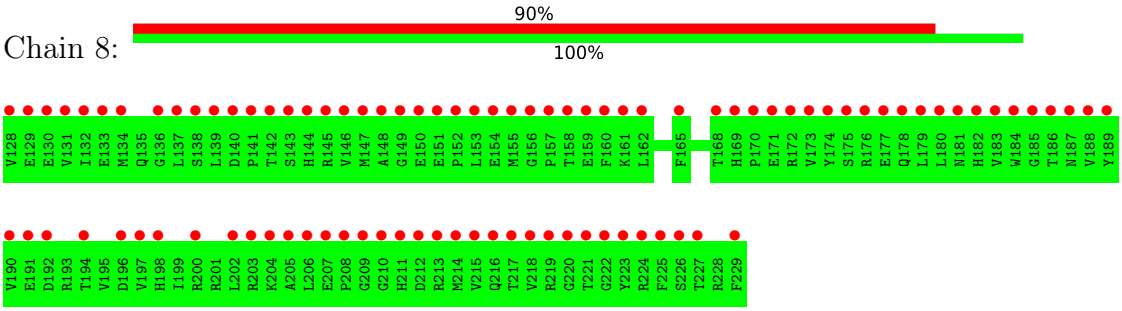
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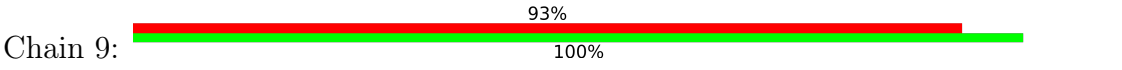
• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

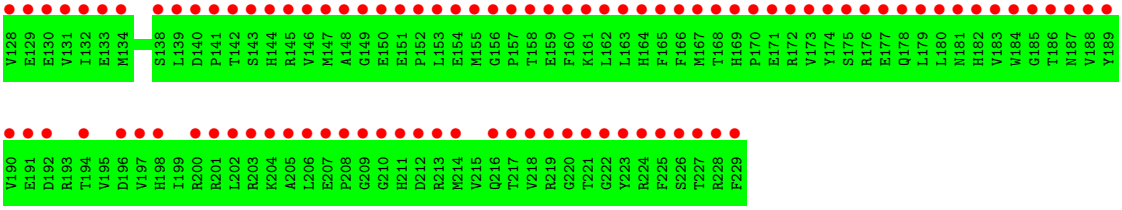


• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB



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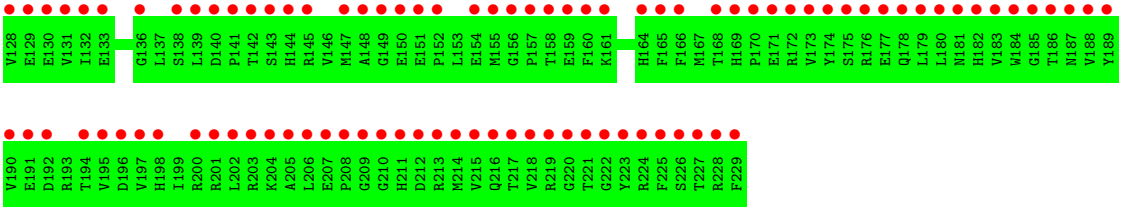




• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

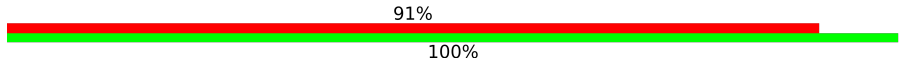
Chain c:

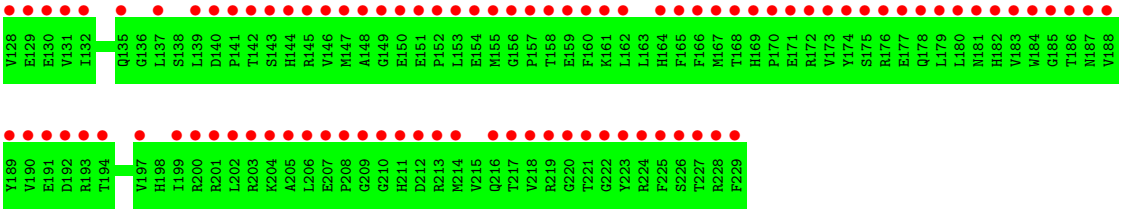




• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

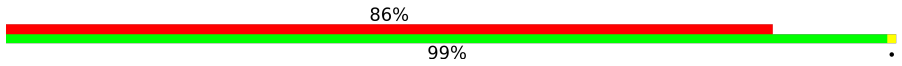
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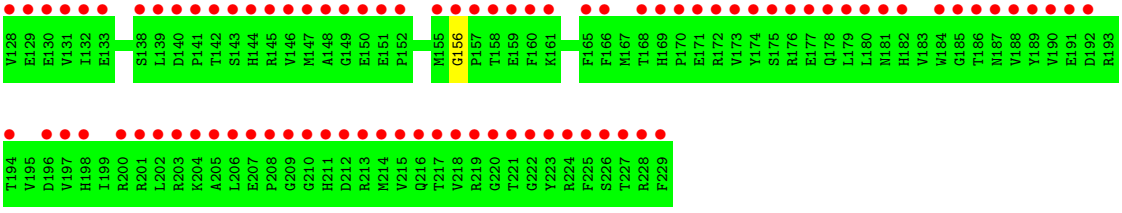




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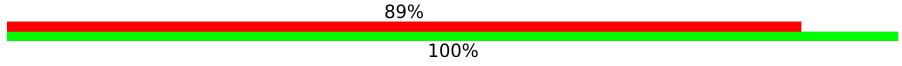
Chain g:

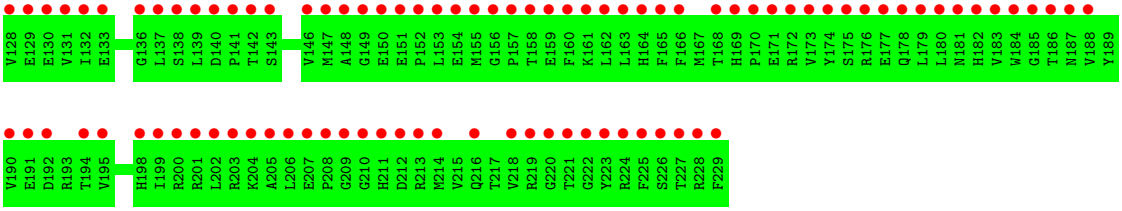




• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

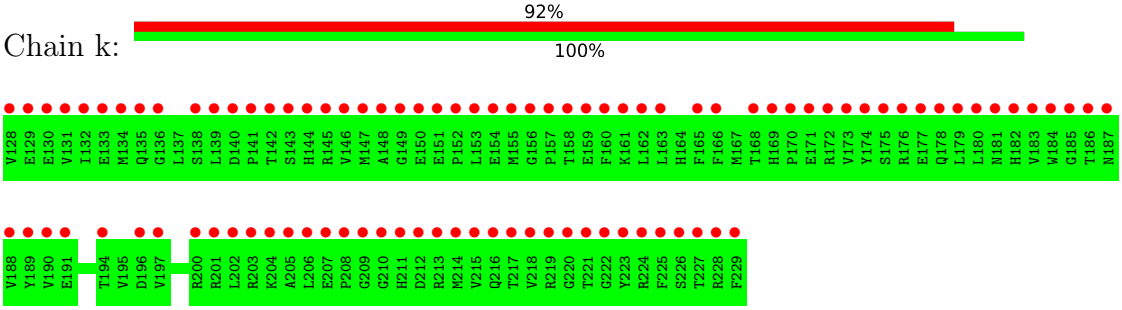
Chain h:





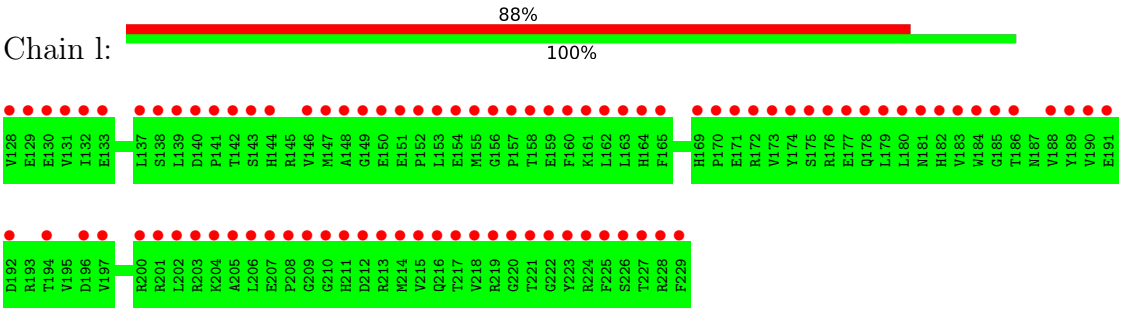
• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain k:



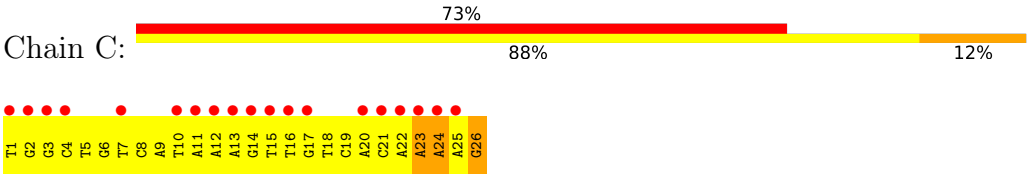
• Molecule 1: Phosphate regulon transcriptional regulatory protein phoB

Chain l:



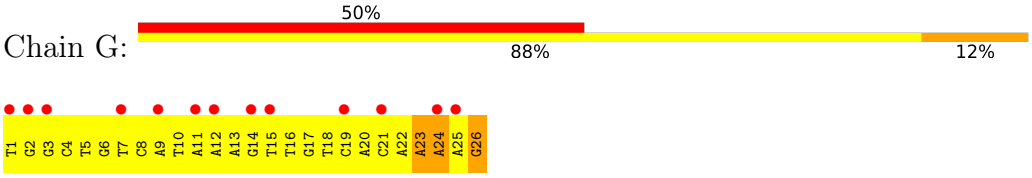
• Molecule 2: PHO BOX DNA (STRAND 1)

Chain C:



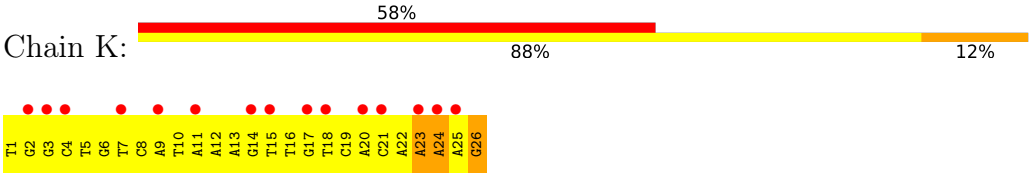
• Molecule 2: PHO BOX DNA (STRAND 1)

Chain G:



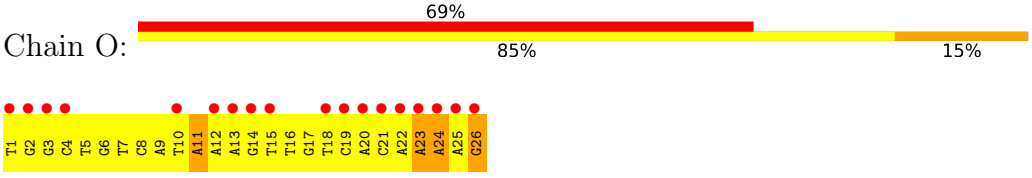
• Molecule 2: PHO BOX DNA (STRAND 1)

Chain K:



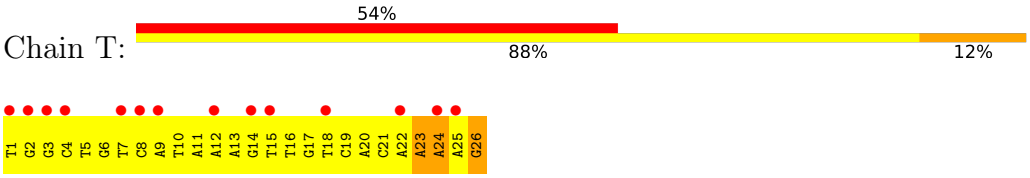
• Molecule 2: PHO BOX DNA (STRAND 1)

Chain O:



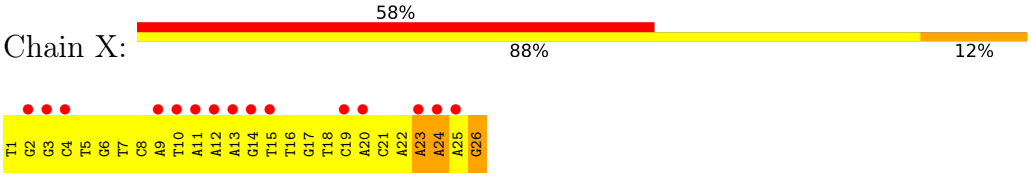
• Molecule 2: PHO BOX DNA (STRAND 1)

Chain T:



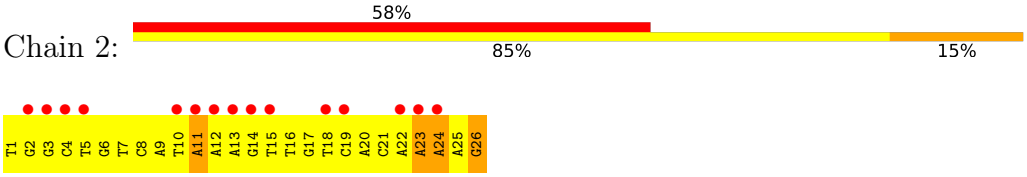
• Molecule 2: PHO BOX DNA (STRAND 1)

Chain X:



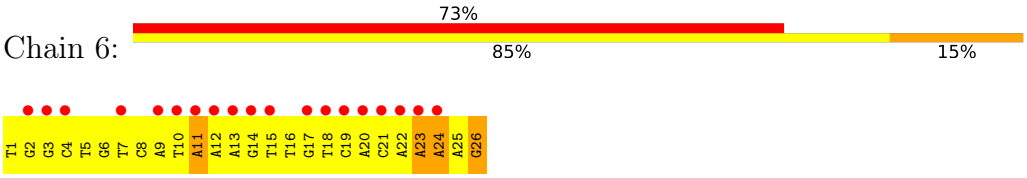
• Molecule 2: PHO BOX DNA (STRAND 1)

Chain 2:



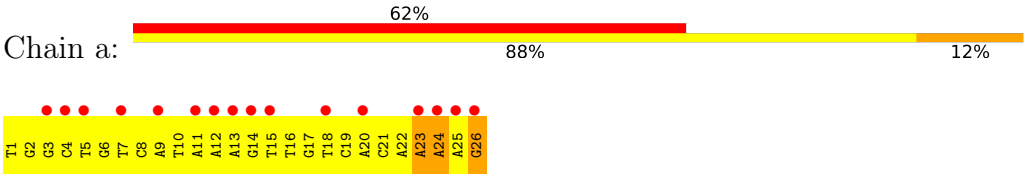
• Molecule 2: PHO BOX DNA (STRAND 1)

Chain 6:



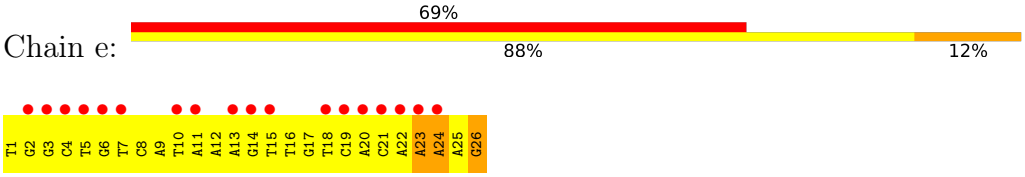
• Molecule 2: PHO BOX DNA (STRAND 1)

Chain a:



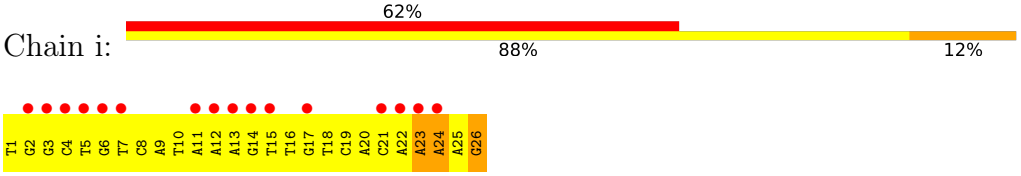
• Molecule 2: PHO BOX DNA (STRAND 1)

Chain e:



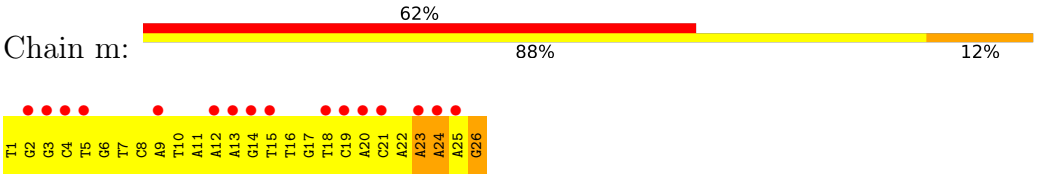
• Molecule 2: PHO BOX DNA (STRAND 1)

Chain i:



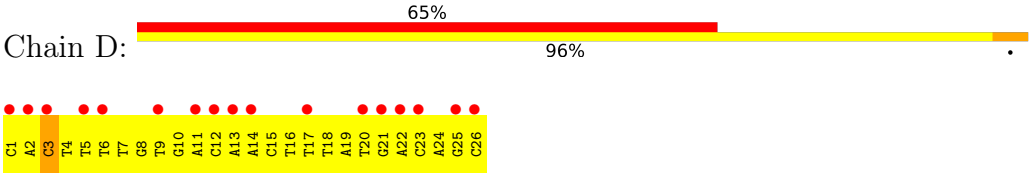
• Molecule 2: PHO BOX DNA (STRAND 1)

Chain m:



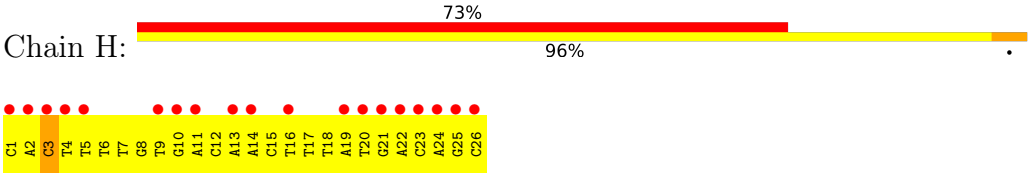
• Molecule 3: PHO BOX DNA (STRAND 2)

Chain D:



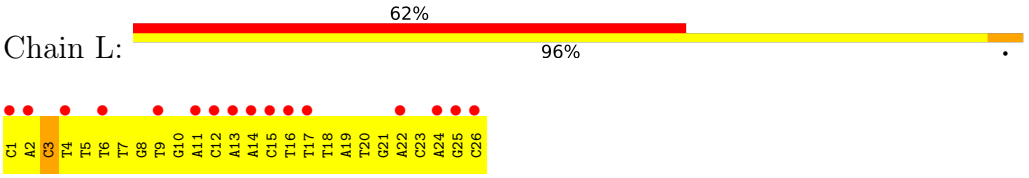
• Molecule 3: PHO BOX DNA (STRAND 2)

Chain H:



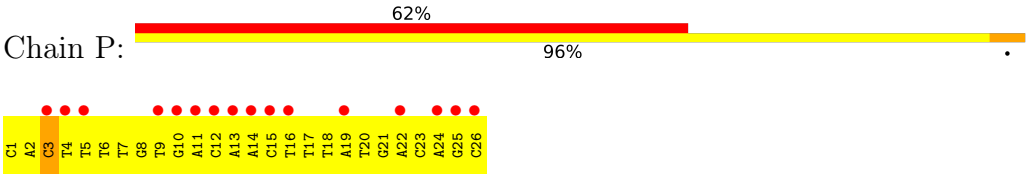
• Molecule 3: PHO BOX DNA (STRAND 2)

Chain L:



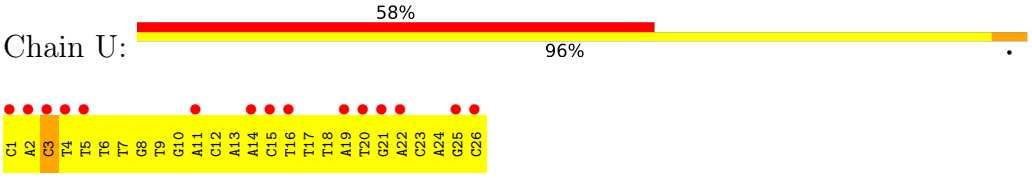
• Molecule 3: PHO BOX DNA (STRAND 2)

Chain P:



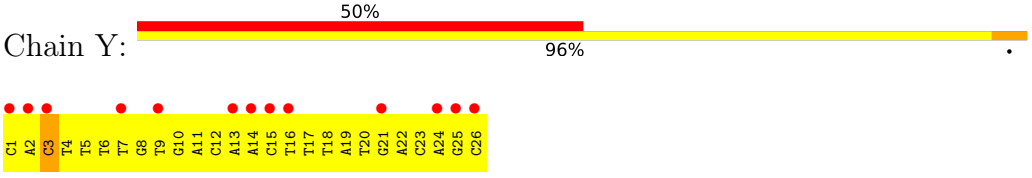
• Molecule 3: PHO BOX DNA (STRAND 2)

Chain U:



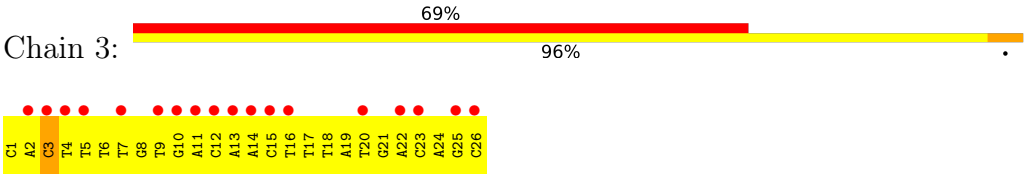
• Molecule 3: PHO BOX DNA (STRAND 2)

Chain Y:



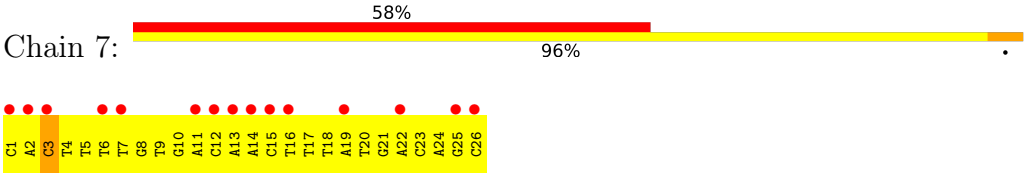
• Molecule 3: PHO BOX DNA (STRAND 2)

Chain 3:



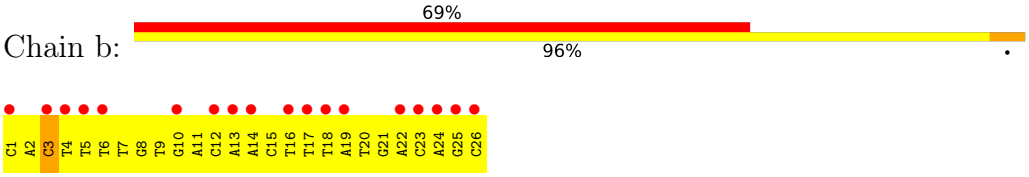
• Molecule 3: PHO BOX DNA (STRAND 2)

Chain 7:



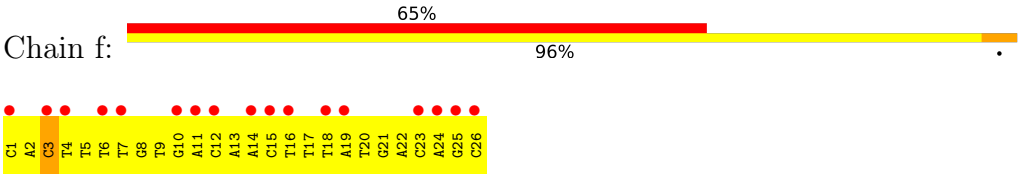
• Molecule 3: PHO BOX DNA (STRAND 2)

Chain b:



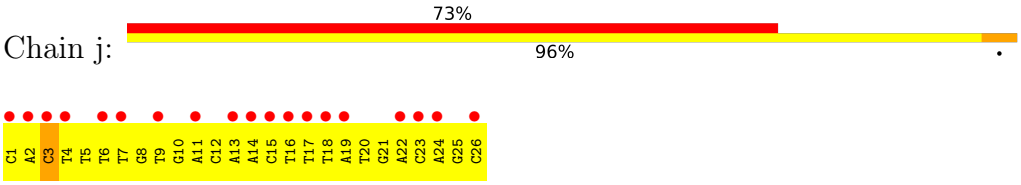
• Molecule 3: PHO BOX DNA (STRAND 2)

Chain f:



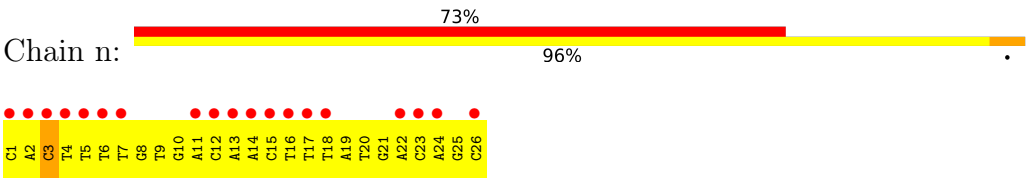
• Molecule 3: PHO BOX DNA (STRAND 2)

Chain j:



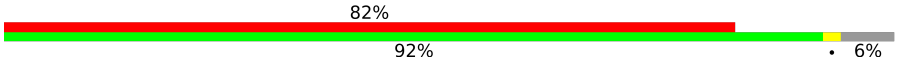
• Molecule 3: PHO BOX DNA (STRAND 2)

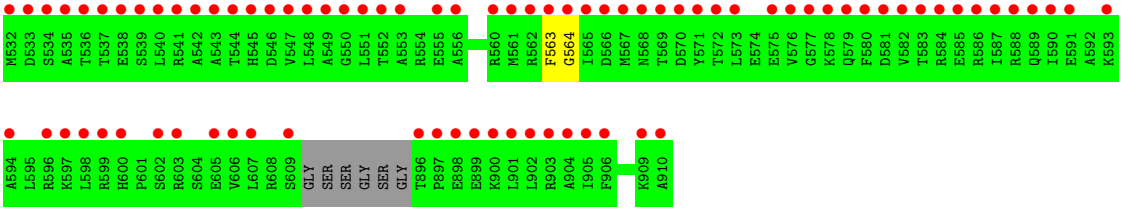
Chain n:



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

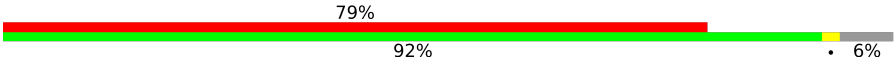
Chain o:

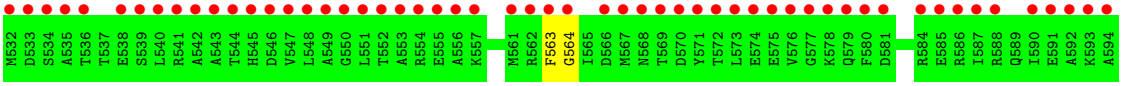


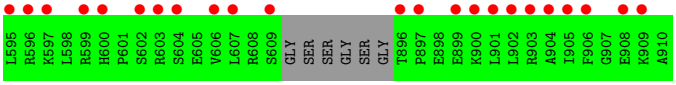


• Molecule 4: RNA polymerase sigma factor rpoD, DNA-directed RNA polymerase subunit beta

Chain q:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	277.30Å 161.40Å 260.10Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	50.00 – 4.33 50.00 – 4.33	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.33) 95.3 (50.00-4.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 4.36Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	(Not available) , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	189.2	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	1.05 , 999.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.012 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.013 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.046 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.028 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.019 for -h,-k,l	Xtriage
F_o,F_c correlation	0.69	EDS
Total number of atoms	15354	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

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

5 Model quality

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	0.92	0/600	0.93	4/925 (0.4%)
2	6	0.91	0/600	0.94	4/925 (0.4%)
2	C	0.91	0/600	0.94	3/925 (0.3%)
2	G	0.95	0/600	0.92	3/925 (0.3%)
2	K	0.91	0/600	0.94	3/925 (0.3%)
2	O	0.93	0/600	0.93	4/925 (0.4%)
2	T	0.95	0/600	0.92	3/925 (0.3%)
2	X	0.91	0/600	0.94	3/925 (0.3%)
2	a	0.95	0/600	0.92	3/925 (0.3%)
2	e	0.90	0/600	0.94	3/925 (0.3%)
2	i	0.90	0/600	0.93	3/925 (0.3%)
2	m	0.95	0/600	0.92	3/925 (0.3%)
3	3	0.91	0/588	0.93	1/905 (0.1%)
3	7	0.92	0/588	0.94	1/905 (0.1%)
3	D	0.91	0/588	0.95	1/905 (0.1%)
3	H	0.95	0/588	0.93	1/905 (0.1%)
3	L	0.90	0/588	0.93	1/905 (0.1%)
3	P	0.91	0/588	0.93	1/905 (0.1%)
3	U	0.95	0/588	0.92	1/905 (0.1%)
3	Y	0.90	0/588	0.93	1/905 (0.1%)
3	b	0.96	0/588	0.93	1/905 (0.1%)
3	f	0.89	0/588	0.93	1/905 (0.1%)
3	j	0.89	0/588	0.93	1/905 (0.1%)
3	n	0.95	0/588	0.93	1/905 (0.1%)
All	All	0.92	0/14256	0.93	51/21960 (0.2%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	3	DC	N1-C1'-C2'	6.84	123.76	113.50
3	H	3	DC	N1-C1'-C2'	6.79	123.68	113.50
2	X	26	DG	C2'-C3'-O3'	-6.77	101.35	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	26	DG	C2'-C3'-O3'	-6.75	101.38	111.50
3	Y	3	DC	N1-C1'-C2'	6.64	123.47	113.50
3	L	3	DC	N1-C1'-C2'	6.63	123.45	113.50
3	j	3	DC	N1-C1'-C2'	6.63	123.45	113.50
3	D	3	DC	N1-C1'-C2'	6.59	123.38	113.50
3	f	3	DC	N1-C1'-C2'	6.57	123.36	113.50
3	7	3	DC	N1-C1'-C2'	6.54	123.31	113.50
3	b	3	DC	N1-C1'-C2'	6.50	123.24	113.50
3	n	3	DC	N1-C1'-C2'	6.46	123.19	113.50
2	G	26	DG	C2'-C3'-O3'	-6.42	101.86	111.50
2	T	26	DG	C2'-C3'-O3'	-6.37	101.95	111.50
3	P	3	DC	N1-C1'-C2'	6.32	122.97	113.50
2	e	26	DG	C2'-C3'-O3'	-6.29	102.06	111.50
2	i	26	DG	C2'-C3'-O3'	-6.28	102.08	111.50
2	6	26	DG	C2'-C3'-O3'	-6.25	102.13	111.50
3	3	3	DC	N1-C1'-C2'	6.24	122.86	113.50
2	C	26	DG	C2'-C3'-O3'	-6.20	102.20	111.50
2	a	26	DG	C2'-C3'-O3'	-6.15	102.27	111.50
2	m	26	DG	C2'-C3'-O3'	-6.14	102.29	111.50
2	2	26	DG	C2'-C3'-O3'	-5.96	102.56	111.50
2	O	26	DG	C2'-C3'-O3'	-5.89	102.66	111.50
2	C	24	DA	C2'-C3'-O3'	-5.68	102.97	111.50
2	m	24	DA	C2'-C3'-O3'	-5.66	103.01	111.50
2	2	23	DA	C2'-C3'-O3'	-5.66	103.01	111.50
2	a	24	DA	C2'-C3'-O3'	-5.65	103.02	111.50
2	O	23	DA	C2'-C3'-O3'	-5.63	103.06	111.50
2	6	24	DA	C2'-C3'-O3'	-5.58	103.12	111.50
2	6	23	DA	C2'-C3'-O3'	-5.53	103.21	111.50
2	i	24	DA	C2'-C3'-O3'	-5.51	103.23	111.50
2	O	24	DA	C2'-C3'-O3'	-5.50	103.25	111.50
2	e	24	DA	C2'-C3'-O3'	-5.49	103.26	111.50
2	2	24	DA	C2'-C3'-O3'	-5.47	103.29	111.50
2	a	23	DA	C2'-C3'-O3'	-5.44	103.34	111.50
2	C	23	DA	C2'-C3'-O3'	-5.43	103.36	111.50
2	m	23	DA	C2'-C3'-O3'	-5.40	103.40	111.50
2	e	23	DA	C2'-C3'-O3'	-5.38	103.44	111.50
2	i	23	DA	C2'-C3'-O3'	-5.37	103.44	111.50
2	O	11	DA	N9-C1'-C2'	5.34	121.51	113.50
2	2	11	DA	N9-C1'-C2'	5.33	121.50	113.50
2	X	24	DA	C2'-C3'-O3'	-5.30	103.55	111.50
2	T	24	DA	C2'-C3'-O3'	-5.29	103.56	111.50
2	G	24	DA	C2'-C3'-O3'	-5.28	103.58	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	24	DA	C2'-C3'-O3'	-5.28	103.59	111.50
2	K	23	DA	C2'-C3'-O3'	-5.26	103.61	111.50
2	X	23	DA	C2'-C3'-O3'	-5.25	103.63	111.50
2	T	23	DA	C2'-C3'-O3'	-5.11	103.84	111.50
2	G	23	DA	C2'-C3'-O3'	-5.03	103.96	111.50
2	6	11	DA	N9-C1'-C2'	5.01	121.02	113.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	102	0	0	0	0
1	4	102	0	0	0	0
1	5	102	0	0	0	0
1	8	102	0	0	0	0
1	9	102	0	0	0	0
1	A	102	0	0	0	0
1	B	102	0	0	0	0
1	E	102	0	0	0	0
1	F	102	0	0	0	0
1	I	102	0	0	0	0
1	J	102	0	0	0	0
1	M	102	0	0	0	0
1	N	102	0	0	0	0
1	R	102	0	0	0	0
1	S	102	0	0	0	0
1	V	102	0	0	0	0
1	W	102	0	0	0	0
1	Z	102	0	0	0	0
1	c	102	0	0	0	0
1	d	102	0	0	0	0
1	g	102	0	0	1	0
1	h	102	0	0	0	0
1	k	102	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	82	2
2	e	534	0	295	77	5
2	i	534	0	295	84	1
2	m	534	0	295	85	2
3	3	526	0	297	70	3
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	71	7
3	f	526	0	297	71	4
3	j	526	0	297	73	2
3	n	526	0	297	73	1
4	o	93	0	0	1	0
4	q	93	0	0	1	0
All	All	15354	0	7104	1812	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 (1812) 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
3:f:14:DA:H2"	3:f:15:DC:H5"	1.27	1.17
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:a:25:DA:H2"	2:a:26:DG:H5"	1.21	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:m:25:DA:H2”	2:m:26:DG:H5”	1.21	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:j:14:DA:H2”	3:j:15:DC:H5”	1.27	1.13
3:P:14:DA:H2”	3:P:15:DC:H5”	1.29	1.11
3:3:14:DA:H2”	3:3:15:DC:H5”	1.29	1.11
3:L:14:DA:H2”	3:L:15:DC:H5”	1.27	1.11
3:H:14:DA:H2”	3:H:15:DC:H5”	1.27	1.10
3:n:14:DA:H2”	3:n:15:DC:H5”	1.27	1.10
2:O:25:DA:H2”	2:O:26:DG:H5”	1.22	1.09
3:b:14:DA:H2”	3:b:15:DC:H5”	1.27	1.09
2:2:25:DA:H2”	2:2:26:DG:H5”	1.22	1.08
2:i:25:DA:H2”	2:i:26:DG:H5”	1.21	1.08
2:e:25:DA:H2”	2:e:26:DG:H5”	1.21	1.08
3:D:14:DA:H2”	3:D:15:DC:H5”	1.27	1.06
3:D:14:DA:C2’	3:D:15:DC:H5”	1.85	1.06
3:7:14:DA:H2”	3:7:15:DC:H5”	1.27	1.06
3:7:14:DA:C2’	3:7:15:DC:H5”	1.85	1.06
3:f:14:DA:C2’	3:f:15:DC:H5”	1.85	1.06
3:j:14:DA:C2’	3:j:15:DC:H5”	1.85	1.06
3:Y:14:DA:C2’	3:Y:15:DC:H5”	1.85	1.06
3:L:14:DA:C2’	3:L:15:DC:H5”	1.85	1.05
3:n:14:DA:C2’	3:n:15:DC:H5”	1.86	1.05
3:b:14:DA:C2’	3:b:15:DC:H5”	1.86	1.05
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:e:24:DA:H4’	2:e:25:DA:OP1	1.62	0.98
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:j:9:DT:H2”	3:j:10:DG:H5”	1.46	0.98
3:n:9:DT:H2”	3:n:10:DG:H5”	1.46	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
3:b:9:DT:H2”	3:b:10:DG:H5”	1.46	0.97
2:a:24:DA:H4’	2:a:25:DA:OP1	1.61	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:f:9:DT:H2"	3:f:10:DG:H5"	1.46	0.97
3:H:9:DT:H2"	3:H:10:DG:H5"	1.44	0.96
2:O:23:DA:H4'	2:O:24:DA:OP1	1.64	0.96
2:T:24:DA:H4'	2:T:25:DA:OP1	1.62	0.96
2:C:24:DA:H4'	2:C:25:DA:OP1	1.61	0.96
3:P:9:DT:H2"	3:P:10:DG:H5"	1.46	0.96
2:i:24:DA:H4'	2:i:25:DA:OP1	1.62	0.95
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:e:23:DA:H4'	2:e:24:DA:OP1	1.65	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:m:24:DA:H4'	2:m:25:DA:OP1	1.61	0.94
2:m:23:DA:H4'	2:m:24:DA:OP1	1.64	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:i:23:DA:H4'	2:i:24:DA:OP1	1.65	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:a:23:DA:H4'	2:a:24:DA:OP1	1.64	0.92
3:j:5:DT:H1'	3:j:6:DT:H5"	1.51	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:a:11:DA:H2"	2:a:12:DA:H5"	1.51	0.91
3:f:5:DT:H1'	3:f:6:DT:H5"	1.51	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:j:14:DA:H2"	3:j:15:DC:C5'	2.00	0.91
2:G:7:DT:H2"	2:G:8:DC:H5'	1.52	0.91
3:U:14:DA:H2"	3:U:15:DC:C5'	2.00	0.91
3:b:14:DA:H2"	3:b:15:DC:C5'	2.00	0.91
3:D:14:DA:H2"	3:D:15:DC:C5'	2.00	0.91
2:C:7:DT:H2"	2:C:8:DC:H5'	1.51	0.91
2:a:7:DT:H2"	2:a:8:DC:H5'	1.51	0.91
2:e:11:DA:H2"	2:e:12:DA:H5"	1.53	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:n:14:DA:H2"	3:n:15:DC:C5'	2.01	0.91
3:7:14:DA:H2"	3:7:15:DC:C5'	2.00	0.91
2:e:6:DG:H2"	2:e:7:DT:H5"	1.53	0.91
3:L:5:DT:H1'	3:L:6:DT:H5"	1.52	0.90
3:b:5:DT:H1'	3:b:6:DT:H5"	1.53	0.90
2:T:25:DA:H1'	2:T:26:DG:O4'	1.71	0.90
2:i:25:DA:H1'	2:i:26:DG:O4'	1.72	0.90
2:C:11:DA:H2"	2:C:12:DA:H5"	1.52	0.90
3:f:14:DA:H2"	3:f:15:DC:C5'	2.00	0.90
2:X:6:DG:H2"	2:X:7:DT:H5"	1.52	0.90
2:m:7:DT:H2"	2:m:8:DC:H5'	1.51	0.90
3:n:5:DT:H1'	3:n:6:DT:H5"	1.54	0.90
2:m:6:DG:H2"	2:m:7:DT:H5"	1.52	0.90
3:H:8:DG:H2"	3:H:9:DT:C5'	2.01	0.90
2:K:25:DA:H1'	2:K:26:DG:O4'	1.72	0.90
2:O:25:DA:H1'	2:O:26:DG:O4'	1.72	0.90
2:T:7:DT:H2"	2:T:8:DC:H5'	1.52	0.90
2:2:11:DA:H2"	2:2:12:DA:H5"	1.50	0.90
2:i:6:DG:H2"	2:i:7:DT:H5"	1.53	0.90
2:i:7:DT:H2"	2:i:8:DC:H5'	1.52	0.90
2:m:24:DA:N1	3:n:5:DT:N3	2.19	0.90
2:G:6:DG:H2"	2:G:7:DT:H5"	1.53	0.90
2:X:7:DT:H2"	2:X:8:DC:H5'	1.53	0.90
2:X:25:DA:H1'	2:X:26:DG:O4'	1.72	0.90
3:3:14:DA:H2"	3:3:15:DC:C5'	2.02	0.90
2:6:11:DA:H2"	2:6:12:DA:H5"	1.53	0.90
2:T:6:DG:H2"	2:T:7:DT:H5"	1.53	0.89
2:e:7:DT:H2"	2:e:8:DC:H5'	1.52	0.89
2:e:25:DA:H1'	2:e:26:DG:O4'	1.72	0.89
2:i:11:DA:H2"	2:i:12:DA:H5"	1.53	0.89
2:m:11:DA:H2"	2:m:12:DA:H5"	1.51	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:13:DA:H1'	2:m:14:DG:H5'	1.53	0.89
2:C:6:DG:H2"	2:C:7:DT:H5"	1.53	0.89
3:Y:8:DG:H2"	3:Y:9:DT:C5'	2.02	0.89
2:2:25:DA:H1'	2:2:26:DG:O4'	1.72	0.89
2:a:13:DA:H1'	2:a:14:DG:H5'	1.54	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:a:25:DA:H1'	2:a:26:DG:O4'	1.72	0.89
2:m:25:DA:H1'	2:m:26:DG:O4'	1.72	0.89
2:2:13:DA:H1'	2:2:14:DG:H5'	1.55	0.89
2:G:13:DA:H1'	2:G:14:DG:H5'	1.55	0.89
3:H:5:DT:H1'	3:H:6:DT:H5"	1.54	0.89
3:U:8:DG:H2"	3:U:9:DT:H5"	1.52	0.89
3:f:8:DG:H2"	3:f:9:DT:C5'	2.03	0.89
3:H:8:DG:H2"	3:H:9:DT:H5"	1.53	0.89
3:P:14:DA:H2"	3:P:15:DC:C5'	2.02	0.89
3:b:8:DG:H2"	3:b:9:DT:H5"	1.54	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:n:8:DG:H2"	3:n:9:DT:C5'	2.02	0.88
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
3:f:8:DG:H2"	3:f:9:DT:H5"	1.55	0.88
2:a:6:DG:H2"	2:a:7:DT:H5"	1.53	0.88
3:D:11:DA:H1'	3:D:12:DC:H5"	1.56	0.88
3:3:8:DG:H2"	3:3:9:DT:C5'	2.04	0.88
3:7:11:DA:H1'	3:7:12:DC:H5"	1.56	0.88
3:j:8:DG:H2"	3:j:9:DT:C5'	2.03	0.88
2:K:7:DT:H2"	2:K:8:DC:H5'	1.53	0.88
3:b:8:DG:H2"	3:b:9:DT:C5'	2.02	0.88
3:P:8:DG:H2"	3:P:9:DT:C5'	2.04	0.88
2:6:25:DA:H1'	2:6:26:DG:O4'	1.72	0.88
3:L:8:DG:H2"	3:L:9:DT:C5'	2.02	0.88
3:L:8:DG:H2"	3:L:9:DT:H5"	1.54	0.88
3:U:8:DG:C2'	3:U:9:DT:H5"	2.04	0.88
3:n:11:DA:H1'	3:n:12:DC:H5"	1.55	0.88
2:O:13:DA:H1'	2:O:14:DG:H5'	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:8:DG:H2”	3:D:9:DT:H5”	1.55	0.87
3:7:8:DG:H2”	3:7:9:DT:H5”	1.55	0.87
3:P:8:DG:H2”	3:P:9:DT:H5”	1.56	0.87
3:7:8:DG:H2”	3:7:9:DT:C5’	2.03	0.87
3:D:8:DG:H2”	3:D:9:DT:C5’	2.03	0.87
3:3:8:DG:H2”	3:3:9:DT:H5”	1.56	0.87
3:b:11:DA:H1’	3:b:12:DC: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
2:T:13:DA:H1’	2:T:14:DG:H5’	1.55	0.87
2:e:13:DA:H1’	2:e:14:DG:H5’	1.56	0.87
3:Y:8:DG:H2”	3:Y:9:DT:H5”	1.55	0.86
3:P:5:DT:H1’	3:P:6:DT:H5”	1.55	0.86
2:X:25:DA:C2’	2:X:26:DG:H5”	2.05	0.86
3:n:8:DG:H2”	3:n:9:DT:H5”	1.54	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
3:j:8:DG:H2”	3:j:9:DT:H5”	1.55	0.86
2:m:25:DA:C2’	2:m:26:DG:H5”	2.05	0.86
3:f:11:DA:H1’	3:f:12:DC:H5”	1.57	0.85
3:n:8:DG:C2’	3:n:9:DT:H5”	2.06	0.85
2:K:25:DA:C2’	2:K:26:DG:H5”	2.05	0.85
3:b:8:DG:C2’	3:b:9:DT:H5”	2.06	0.85
2:i:13:DA:H1’	2:i:14:DG:H5’	1.56	0.85
3:j:11:DA:H1’	3:j:12:DC:H5”	1.57	0.85
3:U:11:DA:H1’	3:U:12:DC:H5”	1.56	0.85
2:e:25:DA:C2’	2:e:26:DG:H5”	2.05	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:a:25:DA:C2’	2:a:26:DG:H5”	2.05	0.85
2:i:25:DA:C2’	2:i:26:DG:H5”	2.05	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:j:8:DG:C2’	3:j:9:DT:H5”	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:3:8:DG:C2'	3:3:9:DT:H5"	2.08	0.83
3:f:8:DG:C2'	3:f:9:DT:H5"	2.07	0.83
2:2:6:DG:H2"	2:2:7:DT:C5'	2.09	0.82
2:a:12:DA:H2"	2:a:13:DA:H5'	1.62	0.82
2:C:5:DT:H5'	2:C:5:DT:H6	1.45	0.82
2:6:5:DT:H5'	2:6:5:DT:H6	1.44	0.82
2:m:12:DA:H2"	2:m:13:DA:H5'	1.62	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:n:13:DA:H2"	3:n:14:DA:OP2	1.81	0.81
2:O:5:DT:H6	2:O:5:DT:H5'	1.46	0.81
3:U:4:DT:H2"	3:U:5:DT:H72	1.63	0.81
2:2:5:DT:H6	2:2:5:DT:H5'	1.46	0.81
3:3:4:DT:H2"	3:3:5:DT:H72	1.63	0.81
2:G:12:DA:H2"	2:G:13:DA:H5'	1.63	0.81
2:O:12:DA:H2"	2:O:13:DA:H5'	1.62	0.81
2:e:12:DA:H2"	2:e:13:DA:H5'	1.63	0.81
2:i:5:DT:H5'	2:i:5:DT:H6	1.45	0.81
2:G:3:DG:H2"	2:G:4:DC:H5'	1.61	0.80
2:O:8:DC:N4	3:P:21:DG:O6	2.12	0.80
3:3:13:DA:H2"	3:3:14:DA:OP2	1.81	0.80
2:T:6:DG:H2"	2:T:7:DT:C5'	2.11	0.80
3:b:13:DA:H2"	3:b:14:DA:OP2	1.81	0.80
2:a:5:DT:H5'	2:a:5:DT:H6	1.45	0.80
2:e:5:DT:H6	2:e:5:DT:H5'	1.45	0.80
2:C:3:DG:H2"	2:C:4:DC:H5'	1.64	0.80
2:2:7:DT:H2"	2:2:8:DC:C5'	2.11	0.80
2:2:12:DA:H2"	2:2:13:DA:H5'	1.62	0.80
2:m:5:DT:H6	2:m:5:DT:H5'	1.45	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:m:6:DG:H2"	2:m:7:DT:C5'	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:7:DT:H2"	2:C:8:DC:C5'	2.12	0.80
2:T:5:DT:H6	2:T:5:DT:H5'	1.47	0.80
2:6:3:DG:H2"	2:6:4:DC:H5'	1.64	0.80
3:7:13:DA:H2"	3:7:14:DA:OP2	1.82	0.80
2:e:6:DG:H2"	2:e:7:DT:C5'	2.12	0.80
3:H:4:DT:H2"	3:H:5:DT:H72	1.63	0.80
2:i:12:DA:H2"	2:i:13:DA:H5'	1.64	0.80
2:C:6:DG:H2"	2:C:7:DT:C5'	2.12	0.80
3:U:13:DA:H2"	3:U:14:DA:OP2	1.81	0.80
3:Y:4:DT:H2"	3:Y:5:DT:H72	1.64	0.80
3:7:4:DT:H2"	3:7:5:DT:H72	1.64	0.80
3:H:13:DA:H2"	3:H:14:DA:OP2	1.82	0.79
2:X:6:DG:H2"	2:X:7:DT:C5'	2.11	0.79
3:D:13:DA:H2"	3:D:14:DA:OP2	1.82	0.79
2:G:6:DG:H2"	2:G:7:DT:C5'	2.11	0.79
2:G:5:DT:H6	2:G:5:DT:H5'	1.46	0.79
2:a:3:DG:H2"	2:a:4:DC:H5'	1.63	0.79
2:6:6:DG:H2"	2:6:7:DT:C5'	2.12	0.79
3:f:4:DT:H2"	3:f:5:DT:H72	1.63	0.79
2:i:6:DG:H2"	2:i:7:DT:C5'	2.12	0.79
2:a:7:DT:H2"	2:a:8:DC:C5'	2.11	0.79
2:m:7:DT:H2"	2:m:8:DC:C5'	2.11	0.79
3:D:4:DT:H2"	3:D:5:DT:H72	1.64	0.79
2:K:5:DT:H5'	2:K:5:DT:H6	1.47	0.79
3:L:4:DT:H2"	3:L:5:DT:H72	1.64	0.79
3:P:13:DA:H2"	3:P:14:DA:OP2	1.81	0.79
2:a:6:DG:H2"	2:a:7:DT:C5'	2.11	0.79
2:K:3:DG:H2"	2:K:4:DC:H5'	1.64	0.79
3:P:11:DA:H2"	3:P:12:DC:C5'	2.13	0.79
3:3:11:DA:H2"	3:3:12:DC:C5'	2.12	0.79
3:Y:13:DA:H2"	3:Y:14:DA:OP2	1.82	0.79
2:O:7:DT:O4	3:P:22:DA:N6	2.14	0.79
2:T:7:DT:H2"	2:T:8:DC:C5'	2.13	0.79
3:n:11:DA:H2"	3:n:12:DC:C5'	2.13	0.79
2:a:12:DA:H2"	2:a:13:DA:C5'	2.13	0.79
2:m:3:DG:H2"	2:m:4:DC:H5'	1.63	0.79
2:X:3:DG:H2"	2:X:4:DC:H5'	1.64	0.78
2:e:3:DG:H2"	2:e:4:DC:H5'	1.64	0.78
2:m:12:DA:H2"	2:m:13:DA:C5'	2.13	0.78
2:T:12:DA:H2"	2:T:13:DA:H5'	1.63	0.78
3:b:11:DA:H2"	3:b:12:DC:C5'	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:7:DT:H2"	2:i:8:DC:C5'	2.13	0.78
2:K:12:DA:H2"	2:K:13:DA:H5'	1.65	0.78
2:O:12:DA:H2"	2:O:13:DA:C5'	2.13	0.78
3:U:16:DT:H2'	3:U:17:DT:H72	1.66	0.78
2:6:12:DA:H2"	2:6:13:DA:C5'	2.13	0.78
3:j:4:DT:H2"	3:j:5:DT:H72	1.63	0.78
2:X:5:DT:H6	2:X:5:DT:H5'	1.48	0.78
2:C:12:DA:H2"	2:C:13:DA:C5'	2.14	0.77
3:D:11:DA:H2"	3:D:12:DC:C5'	2.14	0.77
2:e:7:DT:H2"	2:e:8:DC:C5'	2.13	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:b:4:DT:H2"	3:b:5:DT:H72	1.65	0.77
2:i:3:DG:H2"	2:i:4:DC:H5'	1.64	0.77
2:G:7:DT:H2"	2:G:8:DC:C5'	2.13	0.77
3:L:13:DA:H2"	3:L:14:DA:OP2	1.82	0.77
2:X:7:DT:H2"	2:X:8:DC:C5'	2.14	0.77
2:O:2:DG:H4'	2:O:2:DG:OP1	1.85	0.77
2:X:12:DA:H2"	2:X:13:DA:H5'	1.65	0.77
3:H:16:DT:H2'	3:H:17:DT:H72	1.66	0.77
3:L:11:DA:H2"	3:L:12:DC:C5'	2.15	0.77
3:n:4:DT:H2"	3:n:5:DT:H72	1.64	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
3:f:13:DA:H2"	3:f:14:DA:OP2	1.83	0.77
3:j:13:DA:H2"	3:j:14:DA:OP2	1.83	0.77
2:2:3:DG:H2"	2:2:4:DC:H5'	1.65	0.76
2:e:12:DA:H2"	2:e:13:DA:C5'	2.15	0.76
2:G:12:DA:H2"	2:G:13:DA:C5'	2.15	0.76
2:i:12:DA:H2"	2:i:13:DA:C5'	2.15	0.76
3:j:11:DA:H2"	3:j:12:DC:C5'	2.15	0.76
2:X:2:DG:H4'	2:X:2:DG:OP1	1.86	0.76
3:f:11:DA:H2"	3:f:12:DC:C5'	2.15	0.76
3:L:2:DA:H1'	3:L:3:DC:H5'	1.68	0.76
2:T:12:DA:H2"	2:T:13:DA:C5'	2.15	0.76
3:U:11:DA:H2"	3:U:12:DC:C5'	2.15	0.76
2:i:2:DG:OP1	2:i:2:DG:H4'	1.85	0.76
2:G:2:DG:H4'	2:G:2:DG:OP1	1.85	0.76
2:K:6:DG:H2'	2:K:7:DT:H71	1.67	0.76
2:T:2:DG:OP1	2:T:2:DG:H4'	1.85	0.76
3:3:2:DA:H1'	3:3:3:DC:H5'	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:9:DT:C2'	3:H:10:DG:H5"	2.15	0.76
2:K:2:DG:OP1	2:K:2:DG:H4'	1.86	0.76
2:K:12:DA:H2"	2:K:13:DA:C5'	2.16	0.76
2:e:2:DG:H4'	2:e:2:DG:OP1	1.86	0.76
2:K:7:DT:H2"	2:K:8:DC:C5'	2.14	0.76
3:P:2:DA:H1'	3:P:3:DC:H5'	1.67	0.75
3:D:16:DT:H2'	3:D:17:DT:H72	1.68	0.75
2:m:2:DG:H4'	2:m:2:DG:OP1	1.85	0.75
3:n:16:DT:H2'	3:n:17:DT:H72	1.67	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:n:9:DT:C2'	3:n:10:DG:H5"	2.17	0.75
3:L:9:DT:C2'	3:L:10:DG:H5"	2.17	0.75
3:U:9:DT:C2'	3:U:10:DG:H5"	2.15	0.75
3:b:16:DT:H2'	3:b:17:DT:H72	1.67	0.75
3:f:16:DT:H2'	3:f:17:DT:H72	1.69	0.75
2:a:2:DG:OP1	2:a:2:DG:H4'	1.86	0.75
3:b:9:DT:C2'	3:b:10:DG:H5"	2.17	0.75
3:f:2:DA:H1'	3:f:3:DC:H5'	1.69	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
2:e:1:DT:H2'	2:e:2:DG:C8	2.22	0.74
2:i:1:DT:H2'	2:i:2:DG:C8	2.22	0.74
2:i:6:DG:H2'	2:i:7:DT:H71	1.69	0.74
3:j:2:DA:H1'	3:j:3:DC:H5'	1.69	0.74
3:L:16:DT:H2'	3:L:17:DT:H72	1.69	0.74
2:e:6:DG:H2'	2:e:7:DT:H71	1.70	0.74
2:X:12:DA:H2"	2:X:13:DA:C5'	2.16	0.74
3:j:16:DT:H2'	3:j:17:DT:H72	1.69	0.74
2:K:19:DC:H2"	2:K:20:DA:C8	2.23	0.74
2:O:11:DA:C2'	2:O:12:DA:H5"	2.17	0.74
2:X:6:DG:H2'	2:X:7:DT:H71	1.68	0.74
2:2:1:DT:H2'	2:2:2:DG:C8	2.22	0.74
2:X:19:DC:H2"	2:X:20:DA:C8	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:16:DT:H2'	3:Y:17:DT:H72	1.69	0.74
2:X:1:DT:H2'	2:X:2:DG:C8	2.23	0.74
2:2:11:DA:C2'	2:2:12:DA:H5"	2.17	0.74
3:H:2:DA:H1'	3:H:3:DC:H5'	1.69	0.73
3:Y:9:DT:C2'	3:Y:10:DG:H5"	2.18	0.73
2:K:1:DT:H2'	2:K:2:DG:C8	2.23	0.73
2:C:2:DG:OP1	2:C:2:DG:H4'	1.85	0.73
2:6:2:DG:OP1	2:6:2:DG:H4'	1.85	0.73
2:m:6:DG:H2'	2:m:7:DT:H71	1.70	0.73
3:n:2:DA:H1'	3:n:3:DC:H5'	1.69	0.73
3:3:16:DT:H2'	3:3:17:DT:H72	1.69	0.73
2:m:15:DT:H1'	2:m:16:DT:H5'	1.71	0.73
2:T:6:DG:H2'	2:T:7:DT:H71	1.70	0.73
3:U:2:DA:H1'	3:U:3:DC:H5'	1.68	0.73
2:6:6:DG:H2'	2:6:7:DT:H71	1.70	0.73
3:D:9:DT:C2'	3:D:10:DG:H5"	2.18	0.73
3:b:2:DA:H1'	3:b:3:DC:H5'	1.69	0.73
2:C:6:DG:H2'	2:C:7:DT:H71	1.70	0.73
2:X:11:DA:C2'	2:X:12:DA:H5"	2.18	0.73
3:7:9:DT:C2'	3:7:10:DG:H5"	2.18	0.73
2:a:15:DT:H1'	2:a:16:DT:H5'	1.71	0.73
2:m:1:DT:H2'	2:m:2:DG:C8	2.23	0.73
2:G:15:DT:H1'	2:G:16:DT:H5'	1.69	0.73
3:3:9:DT:C2'	3:3:10:DG:H5"	2.18	0.73
2:a:1:DT:H2'	2:a:2:DG:C8	2.23	0.73
2:a:11:DA:C2'	2:a:12:DA:H5"	2.18	0.72
2:K:11:DA:C2'	2:K:12:DA:H5"	2.18	0.72
2:T:15:DT:H1'	2:T:16:DT:H5'	1.69	0.72
2:G:11:DA:C2'	2:G:12:DA:H5"	2.19	0.72
3:3:8:DG:H1'	3:3:9:DT:H5"	1.72	0.72
2:C:11:DA:C2'	2:C:12:DA:H5"	2.19	0.72
3:U:8:DG:H1'	3:U:9:DT:H5"	1.72	0.72
2:6:11:DA:C2'	2:6:12:DA:H5"	2.19	0.72
2:a:6:DG:H2'	2:a:7:DT:H71	1.70	0.72
3:f:9:DT:C2'	3:f:10:DG:H5"	2.18	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:a:19:DC:H2"	2:a:20:DA:C8	2.25	0.72
2:m:19:DC:H2"	2:m:20:DA:C8	2.25	0.72
2:C:15:DT:H1'	2:C:16:DT:H5'	1.71	0.72
2:i:19:DC:H2"	2:i:20:DA:C8	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:11:DA:C2'	2:m:12:DA:H5"	2.18	0.72
3:j:9:DT:C2'	3:j:10:DG:H5"	2.18	0.72
2:O:19:DC:H5'	2:O:19:DC:H6	1.55	0.72
3:Y:8:DG:H1'	3:Y:9:DT:H5"	1.72	0.72
2:O:19:DC:H2"	2:O:20:DA:C8	2.25	0.71
3:P:9:DT:C2'	3:P:10:DG:H5"	2.18	0.71
2:i:15:DT:H1'	2:i:16:DT:H5'	1.71	0.71
2:O:6:DG:H2'	2:O:7:DT:H71	1.72	0.71
3:P:8:DG:H1'	3:P:9:DT:H5"	1.71	0.71
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:n:8:DG:H1'	3:n:9:DT:H5"	1.72	0.71
3:D:2:DA:H1'	3:D:3:DC:H5'	1.69	0.71
3:H:8:DG:H1'	3:H:9:DT:H5"	1.72	0.71
3:j:8:DG:H1'	3:j:9:DT:H5"	1.72	0.71
2:X:15:DT:H1'	2:X:16:DT:H5'	1.71	0.71
2:K:15:DT:H1'	2:K:16:DT:H5'	1.71	0.71
2:2:6:DG:C2'	2:2:7:DT:H5"	2.20	0.71
2:G:2:DG:H2"	2:G:3:DG:C8	2.26	0.71
2:e:19:DC:H2"	2:e:20:DA:C8	2.25	0.71
3:f:8:DG:H1'	3:f:9:DT:H5"	1.72	0.71
3:L:8:DG:H1'	3:L:9:DT:H5"	1.72	0.71
3:7:2:DA:H1'	3:7:3:DC:H5'	1.70	0.71
3:7:8:DG:H1'	3:7:9:DT:H5"	1.73	0.71
3:b:8:DG:H1'	3:b:9:DT:H5"	1.73	0.71
2:G:19:DC:H2"	2:G:20:DA:C8	2.25	0.71
2:2:15:DT:H1'	2:2:16:DT:H5'	1.72	0.71
2:T:2:DG:H2"	2:T:3:DG:C8	2.26	0.70
2:i:11:DA:C2'	2:i:12:DA:H5"	2.20	0.70
2:T:19:DC:H2"	2:T:20:DA:C8	2.25	0.70
3:D:8:DG:H1'	3:D:9:DT:H5"	1.73	0.70
2:O:6:DG:C2'	2:O:7:DT:H5"	2.20	0.70
2:e:15:DT:H1'	2:e:16:DT:H5'	1.71	0.70
2:m:19:DC:H5'	2:m:19:DC:H6	1.57	0.70
2:2:6:DG:H2'	2:2:7:DT:H71	1.71	0.70
2:X:19:DC:H6	2:X:19:DC:H5'	1.57	0.70
3:L:4:DT:H4'	3:L:5:DT:OP1	1.92	0.70
2:6:19:DC:H2"	2:6:20:DA:C8	2.25	0.69
2:T:19:DC:H6	2:T:19:DC:H5'	1.57	0.69
2:a:6:DG:C2'	2:a:7:DT:H5"	2.22	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
2:a:19:DC:H6	2:a:19:DC:H5'	1.57	0.69
2:i:11:DA:C2	3:j:19:DA:C2	2.81	0.69
3:Y:4:DT:H4'	3:Y:5:DT:OP1	1.92	0.69
2:K:2:DG:H2"	2:K:3:DG:C8	2.28	0.69
3:U:4:DT:H4'	3:U:5:DT:OP1	1.92	0.69
2:e:11:DA:C2'	2:e:12:DA:H5"	2.20	0.69
2:e:2:DG:H2"	2:e:3:DG:C8	2.28	0.69
2:i:2:DG:H2"	2:i: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
3:f:4:DT:H4'	3:f:5:DT:OP1	1.93	0.69
3:j:4:DT:H4'	3:j:5:DT:OP1	1.93	0.69
2:G:6:DG:C2'	2:G:7:DT:H5"	2.23	0.68
2:G:19:DC:H5'	2:G:19:DC:H6	1.57	0.68
2:K:19:DC:H6	2:K:19:DC:H5'	1.57	0.68
2:O:2:DG:H2"	2:O:3:DG:C8	2.28	0.68
2:2:2:DG:H2"	2:2:3:DG:C8	2.29	0.68
2:6:2:DG:H2"	2:6:3:DG:C8	2.28	0.68
2:C:15:DT:H6	2:C:15:DT:H5'	1.58	0.68
2:X:6:DG:C2'	2:X:7:DT:H5"	2.23	0.68
2:6:15:DT:H5'	2:6:15:DT:H6	1.58	0.68
2:m:2:DG:H2"	2:m:3:DG:C8	2.28	0.68
2:C:6:DG:C2'	2:C:7:DT:H5"	2.23	0.68
3:n:4:DT:H4'	3:n:5:DT:OP1	1.93	0.68
2:O:15:DT:H6	2:O:15:DT:H5'	1.59	0.68
3:3:4:DT:H4'	3:3:5:DT:OP1	1.94	0.68
2:a:2:DG:H2"	2:a:3:DG:C8	2.28	0.68
3:H:4:DT:H4'	3:H:5:DT:OP1	1.93	0.68
2:e:6:DG:C2'	2:e:7:DT:H5"	2.23	0.68
2:X:2:DG:H2"	2:X:3:DG:C8	2.28	0.68
3:n:11:DA:C1'	3:n:12:DC:H5"	2.24	0.68
3:b:4:DT:H4'	3:b:5:DT:OP1	1.93	0.67
2:K:6:DG:C2'	2:K:7:DT:H5"	2.23	0.67
3:L:1:DC:H2"	3:L:2:DA:C8	2.29	0.67
3:H:19:DA:H1'	3:H:20:DT:H5"	1.77	0.67
3:P:1:DC:H2"	3:P:2:DA:C8	2.29	0.67
3:P:4:DT:H4'	3:P:5:DT:OP1	1.94	0.67
2:6:19:DC:H6	2:6:19:DC:H5'	1.58	0.67
2:e:19:DC:H5'	2:e:19:DC:H6	1.58	0.67
3:U:7:DT:H2"	3:U:8:DG:H8	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:19:DC:H6	2:i:19:DC:H5'	1.58	0.67
2:C:19:DC:H6	2:C:19:DC:H5'	1.58	0.67
3:b:11:DA:C1'	3:b:12:DC:H5"	2.25	0.67
2:T:6:DG:C2'	2:T:7:DT:H5"	2.23	0.67
2:e:15:DT:H6	2:e:15:DT:H5'	1.59	0.67
3:H:1:DC:H2"	3:H:2:DA:C8	2.30	0.67
3:D:1:DC:H2"	3:D:2:DA:C8	2.30	0.67
3:7:1:DC:H2"	3:7:2:DA:C8	2.30	0.67
3:7:4:DT:H4'	3:7:5:DT:OP1	1.94	0.67
3:D:4:DT:H4'	3:D:5:DT:OP1	1.94	0.67
3:Y:1:DC:H2"	3:Y:2:DA:C8	2.28	0.67
2:i:6:DG:C2'	2:i:7:DT:H5"	2.22	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
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
2:a:15:DT:H5'	2:a:15:DT:H6	1.59	0.66
3:n:1:DC:H2"	3:n:2:DA:C8	2.30	0.66
3:H:11:DA:C1'	3:H:12:DC:H5"	2.25	0.66
2:m:6:DG:C2'	2:m:7:DT:H5"	2.23	0.66
3:n:7:DT:H2"	3:n:8:DG:H8	1.60	0.66
3:U:1:DC:H2"	3:U:2:DA:C8	2.30	0.66
3:b:1:DC:H2"	3:b:2:DA:C8	2.29	0.66
3:b:2:DA:H1'	3:b:3:DC:C5'	2.26	0.66
2:i:15:DT:H5'	2:i:15:DT:H6	1.59	0.66
3:n:2:DA:H1'	3:n:3:DC:C5'	2.26	0.66
3:D:11:DA:C1'	3:D:12:DC:H5"	2.26	0.66
3:L:19:DA:H1'	3:L:20:DT:H5"	1.78	0.66
3:7:11:DA:C1'	3:7:12:DC:H5"	2.26	0.66
3:U:11:DA:C1'	3:U:12:DC:H5"	2.26	0.66
3:f:7:DT:H2"	3:f:8:DG:H8	1.61	0.66
3:U:22:DA:H1'	3:U:23:DC:H5"	1.78	0.66
2:m:15:DT:H6	2:m:15:DT:H5'	1.59	0.66
2:6:11:DA:C2	3:7:19:DA:C2	2.84	0.65
2:G:15:DT:H6	2:G:15:DT:H5'	1.61	0.65
2:T:15:DT:H5'	2:T:15:DT:H6	1.61	0.65
3:f:1:DC:H2"	3:f:2:DA:C8	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:2:DA:H1'	3:H:3:DC:C5'	2.26	0.65
3:L:2:DA:H1'	3:L:3:DC:C5'	2.25	0.65
3:P:22:DA:H1'	3:P:23:DC:H5"	1.79	0.65
3:U:2:DA:H1'	3:U:3:DC:C5'	2.26	0.65
3:3:11:DA:C1'	3:3:12:DC:H5"	2.25	0.65
3:3:11:DA:H2"	3:3:12:DC:H5'	1.78	0.65
3:D:7:DT:H2"	3:D:8:DG:H8	1.61	0.65
2:X:15:DT:H6	2:X:15:DT:H5'	1.61	0.65
2:2:1:DT:H3'	2:2:2:DG:H5"	1.79	0.65
3:3:19:DA:H1'	3:3:20:DT:H5"	1.78	0.65
3:f:19:DA:H1'	3:f:20:DT:H5"	1.79	0.65
3:j:7:DT:H2"	3:j:8:DG:H8	1.61	0.65
3:n:22:DA:H1'	3:n:23:DC:H5"	1.77	0.65
3:b:7:DT:H2"	3:b:8:DG:H8	1.61	0.65
3:j:2:DA:H1'	3:j:3:DC:C5'	2.27	0.65
3:f:2:DA:H1'	3:f:3:DC:C5'	2.27	0.65
3:j:1:DC:H2"	3:j:2:DA:C8	2.31	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:n:11:DA:H2"	3:n:12:DC:H5'	1.79	0.65
2:K:15:DT:H6	2:K:15:DT:H5'	1.61	0.64
3:7:7:DT:H2"	3:7:8:DG:H8	1.61	0.64
3:f:11:DA:C1'	3:f:12:DC:H5"	2.27	0.64
2:C:1:DT:H3'	2:C:2:DG:H5"	1.80	0.64
3:L:7:DT:H2"	3:L:8:DG:H8	1.62	0.64
3:7:2:DA:H1'	3:7:3:DC:C5'	2.27	0.64
3:Y:19:DA:H1'	3:Y:20:DT:H5"	1.78	0.64
3:3:22:DA:H1'	3:3:23:DC:H5"	1.79	0.64
3:n:19:DA:H1'	3:n:20:DT:H5"	1.79	0.64
3:H:22:DA:H1'	3:H:23:DC:H5"	1.79	0.64
2:T:2:DG:OP1	2:T:2:DG:C4'	2.46	0.64
3:U:8:DG:C1'	3:U:9:DT:H5"	2.28	0.64
3:Y:7:DT:H2"	3:Y:8:DG:H8	1.62	0.64
2:6:1:DT:H3'	2:6:2:DG:H5"	1.80	0.64
3:7:22:DA:H1'	3:7:23:DC:H5"	1.79	0.64
3:P:7:DT:H2"	3:P:8:DG:H8	1.62	0.64
2:i:24:DA:C4'	2:i:25:DA:OP1	2.44	0.64
3:D:22:DA:H1'	3:D:23:DC:H5"	1.79	0.64
3:P:19:DA:H1'	3:P:20:DT:H5"	1.78	0.64
3:b:22:DA:H1'	3:b:23:DC:H5"	1.78	0.64
3:L:22:DA:H1'	3:L:23:DC:H5"	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:11:DA:H2"	3:P:12:DC:H5'	1.78	0.64
3:n:10:DG:H1'	3:n:11:DA:H5'	1.80	0.64
2:O:1:DT:H3'	2:O:2:DG:H5"	1.79	0.63
3:b:11:DA:H2"	3:b:12:DC:H5'	1.80	0.63
3:H:11:DA:H2"	3:H:12:DC:H5'	1.80	0.63
3:U:11:DA:H2"	3:U:12:DC:H5'	1.80	0.63
3:j:19:DA:H1'	3:j:20:DT:H5"	1.79	0.63
2:O:2:DG:OP1	2:O:2:DG:C4'	2.46	0.63
2:X:8:DC:H5'	2:X:8:DC:H6	1.64	0.63
3:b:19:DA:H1'	3:b:20:DT:H5"	1.79	0.63
2:G:2:DG:OP1	2:G:2:DG:C4'	2.46	0.63
3:Y:22:DA:H1'	3:Y:23:DC:H5"	1.80	0.63
2:2:2:DG:OP1	2:2:2:DG:C4'	2.46	0.63
3:7:19:DA:H1'	3:7:20:DT:H5"	1.80	0.63
3:b:10:DG:H1'	3:b:11:DA:H5'	1.80	0.63
3:H:16:DT:H6	3:H:16:DT:H5'	1.63	0.63
3:L:11:DA:C1'	3:L:12:DC:H5"	2.27	0.63
3:Y:24:DA:H2"	3:Y:25:DG:OP2	1.99	0.63
3:f:11:DA:H2"	3:f:12:DC:H5'	1.81	0.63
3:D:19:DA:H1'	3:D:20:DT:H5"	1.80	0.63
2:K:11:DA:C2	3:L:19:DA:C2	2.87	0.63
2:C:2:DG:OP1	2:C:2:DG:C4'	2.46	0.63
3:H:8:DG:C1'	3:H:9:DT:H5"	2.28	0.63
2:2:24:DA:C4'	2:2:25:DA:OP1	2.45	0.63
2:i:10:DT:H2"	2:i:11:DA:OP2	1.98	0.63
3:j:11:DA:H2"	3:j:12:DC:H5'	1.80	0.63
2:K:2:DG:OP1	2:K:2:DG:C4'	2.47	0.63
2:X:10:DT:H2"	2:X:11:DA:OP2	1.99	0.63
3:Y:11:DA:C1'	3:Y:12:DC:H5"	2.27	0.63
2:2:5:DT:H2"	2:2:6:DG:C8	2.34	0.63
3:3:7:DT:H2"	3:3:8:DG:H8	1.63	0.63
3:3:17:DT:H1'	3:3:18:DT:H5"	1.81	0.63
2:m:1:DT:H3'	2:m:2:DG:H5"	1.80	0.63
2:K:8:DC:H5'	2:K:8:DC:H6	1.64	0.62
3:U:16:DT:H6	3:U:16:DT:H5'	1.63	0.62
3:Y:8:DG:C1'	3:Y:9:DT:H5"	2.29	0.62
3:Y:11:DA:H2"	3:Y:12:DC:H5'	1.80	0.62
2:6:2:DG:OP1	2:6:2:DG:C4'	2.46	0.62
2:e:2:DG:OP1	2:e:2:DG:C4'	2.46	0.62
2:e:24:DA:C4'	2:e:25:DA:OP1	2.44	0.62
3:L:11:DA:H2"	3:L:12:DC:H5'	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:10:DG:H1'	3:U:11:DA:H5'	1.80	0.62
2:a:1:DT:H3'	2:a:2:DG:H5"	1.80	0.62
3:L:24:DA:H2"	3:L:25:DG:OP2	1.99	0.62
3:P:17:DT:H1'	3:P:18:DT:H5"	1.81	0.62
3:U:9:DT:H2"	3:U:10:DG:C5'	2.27	0.62
2:X:2:DG:OP1	2:X:2:DG:C4'	2.47	0.62
2:i:2:DG:OP1	2:i:2:DG:C4'	2.46	0.62
3:n:8:DG:C1'	3:n:9:DT:H5"	2.29	0.62
3:H:10:DG:H1'	3:H:11:DA:H5'	1.80	0.62
2:a:10:DT:H2"	2:a:11:DA:OP2	2.00	0.62
3:f:22:DA:H1'	3:f:23:DC:H5"	1.80	0.62
2:T:9:DA:H1'	2:T:10:DT:H5'	1.82	0.62
3:j:8:DG:C1'	3:j:9:DT:H5"	2.29	0.62
2:T:1:DT:H3'	2:T:2:DG:H5"	1.81	0.62
3:b:8:DG:C1'	3:b:9:DT:H5"	2.30	0.62
3:D:10:DG:H1'	3:D:11:DA:H5'	1.80	0.62
2:G:8:DC:H5'	2:G:8:DC:H6	1.65	0.62
3:f:10:DG:H1'	3:f:11:DA:H5'	1.82	0.62
2:i:5:DT:H2"	2:i:6:DG:C8	2.35	0.62
2:G:9:DA:H1'	2:G:10:DT:H5'	1.82	0.62
2:X:1:DT:H3'	2:X:2:DG:H5"	1.81	0.62
2:e:5:DT:H2"	2:e:6:DG:C8	2.34	0.62
3:L:16:DT:H5'	3:L:16:DT:H6	1.65	0.62
2:O:5:DT:H2"	2:O:6:DG:C8	2.34	0.62
3:P:8:DG:C1'	3:P:9:DT:H5"	2.29	0.62
3:Y:14:DA:C3'	3:Y:15:DC:H5"	2.29	0.62
3:3:8:DG:C1'	3:3:9:DT:H5"	2.29	0.62
3:j:10:DG:H1'	3:j:11:DA:H5'	1.81	0.62
2:K:1:DT:H3'	2:K:2:DG:H5"	1.81	0.61
2:2:5:DT:H5'	2:2:5:DT:C6	2.34	0.61
3:7:10:DG:H1'	3:7:11:DA:H5'	1.81	0.61
3:j:11:DA:C1'	3:j:12:DC:H5"	2.27	0.61
2:m:8:DC:H5'	2:m:8:DC:H6	1.65	0.61
2:e:1:DT:H3'	2:e:2:DG:H5"	1.81	0.61
2:e:11:DA:C2	3:f:19:DA:C2	2.88	0.61
2:i:1:DT:H3'	2:i:2:DG:H5"	1.81	0.61
3:P:4:DT:H2"	3:P:5:DT:C7	2.30	0.61
3:Y:10:DG:H1'	3:Y:11:DA:H5'	1.82	0.61
2:2:8:DC:H5'	2:2:8:DC:H6	1.64	0.61
2:m:10:DT:H2"	2:m:11:DA:OP2	2.00	0.61
3:L:8:DG:C1'	3:L:9:DT:H5"	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:8:DC:H5'	2:T:8:DC:H6	1.65	0.61
3:Y:16:DT:H6	3:Y:16:DT:H5'	1.65	0.61
2:6:5:DT:H2"	2:6:6:DG:C8	2.35	0.61
2:6:24:DA:C4'	2:6:25:DA:OP1	2.44	0.61
2:a:8:DC:H5'	2:a:8:DC:H6	1.65	0.61
3:f:8:DG:C1'	3:f:9:DT:H5"	2.29	0.61
2:m:1:DT:H3'	2:m:2:DG:C5'	2.30	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
2:a:1:DT:H3'	2:a:2:DG:C5'	2.31	0.61
3:f:4:DT:H2"	3:f:5:DT:C7	2.30	0.61
2:m:2:DG:OP1	2:m:2:DG:C4'	2.47	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
2:a:9:DA:H1'	2:a:10:DT:H5'	1.82	0.61
2:e:10:DT:H2"	2:e:11:DA:OP2	1.99	0.61
3:D:11:DA:H2"	3:D:12:DC:H5'	1.80	0.61
3:L:4:DT:H2"	3:L:5:DT:C7	2.31	0.61
3:3:4:DT:H2"	3:3:5:DT:C7	2.30	0.61
3:b:16:DT:H5'	3:b:16:DT:H6	1.66	0.61
3:j:16:DT:H5'	3:j:16:DT:H6	1.65	0.61
3:j:22:DA:H1'	3:j:23:DC:H5"	1.80	0.61
2:K:10:DT:H2"	2:K:11:DA:OP2	1.99	0.61
2:O:8:DC:H5'	2:O:8:DC:H6	1.65	0.61
2:O:19:DC:H5'	2:O:19:DC:C6	2.36	0.61
2:T:10:DT:H2"	2:T:11:DA:OP2	2.00	0.61
2:X:1:DT:H3'	2:X:2:DG:C5'	2.31	0.61
3:7:4:DT:H2"	3:7:5:DT:C7	2.31	0.61
2:a:2:DG:OP1	2:a:2:DG:C4'	2.47	0.61
3:f:17:DT:H1'	3:f:18:DT:H5"	1.83	0.61
2:m:9:DA:H1'	2:m:10:DT:H5'	1.82	0.61
3:n:11:DA:C2'	3:n:12:DC:H5"	2.31	0.61
2:C:5:DT:H2"	2:C:6:DG:C8	2.35	0.60
3:H:7:DT:H2"	3:H:8:DG:C8	2.36	0.60
3:L:10:DG:H1'	3:L:11:DA:H5'	1.82	0.60
2:2:19:DC:H5'	2:2:19:DC:C6	2.36	0.60
3:3:24:DA:H2"	3:3:25:DG:OP2	2.01	0.60
3:7:17:DT:H1'	3:7:18:DT:H5"	1.82	0.60
3:n:7:DT:H2"	3:n:8:DG:C8	2.36	0.60
3:n:16:DT:H6	3:n:16:DT:H5'	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:10:DT:H2"	2:C:11:DA:OP2	1.99	0.60
2:C:24:DA:C4'	2:C:25:DA:OP1	2.44	0.60
2:K:7:DT:H2"	2:K:8:DC:H6	1.66	0.60
3:P:16:DT:H6	3:P:16:DT:H5'	1.66	0.60
2:6:9:DA:H1'	2:6:10:DT:H5'	1.83	0.60
3:b:9:DT:H2"	3:b:10:DG:C8	2.36	0.60
3:j:5:DT:C1'	3:j:6:DT:H5"	2.29	0.60
2:C:9:DA:H1'	2:C:10:DT:H5'	1.83	0.60
2:T:4:DC:H1'	2:T:5:DT:H5"	1.83	0.60
2:X:5:DT:H2"	2:X:6:DG:C8	2.36	0.60
2:2:1:DT:H3'	2:2:2:DG:C5'	2.30	0.60
2:a:5:DT:H2"	2:a:6:DG:C8	2.36	0.60
3:n:9:DT:H2"	3:n:10:DG:C8	2.36	0.60
3:D:8:DG:C1'	3:D:9:DT:H5"	2.30	0.60
3:D:17:DT:H1'	3:D:18:DT:H5"	1.82	0.60
3:H:4:DT:H2"	3:H:5:DT:C7	2.31	0.60
3:P:9:DT:H2"	3:P:10:DG:C8	2.37	0.60
3:U:4:DT:H2"	3:U:5:DT:C7	2.31	0.60
3:3:10:DG:H1'	3:3:11:DA:H5'	1.83	0.60
3:7:8:DG:C1'	3:7:9:DT:H5"	2.30	0.60
3:b:11:DA:C2'	3:b:12:DC:H5"	2.31	0.60
3:j:17:DT:H1'	3:j:18:DT:H5"	1.82	0.60
2:C:1:DT:H3'	2:C:2:DG:C5'	2.31	0.60
3:D:4:DT:H2"	3:D:5:DT:C7	2.31	0.60
3:U:7:DT:H2"	3:U:8:DG:C8	2.36	0.60
2:X:7:DT:H2"	2:X:8:DC:H6	1.66	0.60
2:T:7:DT:H2"	2:T:8:DC:H6	1.67	0.60
3:U:9:DT:H2"	3:U:10:DG:C8	2.37	0.60
3:3:16:DT:H6	3:3:16:DT:H5'	1.66	0.60
2:6:10:DT:H2"	2:6:11:DA:OP2	1.99	0.60
2:a:5:DT:H5'	2:a:5:DT:C6	2.33	0.60
3:j:4:DT:H2"	3:j:5:DT:C7	2.30	0.60
2:m:5:DT:H2"	2:m:6:DG:C8	2.37	0.60
3:H:17:DT:H1'	3:H:18:DT:H5"	1.84	0.60
3:P:11:DA:C2'	3:P:12:DC:H5"	2.31	0.60
3:b:7:DT:H2"	3:b:8:DG:C8	2.37	0.60
2:e:8:DC:H5'	2:e:8:DC:H6	1.66	0.60
2:i:8:DC:H5'	2:i:8:DC:H6	1.67	0.60
2:m:13:DA:C1'	2:m:14:DG:H5'	2.30	0.60
3:n:24:DA:H2"	3:n:25:DG:OP2	2.00	0.60
3:H:9:DT:H2"	3:H:10:DG:C5'	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:i:5:DT:H5'	2:i:5:DT:C6	2.34	0.60
2:G:10:DT:H2"	2:G:11:DA:OP2	2.00	0.60
3:H:24:DA:H2"	3:H:25:DG:OP2	2.01	0.60
2:O:23:DA:C4'	2:O:24:DA:OP1	2.46	0.60
3:P:10:DG:H1'	3:P:11:DA:H5'	1.83	0.60
2:X:19:DC:H5'	2:X:19:DC:C6	2.37	0.60
2:m:5:DT:H5'	2:m:5:DT:C6	2.33	0.60
2:C:5:DT:H5'	2:C:5:DT:C6	2.33	0.60
2:T:11:DA:C2	3:U:19:DA:C2	2.90	0.60
3:D:16:DT:H5'	3:D:16:DT:H6	1.66	0.59
2:2:12:DA:H1'	2:2:13:DA:H5"	1.84	0.59
2:a:18:DT:H2"	2:a:19:DC:H5'	1.84	0.59
2:G:7:DT:H2"	2:G:8:DC:H6	1.67	0.59
3:H:11:DA:C2'	3:H:12:DC:H5"	2.32	0.59
2:K:5:DT:H2"	2:K:6:DG:C8	2.37	0.59
3:L:17:DT:H1'	3:L:18:DT:H5"	1.84	0.59
2:O:10:DT:H2"	2:O:11:DA:OP2	2.02	0.59
2:6:8:DC:H5'	2:6:8:DC:H6	1.67	0.59
2:6:18:DT:H2"	2:6:19:DC:H5'	1.84	0.59
3:7:16:DT:H6	3:7:16:DT:H5'	1.66	0.59
3:b:24:DA:H2"	3:b:25:DG:OP2	2.01	0.59
3:f:5:DT:C1'	3:f:6:DT:H5"	2.29	0.59
3:f:16:DT:H6	3:f:16:DT:H5'	1.65	0.59
2:G:1:DT:H3'	2:G:2:DG:C5'	2.32	0.59
2:e:9:DA:H1'	2:e:10:DT:H5'	1.83	0.59
2:C:18:DT:H2"	2:C:19:DC:H5'	1.84	0.59
2:K:1:DT:H3'	2:K:2:DG:C5'	2.31	0.59
3:P:24:DA:H2"	3:P:25:DG:OP2	2.01	0.59
3:Y:9:DT:H2"	3:Y:10:DG:C8	2.37	0.59
3:b:5:DT:C1'	3:b:6:DT:H5"	2.31	0.59
2:e:5:DT:H5'	2:e:5:DT:C6	2.34	0.59
2:i:7:DT:H2"	2:i:8:DC:H6	1.67	0.59
3:P:14:DA:C3'	3:P:15:DC:H5"	2.29	0.59
3:3:9:DT:H2"	3:3:10:DG:C8	2.36	0.59
2:6:5:DT:H5'	2:6:5:DT:C6	2.33	0.59
3:b:4:DT:H2"	3:b:5:DT:C7	2.32	0.59
3:b:17:DT:H1'	3:b:18:DT:H5"	1.83	0.59
2:e:7:DT:H2"	2:e:8:DC:H6	1.67	0.59
2:C:8:DC:H5'	2:C:8:DC:H6	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:11:DA:C2'	3:D:12:DC:H5"	2.32	0.59
3:H:9:DT:H2"	3:H:10:DG:C8	2.37	0.59
3:L:9:DT:H2"	3:L:10:DG:C8	2.38	0.59
2:2:10:DT:H2"	2:2:11:DA:OP2	2.01	0.59
3:7:24:DA:H2"	3:7:25:DG:OP2	2.01	0.59
3:D:9:DT:H2"	3:D:10:DG:C8	2.37	0.59
2:K:9:DA:H1'	2:K:10:DT:H5'	1.84	0.59
3:L:11:DA:C2'	3:L:12:DC:H5"	2.32	0.59
2:O:12:DA:H1'	2:O:13:DA:H5"	1.85	0.59
3:U:17:DT:H1'	3:U:18:DT:H5"	1.84	0.59
3:7:9:DT:H2"	3:7:10:DG:C8	2.37	0.59
3:7:11:DA:C2'	3:7:12:DC:H5"	2.33	0.59
2:C:13:DA:C1'	2:C:14:DG:H5'	2.31	0.59
3:D:24:DA:H2"	3:D:25:DG:OP2	2.01	0.59
3:H:5:DT:C1'	3:H:6:DT:H5"	2.32	0.59
2:K:19:DC:H5'	2:K:19:DC:C6	2.37	0.59
3:L:5:DT:H1'	3:L:6:DT:C5'	2.31	0.59
2:X:9:DA:H1'	2:X:10:DT:H5'	1.84	0.59
3:f:24:DA:H2"	3:f:25:DG:OP2	2.01	0.59
2:m:4:DC:H1'	2:m:5:DT:H5"	1.85	0.59
3:n:4:DT:H2"	3:n:5:DT:C7	2.32	0.59
2:e:1:DT:H3'	2:e:2:DG:C5'	2.32	0.59
2:i:9:DA:H1'	2:i:10:DT:H5'	1.83	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
3:b:9:DT:H2"	3:b:10:DG:C5'	2.29	0.59
3:f:9:DT:H2"	3:f:10:DG:C8	2.38	0.59
2:m:18:DT:H2"	2:m:19:DC:H5'	1.85	0.59
2:G:5:DT:H2"	2:G:6:DG:C8	2.38	0.58
2:a:13:DA:C1'	2:a:14:DG:H5'	2.30	0.58
3:j:24:DA:H2"	3:j:25:DG:OP2	2.01	0.58
2:G:4:DC:H1'	2:G:5:DT:H5"	1.84	0.58
3:L:9:DT:H2"	3:L:10:DG:C5'	2.28	0.58
2:a:4:DC:H1'	2:a:5:DT:H5"	1.86	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
2:a:24:DA:C4'	2:a:25:DA:OP1	2.44	0.58
3:b:11:DA:C2'	3:b:12:DC:C5'	2.81	0.58
3:L:7:DT:H2"	3:L:8:DG:C8	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:11:DA:C2'	3:3:12:DC:C5'	2.80	0.58
2:a:19:DC:H5'	2:a:19:DC:C6	2.37	0.58
2:i:1:DT:H3'	2:i:2:DG:C5'	2.32	0.58
3:D:14:DA:C3'	3:D:15:DC:H5"	2.28	0.58
3:P:11:DA:C2'	3:P:12:DC:C5'	2.81	0.58
3:Y:4:DT:H2"	3:Y:5:DT:C7	2.31	0.58
3:Y:7:DT:H2"	3:Y:8:DG:C8	2.39	0.58
2:2:4:DC:H1'	2:2:5:DT:H5"	1.86	0.58
2:a:12:DA:H1'	2:a:13:DA:H5"	1.85	0.58
2:i:18:DT:H2"	2:i:19:DC:H5'	1.85	0.58
3:j:9:DT:H2"	3:j:10:DG:C8	2.38	0.58
3:n:17:DT:H1'	3:n:18:DT:H5"	1.83	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
3:f:11:DA:C2'	3:f:12:DC:H5"	2.33	0.58
2:m:12:DA:H1'	2:m:13:DA:H5"	1.85	0.58
3:n:5:DT:H1'	3:n:6:DT:C5'	2.32	0.58
3:n:9:DT:H2"	3:n:10:DG:C5'	2.29	0.58
2:O:9:DA:H1'	2:O:10:DT:H5'	1.85	0.58
2:e:4:DC:H1'	2:e:5:DT:H5"	1.86	0.58
2:C:7:DT:H2"	2:C:8:DC:H6	1.67	0.58
2:O:4:DC:H1'	2:O:5:DT:H5"	1.86	0.58
3:Y:17:DT:H1'	3:Y:18:DT:H5"	1.84	0.58
2:6:4:DC:H1'	2:6:5:DT:H5"	1.86	0.58
2:a:7:DT:H2"	2:a:8:DC:H6	1.67	0.58
3:b:5:DT:H1'	3:b:6:DT:C5'	2.32	0.58
3:f:5:DT:H1'	3:f:6:DT:C5'	2.30	0.58
3:j:5:DT:H1'	3:j:6:DT:C5'	2.30	0.58
3:j:11:DA:C2'	3:j:12:DC:H5"	2.33	0.58
3:D:11:DA:C2'	3:D:12:DC:C5'	2.82	0.58
3:L:24:DA:H1'	3:L:25:DG:O5'	2.03	0.58
2:O:13:DA:C1'	2:O:14:DG:H5'	2.32	0.58
2:6:7:DT:H2"	2:6:8:DC:H6	1.67	0.58
3:7:11:DA:C2'	3:7:12:DC:C5'	2.82	0.58
3:f:7:DT:H2"	3:f:8:DG:C8	2.38	0.58
3:n:11:DA:C2'	3:n:12:DC:C5'	2.81	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
3:j:7:DT:H2"	3:j:8:DG:C8	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:7:DT:H2”	2:m:8:DC:H6	1.68	0.57
2:C:4:DC:H1’	2:C:5:DT:H5”	1.86	0.57
2:K:23:DA:C4’	2:K:24:DA:OP1	2.48	0.57
2:i:4:DC:H1’	2:i: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
2:2:17:DG:H2”	2:2:18:DT:C5’	2.35	0.57
3:3:7:DT:H2”	3:3:8:DG:C8	2.39	0.57
3:D:5:DT:H1’	3:D:6:DT:C5’	2.30	0.57
2:K:4:DC:H1’	2:K:5:DT:H5”	1.87	0.57
2:T:18:DT:H2”	2:T:19:DC:H5’	1.87	0.57
3:Y:11:DA:C2’	3:Y:12:DC:C5’	2.82	0.57
3:Y:24:DA:H1’	3:Y:25:DG:O5’	2.04	0.57
3:7:7:DT:H2”	3:7:8:DG:C8	2.38	0.57
2:i:17:DG:H2”	2:i:18:DT:C5’	2.35	0.57
2:m:19:DC:H5’	2:m:19:DC:C6	2.37	0.57
3:n:5:DT:C1’	3:n:6:DT:H5”	2.31	0.57
2:G:12:DA:H1’	2:G:13:DA:H5”	1.86	0.57
2:O:18:DT:H2”	2:O:19:DC:H5’	1.86	0.57
2:T:13:DA:C1’	2:T:14:DG:H5’	2.31	0.57
2:T:19:DC:H5’	2:T:19:DC:C6	2.37	0.57
2:X:12:DA:H1’	2:X:13:DA:H5”	1.86	0.57
2:2:9:DA:H1’	2:2:10:DT:H5’	1.85	0.57
2:2:18:DT:H2”	2:2:19:DC:H5’	1.86	0.57
3:7:5:DT:H1’	3:7:6:DT:C5’	2.31	0.57
2:i:19:DC:H5’	2:i:19:DC:C6	2.38	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
2:e:17:DG:H2”	2:e:18:DT:C5’	2.35	0.57
2:C:17:DG:H2”	2:C:18:DT:C5’	2.35	0.57
3:H:10:DG:H2”	3:H:11:DA:O5’	2.05	0.57
2:O:7:DT:H2”	2:O:8:DC:H6	1.70	0.57
2:6:17:DG:H2”	2:6:18:DT:C5’	2.35	0.57
2:e:18:DT:H2”	2:e:19:DC:H5’	1.85	0.57
3:f:24:DA:H1’	3:f:25:DG:O5’	2.05	0.57
2:G:19:DC:H5’	2:G:19:DC:C6	2.38	0.57
2:K:24:DA:C4’	2:K:25:DA:OP1	2.46	0.57
2:e:13:DA:C1’	2:e:14:DG:H5’	2.32	0.57
2:G:18:DT:H2”	2:G:19:DC:H5’	1.86	0.57
2:T:5:DT:H5’	2:T:5:DT:C6	2.35	0.57
3:Y:5:DT:C1’	3:Y:6:DT:H5”	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:19:DC:H5'	2:6:19:DC:C6	2.38	0.57
2:i:12:DA:H1'	2:i:13:DA:H5"	1.87	0.56
3:j:24:DA:H1'	3:j:25:DG:O5'	2.05	0.56
2:O:17:DG:H2"	2:O:18:DT:C5'	2.35	0.56
2:X:2:DG:H5"	2:X:2:DG:H8	1.70	0.56
2:2:13:DA:C1'	2:2:14:DG:H5'	2.32	0.56
3:b:10:DG:H2"	3:b:11:DA:O5'	2.04	0.56
2:e:19:DC:H5'	2:e:19:DC:C6	2.39	0.56
2:m:24:DA:C4'	2:m:25:DA:OP1	2.44	0.56
2:C:19:DC:H5'	2:C:19:DC:C6	2.38	0.56
2:X:5:DT:H5'	2:X:5:DT:C6	2.36	0.56
2:X:18:DT:H2"	2:X:19:DC:H5'	1.87	0.56
3:Y:4:DT:C2'	3:Y:5:DT:H72	2.35	0.56
3:3:4:DT:C2'	3:3:5:DT:H72	2.34	0.56
2:a:17:DG:H2"	2:a:18:DT:C5'	2.35	0.56
2:a:23:DA:C4'	2:a:24:DA:OP1	2.46	0.56
2:m:17:DG:H2"	2:m:18:DT:C5'	2.36	0.56
3:P:7:DT:H2"	3:P:8:DG:C8	2.39	0.56
2:T:2:DG:H5"	2:T:2:DG:H8	1.71	0.56
3:n:4:DT:C2'	3:n:5:DT:H72	2.35	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:n:10:DG:H2"	3:n:11:DA:O5'	2.04	0.56
3:D:24:DA:H1'	3:D:25:DG:O5'	2.05	0.56
3:H:15:DC:H2'	3:H:16:DT:H72	1.88	0.56
3:P:5:DT:C1'	3:P:6:DT:H5"	2.31	0.56
2:e:12:DA:H1'	2:e:13:DA:H5"	1.87	0.56
3:f:11:DA:C2'	3:f:12:DC:C5'	2.83	0.56
3:f:14:DA:C3'	3:f:15:DC:H5"	2.27	0.56
3:H:24:DA:H1'	3:H:25:DG:O5'	2.06	0.56
3:L:11:DA:C2'	3:L:12:DC:C5'	2.82	0.56
3:7:24:DA:H1'	3:7:25:DG:O5'	2.06	0.56
3:D:10:DG:H2"	3:D:11:DA:O5'	2.04	0.56
2:K:2:DG:H5"	2:K:2:DG:H8	1.70	0.56
3:P:6:DT:H2"	3:P:7:DT:O5'	2.06	0.56
3:U:10:DG:H2"	3:U:11:DA:O5'	2.05	0.56
3:3:24:DA:H1'	3:3:25:DG:O5'	2.06	0.56
3:f:10:DG:H2"	3:f:11:DA:O5'	2.05	0.56
3:j:11:DA:C2'	3:j:12:DC:C5'	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7:10:DG:H2”	3:7:11:DA:O5’	2.04	0.55
2:i:13:DA:C1’	2:i:14:DG:H5’	2.32	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
3:b:4:DT:C2’	3:b:5:DT:H72	2.36	0.55
3:n:24:DA:H1’	3:n:25:DG:O5’	2.06	0.55
2:G:2:DG:H5”	2:G:2:DG:H8	1.71	0.55
2:K:18:DT:H2”	2:K:19:DC:H5’	1.87	0.55
3:P:24:DA:H1’	3:P:25:DG:O5’	2.06	0.55
3:b:24:DA:H1’	3:b:25:DG:O5’	2.06	0.55
3:P:10:DG:H2”	3:P:11:DA:O5’	2.07	0.55
3:U:15:DC:H2’	3:U:16:DT:H72	1.88	0.55
3:j:14:DA:C3’	3:j:15:DC:H5”	2.27	0.55
3:L:10:DG:H2”	3:L:11:DA:O5’	2.06	0.55
2:X:17:DG:H2”	2:X:18:DT:C5’	2.37	0.55
2:T:17:DG:H2”	2:T:18:DT:C5’	2.37	0.55
2:X:11:DA:C2	3:Y:19:DA:C2	2.95	0.55
2:m:23:DA:C4’	2:m:24:DA:OP1	2.46	0.55
2:C:24:DA:H1’	2:C:25:DA:H5’	1.88	0.55
3:U:4:DT:C2’	3:U:5:DT:H72	2.34	0.55
3:3:10:DG:H2”	3:3:11:DA:O5’	2.06	0.55
3:f:4:DT:C2’	3:f:5:DT:H72	2.34	0.55
2:X:8:DC:H2”	2:X:9:DA:C8	2.42	0.55
2:2:7:DT:H2”	2:2:8:DC:H6	1.70	0.55
2:2:17:DG:H1’	2:2:18:DT:H5”	1.89	0.55
3:3:6:DT:H2”	3:3:7:DT:O5’	2.06	0.55
2:a:11:DA:C2	3:b:19:DA:C2	2.95	0.55
2:e:16:DT:H2”	2:e:17:DG:C8	2.42	0.55
2:i:16:DT:H2”	2:i:17:DG:C8	2.42	0.55
2:K:5:DT:H5’	2:K:5:DT:C6	2.36	0.54
2:K:8:DC:H2”	2:K:9:DA:C8	2.42	0.54
3:j:9:DT:H2”	3:j:10:DG:C5’	2.29	0.54
2:K:17:DG:H2”	2:K:18:DT:C5’	2.37	0.54
2:6:24:DA:H1’	2:6:25:DA:H5’	1.88	0.54
3:f:9:DT:H2”	3:f:10:DG:C5’	2.29	0.54
2:i:17:DG:H1’	2:i:18:DT:H5”	1.90	0.54
3:Y:9:DT:H2”	3:Y:10:DG:C5’	2.28	0.54
3:7:6:DT:H2”	3:7:7:DT:O5’	2.07	0.54
3:j:15:DC:H2’	3:j:16:DT:H72	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:n:6:DT:H2”	3:n:7:DT:O5’	2.07	0.54
3:n:15:DC:H2”	3:n:16:DT:H5”	1.90	0.54
3:D:6:DT:H2”	3:D:7:DT:O5’	2.07	0.54
2:O:7:DT:C2’	2:O:8:DC:C5’	2.85	0.54
3:P:9:DT:H2”	3:P:10:DG:C5’	2.29	0.54
2:C:23:DA:H1’	2:C:24:DA:H5’	1.90	0.54
3:D:5:DT:C1’	3:D:6:DT:H5”	2.29	0.54
2:O:17:DG:H1’	2:O:18:DT:H5”	1.90	0.54
2:T:24:DA:H1’	2:T:25:DA:H5’	1.89	0.54
3:7:5:DT:C1’	3:7:6:DT:H5”	2.29	0.54
3:b:15:DC:H2”	3:b:16:DT:H5”	1.90	0.54
3:j:4:DT:C2’	3:j:5:DT:H72	2.34	0.54
2:6:23:DA:H1’	2:6:24:DA:H5’	1.90	0.54
2:e:17:DG:H1’	2:e:18:DT:H5”	1.90	0.54
3:f:15:DC:H2’	3:f:16:DT:H72	1.90	0.54
2:C:16:DT:H2”	2:C:17:DG:C8	2.43	0.54
2:G:17:DG:H2”	2:G:18:DT:C5’	2.37	0.54
2:a:24:DA:H1’	2:a:25:DA:H5’	1.88	0.54
3:b:6:DT:H2”	3:b:7:DT:O5’	2.07	0.54
3:j:6:DT:H2”	3:j:7:DT:O5’	2.07	0.54
3:j:10:DG:H2”	3:j:11:DA:O5’	2.05	0.54
2:a:23:DA:H1’	2:a:24:DA:H5’	1.89	0.54
3:H:4:DT:C2’	3:H:5:DT:H72	2.34	0.54
2:6:16:DT:H2”	2:6:17:DG:C8	2.43	0.54
3:D:15:DC:H2’	3:D:16:DT:H72	1.90	0.54
2:2:23:DA:H1’	2:2:24:DA:H5’	1.90	0.54
3:7:4:DT:C2’	3:7:5:DT:H72	2.35	0.54
2:C:2:DG:H5”	2:C:2:DG:H8	1.73	0.53
2:6:2:DG:H5”	2:6:2:DG:H8	1.73	0.53
2:a:2:DG:H5”	2:a:2:DG:H8	1.73	0.53
2:G:5:DT:H5’	2:G:5:DT:C6	2.35	0.53
2:2:2:DG:H5”	2:2:2:DG:H8	1.73	0.53
2:e:24:DA:H1’	2:e:25:DA:H5’	1.90	0.53
3:f:6:DT:H2”	3:f:7:DT:O5’	2.07	0.53
2:i:23:DA:C4’	2:i:24:DA:OP1	2.47	0.53
2:m:24:DA:H1’	2:m:25:DA:H5’	1.89	0.53
3:P:9:DT:H6	3:P:9:DT:H5’	1.74	0.53
2:i:24:DA:H1’	2:i:25:DA:H5’	1.89	0.53
3:n:15:DC:H2’	3:n:16:DT:H72	1.90	0.53
3:D:4:DT:C2’	3:D:5:DT:H72	2.35	0.53
2:G:15:DT:C1’	2:G:16:DT:H5’	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:24:DA:H1'	2:G:25:DA:H5'	1.90	0.53
2:K:17:DG:H1'	2:K:18:DT:H5"	1.91	0.53
3:L:6:DT:H2"	3:L:7:DT:O5'	2.08	0.53
3:Y:10:DG:H2"	3:Y:11:DA:O5'	2.06	0.53
2:2:16:DT:H2"	2:2:17:DG:C8	2.44	0.53
2:6:7:DT:C2'	2:6:8:DC:C5'	2.86	0.53
3:7:15:DC:H2"	3:7:16:DT:H5"	1.90	0.53
3:7:15:DC:H2'	3:7:16:DT:H72	1.91	0.53
2:C:7:DT:C2'	2:C:8:DC:C5'	2.86	0.53
2:K:13:DA:C1'	2:K:14:DG:H5'	2.33	0.53
2:O:8:DC:O2	3:P:21:DG:N2	2.29	0.53
3:3:9:DT:H6	3:3:9:DT:H5'	1.73	0.53
2:6:17:DG:H1'	2:6:18:DT:H5"	1.91	0.53
2:e:2:DG:H5"	2:e:2:DG:H8	1.73	0.53
2:T:15:DT:C1'	2:T:16:DT:H5'	2.37	0.53
2:i:8:DC:H2"	2:i:9:DA:C8	2.44	0.53
3:j:15:DC:H2"	3:j:16:DT:H5"	1.91	0.53
2:m:2:DG:H5"	2:m:2:DG:H8	1.73	0.53
2:K:16:DT:H2"	2:K:17:DG:C8	2.44	0.53
3:P:5:DT:H1'	3:P:6:DT:C5'	2.33	0.53
3:P:18:DT:H1'	3:P:19:DA:H5'	1.90	0.53
3:3:11:DA:H1'	3:3:12:DC:C5'	2.35	0.53
3:3:18:DT:H1'	3:3:19:DA:H5'	1.90	0.53
3:f:15:DC:H2"	3:f:16:DT:H5"	1.91	0.53
3:D:9:DT:H2"	3:D:10:DG:C5'	2.30	0.53
3:D:15:DC:H2"	3:D:16:DT:H5"	1.90	0.53
3:L:12:DC:H2"	3:L:13:DA:C8	2.44	0.53
2:O:2:DG:H5"	2:O:2:DG:H8	1.73	0.53
3:Y:5:DT:H1'	3:Y:6:DT:C5'	2.31	0.53
3:3:5:DT:H1'	3:3:6:DT:C5'	2.32	0.53
2:a:7:DT:C2'	2:a:8:DC:C5'	2.85	0.53
2:i:2:DG:H5"	2:i:2:DG:H8	1.73	0.53
2:m:23:DA:H1'	2:m:24:DA:H5'	1.89	0.53
2:C:17:DG:H1'	2:C:18:DT:H5"	1.91	0.53
3:H:6:DT:H2"	3:H:7:DT:O5'	2.09	0.53
3:L:18:DT:H1'	3:L:19:DA:H5'	1.91	0.53
3:Y:6:DT:H2"	3:Y:7:DT:O5'	2.09	0.53
3:7:9:DT:H2"	3:7:10:DG:C5'	2.30	0.53
2:e:8:DC:H2"	2:e:9:DA:C8	2.44	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)
3:H:15:DC:H2”	3:H:16:DT:H5”	1.91	0.53
3:H:19:DA:H2”	3:H:20:DT:C5’	2.39	0.53
3:U:6:DT:H2”	3:U:7:DT:O5’	2.09	0.53
3:U:15:DC:H2”	3:U:16:DT:H5”	1.91	0.53
2:2:7:DT:C2’	2:2:8:DC:C5’	2.85	0.53
3:3:15:DC:H2’	3:3:16:DT:H72	1.90	0.53
3:b:15:DC:H2’	3:b:16:DT:H72	1.91	0.53
2:O:11:DA:C2	3:P:19:DA:C2	2.97	0.52
3:b:9:DT:C3’	3:b:10:DG:H5”	2.38	0.52
3:b:19:DA:H2”	3:b:20:DT:H5’	1.91	0.52
2:G:17:DG:H1’	2:G:18:DT:H5”	1.91	0.52
3:H:9:DT:C3’	3:H:10:DG:H5”	2.38	0.52
3:L:15:DC:H2’	3:L:16:DT:H72	1.90	0.52
2:X:24:DA:H1’	2:X:25:DA:H5’	1.91	0.52
2:6:23:DA:C4’	2:6:24:DA:OP1	2.46	0.52
2:O:22:DA:H2”	2:O:23:DA:H5’	1.91	0.52
2:O:23:DA:H1’	2:O:24:DA:H5’	1.90	0.52
2:T:17:DG:H1’	2:T:18:DT:H5”	1.91	0.52
2:T:23:DA:H1’	2:T:24:DA:H5’	1.91	0.52
2:T:23:DA:C4’	2:T:24:DA:OP1	2.48	0.52
3:U:5:DT:C1’	3:U:6:DT:H5”	2.32	0.52
3:Y:12:DC:H2”	3:Y:13:DA:C8	2.44	0.52
2:6:8:DC:H2”	2:6:9:DA:C8	2.45	0.52
3:H:18:DT:H1’	3:H:19:DA:H5’	1.91	0.52
2:K:15:DT:C1’	2:K:16:DT:H5’	2.39	0.52
2:T:7:DT:C2’	2:T:8:DC:C5’	2.87	0.52
2:m:7:DT:C2’	2:m:8:DC:C5’	2.86	0.52
2:O:16:DT:H2”	2:O:17:DG:C8	2.44	0.52
2:X:16:DT:H2”	2:X:17:DG:C8	2.44	0.52
2:2:12:DA:C2’	2:2:13:DA:H5”	2.40	0.52
2:a:16:DT:H2”	2:a:17:DG:C8	2.45	0.52
2:m:15:DT:C1’	2:m:16:DT:H5’	2.40	0.52
3:n:19:DA:H2”	3:n:20:DT:H5’	1.91	0.52
2:G:8:DC:H2”	2:G:9:DA:C8	2.45	0.52
3:H:19:DA:H2”	3:H:20:DT:H5’	1.90	0.52
3:P:15:DC:H2’	3:P:16:DT:H72	1.90	0.52
3:H:21:DG:H2”	3:H:22:DA:OP2	2.10	0.52
3:L:15:DC:H2”	3:L:16:DT:H5”	1.92	0.52
2:O:24:DA:H1’	2:O:25:DA:H5’	1.90	0.52
2:T:8:DC:H2”	2:T:9:DA:C8	2.45	0.52
3:Y:14:DA:C1’	3:Y:15:DC:H5”	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:15:DC:H2”	3:Y:16:DT:H5”	1.92	0.52
2:a:17:DG:H1’	2:a:18:DT:H5”	1.92	0.52
3:D:19:DA:H2”	3:D:20:DT:H5’	1.92	0.52
2:G:23:DA:H1’	2:G:24:DA:H5’	1.91	0.52
2:K:24:DA:H1’	2:K:25:DA:H5’	1.91	0.52
3:U:19:DA:H2”	3:U:20:DT:H5’	1.90	0.52
2:m:12:DA:C2’	2:m:13:DA:H5”	2.39	0.52
2:2:7:DT:C2	2:2:8:DC:C5	2.98	0.52
3:b:18:DT:H1’	3:b:19:DA:H5’	1.92	0.52
2:e:22:DA:H2”	2:e:23:DA:H5’	1.92	0.52
3:f:12:DC:H2”	3:f:13:DA:C8	2.45	0.52
3:D:9:DT:C3’	3:D:10:DG:H5”	2.39	0.52
3:U:18:DT:H1’	3:U:19:DA:H5’	1.91	0.52
2:X:7:DT:C2’	2:X:8:DC:C5’	2.88	0.52
2:X:17:DG:H1’	2:X:18:DT:H5”	1.91	0.52
3:Y:15:DC:H2’	3:Y:16:DT:H72	1.90	0.52
2:2:22:DA:H2”	2:2:23:DA:H5’	1.91	0.52
3:7:19:DA:H2”	3:7:20:DT:H5’	1.92	0.52
2:O:24:DA:C4’	2:O:25:DA:OP1	2.45	0.51
3:P:9:DT:C3’	3:P:10:DG:H5”	2.40	0.51
3:P:22:DA:H1’	3:P:23:DC:C5’	2.40	0.51
2:T:3:DG:H2”	2:T:4:DC:C5’	2.38	0.51
2:X:13:DA:C1’	2:X:14:DG:H5’	2.34	0.51
3:3:15:DC:H2”	3:3:16:DT:H5”	1.92	0.51
2:a:15:DT:C1’	2:a:16:DT:H5’	2.40	0.51
2:m:16:DT:H2”	2:m:17:DG:C8	2.45	0.51
3:U:19:DA:H2”	3:U:20:DT:C5’	2.39	0.51
3:U:22:DA:H1’	3:U:23:DC:C5’	2.40	0.51
2:2:8:DC:H2”	2:2:9:DA:C8	2.46	0.51
3:7:9:DT:C3’	3:7:10:DG:H5”	2.39	0.51
3:n:22:DA:H1’	3:n:23:DC:C5’	2.39	0.51
2:G:12:DA:C2’	2:G:13:DA:H5”	2.41	0.51
3:L:22:DA:H1’	3:L:23:DC:C5’	2.41	0.51
3:b:22:DA:H1’	3:b:23:DC:C5’	2.40	0.51
2:e:7:DT:C2	2:e:8:DC:C5	2.98	0.51
3:f:19:DA:H2”	3:f:20:DT:C5’	2.41	0.51
3:j:12:DC:H2”	3:j:13:DA:C8	2.45	0.51
2:C:7:DT:C2	2:C:8:DC:C5	2.99	0.51
2:X:23:DA:C4’	2:X:24:DA:OP1	2.48	0.51
3:Y:18:DT:H1’	3:Y:19:DA:H5’	1.91	0.51
2:6:7:DT:C2	2:6:8:DC:C5	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:18:DT:H1'	3:f:19:DA:H5'	1.93	0.51
3:n:19:DA:H2"	3:n:20:DT:C5'	2.40	0.51
2:C:22:DA:H2"	2:C:23:DA:H5'	1.91	0.51
3:D:11:DA:H1'	3:D:12:DC:C5'	2.35	0.51
3:D:19:DA:H2"	3:D:20:DT:C5'	2.41	0.51
2:G:2:DG:C2'	2:G:3:DG:C8	2.93	0.51
3:U:21:DG:H2"	3:U:22:DA:OP2	2.10	0.51
2:X:7:DT:C2	2:X:8:DC:C5	2.99	0.51
2:2:24:DA:H1'	2:2:25:DA:H5'	1.91	0.51
3:3:9:DT:H2"	3:3:10:DG:C5'	2.29	0.51
2:6:12:DA:C2'	2:6:13:DA:H5"	2.40	0.51
3:7:11:DA:H1'	3:7:12:DC:C5'	2.35	0.51
2:a:12:DA:C2'	2:a:13:DA:H5"	2.39	0.51
2:m:17:DG:H1'	2:m:18:DT:H5"	1.93	0.51
2:C:23:DA:C4'	2:C:24:DA:OP1	2.46	0.51
2:O:12:DA:C2'	2:O:13:DA:H5"	2.40	0.51
2:X:24:DA:C4'	2:X:25:DA:OP1	2.46	0.51
2:2:15:DT:C1'	2:2:16:DT:H5'	2.40	0.51
3:f:19:DA:H2"	3:f:20:DT:H5'	1.92	0.51
2:i:7:DT:C2	2:i:8:DC:C5	2.98	0.51
2:K:7:DT:C2'	2:K:8:DC:C5'	2.88	0.51
3:P:15:DC:H2"	3:P:16:DT:H5"	1.92	0.51
3:U:9:DT:C3'	3:U:10:DG:H5"	2.38	0.51
2:6:22:DA:H2"	2:6:23:DA:H5'	1.91	0.51
3:7:19:DA:H2"	3:7:20:DT:C5'	2.41	0.51
2:a:8:DC:H2"	2:a:9:DA:C8	2.45	0.51
2:i:22:DA:H2"	2:i:23:DA:H5'	1.92	0.51
2:m:25:DA:C2	2:m:26:DG:C4	2.99	0.51
2:K:7:DT:C2	2:K:8:DC:C5	2.99	0.51
3:U:9:DT:H6	3:U:9:DT:H5'	1.76	0.51
3:7:22:DA:H1'	3:7:23:DC:C5'	2.40	0.51
3:b:9:DT:H5'	3:b:9:DT:H6	1.75	0.51
2:i:23:DA:H1'	2:i:24:DA:H5'	1.91	0.51
3:D:22:DA:H1'	3:D:23:DC:C5'	2.40	0.51
2:K:6:DG:H2"	2:K:7:DT:H5'	1.93	0.51
2:O:25:DA:C2	2:O:26:DG:C4	2.99	0.51
3:Y:9:DT:H6	3:Y:9:DT:H5'	1.76	0.51
2:a:22:DA:H2"	2:a:23:DA:H5'	1.92	0.51
2:i:7:DT:C2'	2:i:8:DC:C5'	2.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:16:DT:H2"	2:T:17:DG:C8	2.46	0.51
2:e:23:DA:C4'	2:e:24:DA:OP1	2.47	0.51
3:f:22:DA:H1'	3:f:23:DC:C5'	2.41	0.51
3:j:19:DA:H2"	3:j:20:DT:C5'	2.41	0.51
2:m:22:DA:H2"	2:m:23:DA:H5'	1.92	0.51
3:n:9:DT:H6	3:n:9:DT:H5'	1.75	0.51
3:n:21:DG:H2"	3:n:22:DA:OP2	2.10	0.51
3:D:12:DC:H2"	3:D:13:DA:C8	2.46	0.50
2:G:3:DG:H2"	2:G:4:DC:C5'	2.38	0.50
3:H:22:DA:H1'	3:H:23:DC:C5'	2.40	0.50
2:T:2:DG:C2'	2:T:3:DG:C8	2.93	0.50
2:T:15:DT:H2"	2:T:16:DT:O5'	2.10	0.50
3:U:5:DT:H1'	3:U:6:DT:C5'	2.32	0.50
2:X:23:DA:H1'	2:X:24:DA:H5'	1.93	0.50
2:a:7:DT:C2	2:a:8:DC:C5	3.00	0.50
2:e:23:DA:H1'	2:e:24:DA:H5'	1.91	0.50
3:j:22:DA:H1'	3:j:23:DC:C5'	2.41	0.50
2:m:7:DT:C2	2:m:8:DC:C5	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
2:T:25:DA:C2	2:T:26:DG:C4	2.99	0.50
3:7:12:DC:H2"	3:7:13:DA:C8	2.46	0.50
2:e:15:DT:H2"	2:e:16:DT:O5'	2.12	0.50
3:j:19:DA:H2"	3:j:20:DT:H5'	1.92	0.50
2:m:8:DC:H2"	2:m:9:DA:C8	2.45	0.50
2:m:12:DA:C2'	2:m:13:DA:C5'	2.88	0.50
2:m:15:DT:H2"	2:m:16:DT:O5'	2.11	0.50
3:n:11:DA:H1'	3:n:12:DC:C5'	2.34	0.50
3:n:18:DT:H1'	3:n:19:DA:H5'	1.92	0.50
2:G:7:DT:C2'	2:G:8:DC:C5'	2.87	0.50
2:O:8:DC:H2"	2:O:9:DA:C8	2.46	0.50
2:a:12:DA:C2'	2:a:13:DA:C5'	2.88	0.50
2:a:25:DA:C2	2:a:26:DG:C4	2.99	0.50
3:b:19:DA:H2"	3:b:20:DT:C5'	2.40	0.50
3:b:21:DG:H2"	3:b:22:DA:OP2	2.11	0.50
2:m:11:DA:C2	3:n:19:DA:C2	3.00	0.50
3:H:5:DT:H1'	3:H:6:DT:C5'	2.32	0.50
2:O:6:DG:C2	3:P:24:DA:C2	2.99	0.50
2:2:6:DG:H2"	2:2:7:DT:H5'	1.91	0.50
3:3:12:DC:H2"	3:3:13:DA:C8	2.47	0.50
2:K:25:DA:C2	2:K:26:DG:C4	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:19:DA:H2"	3:L:20:DT:C5'	2.41	0.50
2:O:6:DG:H2"	2:O:7:DT:H5'	1.91	0.50
2:X:15:DT:C1'	2:X:16:DT:H5'	2.39	0.50
3:Y:22:DA:H1'	3:Y:23:DC:C5'	2.41	0.50
3:7:15:DC:H2"	3:7:16:DT:C5'	2.42	0.50
2:a:15:DT:H2"	2:a:16:DT:O5'	2.11	0.50
2:C:15:DT:H2"	2:C:16:DT:O5'	2.12	0.50
3:U:12:DC:H2"	3:U:13:DA:C8	2.47	0.50
3:Y:19:DA:H2"	3:Y:20:DT:H5'	1.92	0.50
3:3:22:DA:H1'	3:3:23:DC:C5'	2.40	0.50
2:6:15:DT:H2"	2:6:16:DT:O5'	2.12	0.50
2:e:7:DT:C2'	2:e:8:DC:C5'	2.86	0.50
2:e:12:DA:C2'	2:e:13:DA:H5"	2.42	0.50
2:i:15:DT:H2"	2:i:16:DT:O5'	2.12	0.50
3:D:15:DC:H2"	3:D:16:DT:C5'	2.42	0.50
2:G:25:DA:C2	2:G:26:DG:C4	2.99	0.50
3:H:9:DT:H6	3:H:9:DT:H5'	1.76	0.50
3:P:12:DC:H2"	3:P:13:DA:C8	2.47	0.50
2:X:25:DA:C2	2:X:26:DG:C4	3.00	0.50
2:6:25:DA:C2	2:6:26:DG:C4	2.99	0.50
3:b:11:DA:H1'	3:b:12:DC:C5'	2.35	0.50
2:e:17:DG:H2"	2:e:18:DT:H5'	1.94	0.50
2:i:17:DG:H2"	2:i:18:DT:H5'	1.94	0.50
2:C:25:DA:C2	2:C:26:DG:C4	2.99	0.50
2:K:15:DT:H2"	2:K:16:DT:O5'	2.11	0.50
3:L:19:DA:H2"	3:L:20:DT:H5'	1.92	0.50
2:O:12:DA:H2"	2:O:13:DA:H5"	1.93	0.50
2:T:12:DA:C2'	2:T:13:DA:H5"	2.41	0.50
3:Y:19:DA:H2"	3:Y:20:DT:C5'	2.41	0.50
2:2:23:DA:C4'	2:2:24:DA:OP1	2.46	0.50
3:7:18:DT:H1'	3:7:19:DA:H5'	1.93	0.50
2:e:25:DA:C2	2:e:26:DG:C4	3.00	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
3:j:18:DT:H1'	3:j:19:DA:H5'	1.93	0.50
2:C:17:DG:H2"	2:C:18:DT:H5'	1.94	0.49
2:G:6:DG:C2'	2:G:7:DT:H71	2.41	0.49
2:K:23:DA:H1'	2:K:24:DA:H5'	1.93	0.49
2:X:11:DA:H2"	2:X:12:DA:C5'	2.34	0.49
2:2:25:DA:C2	2:2:26:DG:C4	2.99	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7:9:DT:H5'	3:7:9:DT:H6	1.77	0.49
3:j:9:DT:H5'	3:j:9:DT:H6	1.77	0.49
3:D:9:DT:H5'	3:D:9:DT:H6	1.77	0.49
3:D:14:DA:C1'	3:D:15:DC:H5"	2.42	0.49
3:H:12:DC:H2"	3:H:13:DA:C8	2.47	0.49
2:K:15:DT:H2'	2:K:16:DT:H72	1.94	0.49
2:a:2:DG:C2'	2:a:3:DG:C8	2.95	0.49
2:i:25:DA:C2	2:i:26:DG:C4	3.00	0.49
2:C:11:DA:H2"	2:C:12:DA:C5'	2.36	0.49
3:P:19:DA:H2"	3:P:20:DT:H5'	1.94	0.49
2:T:7:DT:C2	2:T:8:DC:C5	2.99	0.49
3:3:9:DT:C3'	3:3:10:DG:H5"	2.40	0.49
3:7:14:DA:C1'	3:7:15:DC:H5"	2.42	0.49
2:G:12:DA:H2"	2:G:13:DA:H5"	1.94	0.49
2:K:12:DA:C2'	2:K:13:DA:H5"	2.43	0.49
2:T:22:DA:H2"	2:T:23:DA:H5'	1.94	0.49
2:X:6:DG:C2'	2:X:7:DT:H71	2.39	0.49
3:f:9:DT:H6	3:f:9:DT:H5'	1.77	0.49
2:i:12:DA:C2'	2:i:13:DA:H5"	2.42	0.49
2:m:17:DG:H2"	2:m:18:DT:H5'	1.95	0.49
3:D:18:DT:H1'	3:D:19:DA:H5'	1.93	0.49
2:G:7:DT:C2	2:G:8:DC:C5	3.00	0.49
3:P:21:DG:H2"	3:P:22:DA:OP2	2.12	0.49
2:m:2:DG:C2'	2:m:3:DG:C8	2.95	0.49
3:D:21:DG:H2"	3:D:22:DA:OP2	2.11	0.49
2:G:6:DG:H2"	2:G:7:DT:H5'	1.94	0.49
3:H:13:DA:C2'	3:H:14:DA:OP2	2.57	0.49
2:K:6:DG:C2'	2:K:7:DT:H71	2.39	0.49
2:O:6:DG:C2'	2:O:7:DT:H71	2.42	0.49
2:O:17:DG:H2"	2:O:18:DT:H5'	1.94	0.49
3:3:19:DA:H2"	3:3:20:DT:C5'	2.43	0.49
3:3:21:DG:H2"	3:3:22:DA:OP2	2.12	0.49
3:7:21:DG:H2"	3:7:22:DA:OP2	2.11	0.49
3:b:15:DC:H2"	3:b:16:DT:C5'	2.42	0.49
3:n:15:DC:H2"	3:n:16:DT:C5'	2.42	0.49
2:C:3:DG:H2"	2:C:4:DC:C5'	2.39	0.49
2:C:15:DT:C1'	2:C:16:DT:H5'	2.40	0.49
3:Y:21:DG:H2"	3:Y:22:DA:OP2	2.13	0.49
3:3:19:DA:H2"	3:3:20:DT:H5'	1.94	0.49
2:a:6:DG:C2'	2:a:7:DT:H71	2.42	0.49
2:a:17:DG:H2"	2:a:18:DT:H5'	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:14:DA:C1'	3:f:15:DC:H5"	2.42	0.49
3:L:14:DA:C1'	3:L:15:DC:H5"	2.39	0.49
2:O:15:DT:H2"	2:O:16:DT:O5'	2.13	0.49
2:X:15:DT:H2"	2:X:16:DT:O5'	2.11	0.49
2:2:11:DA:C2	3:3:19:DA:C2	3.01	0.49
2:2:15:DT:H2"	2:2:16:DT:O5'	2.13	0.49
2:C:12:DA:C2'	2:C:13:DA:C5'	2.89	0.49
2:K:22:DA:H2"	2:K:23:DA:H5'	1.94	0.49
2:O:11:DA:H2"	2:O:12:DA:C5'	2.33	0.49
2:i:6:DG:H2"	2:i:7:DT:H5'	1.93	0.49
3:U:14:DA:C3'	3:U:15:DC:H5"	2.31	0.49
2:2:17:DG:H2"	2:2:18:DT:H5'	1.94	0.49
2:6:12:DA:C2'	2:6:13:DA:C5'	2.89	0.49
3:L:9:DT:H5'	3:L:9:DT:H6	1.76	0.48
2:X:12:DA:C2'	2:X:13:DA:H5"	2.43	0.48
3:Y:9:DT:C3'	3:Y:10:DG:H5"	2.41	0.48
3:b:12:DC:H2"	3:b:13:DA:C8	2.47	0.48
2:e:6:DG:C2'	2:e:7:DT:H71	2.41	0.48
2:e:15:DT:C1'	2:e:16:DT:H5'	2.40	0.48
3:f:21:DG:H2"	3:f:22:DA:OP2	2.12	0.48
3:f:11:DA:H1'	3:f:12:DC:C5'	2.36	0.48
3:n:14:DA:C1'	3:n:15:DC:H5"	2.42	0.48
2:C:15:DT:H2'	2:C:16:DT:H72	1.96	0.48
2:X:22:DA:H2"	2:X:23:DA:H5'	1.94	0.48
3:3:14:DA:C1'	3:3:15:DC:H5"	2.42	0.48
3:f:15:DC:H2"	3:f:16:DT:C5'	2.42	0.48
3:j:14:DA:C1'	3:j:15:DC:H5"	2.42	0.48
3:L:21:DG:H2"	3:L:22:DA:OP2	2.13	0.48
2:O:15:DT:C1'	2:O:16:DT:H5'	2.41	0.48
2:i:2:DG:C2'	2:i:3:DG:C8	2.95	0.48
2:K:2:DG:C2'	2:K:3:DG:C8	2.95	0.48
3:L:9:DT:C3'	3:L:10:DG:H5"	2.41	0.48
3:P:11:DA:H1'	3:P:12:DC:C5'	2.35	0.48
3:U:11:DA:H1'	3:U:12:DC:C5'	2.35	0.48
2:6:15:DT:C1'	2:6:16:DT:H5'	2.40	0.48
2:a:3:DG:H2"	2:a:4:DC:C5'	2.39	0.48
2:e:2:DG:C2'	2:e:3:DG:C8	2.95	0.48
2:i:15:DT:H2'	2:i:16:DT:H72	1.95	0.48
3:j:15:DC:H2"	3:j:16:DT:C5'	2.42	0.48
3:Y:24:DA:H1'	3:Y:25:DG:C5'	2.44	0.48
2:6:2:DG:C2'	2:6:3:DG:C8	2.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:6:DG:H2”	2:e:7:DT:H5’	1.93	0.48
3:n:12:DC:H2”	3:n:13:DA:C8	2.47	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
2:e:12:DA:C2’	2:e:13:DA:C5’	2.90	0.48
3:j:21:DG:H2”	3:j:22:DA:OP2	2.12	0.48
3:H:15:DC:H2”	3:H:16:DT:C5’	2.43	0.48
2:K:3:DG:H2”	2:K:4:DC:C5’	2.40	0.48
2:2:7:DT:C2’	2:2:8:DC:H5”	2.44	0.48
2:2:12:DA:C2’	2:2:13:DA:C5’	2.89	0.48
2:6:15:DT:H2’	2:6:16:DT:H72	1.96	0.48
3:b:14:DA:C1’	3:b:15:DC:H5”	2.42	0.48
4:q:563:PHE:CA	4:q:564:GLY:CA	2.91	0.48
3:P:15:DC:H2”	3:P:16:DT:C5’	2.44	0.48
3:U:15:DC:H2”	3:U:16:DT:C5’	2.43	0.48
2:2:11:DA:H2”	2:2:12:DA:C5’	2.33	0.48
3:j:11:DA:H1’	3:j:12:DC:C5’	2.36	0.48
2:X:15:DT:H2’	2:X:16:DT:H72	1.94	0.47
3:Y:15:DC:H2”	3:Y:16:DT:C5’	2.44	0.47
2:2:3:DG:H2”	2:2:4:DC:C5’	2.41	0.47
2:a:7:DT:C2’	2:a:8:DC:H5”	2.44	0.47
2:C:2:DG:C2’	2:C:3:DG:C8	2.95	0.47
3:L:11:DA:H1’	3:L:12:DC:C5’	2.36	0.47
3:L:15:DC:H2”	3:L:16:DT:C5’	2.44	0.47
3:P:19:DA:H2”	3:P:20:DT:C5’	2.43	0.47
2:T:6:DG:C2’	2:T:7:DT:H71	2.41	0.47
3:f:8:DG:H2”	3:f:9:DT:H5’	1.94	0.47
2:i:6:DG:C2’	2:i:7:DT:H71	2.41	0.47
2:i:12:DA:C2’	2:i:13:DA:C5’	2.90	0.47
3:j:9:DT:C3’	3:j:10:DG:H5”	2.41	0.47
3:H:14:DA:C1’	3:H:15:DC:H5”	2.42	0.47
2:K:11:DA:H2”	2:K:12:DA:C5’	2.34	0.47
3:L:10:DG:H2”	3:L:11:DA:H8	1.80	0.47
3:n:13:DA:C2’	3:n:14:DA:OP2	2.56	0.47
2:m:3:DG:H2”	2:m:4:DC:C5’	2.38	0.47
2:C:7:DT:C2’	2:C:8:DC:H5”	2.44	0.47
3:H:8:DG:H2”	3:H:9:DT:H5’	1.92	0.47
3:L:24:DA:H1’	3:L:25:DG:C5’	2.44	0.47
3:Y:10:DG:H2”	3:Y:11:DA:H8	1.79	0.47
2:i:15:DT:C1’	2:i:16:DT:H5’	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:12:DA:C2'	2:G:13:DA:C5'	2.89	0.47
2:G:17:DG:H2"	2:G:18:DT:H5'	1.96	0.47
3:3:15:DC:H2"	3:3:16:DT:C5'	2.45	0.47
2:m:7:DT:C2'	2:m:8:DC:H5"	2.44	0.47
2:T:17:DG:H2"	2:T:18:DT:H5'	1.97	0.47
2:6:7:DT:C2'	2:6:8:DC:H5"	2.44	0.47
2:a:15:DT:H2'	2:a:16:DT:H72	1.97	0.47
2:e:3:DG:H2"	2:e:4:DC:C5'	2.40	0.47
2:e:7:DT:C2'	2:e:8:DC:H5"	2.45	0.47
2:e:15:DT:H2'	2:e:16:DT:H72	1.95	0.47
2:i:7:DT:C2'	2:i:8:DC:H5"	2.45	0.47
4:o:563:PHE:CA	4:o:564:GLY:CA	2.93	0.47
2:i:3:DG:C2'	2:i:4:DC:H5'	2.42	0.47
2:K:17:DG:H2"	2:K:18:DT:H5'	1.96	0.47
3:U:24:DA:H1'	3:U:25:DG:C5'	2.45	0.47
3:Y:11:DA:H1'	3:Y:12:DC:C5'	2.36	0.47
3:3:10:DG:H2"	3:3:11:DA:H8	1.79	0.47
3:f:24:DA:H1'	3:f:25:DG:C5'	2.46	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:b:24:DA:H1'	3:b:25:DG:C5'	2.45	0.46
3:j:4:DT:H2'	3:j:4:DT:O5'	2.16	0.46
3:P:10:DG:H2"	3:P:11:DA:H8	1.79	0.46
3:f:4:DT:H2'	3:f:4:DT:O5'	2.16	0.46
2:m:15:DT:H2'	2:m:16:DT:H72	1.97	0.46
3:n:24:DA:H1'	3:n:25:DG:C5'	2.46	0.46
2:O:6:DG:N2	3:P:24:DA:C2	2.83	0.46
3:3:5:DT:H2"	3:3:6:DT:H5'	1.98	0.46
2:i:4:DC:C2'	2:i:5:DT:H71	2.46	0.46
2:m:6:DG:H2"	2:m:7:DT:H5'	1.93	0.46
3:D:10:DG:H2"	3:D:11:DA:H8	1.81	0.46
3:H:11:DA:H1'	3:H:12:DC:C5'	2.35	0.46
2:X:20:DA:H2"	2:X:21:DC:OP2	2.16	0.46
3:7:10:DG:H2"	3:7:11:DA:H8	1.81	0.46
3:D:8:DG:H2"	3:D:9:DT:H5'	1.94	0.46
3:H:24:DA:H1'	3:H:25:DG:C5'	2.45	0.46
2:O:2:DG:C2'	2:O:3:DG:C8	2.96	0.46
3:U:14:DA:C1'	3:U:15:DC:H5"	2.42	0.46
3:3:25:DG:C4	3:3:26:DC:C4	3.04	0.46
2:6:3:DG:C2'	2:6:4:DC:H5'	2.42	0.46
3:7:8:DG:H2"	3:7:9:DT:H5'	1.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:20:DA:H2”	2:e:21:DC:OP2	2.15	0.46
2:i:17:DG:C2’	2:i:18:DT:H5”	2.46	0.46
2:m:11:DA:H2”	2:m:12:DA:C5’	2.34	0.46
3:P:8:DG:H2”	3:P:9:DT:H5’	1.95	0.46
3:b:5:DT:H2”	3:b:6:DT:H5’	1.98	0.46
3:f:25:DG:C4	3:f:26:DC:C4	3.04	0.46
2:m:6:DG:C2’	2:m:7:DT:H71	2.42	0.46
2:C:3:DG:C2’	2:C:4:DC:H5’	2.42	0.46
2:O:3:DG:H2”	2:O:4:DC:C5’	2.41	0.46
3:P:4:DT:H2’	3:P:4:DT:O5’	2.16	0.46
2:T:3:DG:C2’	2:T:4:DC:H5’	2.39	0.46
2:X:7:DT:H2”	2:X:8:DC:C6	2.50	0.46
2:a:24:DA:H1’	2:a:25:DA:C5’	2.46	0.46
2:i:20:DA:H2”	2:i:21:DC:OP2	2.15	0.46
3:n:10:DG:H2”	3:n:11:DA:H8	1.80	0.46
2:C:4:DC:C2’	2:C:5:DT:H71	2.46	0.46
2:2:2:DG:H2”	2:2:3:DG:O5’	2.16	0.46
2:a:6:DG:H2”	2:a:7:DT:H5’	1.93	0.46
2:i:3:DG:H2”	2:i:4:DC:C5’	2.40	0.46
3:H:10:DG:H2”	3:H:11:DA:H8	1.80	0.46
2:X:6:DG:H2”	2:X:7:DT:H5’	1.93	0.46
2:X:17:DG:H2”	2:X:18:DT:H5’	1.96	0.46
2:2:15:DT:H2’	2:2:16:DT:H72	1.98	0.46
2:6:4:DC:C2’	2:6:5:DT:H71	2.46	0.46
3:j:24:DA:H1’	3:j:25:DG:C5’	2.46	0.46
2:m:2:DG:H2”	2:m:3:DG:O5’	2.16	0.46
2:O:3:DG:C2’	2:O:4:DC:H5’	2.43	0.45
3:U:10:DG:H2”	3:U:11:DA:H8	1.81	0.45
3:n:5:DT:H2”	3:n:6:DT:H5’	1.98	0.45
3:L:14:DA:C3’	3:L:15:DC:H5”	2.29	0.45
2:T:7:DT:C2’	2:T:8:DC:H5”	2.46	0.45
3:Y:23:DC:H2”	3:Y:24:DA:C8	2.52	0.45
3:f:9:DT:C3’	3:f:10:DG:H5”	2.40	0.45
3:f:23:DC:H2”	3:f:24:DA:C8	2.51	0.45
2:m:24:DA:H1’	2:m:25:DA:C5’	2.46	0.45
3:n:9:DT:C3’	3:n:10:DG:H5”	2.38	0.45
2:O:15:DT:H2’	2:O:16:DT:H72	1.98	0.45
3:P:25:DG:C4	3:P:26:DC:C4	3.04	0.45
2:a:11:DA:H2”	2:a:12:DA:C5’	2.34	0.45
3:j:25:DG:C4	3:j:26:DC:C4	3.04	0.45
3:D:24:DA:H1’	3:D:25:DG:C5’	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:16:DT:H2'	3:H:17:DT:C7	2.42	0.45
2:K:15:DT:H2"	2:K:16:DT:C5'	2.46	0.45
3:P:5:DT:H2"	3:P:6:DT:H5'	1.98	0.45
3:P:16:DT:H2'	3:P:17:DT:C7	2.44	0.45
3:Y:4:DT:O5'	3:Y:4:DT:H2'	2.17	0.45
3:b:10:DG:H2"	3:b:11:DA:H8	1.80	0.45
1:g:156:GLY:CA	2:i:5:DT:OP1	2.65	0.45
3:j:23:DC:H2"	3:j:24:DA:C8	2.51	0.45
2:G:7:DT:C2'	2:G:8:DC:H5"	2.46	0.45
2:G:15:DT:H2"	2:G:16:DT:C5'	2.47	0.45
2:K:12:DA:C2'	2:K:13:DA:C5'	2.91	0.45
2:O:2:DG:H2"	2:O:3:DG:O5'	2.16	0.45
3:P:14:DA:C1'	3:P:15:DC:H5"	2.42	0.45
2:X:12:DA:H2"	2:X:13:DA:H5"	1.96	0.45
2:X:15:DT:H2"	2:X:16:DT:C5'	2.46	0.45
3:b:8:DG:H2"	3:b:9:DT:H5'	1.94	0.45
2:e:4:DC:C2'	2:e:5:DT:H71	2.46	0.45
2:e:17:DG:C2'	2:e:18:DT:H5"	2.46	0.45
3:f:10:DG:H2"	3:f:11:DA:H8	1.81	0.45
3:f:16:DT:H2'	3:f:17:DT:C7	2.44	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:a:2:DG:H2"	2:a:3:DG:O5'	2.17	0.45
3:n:8:DG:H2"	3:n:9:DT:H5'	1.93	0.45
2:K:2:DG:H2"	2:K:3:DG:H8	1.80	0.45
3:3:24:DA:H1'	3:3:25:DG:C5'	2.47	0.45
2:G:24:DA:H1'	2:G:25:DA:C5'	2.47	0.45
2:2:2:DG:H2"	2:2:3:DG:H8	1.80	0.45
3:j:5:DT:H2"	3:j:6:DT:H5'	1.99	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:K:3:DG:C2'	2:K:4:DC:H5'	2.42	0.45
2:K:7:DT:C2'	2:K:8:DC:H5"	2.46	0.45
3:L:23:DC:H2"	3:L:24:DA:C8	2.52	0.45
2:T:15:DT:H2'	2:T:16:DT:H72	1.98	0.45
2:X:7:DT:C2'	2:X:8:DC:H5"	2.46	0.45
3:3:4:DT:H2'	3:3:4:DT:O5'	2.16	0.45
3:j:10:DG:H2"	3:j:11:DA:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:25:DG:C4	3:D:26:DC:C4	3.05	0.45
2:G:15:DT:H2'	2:G:16:DT:H72	1.98	0.45
2:K:20:DA:H2"	2:K:21:DC:OP2	2.16	0.45
2:O:20:DA:H2"	2:O:21:DC:OP2	2.18	0.45
2:X:2:DG:C8	2:X:2:DG:H5"	2.52	0.45
3:7:4:DT:H2'	3:7:4:DT:O5'	2.16	0.45
3:7:5:DT:H2"	3:7:6:DT:H5'	1.98	0.45
3:7:25:DG:C4	3:7:26:DC:C4	3.05	0.45
2:a:2:DG:H2"	2:a:3:DG:H8	1.80	0.45
2:a:4:DC:C2'	2:a:5:DT:H71	2.47	0.45
2:a:17:DG:C2'	2:a:18:DT:H5"	2.48	0.45
2:i:24:DA:H1'	2:i:25:DA:C5'	2.47	0.45
3:D:23:DC:H2"	3:D:24:DA:C8	2.52	0.44
3:L:25:DG:C4	3:L:26:DC:C4	3.05	0.44
2:2:17:DG:C2'	2:2:18:DT:H5"	2.47	0.44
2:m:2:DG:H2"	2:m:3:DG:H8	1.79	0.44
2:O:17:DG:C2'	2:O:18:DT:H5"	2.47	0.44
3:Y:25:DG:C4	3:Y:26:DC:C4	3.05	0.44
2:2:4:DC:C2'	2:2:5:DT:H71	2.47	0.44
2:6:20:DA:H2"	2:6:21:DC:OP2	2.16	0.44
3:7:23:DC:H2"	3:7:24:DA:C8	2.52	0.44
2:e:24:DA:H1'	2:e:25:DA:C5'	2.47	0.44
2:C:17:DG:C2'	2:C:18:DT:H5"	2.47	0.44
2:C:20:DA:H2"	2:C:21:DC:OP2	2.15	0.44
2:m:4:DC:C2'	2:m:5:DT:H71	2.48	0.44
2:C:6:DG:H2"	2:C:7:DT:H5'	1.93	0.44
3:H:25:DG:C4	3:H:26:DC:C4	3.05	0.44
2:K:4:DC:C2'	2:K:5:DT:H71	2.48	0.44
3:P:24:DA:H1'	3:P:25:DG:C5'	2.47	0.44
3:U:8:DG:H2"	3:U:9:DT:H5'	1.92	0.44
3:U:16:DT:H2'	3:U:17:DT:C7	2.42	0.44
3:L:4:DT:O5'	3:L:4:DT:H2'	2.17	0.44
2:2:6:DG:C2'	2:2:7:DT:H71	2.42	0.44
2:6:6:DG:H2"	2:6:7:DT:H5'	1.93	0.44
3:j:16:DT:H2'	3:j:17:DT:C7	2.44	0.44
2:C:24:DA:H1'	2:C:25:DA:C5'	2.46	0.44
2:K:7:DT:H2"	2:K:8:DC:C6	2.50	0.44
2:T:15:DT:H2"	2:T:16:DT:C5'	2.47	0.44
2:X:15:DT:C2'	2:X:16:DT:H5'	2.48	0.44
2:i:7:DT:H2"	2:i:8:DC:C6	2.51	0.44
2:m:17:DG:C2'	2:m:18:DT:H5"	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:5:DT:H2"	3:H:6:DT:H5'	2.00	0.44
3:U:4:DT:H2'	3:U:4:DT:O5'	2.18	0.44
2:K:15:DT:C2'	2:K:16:DT:H5'	2.48	0.44
2:O:24:DA:H1'	2:O:25:DA:C5'	2.48	0.44
3:U:25:DG:C4	3:U:26:DC:C4	3.05	0.44
2:X:4:DC:C2'	2:X:5:DT:H71	2.48	0.44
3:3:8:DG:H2"	3:3:9:DT:H5'	1.95	0.44
2:m:15:DT:H2"	2:m:16:DT:C5'	2.48	0.44
2:C:7:DT:H2"	2:C:8:DC:C6	2.51	0.44
2:O:4:DC:C2'	2:O:5:DT:H71	2.47	0.44
2:T:20:DA:H2"	2:T:21:DC:OP2	2.18	0.44
2:T:24:DA:H1'	2:T:25:DA:C5'	2.47	0.44
2:X:17:DG:C2'	2:X:18:DT:H5"	2.48	0.44
2:6:24:DA:H1'	2:6:25:DA:C5'	2.46	0.44
3:f:5:DT:H2"	3:f:6:DT:H5'	1.98	0.44
2:C:6:DG:C2'	2:C:7:DT:H71	2.42	0.43
3:L:5:DT:H2"	3:L:6:DT:H5'	2.00	0.43
2:T:2:DG:C8	2:T:2:DG:H5"	2.53	0.43
2:T:2:DG:H2"	2:T:3:DG:O5'	2.18	0.43
2:T:6:DG:H2"	2:T:7:DT:H5'	1.93	0.43
2:T:23:DA:H1'	2:T:24:DA:C8	2.53	0.43
2:2:24:DA:H1'	2:2:25:DA:C5'	2.48	0.43
3:3:16:DT:H2"	3:3:17:DT:C6	2.53	0.43
2:i:15:DT:H2"	2:i:16:DT:C5'	2.48	0.43
2:m:7:DT:H2"	2:m:8:DC:C6	2.52	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
3:b:25:DG:C4	3:b:26:DC:C4	3.06	0.43
3:n:4:DT:H2'	3:n:4:DT:O5'	2.18	0.43
2:G:2:DG:H2"	2:G:3:DG:O5'	2.18	0.43
2:G:23:DA:H1'	2:G:24:DA:C8	2.53	0.43
3:P:16:DT:H2"	3:P:17:DT:C6	2.54	0.43
2:a:20:DA:H2"	2:a:21:DC:OP2	2.17	0.43
3:b:4:DT:H2'	3:b:4:DT:O5'	2.18	0.43
2:e:3:DG:C5	2:e:4:DC:C4	3.06	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
2:a:15:DT:H2"	2:a:16:DT:C5'	2.48	0.43
2:e:15:DT:H2"	2:e:16:DT:C5'	2.49	0.43
3:D:23:DC:H6	3:D:23:DC:H5'	1.83	0.43
3:L:19:DA:C1'	3:L:20:DT:H5"	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:3:DG:C5	2:O:4:DC:C4	3.06	0.43
3:Y:14:DA:H1'	3:Y:15:DC:H5"	2.00	0.43
2:6:7:DT:H2"	2:6:8:DC:C6	2.52	0.43
3:7:23:DC:H6	3:7:23:DC:H5'	1.84	0.43
3:n:16:DT:H2'	3:n:17:DT:C7	2.43	0.43
3:n:25:DG:C4	3:n:26:DC:C4	3.06	0.43
2:G:17:DG:C2'	2:G:18:DT:H5"	2.49	0.43
3:H:4:DT:H2'	3:H:4:DT:O5'	2.18	0.43
2:T:2:DG:H2"	2:T:3:DG:H8	1.78	0.43
2:6:6:DG:C2'	2:6:7:DT:H71	2.42	0.43
2:i:3:DG:C5	2:i:4:DC:C4	3.06	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
3:b:23:DC:H2"	3:b:24:DA:C8	2.53	0.43
2:C:3:DG:C5	2:C:4:DC:C4	3.07	0.43
3:D:16:DT:H2'	3:D:17:DT:C7	2.44	0.43
2:T:4:DC:H1'	2:T:5:DT:C5'	2.49	0.43
3:7:16:DT:H2'	3:7:17:DT:C7	2.44	0.43
2:i:11:DA:H2"	2:i:12:DA:C5'	2.36	0.43
2:T:4:DC:C2'	2:T:5:DT:H71	2.49	0.43
2:X:15:DT:H2"	2:X:16:DT:H5'	2.01	0.43
2:X:24:DA:H1'	2:X:25:DA:C5'	2.48	0.43
2:2:20:DA:H2"	2:2:21:DC:OP2	2.18	0.43
3:3:13:DA:C2'	3:3:14:DA:OP2	2.56	0.43
3:b:23:DC:H6	3:b:23:DC:H5'	1.84	0.43
2:C:15:DT:H2"	2:C:16:DT:C5'	2.49	0.43
2:K:2:DG:C8	2:K:2:DG:H5"	2.52	0.43
3:U:19:DA:C1'	3:U:20:DT:H5"	2.46	0.43
2:a:7:DT:H2"	2:a:8:DC:C6	2.51	0.43
3:b:19:DA:C1'	3:b:20:DT:H5"	2.49	0.43
2:i:2:DG:H2"	2:i:3:DG:O5'	2.18	0.43
2:i:23:DA:H1'	2:i:24:DA:C8	2.54	0.43
3:n:23:DC:H2"	3:n:24:DA:C8	2.54	0.43
2:K:3:DG:C5	2:K:4:DC:C4	3.07	0.42
2:O:12:DA:C2'	2:O:13:DA:C5'	2.89	0.42
3:U:5:DT:H2"	3:U:6:DT:H5'	2.00	0.42
3:U:23:DC:H2"	3:U:24:DA:C8	2.54	0.42
3:Y:5:DT:H2"	3:Y:6:DT:H5'	2.00	0.42
3:Y:16:DT:H2"	3:Y:17:DT:C6	2.54	0.42
3:Y:19:DA:C1'	3:Y:20:DT:H5"	2.48	0.42
2:6:15:DT:H2"	2:6:16:DT:C5'	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:3:DG:C5	2:a:4:DC:C4	3.07	0.42
2:e:2:DG:H2"	2:e:3:DG:O5'	2.19	0.42
2:m:3:DG:C5	2:m:4:DC:C4	3.08	0.42
2:m:20:DA:H2"	2:m:21:DC:OP2	2.18	0.42
3:n:19:DA:C1'	3:n:20:DT:H5"	2.48	0.42
2:2:15:DT:H2"	2:2:16:DT:C5'	2.49	0.42
2:e:23:DA:H1'	2:e:24:DA:C8	2.54	0.42
3:f:12:DC:H5'	3:f:12:DC:H6	1.85	0.42
3:f:23:DC:H5'	3:f:23:DC:H6	1.84	0.42
3:j:12:DC:H5'	3:j:12:DC:H6	1.84	0.42
2:G:20:DA:H2"	2:G:21:DC:OP2	2.19	0.42
3:H:23:DC:H2"	3:H:24:DA:C8	2.54	0.42
2:K:2:DG:H2"	2:K:3:DG:O5'	2.19	0.42
2:K:24:DA:H1'	2:K:25:DA:C5'	2.49	0.42
3:L:14:DA:H1'	3:L:15:DC:H5"	2.00	0.42
2:O:23:DA:H1'	2:O:24:DA:C8	2.54	0.42
2:6:23:DA:H1'	2:6:24:DA:C8	2.54	0.42
3:b:16:DT:H2'	3:b:17:DT:C7	2.43	0.42
2:m:25:DA:C4	2:m:26:DG:C8	3.07	0.42
2:K:17:DG:C2'	2:K:18:DT:H5"	2.48	0.42
2:T:11:DA:H2"	2:T:12:DA:C5'	2.35	0.42
3:b:16:DT:C2'	3:b:17:DT:H72	2.46	0.42
2:i:6:DG:C2	3:j:24:DA:C2	3.06	0.42
3:D:5:DT:H2"	3:D:6:DT:C5'	2.50	0.42
3:D:12:DC:H5'	3:D:12:DC:H6	1.84	0.42
3:U:16:DT:H2"	3:U:17:DT:C6	2.54	0.42
3:3:23:DC:H2"	3:3:24:DA:C8	2.54	0.42
3:7:5:DT:H2"	3:7:6:DT:C5'	2.50	0.42
3:H:16:DT:H2"	3:H:17:DT:C6	2.54	0.42
3:L:8:DG:H2"	3:L:9:DT:H5'	1.94	0.42
2:X:2:DG:H2"	2:X:3:DG:O5'	2.19	0.42
2:a:2:DG:C8	2:a:2:DG:H5"	2.55	0.42
2:C:2:DG:H2"	2:C:3:DG:H8	1.80	0.42
2:T:3:DG:C5	2:T:4:DC:C4	3.07	0.42
3:U:14:DA:H1'	3:U:15:DC:H5"	2.02	0.42
3:Y:13:DA:C2'	3:Y:14:DA:OP2	2.56	0.42
2:2:23:DA:H1'	2:2:24:DA:C8	2.55	0.42
3:3:5:DT:H2"	3:3:6:DT:C5'	2.50	0.42
3:7:12:DC:H5'	3:7:12:DC:H6	1.84	0.42
2:G:3:DG:C5	2:G:4:DC:C4	3.07	0.42
2:G:15:DT:C2'	2:G:16:DT:H5'	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:15:DT:C2'	2:T:16:DT:H5'	2.49	0.42
2:T:25:DA:C4	2:T:26:DG:C8	3.08	0.42
2:X:12:DA:C2'	2:X:13:DA:C5'	2.91	0.42
3:3:16:DT:H2'	3:3:17:DT:C7	2.44	0.42
2:a:25:DA:C4	2:a:26:DG:C8	3.08	0.42
3:j:16:DT:H2"	3:j:17:DT:C6	2.55	0.42
2:m:3:DG:C2'	2:m:4:DC:H5'	2.40	0.42
2:G:25:DA:C4	2:G:26:DG:C8	3.08	0.42
3:P:23:DC:H2"	3:P:24:DA:C8	2.54	0.42
2:T:17:DG:C2'	2:T:18:DT:H5"	2.49	0.42
3:U:13:DA:C2'	3:U:14:DA:OP2	2.57	0.42
2:a:3:DG:C2'	2:a:4:DC:H5'	2.41	0.42
3:f:16:DT:H2"	3:f:17:DT:C6	2.55	0.42
3:f:19:DA:C1'	3:f:20:DT:H5"	2.48	0.42
2:i:15:DT:C2'	2:i:16:DT:H5'	2.50	0.42
2:m:2:DG:C8	2:m:2:DG:H5"	2.55	0.42
2:C:23:DA:H1'	2:C:24:DA:C8	2.55	0.42
2:K:15:DT:H2"	2:K:16:DT:H5'	2.01	0.42
2:O:15:DT:H2"	2:O:16:DT:C5'	2.49	0.42
3:Y:8:DG:H2"	3:Y:9:DT:H5'	1.94	0.42
3:Y:24:DA:H1'	3:Y:25:DG:H5'	2.02	0.42
2:i:23:DA:C4	2:i:24:DA:N7	2.88	0.42
2:m:23:DA:H1'	2:m:24:DA:C8	2.55	0.42
2:O:15:DT:C2'	2:O:16:DT:H5'	2.50	0.41
2:X:3:DG:C2'	2:X:4:DC:H5'	2.42	0.41
2:e:23:DA:C4	2:e:24:DA:N7	2.88	0.41
2:G:4:DC:H1'	2:G:5:DT:C5'	2.49	0.41
2:K:23:DA:H1'	2:K:24:DA:C8	2.55	0.41
3:L:16:DT:H2"	3:L:17:DT:C6	2.55	0.41
3:P:5:DT:H2"	3:P:6:DT:C5'	2.50	0.41
2:X:3:DG:C5	2:X:4:DC:C4	3.07	0.41
2:6:25:DA:C4	2:6:26:DG:C8	3.08	0.41
2:G:2:DG:C8	2:G:2:DG:H5"	2.53	0.41
2:G:7:DT:H2"	2:G:8:DC:C6	2.51	0.41
3:U:23:DC:H6	3:U:23:DC:H5'	1.86	0.41
2:2:15:DT:C2'	2:2:16:DT:H5'	2.50	0.41
2:2:25:DA:C4	2:2:26:DG:C8	3.08	0.41
3:b:5:DT:H2"	3:b:6:DT:C5'	2.50	0.41
3:f:5:DT:H2"	3:f:6:DT:C5'	2.51	0.41
3:j:8:DG:H2"	3:j:9:DT:H5'	1.94	0.41
3:j:23:DC:H6	3:j:23:DC:H5'	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:23:DA:C4	2:m:24:DA:N7	2.89	0.41
3:n:23:DC:H5'	3:n:23:DC:H6	1.84	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:a:23:DA:H1'	2:a:24:DA:C8	2.55	0.41
2:e:15:DT:C2'	2:e:16:DT:H5'	2.50	0.41
3:n:16:DT:C2'	3:n:17:DT:H72	2.45	0.41
2:C:25:DA:C4	2:C:26:DG:C8	3.09	0.41
3:H:15:DC:C2'	3:H:16:DT:H72	2.51	0.41
2:K:23:DA:C4	2:K:24:DA:N7	2.89	0.41
3:U:24:DA:H1'	3:U:25:DG:H5'	2.02	0.41
2:6:2:DG:H2"	2:6:3:DG:H8	1.80	0.41
2:a:23:DA:C4	2:a:24:DA:N7	2.89	0.41
3:b:14:DA:H1'	3:b:15:DC:H5"	2.02	0.41
2:C:23:DA:C4	2:C:24:DA:N7	2.88	0.41
2:G:2:DG:H2"	2:G:3:DG:H8	1.78	0.41
3:H:24:DA:H1'	3:H:25:DG:H5'	2.02	0.41
2:O:23:DA:C4	2:O:24:DA:N7	2.88	0.41
3:P:23:DC:H5'	3:P:23:DC:H6	1.85	0.41
3:b:16:DT:H2"	3:b:17:DT:C6	2.56	0.41
2:i:6:DG:N2	3:j:24:DA:C2	2.89	0.41
3:n:16:DT:H2"	3:n:17:DT:C6	2.56	0.41
3:L:24:DA:H1'	3:L:25:DG:H5'	2.02	0.41
2:X:23:DA:H1'	2:X:24:DA:C8	2.55	0.41
2:2:23:DA:C4	2:2:24:DA:N7	2.88	0.41
2:i:2:DG:H2"	2:i:3:DG:H8	1.80	0.41
3:n:5:DT:H2"	3:n:6:DT:C5'	2.50	0.41
3:3:19:DA:C1'	3:3:20:DT:H5"	2.48	0.41
2:6:23:DA:C4	2:6:24:DA:N7	2.88	0.41
3:7:19:DA:C1'	3:7:20:DT:H5"	2.49	0.41
2:a:8:DC:H2"	2:a:9:DA:O5'	2.20	0.41
2:a:15:DT:C2'	2:a:16:DT:H5'	2.50	0.41
3:b:12:DC:H5'	3:b:12:DC:H6	1.85	0.41
2:e:2:DG:H2"	2:e:3:DG:H8	1.80	0.41
3:j:5:DT:H2"	3:j:6:DT:C5'	2.51	0.41
2:m:12:DA:C1'	2:m:13:DA:H5"	2.50	0.41
3:n:14:DA:H1'	3:n:15:DC:H5"	2.02	0.41
2:C:8:DC:H2"	2:C:9:DA:O5'	2.21	0.41
3:D:19:DA:C1'	3:D:20:DT:H5"	2.49	0.41
3:H:19:DA:C1'	3:H:20:DT:H5"	2.46	0.41
2:O:25:DA:C4	2:O:26:DG:C8	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:19:DA:C1'	3:P:20:DT:H5"	2.48	0.41
2:T:23:DA:C4	2:T:24:DA:N7	2.89	0.41
2:X:3:DG:H2"	2:X:4:DC:C5'	2.40	0.41
2:X:25:DA:C4	2:X:26:DG:C8	3.09	0.41
3:Y:12:DC:H5'	3:Y:12:DC:H6	1.85	0.41
2:6:8:DC:H2"	2:6:9:DA:O5'	2.21	0.41
3:b:24:DA:H1'	3:b:25:DG:H5'	2.03	0.41
2:i:2:DG:C8	2:i:2:DG:H5"	2.54	0.41
3:j:19:DA:C1'	3:j:20:DT:H5"	2.48	0.41
2:m:4:DC:H1'	2:m:5:DT:C5'	2.50	0.41
3:n:24:DA:H1'	3:n:25:DG:H5'	2.03	0.41
3:D:16:DT:H2"	3:D:17:DT:C6	2.56	0.41
3:H:23:DC:H5'	3:H:23:DC:H6	1.86	0.41
2:K:25:DA:C4	2:K:26:DG:C8	3.09	0.41
2:T:7:DT:H2"	2:T:8:DC:C6	2.51	0.41
2:X:23:DA:C4	2:X:24:DA:N7	2.88	0.41
3:Y:16:DT:H2'	3:Y:17:DT:C7	2.44	0.41
3:3:14:DA:H1'	3:3:15:DC:H5"	2.02	0.41
3:7:16:DT:H2"	3:7:17:DT:C6	2.56	0.41
2:e:4:DC:H1'	2:e:5:DT:C5'	2.51	0.41
3:f:16:DT:C2'	3:f:17:DT:H72	2.47	0.41
3:j:14:DA:H1'	3:j:15:DC:H5"	2.02	0.41
2:m:15:DT:C2'	2:m:16:DT:H5'	2.50	0.41
3:n:12:DC:H5'	3:n:12:DC:H6	1.85	0.41
2:T:12:DA:C1'	2:T:13:DA:H5"	2.51	0.40
3:j:25:DG:C5	3:j:26:DC:C4	3.10	0.40
2:G:23:DA:C4	2:G:24:DA:N7	2.88	0.40
3:f:25:DG:C5	3:f:26:DC:C4	3.10	0.40
2:i:25:DA:C4	2:i:26:DG:C8	3.10	0.40
2:m:4:DC:H2"	2:m:5:DT:OP2	2.21	0.40
3:H:12:DC:H5'	3:H:12:DC:H6	1.86	0.40
2:e:25:DA:C4	2:e:26:DG:C8	3.10	0.40
2:i:4:DC:H2"	2:i:5:DT:H71	2.03	0.40
2:C:15:DT:C2'	2:C:16:DT:H5'	2.51	0.40
2:G:3:DG:C2'	2:G:4:DC:C5'	3.00	0.40
2:O:4:DC:H1'	2:O:5:DT:C5'	2.51	0.40
2:X:4:DC:H1'	2:X:5:DT:C5'	2.52	0.40
2:6:4:DC:H2"	2:6:5:DT:H71	2.04	0.40
2:a:4:DC:H1'	2:a:5:DT:C5'	2.51	0.40
2:m:8:DC:H2"	2:m:9:DA:O5'	2.20	0.40
3:L:23:DC:H5'	3:L:23:DC:H6	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:23:DC:H5'	3:3:23:DC:H6	1.85	0.40
2:6:15:DT:C2'	2:6:16:DT:H5'	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:1:DC:N4	2:X:2:DG:N1[2_456]	0.94	1.26
2:K:2:DG:N1	3:U:1:DC:N4[2_556]	0.97	1.23
2:K:2:DG:N2	3:U:1:DC:N3[2_556]	1.36	0.84
3:H:1:DC:N3	2:X:2:DG:N2[2_456]	1.37	0.83
2:K:2:DG:C6	3:U:1:DC:N4[2_556]	1.43	0.77
2:G:2:DG:O6	3:Y:1:DC:N4[4_456]	1.45	0.75
2:G:2:DG:N1	3:Y:1:DC:N4[4_456]	1.46	0.74
3:b:1:DC:N4	2:e:2:DG:N1[4_446]	1.47	0.73
3:P:1:DC:O5'	3:3:26:DC:O3'[3_555]	1.50	0.70
3:L:1:DC:N4	2:T:2:DG:O6[4_446]	1.51	0.69
2:G:2:DG:C6	3:Y:1:DC:N4[4_456]	1.52	0.68
3:H:1:DC:N4	2:X:2:DG:C6[2_456]	1.60	0.60
2:K:2:DG:N1	3:U:1:DC:C4[2_556]	1.60	0.60
3:P:26:DC:O3'	3:3:1:DC:O5'[3_545]	1.69	0.51
2:G:2:DG:N2	3:Y:1:DC:N3[4_456]	1.73	0.47
2:G:2:DG:N1	3:Y:1:DC:C4[4_456]	1.73	0.47
3:L:1:DC:N4	2:T:2:DG:N1[4_446]	1.74	0.46
2:K:2:DG:O6	3:U:1:DC:N4[2_556]	1.75	0.45
2:G:2:DG:N1	3:Y:1:DC:N3[4_456]	1.76	0.44
3:H:1:DC:C4	2:X:2:DG:N1[2_456]	1.76	0.44
3:b:1:DC:N3	2:e:2:DG:N2[4_446]	1.78	0.42
3:L:1:DC:N4	2:T:2:DG:C6[4_446]	1.80	0.40
3:L:1:DC:N3	2:T:2:DG:N1[4_446]	1.84	0.36
2:a:2:DG:O6	3:f:1:DC:N4[2_456]	1.86	0.34
2:K:2:DG:C2	3:U:1:DC:N3[2_556]	1.87	0.33
2:i:2:DG:N1	3:n:1:DC:N4[2_557]	1.90	0.30
2:G:2:DG:C2	3:Y:1:DC:N3[4_456]	1.94	0.26
2:G:1:DT:O4	3:Y:2:DA:N6[4_456]	1.95	0.25
3:H:1:DC:N4	2:X:2:DG:O6[2_456]	1.95	0.25
2:K:2:DG:N2	3:U:1:DC:C2[2_556]	1.97	0.23
3:L:1:DC:N3	2:T:2:DG:N2[4_446]	1.97	0.23
2:K:2:DG:N1	3:U:1:DC:N3[2_556]	1.99	0.21
3:L:2:DA:N6	2:T:1:DT:O4[4_446]	1.99	0.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:j:1:DC:N4	2:m:2:DG:O6[4_447]	1.99	0.21
2:G:2:DG:N2	3:Y:1:DC:C2[4_456]	2.01	0.19
3:j:1:DC:N4	2:m:2:DG:N1[4_447]	2.01	0.19
3:b:1:DC:N4	2:e:2:DG:C6[4_446]	2.02	0.18
2:G:2:DG:N2	3:Y:1:DC:O2[4_456]	2.03	0.17
3:L:1:DC:C4	2:T:2:DG:N1[4_446]	2.03	0.17
3:H:1:DC:N3	2:X:2:DG:C2[2_456]	2.04	0.16
3:b:26:DC:O3'	3:f:1:DC:C5'[2_456]	2.05	0.15
3:P:1:DC:C5'	3:3:26:DC:O3'[3_555]	2.07	0.13
3:b:1:DC:N4	2:e:2:DG:O6[4_446]	2.09	0.11
3:L:1:DC:O2	2:T:2:DG:N2[4_446]	2.11	0.09
2:G:1:DT:N3	3:Y:2:DA:N1[4_456]	2.13	0.07
3:H:1:DC:C2	2:X:2:DG:N2[2_456]	2.14	0.06
2:a:2:DG:N1	3:f:1:DC:N4[2_456]	2.15	0.05
3:b:1:DC:C4	2:e:2:DG:N1[4_446]	2.15	0.05
3:b:26:DC:O3'	3:f:1:DC:O5'[2_456]	2.18	0.02
3:H:1:DC:N3	2:X:2:DG:N1[2_456]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

5.3.2 Protein sidechains (i)

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	8.23	92 (90%)	0	1	56, 70, 90, 95	0
1	4	102/102 (100%)	7.95	89 (87%)	0	1	60, 73, 89, 91	0
1	5	102/102 (100%)	7.83	91 (89%)	0	1	56, 70, 90, 95	0
1	8	102/102 (100%)	8.66	92 (90%)	0	1	60, 73, 89, 91	0
1	9	102/102 (100%)	9.84	95 (93%)	0	1	56, 70, 90, 95	0
1	A	102/102 (100%)	8.97	92 (90%)	0	1	60, 73, 89, 91	0
1	B	102/102 (100%)	8.20	90 (88%)	0	1	56, 70, 90, 95	0
1	E	102/102 (100%)	9.26	89 (87%)	0	1	60, 73, 89, 91	0
1	F	102/102 (100%)	8.27	90 (88%)	0	1	56, 70, 90, 95	0
1	I	102/102 (100%)	9.41	89 (87%)	0	1	60, 73, 89, 91	0
1	J	102/102 (100%)	7.86	94 (92%)	0	1	56, 70, 90, 95	0
1	M	102/102 (100%)	9.39	96 (94%)	0	1	60, 73, 89, 91	0
1	N	102/102 (100%)	8.56	93 (91%)	0	1	56, 70, 90, 95	0
1	R	102/102 (100%)	9.52	88 (86%)	0	1	60, 73, 89, 91	0
1	S	102/102 (100%)	8.39	91 (89%)	0	1	56, 70, 90, 95	0
1	V	102/102 (100%)	8.77	89 (87%)	0	1	60, 73, 89, 91	0
1	W	102/102 (100%)	7.53	97 (95%)	0	0	56, 70, 90, 95	0
1	Z	102/102 (100%)	9.21	93 (91%)	0	1	60, 73, 89, 91	0
1	c	102/102 (100%)	8.60	92 (90%)	0	1	60, 73, 89, 91	0
1	d	102/102 (100%)	8.59	93 (91%)	0	1	56, 70, 90, 95	0
1	g	102/102 (100%)	8.67	88 (86%)	0	1	60, 73, 89, 91	0
1	h	102/102 (100%)	8.80	91 (89%)	0	1	56, 70, 90, 95	0
1	k	102/102 (100%)	9.33	94 (92%)	0	1	60, 73, 89, 91	0
1	l	102/102 (100%)	8.74	90 (88%)	0	1	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%)	2.39	15 (57%)	0	1	62, 79, 87, 88	0
2	6	26/26 (100%)	2.78	19 (73%)	0	1	62, 79, 87, 88	0
2	C	26/26 (100%)	2.63	19 (73%)	0	1	62, 79, 87, 88	0
2	G	26/26 (100%)	2.16	13 (50%)	0	1	62, 79, 87, 88	0
2	K	26/26 (100%)	2.30	15 (57%)	0	1	62, 79, 87, 88	0
2	O	26/26 (100%)	2.52	18 (69%)	0	1	62, 79, 87, 88	0
2	T	26/26 (100%)	2.17	14 (53%)	0	1	62, 79, 87, 88	0
2	X	26/26 (100%)	2.32	15 (57%)	0	1	62, 79, 87, 88	0
2	a	26/26 (100%)	2.51	16 (61%)	0	1	62, 79, 87, 88	0
2	e	26/26 (100%)	2.57	18 (69%)	0	1	62, 79, 87, 88	0
2	i	26/26 (100%)	2.47	16 (61%)	0	1	62, 79, 87, 88	0
2	m	26/26 (100%)	2.45	16 (61%)	0	1	62, 79, 87, 88	0
3	3	26/26 (100%)	2.39	18 (69%)	0	1	61, 79, 93, 94	0
3	7	26/26 (100%)	2.48	15 (57%)	0	1	61, 79, 93, 94	0
3	D	26/26 (100%)	2.53	17 (65%)	0	1	61, 79, 93, 94	0
3	H	26/26 (100%)	2.56	19 (73%)	0	1	61, 79, 93, 94	0
3	L	26/26 (100%)	2.31	16 (61%)	0	1	61, 79, 93, 94	0
3	P	26/26 (100%)	2.39	16 (61%)	0	1	61, 79, 93, 94	0
3	U	26/26 (100%)	2.40	15 (57%)	0	1	61, 79, 93, 94	0
3	Y	26/26 (100%)	2.30	13 (50%)	0	1	61, 79, 93, 94	0
3	b	26/26 (100%)	2.64	18 (69%)	0	1	61, 79, 93, 94	0
3	f	26/26 (100%)	2.44	17 (65%)	0	1	61, 79, 93, 94	0
3	j	26/26 (100%)	2.45	19 (73%)	0	1	61, 79, 93, 94	0
3	n	26/26 (100%)	2.55	19 (73%)	0	1	61, 79, 93, 94	0
4	o	93/99 (93%)	9.66	81 (87%)	0	1	19, 23, 79, 88	0
4	q	93/99 (93%)	9.13	78 (83%)	0	1	19, 23, 79, 88	0
All	All	3258/3270 (99%)	7.54	2753 (84%)	0	1	19, 73, 90, 95	0

All (2753) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	225	PHE	83.8
4	o	572	THR	69.0

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Mol	Chain	Res	Type	RSRZ
1	R	182	HIS	48.4
1	1	128	VAL	48.0
1	8	151	GLU	46.6
1	E	208	PRO	46.0
1	B	170	PRO	44.2
1	4	168	THR	43.9
4	q	603	ARG	43.3
1	9	173	VAL	42.3
1	9	161	LYS	41.7
1	R	128	VAL	41.5
1	M	159	GLU	41.5
1	1	129	GLU	41.4
1	M	178	GLN	39.4
1	9	128	VAL	38.8
1	h	149	GLY	38.6
1	Z	178	GLN	37.3
1	l	149	GLY	37.0
4	q	561	MET	36.0
1	9	189	TYR	35.9
1	g	146	VAL	35.8
1	S	227	THR	35.6
1	I	201	ARG	35.5
1	h	229	PHE	35.4
1	l	161	LYS	35.2
1	k	190	VAL	34.4
1	Z	222	GLY	33.5
1	V	205	ALA	33.5
1	k	175	SER	33.3
1	l	218	VAL	33.1
4	o	533	ASP	31.8
1	R	209	GLY	31.8
1	k	133	GLU	31.7
1	l	129	GLU	31.1
1	l	169	HIS	30.9
1	V	192	ASP	30.9
1	I	128	VAL	30.7
1	I	204	LYS	30.7
4	o	571	TYR	30.5
1	8	175	SER	30.2
4	q	543	ALA	30.2
1	k	222	GLY	30.0
4	q	542	ALA	29.8

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Mol	Chain	Res	Type	RSRZ
1	8	149	GLY	29.7
4	q	575	GLU	29.4
1	k	188	VAL	29.4
1	c	149	GLY	29.4
1	A	188	VAL	29.3
1	A	130	GLU	29.3
1	V	212	ASP	28.8
4	o	603	ARG	28.7
1	5	170	PRO	28.6
1	g	149	GLY	28.5
4	q	906	PHE	28.4
1	g	178	GLN	28.3
1	4	186	THR	28.1
4	o	536	THR	27.7
1	E	188	VAL	27.5
1	R	208	PRO	27.3
1	M	222	GLY	27.0
1	4	188	VAL	27.0
1	l	128	VAL	26.9
1	N	128	VAL	26.5
1	I	205	ALA	26.4
1	c	148	ALA	26.3
4	q	574	GLU	26.2
4	o	581	ASP	26.1
1	M	171	GLU	25.9
1	I	209	GLY	25.8
1	I	158	THR	25.7
1	S	187	ASN	25.7
1	1	133	GLU	25.7
1	A	159	GLU	25.5
1	h	180	LEU	25.3
1	A	227	THR	25.3
1	N	129	GLU	25.3
1	9	191	GLU	25.3
4	q	576	VAL	25.2
1	S	228	ARG	25.2
1	R	181	ASN	25.2
1	M	129	GLU	25.0
4	o	562	ARG	25.0
1	M	149	GLY	25.0
1	R	226	SER	25.0
1	4	159	GLU	25.0

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Mol	Chain	Res	Type	RSRZ
4	o	551	LEU	25.0
1	A	168	THR	24.9
1	A	161	LYS	24.8
1	g	185	GLY	24.8
1	E	209	GLY	24.7
4	q	570	ASP	24.7
1	M	142	THR	24.6
1	V	204	LYS	24.6
4	q	609	SER	24.3
1	I	151	GLU	24.3
1	9	129	GLU	24.3
1	h	169	HIS	24.2
1	E	186	THR	24.2
1	d	186	THR	24.2
1	8	144	HIS	24.2
1	R	136	GLY	23.9
1	B	130	GLU	23.8
1	E	201	ARG	23.7
1	c	185	GLY	23.7
1	h	212	ASP	23.6
1	V	201	ARG	23.6
1	A	151	GLU	23.4
1	9	171	GLU	23.0
1	c	178	GLN	22.9
1	R	205	ALA	22.8
1	I	200	ARG	22.8
1	I	203	ARG	22.7
1	h	128	VAL	22.7
1	V	169	HIS	22.7
1	g	145	ARG	22.5
1	F	211	HIS	22.5
1	h	173	VAL	22.5
1	N	199	ILE	22.5
1	d	192	ASP	22.4
4	o	537	THR	22.4
1	8	172	ARG	22.3
1	4	140	ASP	22.2
1	B	161	LYS	22.1
1	F	187	ASN	22.0
1	d	183	VAL	21.9
1	5	229	PHE	21.9
1	N	229	PHE	21.9

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Mol	Chain	Res	Type	RSRZ
1	V	151	GLU	21.7
1	R	164	HIS	21.7
1	k	225	PHE	21.7
1	g	158	THR	21.6
1	k	150	GLU	21.6
1	g	143	SER	21.5
1	d	129	GLU	21.4
1	J	223	TYR	21.2
1	N	173	VAL	21.2
1	9	186	THR	21.1
1	N	131	VAL	21.1
1	F	213	ARG	21.1
1	A	182	HIS	21.0
1	g	148	ALA	20.9
1	R	185	GLY	20.9
1	d	228	ARG	20.8
1	9	212	ASP	20.7
1	E	150	GLU	20.7
1	5	129	GLU	20.7
1	M	183	VAL	20.7
4	o	539	SER	20.7
1	I	142	THR	20.6
1	W	146	VAL	20.5
1	M	148	ALA	20.5
1	B	224	ARG	20.5
1	d	149	GLY	20.4
1	J	132	ILE	20.4
1	l	220	GLY	20.4
1	9	210	GLY	20.4
1	A	131	VAL	20.3
1	E	227	THR	20.3
1	J	130	GLU	20.1
1	V	158	THR	19.9
1	9	169	HIS	19.9
1	E	185	GLY	19.8
1	c	205	ALA	19.8
4	q	533	ASP	19.8
1	1	203	ARG	19.7
1	S	229	PHE	19.7
1	F	186	THR	19.7
1	S	209	GLY	19.7
1	5	189	TYR	19.7

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Mol	Chain	Res	Type	RSRZ
1	R	171	GLU	19.6
1	M	184	TRP	19.5
1	S	157	PRO	19.5
1	g	157	PRO	19.5
1	I	173	VAL	19.5
1	4	182	HIS	19.5
1	A	158	THR	19.5
1	I	171	GLU	19.3
1	8	148	ALA	19.2
1	R	222	GLY	19.2
1	k	157	PRO	19.2
1	1	132	ILE	19.2
1	S	186	THR	19.2
1	E	129	GLU	19.1
4	o	602	SER	19.1
1	E	225	PHE	19.1
1	k	178	GLN	19.0
1	F	228	ARG	19.0
1	k	174	TYR	19.0
1	A	205	ALA	18.9
4	o	897	PRO	18.9
1	B	209	GLY	18.9
1	S	181	ASN	18.9
1	Z	210	GLY	18.8
1	4	143	SER	18.8
1	h	219	ARG	18.8
1	h	183	VAL	18.7
1	M	139	LEU	18.7
1	k	149	GLY	18.7
1	V	130	GLU	18.7
1	N	174	TYR	18.6
1	M	158	THR	18.6
1	d	203	ARG	18.5
1	E	181	ASN	18.5
1	h	181	ASN	18.5
1	d	212	ASP	18.5
1	c	177	GLU	18.5
1	9	181	ASN	18.4
1	l	190	VAL	18.4
1	d	204	LYS	18.4
1	W	212	ASP	18.4
1	S	183	VAL	18.3

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Mol	Chain	Res	Type	RSRZ
1	V	191	GLU	18.3
1	M	161	LYS	18.2
1	k	128	VAL	18.2
1	F	181	ASN	18.1
1	S	213	ARG	18.1
1	J	164	HIS	18.1
1	N	203	ARG	18.1
1	4	157	PRO	18.0
1	5	158	THR	17.9
4	o	569	THR	17.9
1	E	228	ARG	17.9
4	o	532	MET	17.9
1	V	206	LEU	17.9
1	1	225	PHE	17.9
1	8	225	PHE	17.9
1	8	142	THR	17.9
1	A	129	GLU	17.8
1	9	158	THR	17.8
1	I	169	HIS	17.8
1	l	130	GLU	17.7
1	h	129	GLU	17.6
1	k	148	ALA	17.6
1	B	212	ASP	17.6
1	9	130	GLU	17.6
1	W	229	PHE	17.6
1	5	155	MET	17.5
1	N	222	GLY	17.5
1	k	227	THR	17.5
4	o	564	GLY	17.5
1	4	185	GLY	17.4
1	J	133	GLU	17.4
1	h	178	GLN	17.4
1	l	186	THR	17.4
1	d	130	GLU	17.3
1	k	189	TYR	17.3
1	F	151	GLU	17.3
1	1	227	THR	17.3
1	J	157	PRO	17.2
1	W	157	PRO	17.2
1	h	192	ASP	17.2
1	A	149	GLY	17.2
1	g	190	VAL	17.2

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Mol	Chain	Res	Type	RSRZ
1	I	130	GLU	17.2
1	Z	200	ARG	17.2
1	R	170	PRO	17.1
1	I	172	ARG	17.1
1	A	140	ASP	17.1
1	V	152	PRO	17.1
1	c	186	THR	17.1
1	Z	226	SER	17.0
1	E	184	TRP	17.0
1	B	150	GLU	17.0
1	S	221	THR	17.0
1	B	159	GLU	17.0
1	M	157	PRO	17.0
1	c	151	GLU	17.0
1	c	201	ARG	16.9
1	R	169	HIS	16.9
1	d	173	VAL	16.8
1	1	152	PRO	16.8
4	o	567	MET	16.8
1	R	187	ASN	16.8
1	A	187	ASN	16.8
1	h	211	HIS	16.8
1	1	221	THR	16.7
1	5	177	GLU	16.7
1	8	213	ARG	16.7
1	F	158	THR	16.7
1	B	205	ALA	16.7
1	Z	216	GLN	16.6
1	d	158	THR	16.6
1	E	173	VAL	16.6
1	9	155	MET	16.6
1	E	190	VAL	16.6
1	8	130	GLU	16.6
1	g	189	TYR	16.6
1	h	204	LYS	16.6
1	Z	202	LEU	16.5
1	M	130	GLU	16.5
1	g	192	ASP	16.5
1	E	226	SER	16.5
1	1	222	GLY	16.4
1	E	157	PRO	16.4
1	5	159	GLU	16.4

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Mol	Chain	Res	Type	RSRZ
1	N	180	LEU	16.4
1	W	164	HIS	16.4
1	W	149	GLY	16.4
1	I	226	SER	16.4
1	V	157	PRO	16.3
1	g	184	TRP	16.3
1	c	183	VAL	16.2
1	N	183	VAL	16.2
1	R	159	GLU	16.2
1	1	229	PHE	16.2
1	h	182	HIS	16.2
1	F	227	THR	16.2
1	S	210	GLY	16.1
1	A	160	PHE	16.1
1	1	186	THR	16.1
1	A	142	THR	16.1
1	9	170	PRO	16.1
1	l	219	ARG	16.1
1	l	227	THR	16.0
1	S	205	ALA	15.9
1	d	227	THR	15.9
1	1	205	ALA	15.9
1	M	175	SER	15.9
1	1	185	GLY	15.9
1	Z	177	GLU	15.9
1	Z	214	MET	15.9
1	8	159	GLU	15.8
1	J	205	ALA	15.8
1	c	200	ARG	15.8
1	J	222	GLY	15.7
1	F	182	HIS	15.7
1	F	205	ALA	15.7
1	B	158	THR	15.7
1	A	226	SER	15.7
1	Z	145	ARG	15.7
1	5	150	GLU	15.6
1	c	142	THR	15.6
1	1	183	VAL	15.6
4	q	532	MET	15.6
1	g	130	GLU	15.5
1	9	180	LEU	15.5
1	9	172	ARG	15.5

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Mol	Chain	Res	Type	RSRZ
1	Z	223	TYR	15.5
4	q	551	LEU	15.5
1	l	177	GLU	15.5
4	q	539	SER	15.4
1	8	186	THR	15.4
1	E	205	ALA	15.4
1	h	186	THR	15.4
1	l	150	GLU	15.4
1	I	210	GLY	15.4
1	d	159	GLU	15.3
1	d	229	PHE	15.3
1	E	141	PRO	15.3
1	S	140	ASP	15.3
1	J	226	SER	15.3
1	E	200	ARG	15.3
1	d	169	HIS	15.3
1	8	181	ASN	15.3
1	V	173	VAL	15.2
1	Z	183	VAL	15.2
1	k	145	ARG	15.2
1	R	227	THR	15.2
1	d	181	ASN	15.2
1	k	226	SER	15.2
1	F	207	GLU	15.2
1	E	213	ARG	15.1
1	4	158	THR	15.1
4	o	573	LEU	15.1
1	8	210	GLY	15.1
1	M	136	GLY	15.1
1	d	180	LEU	15.1
1	W	187	ASN	15.0
1	M	186	THR	15.0
1	V	190	VAL	15.0
1	g	147	MET	15.0
1	I	213	ARG	15.0
1	g	170	PRO	15.0
1	Z	128	VAL	15.0
1	R	225	PHE	15.0
1	8	152	PRO	14.9
1	B	149	GLY	14.9
1	4	181	ASN	14.9
1	l	159	GLU	14.9

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Mol	Chain	Res	Type	RSRZ
1	V	210	GLY	14.9
1	Z	181	ASN	14.9
1	4	190	VAL	14.9
1	I	190	VAL	14.8
1	9	205	ALA	14.8
1	k	140	ASP	14.8
1	R	186	THR	14.8
1	N	170	PRO	14.8
4	q	550	GLY	14.8
1	h	131	VAL	14.7
1	A	197	VAL	14.7
1	c	210	GLY	14.6
4	q	905	ILE	14.6
1	V	131	VAL	14.6
1	l	170	PRO	14.6
1	S	158	THR	14.6
1	5	187	ASN	14.6
1	8	222	GLY	14.6
1	B	229	PHE	14.6
1	h	191	GLU	14.6
1	h	177	GLU	14.6
1	R	157	PRO	14.5
1	B	129	GLU	14.5
1	l	210	GLY	14.5
1	M	224	ARG	14.5
1	l	148	ALA	14.5
1	N	155	MET	14.4
1	Z	190	VAL	14.4
1	V	172	ARG	14.4
1	B	189	TYR	14.3
1	F	164	HIS	14.3
1	8	143	SER	14.3
1	I	131	VAL	14.3
1	F	196	ASP	14.3
4	q	552	THR	14.3
1	4	178	GLN	14.3
1	c	140	ASP	14.3
1	M	200	ARG	14.2
1	Z	186	THR	14.2
1	B	200	ARG	14.2
1	R	196	ASP	14.2
1	h	205	ALA	14.2

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Mol	Chain	Res	Type	RSRZ
1	8	140	ASP	14.1
1	Z	187	ASN	14.1
1	9	213	ARG	14.1
1	k	186	THR	14.1
4	q	600	HIS	14.1
1	d	139	LEU	14.1
1	1	151	GLU	14.0
1	S	184	TRP	14.0
1	W	158	THR	14.0
1	J	149	GLY	14.0
1	S	222	GLY	14.0
1	c	158	THR	14.0
1	Z	224	ARG	14.0
4	o	904	ALA	14.0
1	g	191	GLU	13.9
1	E	182	HIS	13.9
1	A	186	THR	13.9
1	h	213	ARG	13.9
1	1	181	ASN	13.9
4	o	568	ASN	13.9
1	R	142	THR	13.9
1	5	205	ALA	13.9
1	M	205	ALA	13.8
1	c	187	ASN	13.8
1	V	175	SER	13.8
1	c	175	SER	13.8
1	J	227	THR	13.8
1	B	148	ALA	13.8
1	R	188	VAL	13.8
1	V	142	THR	13.8
1	l	182	HIS	13.7
1	F	209	GLY	13.7
1	Z	159	GLU	13.7
1	k	207	GLU	13.7
1	Z	173	VAL	13.7
1	8	215	VAL	13.6
1	N	205	ALA	13.6
1	5	178	GLN	13.6
1	M	143	SER	13.6
1	g	171	GLU	13.6
1	V	128	VAL	13.6
1	c	209	GLY	13.6

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Mol	Chain	Res	Type	RSRZ
1	J	229	PHE	13.6
1	d	156	GLY	13.6
1	E	176	ARG	13.6
1	W	181	ASN	13.6
1	W	182	HIS	13.6
1	g	205	ALA	13.6
1	4	212	ASP	13.5
1	d	131	VAL	13.5
1	W	186	THR	13.5
1	N	218	VAL	13.5
1	d	221	THR	13.5
1	V	226	SER	13.5
1	R	178	GLN	13.5
1	Z	184	TRP	13.5
1	h	156	GLY	13.5
1	I	181	ASN	13.5
1	W	222	GLY	13.5
1	k	158	THR	13.5
1	W	151	GLU	13.4
1	A	164	HIS	13.4
1	B	175	SER	13.4
1	W	140	ASP	13.4
1	h	170	PRO	13.4
1	c	225	PHE	13.4
1	M	173	VAL	13.4
1	5	207	GLU	13.4
1	I	143	SER	13.3
4	o	899	GLU	13.3
1	A	209	GLY	13.3
1	d	187	ASN	13.3
1	I	129	GLU	13.3
1	W	227	THR	13.3
1	V	182	HIS	13.3
1	4	128	VAL	13.3
1	8	189	TYR	13.3
1	5	130	GLU	13.2
1	d	191	GLU	13.2
1	h	222	GLY	13.2
4	q	604	SER	13.2
1	S	170	PRO	13.2
1	5	206	LEU	13.2
1	V	200	ARG	13.2

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Mol	Chain	Res	Type	RSRZ
4	o	535	ALA	13.2
1	Z	149	GLY	13.2
1	l	205	ALA	13.1
1	Z	185	GLY	13.1
1	g	200	ARG	13.1
1	c	184	TRP	13.1
1	c	191	GLU	13.1
1	N	157	PRO	13.1
1	8	157	PRO	13.1
1	F	155	MET	13.1
1	W	148	ALA	13.1
1	1	188	VAL	13.1
1	l	206	LEU	13.0
1	5	161	LYS	13.0
1	I	229	PHE	13.0
4	o	896	THR	13.0
1	S	161	LYS	13.0
1	Z	196	ASP	13.0
1	8	188	VAL	13.0
4	q	553	ALA	12.9
1	J	203	ARG	12.9
1	N	224	ARG	12.9
1	V	203	ARG	12.9
1	B	204	LYS	12.9
1	9	219	ARG	12.9
1	g	159	GLU	12.9
1	l	222	GLY	12.9
1	S	164	HIS	12.9
1	Z	182	HIS	12.8
1	5	204	LYS	12.8
1	h	221	THR	12.8
1	V	140	ASP	12.8
1	l	213	ARG	12.8
1	d	157	PRO	12.8
1	F	161	LYS	12.8
1	J	161	LYS	12.8
1	V	208	PRO	12.8
1	E	212	ASP	12.8
1	B	171	GLU	12.8
1	d	226	SER	12.8
1	J	183	VAL	12.7
1	k	159	GLU	12.7

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Mol	Chain	Res	Type	RSRZ
4	q	581	ASP	12.7
1	N	130	GLU	12.7
1	A	206	LEU	12.7
1	A	143	SER	12.7
1	N	190	VAL	12.6
1	k	181	ASN	12.6
1	k	213	ARG	12.6
1	V	171	GLU	12.6
1	8	150	GLU	12.6
1	5	151	GLU	12.6
4	q	538	GLU	12.6
1	8	187	ASN	12.6
1	A	204	LYS	12.6
1	9	141	PRO	12.6
1	F	191	GLU	12.5
1	F	149	GLY	12.5
1	c	213	ARG	12.5
1	9	207	GLU	12.5
1	E	187	ASN	12.5
1	5	190	VAL	12.5
1	R	158	THR	12.5
1	I	157	PRO	12.5
1	l	204	LYS	12.5
1	l	171	GLU	12.4
1	S	128	VAL	12.4
1	F	225	PHE	12.4
1	5	164	HIS	12.4
1	9	206	LEU	12.4
1	N	182	HIS	12.4
1	c	224	ARG	12.4
1	F	204	LYS	12.4
1	Z	205	ALA	12.4
1	c	207	GLU	12.3
1	9	228	ARG	12.3
1	B	187	ASN	12.3
1	I	148	ALA	12.3
1	4	161	LYS	12.3
1	d	182	HIS	12.3
1	k	183	VAL	12.3
1	9	203	ARG	12.3
1	h	203	ARG	12.3
1	S	185	GLY	12.2

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Mol	Chain	Res	Type	RSRZ
1	J	181	ASN	12.2
4	o	910	ALA	12.2
1	S	129	GLU	12.2
1	I	155	MET	12.2
1	d	219	ARG	12.2
1	E	222	GLY	12.2
1	F	157	PRO	12.2
1	1	149	GLY	12.2
1	c	157	PRO	12.2
1	d	188	VAL	12.2
1	W	150	GLU	12.2
1	N	169	HIS	12.2
1	E	207	GLU	12.2
1	R	212	ASP	12.1
1	J	170	PRO	12.1
1	g	204	LYS	12.1
1	8	214	MET	12.1
1	5	222	GLY	12.1
1	F	208	PRO	12.1
1	I	212	ASP	12.1
4	q	548	LEU	12.1
1	1	130	GLU	12.1
1	k	177	GLU	12.1
1	R	221	THR	12.0
1	I	176	ARG	12.0
4	o	607	LEU	12.0
1	d	185	GLY	12.0
1	B	160	PHE	12.0
1	J	146	VAL	12.0
1	I	159	GLU	12.0
1	g	150	GLU	12.0
4	o	565	ILE	12.0
1	F	210	GLY	11.9
1	N	192	ASP	11.9
1	N	208	PRO	11.9
1	I	197	VAL	11.9
1	9	168	THR	11.9
1	B	225	PHE	11.9
1	S	226	SER	11.9
1	J	148	ALA	11.9
4	o	549	ALA	11.9
1	F	150	GLU	11.9

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Mol	Chain	Res	Type	RSRZ
1	F	183	VAL	11.8
1	8	185	GLY	11.8
1	J	189	TYR	11.8
1	1	157	PRO	11.8
1	W	190	VAL	11.7
1	E	149	GLY	11.7
1	S	149	GLY	11.7
1	A	174	TYR	11.7
1	F	221	THR	11.7
1	M	131	VAL	11.7
1	R	183	VAL	11.7
4	o	534	SER	11.7
1	h	158	THR	11.7
1	A	225	PHE	11.7
1	k	187	ASN	11.7
1	4	175	SER	11.7
1	8	128	VAL	11.7
1	g	131	VAL	11.7
1	E	151	GLU	11.7
1	R	175	SER	11.7
1	N	191	GLU	11.6
1	Z	211	HIS	11.6
1	8	174	TYR	11.6
1	9	160	PHE	11.6
1	F	203	ARG	11.6
1	g	172	ARG	11.6
1	N	159	GLU	11.6
1	1	184	TRP	11.6
4	o	552	THR	11.6
1	S	130	GLU	11.6
1	4	197	VAL	11.6
1	N	181	ASN	11.6
1	J	158	THR	11.5
1	M	212	ASP	11.5
1	Z	143	SER	11.5
1	c	176	ARG	11.5
1	W	206	LEU	11.5
1	F	159	GLU	11.5
1	W	205	ALA	11.5
1	B	157	PRO	11.5
1	I	180	LEU	11.5
4	q	602	SER	11.5

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Mol	Chain	Res	Type	RSRZ
1	F	130	GLU	11.5
1	c	222	GLY	11.5
1	J	228	ARG	11.5
1	R	190	VAL	11.5
1	S	204	LYS	11.4
1	M	138	SER	11.4
1	5	210	GLY	11.4
1	g	203	ARG	11.4
1	M	203	ARG	11.4
1	k	210	GLY	11.4
1	E	148	ALA	11.4
1	M	211	HIS	11.4
1	N	184	TRP	11.4
1	F	185	GLY	11.4
1	M	196	ASP	11.4
1	E	183	VAL	11.4
1	k	200	ARG	11.4
1	c	204	LYS	11.4
1	B	210	GLY	11.4
1	4	144	HIS	11.3
1	F	190	VAL	11.3
1	I	221	THR	11.3
1	F	140	ASP	11.3
1	A	223	TYR	11.3
1	N	171	GLU	11.3
1	c	159	GLU	11.3
4	q	549	ALA	11.3
1	c	227	THR	11.3
1	h	227	THR	11.3
1	c	203	ARG	11.3
1	5	149	GLY	11.3
1	9	229	PHE	11.3
1	g	187	ASN	11.3
1	M	180	LEU	11.3
1	M	187	ASN	11.2
1	d	222	GLY	11.2
1	E	224	ARG	11.2
1	N	219	ARG	11.2
4	q	580	PHE	11.2
1	k	196	ASP	11.2
1	9	218	VAL	11.2
1	I	170	PRO	11.1

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Mol	Chain	Res	Type	RSRZ
1	5	225	PHE	11.1
1	E	175	SER	11.1
4	q	534	SER	11.1
1	1	155	MET	11.1
1	c	171	GLU	11.1
1	g	210	GLY	11.1
1	E	169	HIS	11.1
1	d	128	VAL	11.1
1	N	207	GLU	11.1
1	S	151	GLU	11.1
1	V	229	PHE	11.1
1	W	203	ARG	11.1
1	I	192	ASP	11.0
1	l	172	ARG	11.0
1	N	151	GLU	11.0
1	R	184	TRP	11.0
4	q	573	LEU	11.0
1	A	201	ARG	11.0
1	B	207	GLU	11.0
1	c	212	ASP	11.0
4	q	562	ARG	11.0
1	1	204	LYS	11.0
1	4	171	GLU	11.0
1	4	210	GLY	11.0
1	A	175	SER	11.0
1	V	222	GLY	11.0
1	5	224	ARG	11.0
1	S	139	LEU	10.9
1	8	204	LYS	10.9
1	E	158	THR	10.9
1	l	203	ARG	10.9
1	k	131	VAL	10.9
1	1	207	GLU	10.9
1	Z	131	VAL	10.9
1	E	210	GLY	10.9
1	l	178	GLN	10.9
1	Z	130	GLU	10.9
1	N	213	ARG	10.9
1	Z	142	THR	10.9
1	M	181	ASN	10.8
1	g	188	VAL	10.8
1	F	229	PHE	10.8

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Mol	Chain	Res	Type	RSRZ
1	N	212	ASP	10.8
1	8	224	ARG	10.8
1	V	181	ASN	10.8
1	d	207	GLU	10.8
1	M	141	PRO	10.8
1	5	131	VAL	10.8
1	5	173	VAL	10.8
1	9	175	SER	10.8
1	E	172	ARG	10.8
1	Z	157	PRO	10.8
1	M	172	ARG	10.8
1	F	129	GLU	10.8
1	9	221	THR	10.8
1	R	180	LEU	10.8
1	5	220	GLY	10.7
4	o	566	ASP	10.7
1	A	214	MET	10.7
1	9	204	LYS	10.7
1	N	136	GLY	10.7
1	4	184	TRP	10.7
1	9	164	HIS	10.7
4	q	896	THR	10.7
1	B	186	THR	10.6
1	5	157	PRO	10.6
1	J	159	GLU	10.6
1	N	226	SER	10.6
1	S	225	PHE	10.6
1	d	165	PHE	10.6
1	l	181	ASN	10.6
1	g	177	GLU	10.6
1	8	212	ASP	10.6
1	R	204	LYS	10.6
1	F	132	ILE	10.6
4	o	540	LEU	10.6
1	R	148	ALA	10.6
1	h	175	SER	10.6
1	k	144	HIS	10.6
1	J	186	THR	10.6
1	k	191	GLU	10.6
1	h	174	TYR	10.6
1	k	180	LEU	10.6
1	1	156	GLY	10.5

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Mol	Chain	Res	Type	RSRZ
1	I	184	TRP	10.5
1	c	155	MET	10.5
1	B	203	ARG	10.5
1	J	138	SER	10.5
1	A	212	ASP	10.5
1	J	213	ARG	10.5
1	1	200	ARG	10.5
1	9	157	PRO	10.5
1	B	164	HIS	10.5
1	Z	206	LEU	10.5
1	V	227	THR	10.5
1	E	180	LEU	10.5
1	M	207	GLU	10.5
1	R	173	VAL	10.5
1	g	151	GLU	10.5
1	5	186	THR	10.5
1	h	206	LEU	10.4
1	1	190	VAL	10.4
1	8	161	LYS	10.4
1	B	140	ASP	10.4
1	N	196	ASP	10.4
1	l	221	THR	10.4
1	g	142	THR	10.4
1	M	225	PHE	10.4
1	8	203	ARG	10.4
1	E	214	MET	10.4
1	h	130	GLU	10.4
1	A	184	TRP	10.4
1	Z	207	GLU	10.4
1	c	131	VAL	10.4
1	d	155	MET	10.4
1	c	208	PRO	10.4
1	8	191	GLU	10.4
1	B	128	VAL	10.4
1	9	227	THR	10.3
1	h	176	ARG	10.3
1	E	229	PHE	10.3
1	c	170	PRO	10.3
1	9	151	GLU	10.3
1	g	141	PRO	10.3
1	N	161	LYS	10.3
1	S	141	PRO	10.3

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Mol	Chain	Res	Type	RSRZ
1	J	201	ARG	10.3
1	4	203	ARG	10.3
1	S	220	GLY	10.3
1	R	197	VAL	10.3
1	M	201	ARG	10.3
1	J	212	ASP	10.3
1	N	227	THR	10.3
1	8	211	HIS	10.2
4	o	576	VAL	10.2
1	4	164	HIS	10.2
1	S	180	LEU	10.2
1	N	200	ARG	10.2
1	g	224	ARG	10.2
1	I	132	ILE	10.2
1	A	185	GLY	10.2
1	9	202	LEU	10.2
1	E	221	THR	10.2
1	g	186	THR	10.2
1	R	189	TYR	10.2
1	N	152	PRO	10.2
1	4	201	ARG	10.2
1	k	205	ALA	10.2
1	l	207	GLU	10.2
1	A	208	PRO	10.2
1	W	204	LYS	10.2
1	8	131	VAL	10.1
4	o	580	PHE	10.2
1	F	141	PRO	10.1
1	g	212	ASP	10.1
4	q	535	ALA	10.1
1	I	141	PRO	10.1
1	F	131	VAL	10.0
1	R	149	GLY	10.0
1	9	176	ARG	10.0
1	k	212	ASP	10.0
1	g	226	SER	10.0
1	N	221	THR	10.0
1	4	207	GLU	10.0
1	E	140	ASP	10.0
1	W	223	TYR	10.0
1	g	218	VAL	10.0
1	l	131	VAL	10.0

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Mol	Chain	Res	Type	RSRZ
1	8	178	GLN	10.0
1	J	204	LYS	10.0
1	4	170	PRO	10.0
1	5	203	ARG	10.0
1	R	130	GLU	9.9
1	F	222	GLY	9.9
1	W	173	VAL	9.9
1	W	130	GLU	9.9
1	F	148	ALA	9.9
1	E	197	VAL	9.9
1	W	226	SER	9.9
1	S	159	GLU	9.8
1	c	128	VAL	9.8
1	Z	158	THR	9.8
4	o	553	ALA	9.8
1	B	173	VAL	9.8
1	R	210	GLY	9.8
1	1	131	VAL	9.8
1	h	210	GLY	9.8
1	8	190	VAL	9.8
1	I	191	GLU	9.8
1	J	207	GLU	9.8
1	A	181	ASN	9.8
1	F	226	SER	9.8
1	l	183	VAL	9.8
1	I	214	MET	9.8
1	g	140	ASP	9.7
1	B	190	VAL	9.7
1	F	201	ARG	9.7
1	J	175	SER	9.7
1	J	140	ASP	9.7
1	I	211	HIS	9.7
1	d	211	HIS	9.7
1	V	180	LEU	9.7
1	8	158	THR	9.7
1	4	187	ASN	9.7
1	g	225	PHE	9.7
1	B	226	SER	9.7
1	N	204	LYS	9.6
1	k	170	PRO	9.6
1	c	226	SER	9.6
1	9	140	ASP	9.6

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Mol	Chain	Res	Type	RSRZ
1	N	225	PHE	9.6
1	9	177	GLU	9.6
1	5	197	VAL	9.6
1	N	165	PHE	9.6
1	8	227	THR	9.5
1	4	224	ARG	9.5
1	B	184	TRP	9.5
1	9	142	THR	9.5
4	q	545	HIS	9.5
1	M	210	GLY	9.5
1	Z	215	VAL	9.5
1	5	180	LEU	9.5
1	d	184	TRP	9.5
1	c	206	LEU	9.5
1	F	184	TRP	9.5
1	J	221	THR	9.5
1	W	143	SER	9.5
1	5	227	THR	9.5
1	B	206	LEU	9.4
1	I	178	GLN	9.4
1	I	187	ASN	9.4
4	q	569	THR	9.4
1	9	156	GLY	9.4
1	S	175	SER	9.4
1	S	150	GLU	9.4
1	4	177	GLU	9.4
1	5	226	SER	9.4
1	9	178	GLN	9.4
1	W	207	GLU	9.4
1	c	172	ARG	9.4
4	q	578	LYS	9.4
1	I	208	PRO	9.3
1	5	209	GLY	9.3
1	g	129	GLU	9.3
1	d	205	ALA	9.3
1	Z	171	GLU	9.3
1	k	155	MET	9.3
1	M	144	HIS	9.3
1	J	143	SER	9.3
1	V	178	GLN	9.3
1	Z	140	ASP	9.3
1	A	132	ILE	9.3

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Mol	Chain	Res	Type	RSRZ
4	o	597	LYS	9.3
1	A	173	VAL	9.3
1	V	159	GLU	9.3
1	F	200	ARG	9.3
1	4	206	LEU	9.3
1	B	131	VAL	9.3
1	E	203	ARG	9.3
1	d	170	PRO	9.3
1	F	212	ASP	9.2
1	l	140	ASP	9.2
1	1	142	THR	9.2
1	J	220	GLY	9.2
1	N	210	GLY	9.2
1	g	155	MET	9.2
1	E	142	THR	9.2
4	q	536	THR	9.2
1	k	184	TRP	9.2
1	W	129	GLU	9.2
1	4	191	GLU	9.2
1	h	155	MET	9.2
1	B	180	LEU	9.2
1	g	201	ARG	9.2
4	q	593	LYS	9.2
1	c	197	VAL	9.1
1	R	207	GLU	9.1
1	h	150	GLU	9.1
1	W	131	VAL	9.1
1	9	187	ASN	9.1
1	Z	148	ALA	9.1
1	N	142	THR	9.1
1	S	148	ALA	9.1
1	4	189	TYR	9.1
1	W	201	ARG	9.1
1	d	210	GLY	9.1
1	5	132	ILE	9.1
1	4	151	GLU	9.0
1	g	156	GLY	9.0
1	Z	180	LEU	9.0
4	o	900	LYS	9.0
1	d	172	ARG	9.0
4	q	900	LYS	9.0
1	B	182	HIS	9.0

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Mol	Chain	Res	Type	RSRZ
1	F	206	LEU	9.0
1	d	190	VAL	9.0
1	A	213	ARG	9.0
1	8	180	LEU	8.9
1	4	156	GLY	8.9
1	Z	150	GLU	8.9
1	d	218	VAL	8.9
1	5	181	ASN	8.9
1	S	206	LEU	8.9
1	c	161	LYS	8.9
4	q	904	ALA	8.9
1	8	200	ARG	8.9
1	J	180	LEU	8.9
1	4	214	MET	8.9
1	I	175	SER	8.9
1	k	136	GLY	8.8
1	Z	201	ARG	8.8
1	c	192	ASP	8.8
1	B	215	VAL	8.8
1	W	218	VAL	8.8
1	S	207	GLU	8.8
1	h	133	GLU	8.8
1	I	144	HIS	8.8
1	8	134	MET	8.8
1	A	144	HIS	8.8
1	V	185	GLY	8.8
1	A	203	ARG	8.8
1	h	132	ILE	8.8
1	W	141	PRO	8.8
1	V	177	GLU	8.8
1	8	226	SER	8.8
1	A	221	THR	8.8
1	k	185	GLY	8.8
1	l	185	GLY	8.8
1	I	149	GLY	8.8
1	S	203	ARG	8.8
1	k	214	MET	8.7
1	5	182	HIS	8.7
1	h	179	LEU	8.7
1	E	130	GLU	8.7
1	c	150	GLU	8.7
1	A	178	GLN	8.7

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Mol	Chain	Res	Type	RSRZ
1	I	188	VAL	8.7
1	l	180	LEU	8.7
1	V	174	TYR	8.7
1	4	228	ARG	8.7
1	W	220	GLY	8.7
1	l	228	ARG	8.7
1	F	162	LEU	8.7
1	B	216	GLN	8.7
1	B	222	GLY	8.7
1	I	222	GLY	8.7
1	k	173	VAL	8.7
1	A	207	GLU	8.6
1	5	208	PRO	8.6
1	1	210	GLY	8.6
1	5	128	VAL	8.6
1	R	211	HIS	8.6
1	J	162	LEU	8.6
1	S	208	PRO	8.6
1	h	153	LEU	8.6
1	9	183	VAL	8.6
1	V	145	ARG	8.6
1	k	182	HIS	8.6
4	q	594	ALA	8.6
4	q	546	ASP	8.6
1	S	189	TYR	8.6
1	c	132	ILE	8.5
1	M	190	VAL	8.5
1	c	194	THR	8.5
1	k	204	LYS	8.5
1	F	220	GLY	8.5
1	W	159	GLU	8.5
1	I	207	GLU	8.5
1	k	171	GLU	8.5
1	d	194	THR	8.5
1	R	201	ARG	8.5
4	o	903	ARG	8.5
1	M	182	HIS	8.5
1	J	218	VAL	8.5
1	5	219	ARG	8.4
1	1	212	ASP	8.4
1	c	229	PHE	8.4
1	k	203	ARG	8.4

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Mol	Chain	Res	Type	RSRZ
1	R	161	LYS	8.4
1	E	143	SER	8.4
1	V	143	SER	8.4
1	1	206	LEU	8.4
1	F	154	GLU	8.4
1	h	164	HIS	8.4
1	N	156	GLY	8.4
1	J	151	GLU	8.4
1	S	143	SER	8.4
1	c	211	HIS	8.4
1	R	213	ARG	8.4
1	V	213	ARG	8.4
1	R	176	ARG	8.4
1	c	143	SER	8.4
1	A	210	GLY	8.4
1	d	146	VAL	8.3
1	l	154	GLU	8.3
1	J	182	HIS	8.3
1	M	189	TYR	8.3
1	R	143	SER	8.3
1	9	153	LEU	8.3
1	8	173	VAL	8.3
1	R	200	ARG	8.3
1	W	171	GLU	8.3
4	o	589	GLN	8.3
1	Z	213	ARG	8.3
1	g	161	LYS	8.3
1	h	165	PHE	8.2
1	c	214	MET	8.2
1	c	220	GLY	8.2
1	F	170	PRO	8.2
1	I	206	LEU	8.2
1	J	219	ARG	8.2
1	5	200	ARG	8.2
1	A	222	GLY	8.2
1	9	185	GLY	8.2
1	M	213	ARG	8.2
1	S	147	MET	8.2
1	W	170	PRO	8.2
1	4	211	HIS	8.2
1	B	220	GLY	8.2
1	E	206	LEU	8.2

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Mol	Chain	Res	Type	RSRZ
1	l	229	PHE	8.2
1	W	219	ARG	8.2
1	g	229	PHE	8.2
1	A	157	PRO	8.2
1	R	229	PHE	8.2
1	h	148	ALA	8.1
1	E	204	LYS	8.1
1	5	221	THR	8.1
1	A	148	ALA	8.1
1	4	167	MET	8.1
1	N	132	ILE	8.1
1	5	175	SER	8.1
1	8	206	LEU	8.1
4	o	587	ILE	8.1
1	d	213	ARG	8.1
1	S	190	VAL	8.1
4	o	606	VAL	8.1
1	F	180	LEU	8.1
1	1	153	LEU	8.1
1	k	143	SER	8.1
1	1	169	HIS	8.1
1	N	141	PRO	8.1
1	R	177	GLU	8.1
1	h	161	LYS	8.1
1	V	170	PRO	8.1
1	Z	229	PHE	8.1
4	o	906	PHE	8.1
1	W	183	VAL	8.0
1	E	155	MET	8.0
1	V	209	GLY	8.0
1	Z	189	TYR	8.0
1	g	152	PRO	8.0
1	V	176	ARG	8.0
1	Z	212	ASP	8.0
1	5	169	HIS	8.0
1	Z	170	PRO	8.0
1	4	227	THR	8.0
1	k	208	PRO	8.0
1	B	178	GLN	8.0
1	R	228	ARG	8.0
1	g	206	LEU	8.0
1	M	179	LEU	8.0

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Mol	Chain	Res	Type	RSRZ
1	R	191	GLU	8.0
4	o	555	GLU	8.0
1	1	178	GLN	8.0
1	J	187	ASN	7.9
4	o	582	VAL	7.9
1	V	149	GLY	7.9
4	q	566	ASP	7.9
1	V	211	HIS	7.9
1	l	155	MET	7.9
1	Z	175	SER	7.9
1	R	194	THR	7.9
1	B	219	ARG	7.9
1	8	154	GLU	7.9
1	8	177	GLU	7.9
1	A	170	PRO	7.9
1	h	157	PRO	7.9
1	8	182	HIS	7.9
1	5	202	LEU	7.9
1	E	159	GLU	7.9
1	1	170	PRO	7.9
1	W	155	MET	7.9
1	A	229	PHE	7.9
1	R	214	MET	7.9
1	S	197	VAL	7.8
1	d	206	LEU	7.8
1	4	222	GLY	7.8
1	d	220	GLY	7.8
1	B	151	GLU	7.8
1	R	219	ARG	7.8
1	1	182	HIS	7.8
1	5	188	VAL	7.8
1	c	141	PRO	7.8
1	9	143	SER	7.8
1	c	221	THR	7.8
1	S	131	VAL	7.8
1	F	214	MET	7.8
1	V	214	MET	7.8
1	l	139	LEU	7.8
1	E	178	GLN	7.8
1	I	177	GLU	7.8
1	M	226	SER	7.8
4	q	555	GLU	7.8

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Mol	Chain	Res	Type	RSRZ
1	J	190	VAL	7.8
1	l	173	VAL	7.8
1	M	156	GLY	7.7
1	Z	136	GLY	7.7
1	k	179	LEU	7.7
1	9	188	VAL	7.7
1	S	212	ASP	7.7
1	k	134	MET	7.7
1	A	191	GLU	7.7
4	q	585	GLU	7.7
1	F	143	SER	7.7
1	V	187	ASN	7.7
1	W	138	SER	7.7
1	d	153	LEU	7.7
1	g	181	ASN	7.7
4	q	590	ILE	7.7
1	J	209	GLY	7.7
1	V	197	VAL	7.7
1	9	220	GLY	7.7
1	S	177	GLU	7.7
1	1	180	LEU	7.7
1	F	189	TYR	7.6
1	V	188	VAL	7.6
1	E	191	GLU	7.6
1	A	141	PRO	7.6
1	k	206	LEU	7.6
4	q	599	ARG	7.6
1	I	227	THR	7.6
1	h	228	ARG	7.6
1	l	212	ASP	7.6
1	F	128	VAL	7.6
1	1	187	ASN	7.6
1	h	226	SER	7.6
1	M	185	GLY	7.6
4	q	563	PHE	7.5
1	B	155	MET	7.5
1	A	180	LEU	7.5
1	c	181	ASN	7.5
1	A	133	GLU	7.5
1	I	150	GLU	7.5
1	J	141	PRO	7.5
1	J	142	THR	7.5

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Mol	Chain	Res	Type	RSRZ
1	9	217	THR	7.5
1	M	208	PRO	7.5
1	4	141	PRO	7.5
1	d	208	PRO	7.5
1	M	191	GLU	7.5
1	J	160	PHE	7.5
1	M	206	LEU	7.5
1	W	142	THR	7.5
1	d	177	GLU	7.5
1	Z	174	TYR	7.5
1	J	194	THR	7.5
1	4	173	VAL	7.5
1	S	160	PHE	7.5
1	W	180	LEU	7.5
1	4	183	VAL	7.4
1	W	185	GLY	7.4
1	B	192	ASP	7.4
1	5	185	GLY	7.4
1	J	216	GLN	7.4
1	Z	227	THR	7.4
1	E	220	GLY	7.4
1	B	181	ASN	7.4
1	h	171	GLU	7.4
1	d	141	PRO	7.4
1	R	139	LEU	7.4
1	l	214	MET	7.3
1	M	216	GLN	7.3
1	d	209	GLY	7.3
1	A	220	GLY	7.3
1	B	194	THR	7.3
1	R	203	ARG	7.3
1	B	208	PRO	7.3
1	A	211	HIS	7.3
1	N	148	ALA	7.3
1	S	178	GLN	7.3
1	1	211	HIS	7.3
1	g	211	HIS	7.3
1	N	220	GLY	7.3
1	N	211	HIS	7.2
1	Z	169	HIS	7.2
1	9	208	PRO	7.2
1	d	152	PRO	7.2

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Mol	Chain	Res	Type	RSRZ
1	J	147	MET	7.2
1	B	143	SER	7.2
1	g	144	HIS	7.2
1	k	130	GLU	7.2
1	k	135	GLN	7.2
1	l	176	ARG	7.2
1	9	174	TYR	7.2
1	Z	138	SER	7.2
1	h	208	PRO	7.2
1	l	157	PRO	7.2
1	R	179	LEU	7.2
1	J	171	GLU	7.2
1	I	164	HIS	7.2
1	N	209	GLY	7.2
1	c	169	HIS	7.2
1	V	139	LEU	7.1
1	k	138	SER	7.1
1	5	191	GLU	7.1
1	9	222	GLY	7.1
1	1	165	PHE	7.1
1	Z	203	ARG	7.1
1	A	171	GLU	7.1
1	4	155	MET	7.1
4	o	594	ALA	7.1
1	Z	155	MET	7.1
4	o	898	GLU	7.1
1	l	217	THR	7.1
1	S	152	PRO	7.1
4	q	897	PRO	7.1
1	N	179	LEU	7.1
1	F	218	VAL	7.1
1	9	194	THR	7.1
1	g	207	GLU	7.1
1	I	182	HIS	7.1
1	F	223	TYR	7.0
1	1	154	GLU	7.0
1	l	192	ASP	7.0
2	e	4	DC	7.0
1	1	192	ASP	7.0
1	8	179	LEU	7.0
1	5	160	PHE	7.0
1	4	142	THR	7.0

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Mol	Chain	Res	Type	RSRZ
1	g	227	THR	7.0
1	1	197	VAL	7.0
1	9	214	MET	7.0
1	N	185	GLY	7.0
1	E	161	LYS	7.0
1	N	189	TYR	7.0
1	l	189	TYR	7.0
1	B	214	MET	7.0
1	1	226	SER	7.0
1	8	160	PHE	7.0
1	k	147	MET	7.0
1	J	191	GLU	7.0
1	1	168	THR	7.0
1	8	170	PRO	7.0
1	d	175	SER	7.0
1	l	175	SER	7.0
1	W	213	ARG	7.0
4	o	548	LEU	6.9
1	l	151	GLU	6.9
1	4	223	TYR	6.9
1	S	155	MET	6.9
1	1	214	MET	6.9
3	D	13	DA	6.9
1	E	145	ARG	6.9
1	B	188	VAL	6.9
1	9	209	GLY	6.9
1	h	159	GLU	6.9
1	k	172	ARG	6.9
1	M	197	VAL	6.9
1	V	179	LEU	6.9
1	E	219	ARG	6.9
1	g	209	GLY	6.9
1	I	174	TYR	6.9
1	9	149	GLY	6.8
1	g	208	PRO	6.8
1	l	156	GLY	6.8
1	4	147	MET	6.8
1	k	151	GLU	6.8
1	M	128	VAL	6.8
1	W	176	ARG	6.8
1	F	152	PRO	6.8
1	1	161	LYS	6.8

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Mol	Chain	Res	Type	RSRZ
1	8	205	ALA	6.8
1	d	171	GLU	6.8
1	V	129	GLU	6.8
1	E	144	HIS	6.8
1	W	228	ARG	6.8
1	N	158	THR	6.8
1	g	214	MET	6.8
1	M	204	LYS	6.8
1	W	153	LEU	6.7
1	5	148	ALA	6.7
1	9	159	GLU	6.7
1	h	223	TYR	6.7
1	g	197	VAL	6.7
1	h	152	PRO	6.7
1	h	142	THR	6.7
1	M	150	GLU	6.7
1	J	131	VAL	6.7
1	M	147	MET	6.7
1	R	160	PHE	6.7
1	S	216	GLN	6.7
1	B	197	VAL	6.7
1	V	144	HIS	6.7
1	4	149	GLY	6.7
1	N	228	ARG	6.7
1	M	174	TYR	6.7
1	5	156	GLY	6.7
1	5	228	ARG	6.7
1	S	217	THR	6.7
1	h	185	GLY	6.7
1	W	175	SER	6.7
1	4	225	PHE	6.7
1	B	141	PRO	6.6
1	S	182	HIS	6.6
1	W	128	VAL	6.6
1	8	207	GLU	6.6
1	M	169	HIS	6.6
1	F	197	VAL	6.6
1	J	184	TRP	6.6
1	B	147	MET	6.6
1	g	132	ILE	6.6
1	g	220	GLY	6.6
1	1	171	GLU	6.6

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Mol	Chain	Res	Type	RSRZ
1	9	165	PHE	6.6
1	V	183	VAL	6.6
1	E	170	PRO	6.6
1	l	143	SER	6.6
1	5	140	ASP	6.6
1	A	155	MET	6.6
1	Z	129	GLU	6.6
1	M	199	ILE	6.6
1	J	206	LEU	6.6
1	W	209	GLY	6.6
1	g	176	ARG	6.6
1	R	216	GLN	6.6
1	Z	179	LEU	6.5
1	9	223	TYR	6.5
4	o	593	LYS	6.5
1	N	186	THR	6.5
1	h	147	MET	6.5
1	A	200	ARG	6.5
1	k	201	ARG	6.5
4	q	554	ARG	6.5
1	J	185	GLY	6.5
4	q	588	ARG	6.5
1	J	165	PHE	6.5
1	W	188	VAL	6.5
1	9	152	PRO	6.5
1	B	165	PHE	6.5
1	V	225	PHE	6.5
1	k	229	PHE	6.5
1	W	214	MET	6.4
1	l	225	PHE	6.4
1	9	131	VAL	6.4
1	V	221	THR	6.4
1	1	194	THR	6.4
1	1	213	ARG	6.4
1	4	219	ARG	6.4
1	4	229	PHE	6.4
3	U	14	DA	6.4
1	V	148	ALA	6.4
1	R	141	PRO	6.4
1	l	158	THR	6.4
1	N	223	TYR	6.4
1	W	147	MET	6.4

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Mol	Chain	Res	Type	RSRZ
1	4	129	GLU	6.4
1	9	197	VAL	6.4
1	V	164	HIS	6.4
1	c	145	ARG	6.4
1	M	140	ASP	6.4
1	A	228	ARG	6.4
1	N	206	LEU	6.4
1	J	144	HIS	6.3
4	o	600	HIS	6.3
1	1	158	THR	6.3
1	h	172	ARG	6.3
1	Z	156	GLY	6.3
1	M	229	PHE	6.3
1	F	175	SER	6.3
1	W	189	TYR	6.3
1	W	221	THR	6.3
1	J	134	MET	6.3
1	9	226	SER	6.3
1	J	153	LEU	6.3
4	q	596	ARG	6.3
1	c	129	GLU	6.3
1	N	164	HIS	6.3
1	E	202	LEU	6.3
1	c	156	GLY	6.3
1	E	194	THR	6.3
1	W	177	GLU	6.3
1	9	150	GLU	6.3
1	h	207	GLU	6.3
1	R	172	ARG	6.3
1	k	224	ARG	6.3
1	l	226	SER	6.2
1	S	176	ARG	6.2
1	4	204	LYS	6.2
1	S	201	ARG	6.2
1	M	188	VAL	6.2
1	9	148	ALA	6.2
1	F	219	ARG	6.2
1	R	155	MET	6.2
1	N	143	SER	6.2
1	d	161	LYS	6.2
1	l	200	ARG	6.2
1	A	183	VAL	6.2

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Mol	Chain	Res	Type	RSRZ
1	F	142	THR	6.2
1	W	132	ILE	6.2
1	F	147	MET	6.2
1	B	227	THR	6.2
4	q	541	ARG	6.2
1	W	134	MET	6.2
1	W	191	GLU	6.2
1	5	192	ASP	6.2
4	o	578	LYS	6.2
1	9	224	ARG	6.1
1	M	218	VAL	6.1
1	E	196	ASP	6.1
1	d	224	ARG	6.1
1	N	214	MET	6.1
1	F	160	PHE	6.1
1	d	200	ARG	6.1
1	1	223	TYR	6.1
1	8	208	PRO	6.1
4	o	538	GLU	6.1
1	E	168	THR	6.1
1	V	136	GLY	6.1
4	o	577	GLY	6.1
1	c	189	TYR	6.1
1	J	129	GLU	6.1
1	I	183	VAL	6.1
1	J	188	VAL	6.1
1	V	147	MET	6.1
1	B	221	THR	6.1
1	N	187	ASN	6.1
1	M	228	ARG	6.1
1	4	148	ALA	6.0
1	S	214	MET	6.0
1	I	189	TYR	6.0
1	c	219	ARG	6.0
1	d	176	ARG	6.0
1	k	223	TYR	6.0
1	d	214	MET	6.0
1	N	166	PHE	6.0
1	5	194	THR	6.0
1	S	162	LEU	6.0
4	q	592	ALA	6.0
1	N	140	ASP	6.0

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Mol	Chain	Res	Type	RSRZ
1	c	164	HIS	6.0
1	g	221	THR	6.0
1	S	219	ARG	6.0
1	l	184	TRP	6.0
1	4	221	THR	5.9
1	l	152	PRO	5.9
1	M	214	MET	5.9
1	W	224	ARG	5.9
1	J	176	ARG	5.9
1	S	194	THR	5.9
1	g	173	VAL	5.9
4	o	545	HIS	5.9
1	8	155	MET	5.9
1	W	179	LEU	5.9
1	d	223	TYR	5.9
1	F	216	GLN	5.9
1	8	141	PRO	5.9
1	d	160	PHE	5.9
1	W	194	THR	5.9
1	R	174	TYR	5.8
1	J	150	GLU	5.8
1	V	155	MET	5.8
1	W	225	PHE	5.8
1	W	154	GLU	5.8
1	9	184	TRP	5.8
1	J	200	ARG	5.8
1	S	132	ILE	5.8
1	I	179	LEU	5.8
1	l	194	THR	5.8
1	g	216	GLN	5.8
1	k	176	ARG	5.8
1	J	179	LEU	5.8
1	S	142	THR	5.8
1	Z	141	PRO	5.8
1	A	219	ARG	5.8
1	B	162	LEU	5.8
1	c	179	LEU	5.8
1	A	194	THR	5.8
1	J	210	GLY	5.8
1	c	130	GLU	5.8
4	q	591	GLU	5.8
3	n	14	DA	5.8

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Mol	Chain	Res	Type	RSRZ
1	1	174	TYR	5.7
1	1	143	SER	5.7
1	1	166	PHE	5.7
1	h	225	PHE	5.7
1	1	175	SER	5.7
4	q	540	LEU	5.7
1	J	197	VAL	5.7
1	W	208	PRO	5.7
1	Z	147	MET	5.7
1	8	192	ASP	5.7
1	M	132	ILE	5.7
1	I	186	THR	5.7
1	k	220	GLY	5.7
1	4	208	PRO	5.7
1	d	178	GLN	5.7
1	k	169	HIS	5.7
1	c	180	LEU	5.7
1	E	215	VAL	5.7
1	E	164	HIS	5.6
1	9	225	PHE	5.6
1	g	213	ARG	5.6
1	J	224	ARG	5.6
1	W	156	GLY	5.6
4	o	586	ARG	5.6
1	c	173	VAL	5.6
1	B	196	ASP	5.6
1	R	202	LEU	5.6
1	5	176	ARG	5.6
1	4	213	ARG	5.6
1	g	194	THR	5.6
1	k	221	THR	5.6
1	J	192	ASP	5.6
2	a	4	DC	5.6
1	S	200	ARG	5.6
1	1	218	VAL	5.6
1	4	209	GLY	5.6
1	5	183	VAL	5.6
1	1	167	MET	5.6
1	M	194	THR	5.6
1	M	227	THR	5.6
3	H	1	DC	5.6
1	l	164	HIS	5.5

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Mol	Chain	Res	Type	RSRZ
1	k	165	PHE	5.5
1	M	209	GLY	5.5
1	V	150	GLU	5.5
1	1	148	ALA	5.5
4	q	909	LYS	5.5
1	c	174	TYR	5.5
1	F	217	THR	5.5
1	J	214	MET	5.5
1	N	147	MET	5.5
1	l	201	ARG	5.5
1	J	208	PRO	5.5
4	o	570	ASP	5.5
1	Z	228	ARG	5.5
1	8	184	TRP	5.5
1	Z	176	ARG	5.5
1	4	180	LEU	5.5
1	k	152	PRO	5.5
1	4	205	ALA	5.5
1	R	224	ARG	5.5
1	8	139	LEU	5.5
1	N	197	VAL	5.4
1	Z	204	LYS	5.4
4	o	905	ILE	5.4
1	A	177	GLU	5.4
1	R	151	GLU	5.4
1	4	200	ARG	5.4
1	5	201	ARG	5.4
1	I	220	GLY	5.4
4	o	542	ALA	5.4
1	M	160	PHE	5.4
1	R	206	LEU	5.4
1	E	211	HIS	5.4
1	R	144	HIS	5.4
1	8	171	GLU	5.4
1	d	174	TYR	5.4
1	d	225	PHE	5.4
1	A	145	ARG	5.4
1	I	133	GLU	5.4
1	M	215	VAL	5.4
1	B	223	TYR	5.4
1	5	141	PRO	5.4
1	5	136	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	W	178	GLN	5.4
1	B	169	HIS	5.4
4	q	908	GLU	5.4
4	o	541	ARG	5.4
1	5	214	MET	5.4
1	c	147	MET	5.4
1	B	142	THR	5.4
1	l	208	PRO	5.4
1	1	179	LEU	5.4
1	c	216	GLN	5.4
1	B	154	GLU	5.4
1	h	151	GLU	5.3
1	l	153	LEU	5.3
1	l	142	THR	5.3
4	q	587	ILE	5.3
1	E	174	TYR	5.3
1	B	152	PRO	5.3
1	1	208	PRO	5.3
1	W	162	LEU	5.3
1	B	228	ARG	5.3
1	R	129	GLU	5.3
1	1	201	ARG	5.3
4	o	543	ALA	5.3
1	k	215	VAL	5.3
1	V	228	ARG	5.3
1	N	177	GLU	5.3
1	8	138	SER	5.3
2	m	4	DC	5.3
2	2	12	DA	5.3
1	W	165	PHE	5.3
1	W	184	TRP	5.3
1	Z	199	ILE	5.3
1	d	142	THR	5.3
1	I	199	ILE	5.3
1	I	194	THR	5.3
1	V	224	ARG	5.3
1	4	145	ARG	5.3
1	8	156	GLY	5.3
1	A	169	HIS	5.3
1	W	217	THR	5.2
1	8	219	ARG	5.2
1	B	174	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
2	i	4	DC	5.2
1	h	140	ASP	5.2
1	F	179	LEU	5.2
1	k	156	GLY	5.2
1	E	177	GLU	5.2
4	o	563	PHE	5.2
1	V	186	THR	5.2
1	h	154	GLU	5.2
2	O	19	DC	5.2
1	N	172	ARG	5.2
1	B	218	VAL	5.2
1	A	198	HIS	5.2
1	9	154	GLU	5.2
4	q	899	GLU	5.2
1	g	215	VAL	5.2
1	h	220	GLY	5.2
1	5	165	PHE	5.2
4	q	571	TYR	5.1
1	Z	172	ARG	5.1
1	4	131	VAL	5.1
1	S	169	HIS	5.1
1	5	147	MET	5.1
1	V	141	PRO	5.1
1	J	139	LEU	5.1
1	V	184	TRP	5.1
1	4	174	TYR	5.1
1	l	223	TYR	5.1
1	4	136	GLY	5.1
1	E	136	GLY	5.1
1	d	201	ARG	5.1
1	Z	161	LYS	5.1
1	V	133	GLU	5.1
1	4	179	LEU	5.1
1	J	215	VAL	5.1
1	c	218	VAL	5.1
1	B	217	THR	5.0
4	o	590	ILE	5.0
1	h	143	SER	5.0
1	Z	133	GLU	5.0
1	A	224	ARG	5.0
1	R	220	GLY	5.0
3	U	1	DC	5.0

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Mol	Chain	Res	Type	RSRZ
1	I	196	ASP	5.0
1	d	151	GLU	5.0
1	I	168	THR	5.0
1	l	179	LEU	5.0
1	W	210	GLY	5.0
1	5	216	GLN	5.0
3	b	1	DC	5.0
3	7	11	DA	5.0
4	o	909	LYS	5.0
1	I	140	ASP	4.9
1	k	216	GLN	4.9
4	o	547	VAL	4.9
1	k	139	LEU	4.9
1	M	165	PHE	4.9
4	o	575	GLU	4.9
1	k	141	PRO	4.9
1	A	192	ASP	4.9
1	1	176	ARG	4.9
1	h	139	LEU	4.9
1	W	160	PHE	4.9
1	W	216	GLN	4.9
1	h	200	ARG	4.9
1	c	154	GLU	4.9
1	N	178	GLN	4.9
1	E	131	VAL	4.9
1	9	144	HIS	4.9
1	g	169	HIS	4.9
1	g	222	GLY	4.9
1	g	174	TYR	4.9
1	B	176	ARG	4.9
1	V	168	THR	4.9
1	g	219	ARG	4.9
1	F	165	PHE	4.8
3	b	14	DA	4.8
1	J	195	VAL	4.8
1	J	155	MET	4.8
1	S	171	GLU	4.8
1	4	150	GLU	4.8
1	A	218	VAL	4.8
3	7	13	DA	4.8
1	8	132	ILE	4.8
1	I	160	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
1	J	177	GLU	4.8
1	5	179	LEU	4.8
1	h	184	TRP	4.8
1	c	182	HIS	4.8
3	Y	1	DC	4.8
4	q	597	LYS	4.8
1	c	152	PRO	4.8
1	N	150	GLU	4.7
1	5	212	ASP	4.7
1	h	201	ARG	4.7
1	9	132	ILE	4.7
1	9	167	MET	4.7
3	U	3	DC	4.7
1	Z	218	VAL	4.7
1	Z	132	ILE	4.7
1	d	179	LEU	4.7
1	N	201	ARG	4.7
1	l	216	GLN	4.7
1	d	147	MET	4.7
1	1	217	THR	4.7
1	k	160	PHE	4.7
1	S	179	LEU	4.7
1	V	138	SER	4.7
1	F	133	GLU	4.7
1	8	194	THR	4.7
1	E	152	PRO	4.7
1	h	194	THR	4.7
1	R	132	ILE	4.7
1	V	207	GLU	4.7
1	h	224	ARG	4.7
1	g	128	VAL	4.6
1	I	225	PHE	4.6
3	H	22	DA	4.6
1	g	196	ASP	4.6
1	k	197	VAL	4.6
1	1	147	MET	4.6
1	4	132	ILE	4.6
4	o	550	GLY	4.6
1	1	160	PHE	4.6
1	4	176	ARG	4.6
1	N	188	VAL	4.6
1	5	143	SER	4.6

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Mol	Chain	Res	Type	RSRZ
2	C	24	DA	4.6
1	S	163	LEU	4.6
1	J	168	THR	4.6
1	k	217	THR	4.6
2	6	21	DC	4.6
1	W	200	ARG	4.6
1	d	135	GLN	4.6
4	o	579	GLN	4.6
1	B	213	ARG	4.6
4	o	561	MET	4.6
1	c	223	TYR	4.6
2	6	18	DT	4.6
1	F	188	VAL	4.6
1	g	139	LEU	4.6
1	1	177	GLU	4.6
1	4	169	HIS	4.6
1	4	194	THR	4.5
1	9	179	LEU	4.5
1	M	220	GLY	4.5
1	h	141	PRO	4.5
3	D	25	DG	4.5
1	8	176	ARG	4.5
1	S	188	VAL	4.5
1	8	146	VAL	4.5
1	l	163	LEU	4.5
1	I	152	PRO	4.5
1	I	145	ARG	4.5
1	1	159	GLU	4.5
1	4	133	GLU	4.5
3	P	14	DA	4.5
1	8	147	MET	4.5
1	V	194	THR	4.5
1	4	172	ARG	4.5
1	A	179	LEU	4.5
1	l	133	GLU	4.5
1	I	147	MET	4.5
1	Z	188	VAL	4.5
2	2	23	DA	4.5
1	I	185	GLY	4.5
1	A	152	PRO	4.5
1	d	193	ARG	4.5
1	S	211	HIS	4.5

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Mol	Chain	Res	Type	RSRZ
1	h	160	PHE	4.5
1	d	148	ALA	4.5
1	B	179	LEU	4.4
1	9	162	LEU	4.4
1	W	167	MET	4.4
1	Z	160	PHE	4.4
4	o	556	ALA	4.4
4	o	591	GLU	4.4
2	G	12	DA	4.4
1	I	216	GLN	4.4
1	F	136	GLY	4.4
1	I	219	ARG	4.4
1	l	141	PRO	4.4
1	M	164	HIS	4.4
1	M	177	GLU	4.4
1	l	160	PHE	4.4
1	B	156	GLY	4.4
1	R	133	GLU	4.4
2	C	4	DC	4.4
1	h	166	PHE	4.4
1	W	161	LYS	4.4
2	O	23	DA	4.4
2	X	23	DA	4.4
3	H	14	DA	4.4
1	5	138	SER	4.3
1	l	138	SER	4.3
1	1	191	GLU	4.3
1	Z	137	LEU	4.3
4	o	599	ARG	4.3
1	B	185	GLY	4.3
1	W	195	VAL	4.3
1	E	154	GLU	4.3
1	k	129	GLU	4.3
4	o	605	GLU	4.3
1	9	139	LEU	4.3
1	4	135	GLN	4.3
3	D	22	DA	4.3
1	4	220	GLY	4.3
3	n	1	DC	4.3
1	5	152	PRO	4.3
1	k	194	THR	4.3
1	R	140	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
4	o	584	ARG	4.3
2	C	22	DA	4.3
1	W	152	PRO	4.3
1	Z	144	HIS	4.3
1	W	196	ASP	4.3
1	E	160	PHE	4.3
1	M	152	PRO	4.3
1	N	176	ARG	4.3
1	1	140	ASP	4.3
1	B	183	VAL	4.3
1	l	144	HIS	4.3
1	J	178	GLN	4.3
1	1	141	PRO	4.2
1	1	164	HIS	4.2
1	M	195	VAL	4.2
1	M	155	MET	4.2
4	o	583	THR	4.2
1	I	136	GLY	4.2
1	k	161	LYS	4.2
1	l	165	PHE	4.2
1	N	146	VAL	4.2
1	Z	197	VAL	4.2
1	c	202	LEU	4.2
1	k	146	VAL	4.2
3	j	3	DC	4.2
1	5	195	VAL	4.2
2	6	11	DA	4.2
2	m	24	DA	4.2
2	O	2	DG	4.2
1	d	143	SER	4.2
1	d	189	TYR	4.2
3	P	26	DC	4.2
1	1	224	ARG	4.2
1	8	169	HIS	4.2
1	S	191	GLU	4.2
1	9	216	GLN	4.2
1	1	219	ARG	4.2
1	5	162	LEU	4.2
1	S	196	ASP	4.2
3	n	22	DA	4.2
1	5	223	TYR	4.2
1	8	197	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	c	168	THR	4.2
2	G	9	DA	4.1
3	7	22	DA	4.1
3	b	22	DA	4.1
1	B	177	GLU	4.1
1	M	145	ARG	4.1
1	A	167	MET	4.1
3	7	26	DC	4.1
1	5	211	HIS	4.1
1	k	211	HIS	4.1
1	Z	191	GLU	4.1
3	L	1	DC	4.1
3	f	23	DC	4.1
2	a	12	DA	4.1
1	E	147	MET	4.1
1	W	168	THR	4.1
3	b	6	DT	4.1
1	1	228	ARG	4.1
1	9	182	HIS	4.1
1	J	167	MET	4.1
1	I	223	TYR	4.1
3	Y	2	DA	4.1
1	4	218	VAL	4.1
1	5	215	VAL	4.1
2	i	13	DA	4.1
1	N	202	LEU	4.1
1	k	153	LEU	4.1
4	o	588	ARG	4.1
2	C	3	DG	4.1
1	1	196	ASP	4.0
1	E	216	GLN	4.0
1	5	172	ARG	4.0
1	1	189	TYR	4.0
1	c	215	VAL	4.0
2	i	3	DG	4.0
1	c	217	THR	4.0
1	Z	152	PRO	4.0
4	q	901	LEU	4.0
3	H	3	DC	4.0
1	1	173	VAL	4.0
1	l	209	GLY	4.0
1	M	202	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
3	H	25	DG	4.0
1	c	166	PHE	4.0
2	T	24	DA	4.0
2	6	10	DT	4.0
1	5	163	LEU	4.0
2	2	24	DA	4.0
1	4	130	GLU	3.9
1	g	180	LEU	3.9
1	J	196	ASP	3.9
1	S	138	SER	3.9
1	5	139	LEU	3.9
4	o	544	THR	3.9
1	S	218	VAL	3.9
3	7	1	DC	3.9
1	W	169	HIS	3.9
1	F	173	VAL	3.9
1	J	163	LEU	3.9
1	Z	151	GLU	3.9
2	e	3	DG	3.9
1	F	163	LEU	3.9
1	h	218	VAL	3.9
1	8	209	GLY	3.9
1	V	216	GLN	3.9
1	5	184	TRP	3.9
2	6	24	DA	3.9
1	E	139	LEU	3.9
1	V	215	VAL	3.9
1	Z	217	THR	3.9
3	7	15	DC	3.9
1	R	150	GLU	3.9
1	g	168	THR	3.8
2	C	12	DA	3.8
1	B	166	PHE	3.8
1	c	160	PHE	3.8
2	i	11	DA	3.8
1	1	172	ARG	3.8
1	9	163	LEU	3.8
4	q	902	LEU	3.8
1	B	168	THR	3.8
1	S	153	LEU	3.8
1	8	229	PHE	3.8
1	J	156	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	l	188	VAL	3.8
3	f	24	DA	3.8
1	N	154	GLU	3.8
1	5	171	GLU	3.8
2	X	11	DA	3.8
1	4	139	LEU	3.8
1	1	209	GLY	3.8
2	X	24	DA	3.8
1	1	198	HIS	3.8
1	V	219	ARG	3.8
4	q	903	ARG	3.8
1	F	194	THR	3.7
2	G	1	DT	3.7
3	f	3	DC	3.7
1	J	193	ARG	3.7
1	Z	220	GLY	3.7
1	N	175	SER	3.7
1	M	168	THR	3.7
1	Z	194	THR	3.7
4	o	902	LEU	3.7
1	8	220	GLY	3.7
1	4	226	SER	3.7
4	o	901	LEU	3.7
1	A	190	VAL	3.7
1	F	144	HIS	3.7
1	V	132	ILE	3.7
1	g	182	HIS	3.7
1	E	189	TYR	3.7
1	1	199	ILE	3.7
2	C	21	DC	3.7
3	D	14	DA	3.7
1	c	196	ASP	3.7
1	B	172	ARG	3.7
1	J	145	ARG	3.7
1	N	160	PHE	3.7
4	q	595	LEU	3.7
2	O	12	DA	3.7
3	L	14	DA	3.7
1	l	197	VAL	3.6
1	8	136	GLY	3.6
3	j	24	DA	3.6
3	D	1	DC	3.6

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Mol	Chain	Res	Type	RSRZ
1	W	135	GLN	3.6
1	k	168	THR	3.6
2	a	15	DT	3.6
1	8	223	TYR	3.6
2	a	23	DA	3.6
1	F	168	THR	3.6
2	i	5	DT	3.6
4	q	572	THR	3.6
1	M	151	GLU	3.6
1	9	201	ARG	3.6
2	a	24	DA	3.6
1	A	215	VAL	3.6
1	J	225	PHE	3.6
1	W	197	VAL	3.6
2	a	5	DT	3.6
1	R	223	TYR	3.6
1	Z	221	THR	3.6
2	6	23	DA	3.6
1	F	156	GLY	3.6
2	6	15	DT	3.6
2	m	18	DT	3.6
1	E	162	LEU	3.6
1	M	166	PHE	3.6
1	Z	165	PHE	3.6
1	J	198	HIS	3.6
1	l	191	GLU	3.6
1	k	219	ARG	3.5
1	S	167	MET	3.5
1	R	168	THR	3.5
1	A	135	GLN	3.5
3	b	13	DA	3.5
2	T	3	DG	3.5
3	Y	3	DC	3.5
1	E	132	ILE	3.5
1	c	133	GLU	3.5
1	A	216	GLN	3.5
2	6	20	DA	3.5
3	3	5	DT	3.5
1	F	202	LEU	3.5
1	d	202	LEU	3.5
1	F	178	GLN	3.5
1	h	216	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
2	C	11	DA	3.5
1	g	179	LEU	3.5
3	H	13	DA	3.5
1	J	152	PRO	3.5
1	8	145	ARG	3.5
1	l	215	VAL	3.5
1	A	156	GLY	3.5
3	L	4	DT	3.5
1	g	175	SER	3.5
1	N	217	THR	3.5
1	5	142	THR	3.5
1	g	217	THR	3.5
2	X	20	DA	3.5
1	V	189	TYR	3.5
1	l	162	LEU	3.4
1	Z	164	HIS	3.4
2	e	5	DT	3.4
2	e	15	DT	3.4
1	h	214	MET	3.4
4	o	585	GLU	3.4
1	k	132	ILE	3.4
2	C	14	DG	3.4
1	1	163	LEU	3.4
2	a	13	DA	3.4
1	g	198	HIS	3.4
1	R	138	SER	3.4
2	O	24	DA	3.4
2	m	20	DA	3.4
1	E	166	PHE	3.4
1	V	195	VAL	3.4
1	1	216	GLN	3.4
1	c	195	VAL	3.4
2	2	14	DG	3.4
2	m	23	DA	3.4
3	P	13	DA	3.4
1	c	144	HIS	3.4
1	E	171	GLU	3.4
1	W	133	GLU	3.4
1	Z	208	PRO	3.4
1	V	220	GLY	3.4
1	I	139	LEU	3.4
1	F	135	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	V	196	ASP	3.4
1	l	147	MET	3.4
1	N	137	LEU	3.4
1	M	146	VAL	3.3
1	1	136	GLY	3.3
1	d	162	LEU	3.3
2	O	21	DC	3.3
2	T	4	DC	3.3
4	o	546	ASP	3.3
2	T	25	DA	3.3
3	3	22	DA	3.3
3	b	24	DA	3.3
1	8	218	VAL	3.3
3	P	10	DG	3.3
3	Y	25	DG	3.3
2	m	15	DT	3.3
3	3	12	DC	3.3
1	E	138	SER	3.3
1	g	138	SER	3.3
1	N	168	THR	3.3
2	K	23	DA	3.3
3	j	14	DA	3.3
1	R	215	VAL	3.3
1	B	133	GLU	3.3
1	S	192	ASP	3.3
1	J	217	THR	3.3
1	d	168	THR	3.3
1	l	224	ARG	3.3
1	B	139	LEU	3.3
1	8	196	ASP	3.3
1	S	215	VAL	3.3
1	B	138	SER	3.3
1	S	168	THR	3.3
1	V	137	LEU	3.3
2	K	11	DA	3.3
2	6	12	DA	3.3
1	S	173	VAL	3.3
1	1	138	SER	3.3
1	k	142	THR	3.3
2	K	24	DA	3.2
3	L	13	DA	3.2
1	M	135	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	224	ARG	3.2
1	W	215	VAL	3.2
1	9	145	ARG	3.2
1	4	152	PRO	3.2
3	3	16	DT	3.2
1	l	211	HIS	3.2
2	K	4	DC	3.2
2	G	25	DA	3.2
2	O	22	DA	3.2
1	W	139	LEU	3.2
3	j	16	DT	3.2
1	9	192	ASP	3.2
2	2	19	DC	3.2
4	q	577	GLY	3.2
1	F	171	GLU	3.2
1	d	199	ILE	3.2
2	K	3	DG	3.2
3	3	26	DC	3.2
1	S	144	HIS	3.2
1	8	183	VAL	3.2
3	j	4	DT	3.2
3	j	23	DC	3.2
1	g	165	PHE	3.2
1	8	168	THR	3.2
1	8	217	THR	3.2
1	k	228	ARG	3.2
4	q	547	VAL	3.2
3	H	11	DA	3.2
4	q	567	MET	3.2
3	D	3	DC	3.2
3	f	25	DG	3.2
1	S	165	PHE	3.2
2	m	12	DA	3.2
2	m	5	DT	3.2
3	b	16	DT	3.2
2	a	3	DG	3.2
1	l	146	VAL	3.2
1	A	150	GLU	3.1
2	G	7	DT	3.1
1	S	223	TYR	3.1
1	d	166	PHE	3.1
1	A	136	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	9	200	ARG	3.1
2	G	2	DG	3.1
1	B	198	HIS	3.1
1	1	144	HIS	3.1
1	M	133	GLU	3.1
2	e	20	DA	3.1
3	U	22	DA	3.1
3	3	13	DA	3.1
1	E	156	GLY	3.1
1	c	188	VAL	3.1
2	i	15	DT	3.1
1	h	162	LEU	3.1
1	V	223	TYR	3.1
2	T	18	DT	3.1
3	f	6	DT	3.1
1	d	154	GLU	3.1
2	2	4	DC	3.1
2	K	25	DA	3.1
2	K	14	DG	3.1
2	6	2	DG	3.1
1	A	139	LEU	3.1
1	S	202	LEU	3.1
1	8	137	LEU	3.1
3	b	26	DC	3.1
2	i	12	DA	3.1
4	o	609	SER	3.1
1	k	163	LEU	3.1
4	q	606	VAL	3.1
4	q	579	GLN	3.1
3	3	11	DA	3.1
3	n	13	DA	3.1
2	i	2	DG	3.1
1	1	139	LEU	3.1
3	D	26	DC	3.1
1	V	218	VAL	3.1
1	h	136	GLY	3.0
1	h	209	GLY	3.0
1	k	202	LEU	3.0
2	e	11	DA	3.0
2	e	22	DA	3.0
2	i	22	DA	3.0
3	n	16	DT	3.0

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Mol	Chain	Res	Type	RSRZ
3	P	12	DC	3.0
1	l	132	ILE	3.0
1	l	174	TYR	3.0
1	E	179	LEU	3.0
1	l	202	LEU	3.0
2	6	14	DG	3.0
2	6	22	DA	3.0
3	L	2	DA	3.0
3	Y	14	DA	3.0
3	U	16	DT	3.0
3	n	23	DC	3.0
1	Z	198	HIS	3.0
1	Z	162	LEU	3.0
2	C	2	DG	3.0
3	7	25	DG	3.0
2	G	11	DA	3.0
2	e	24	DA	3.0
3	j	6	DT	3.0
1	M	219	ARG	3.0
1	B	202	LEU	3.0
1	W	163	LEU	3.0
1	d	164	HIS	3.0
3	D	5	DT	3.0
3	L	16	DT	3.0
3	f	16	DT	3.0
2	T	8	DC	3.0
2	i	24	DA	3.0
3	Y	15	DC	3.0
2	X	3	DG	3.0
1	A	134	MET	3.0
1	h	168	THR	3.0
1	l	196	ASP	3.0
3	n	2	DA	3.0
1	1	162	LEU	3.0
1	N	133	GLU	3.0
1	J	202	LEU	3.0
1	N	153	LEU	3.0
2	2	13	DA	3.0
3	D	2	DA	3.0
3	H	2	DA	3.0
2	K	15	DT	3.0
1	B	201	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	9	190	VAL	3.0
2	X	2	DG	3.0
2	a	14	DG	3.0
1	h	202	LEU	2.9
2	X	9	DA	2.9
2	X	25	DA	2.9
2	a	20	DA	2.9
3	3	14	DA	2.9
1	5	166	PHE	2.9
2	2	18	DT	2.9
1	A	138	SER	2.9
3	7	14	DA	2.9
1	N	144	HIS	2.9
1	c	198	HIS	2.9
3	j	26	DC	2.9
1	F	138	SER	2.9
1	Z	139	LEU	2.9
2	2	15	DT	2.9
2	O	4	DC	2.9
1	M	176	ARG	2.9
1	k	162	LEU	2.9
3	j	19	DA	2.9
3	n	6	DT	2.9
1	E	134	MET	2.9
1	d	140	ASP	2.9
3	U	25	DG	2.9
1	I	153	LEU	2.9
1	1	202	LEU	2.9
1	M	217	THR	2.9
2	C	23	DA	2.9
2	m	13	DA	2.9
3	D	11	DA	2.9
3	f	11	DA	2.9
2	O	1	DT	2.9
2	K	9	DA	2.9
3	f	1	DC	2.9
1	4	198	HIS	2.9
2	e	2	DG	2.9
1	8	133	GLU	2.9
1	V	153	LEU	2.9
3	3	9	DT	2.8
2	i	23	DA	2.8

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Mol	Chain	Res	Type	RSRZ
1	9	166	PHE	2.8
1	A	176	ARG	2.8
1	E	218	VAL	2.8
2	X	15	DT	2.8
3	D	20	DT	2.8
1	5	144	HIS	2.8
2	C	20	DA	2.8
3	U	21	DG	2.8
1	S	136	GLY	2.8
1	9	211	HIS	2.8
2	K	2	DG	2.8
3	Y	24	DA	2.8
1	N	162	LEU	2.8
1	B	195	VAL	2.8
1	A	189	TYR	2.8
2	6	19	DC	2.8
3	L	12	DC	2.8
1	N	139	LEU	2.8
1	4	160	PHE	2.8
1	8	165	PHE	2.8
2	O	14	DG	2.8
1	I	224	ARG	2.8
1	W	144	HIS	2.8
1	c	228	ARG	2.8
1	h	188	VAL	2.8
2	a	9	DA	2.8
2	m	9	DA	2.8
1	V	154	GLU	2.8
1	8	129	GLU	2.8
3	P	16	DT	2.8
2	6	4	DC	2.8
1	J	166	PHE	2.8
3	H	21	DG	2.8
2	O	18	DT	2.8
3	P	5	DT	2.8
3	P	11	DA	2.8
1	4	216	GLN	2.8
1	4	146	VAL	2.7
3	D	21	DG	2.7
1	5	198	HIS	2.7
1	I	162	LEU	2.7
1	M	221	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	202	LEU	2.7
1	I	137	LEU	2.7
1	4	192	ASP	2.7
1	A	147	MET	2.7
1	h	137	LEU	2.7
1	9	198	HIS	2.7
2	m	21	DC	2.7
3	P	3	DC	2.7
1	S	166	PHE	2.7
2	K	20	DA	2.7
3	n	24	DA	2.7
1	B	132	ILE	2.7
1	5	213	ARG	2.7
1	8	153	LEU	2.7
2	O	3	DG	2.7
2	e	14	DG	2.7
3	f	10	DG	2.7
1	M	198	HIS	2.7
3	U	26	DC	2.7
1	h	199	ILE	2.7
4	q	586	ARG	2.7
1	N	194	THR	2.7
1	g	166	PHE	2.7
3	n	3	DC	2.7
3	n	15	DC	2.7
4	q	556	ALA	2.7
3	P	25	DG	2.7
1	Z	166	PHE	2.7
2	X	14	DG	2.7
1	F	166	PHE	2.7
3	f	26	DC	2.6
1	J	173	VAL	2.6
1	d	197	VAL	2.6
1	9	134	MET	2.6
2	X	12	DA	2.6
1	8	216	GLN	2.6
2	6	9	DA	2.6
3	U	11	DA	2.6
3	j	1	DC	2.6
1	Z	163	LEU	2.6
1	5	196	ASP	2.6
2	O	15	DT	2.6

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Mol	Chain	Res	Type	RSRZ
2	2	10	DT	2.6
3	b	5	DT	2.6
3	j	18	DT	2.6
2	a	25	DA	2.6
2	i	6	DG	2.6
2	m	25	DA	2.6
1	g	223	TYR	2.6
2	T	7	DT	2.6
3	L	15	DC	2.6
3	P	15	DC	2.6
1	Z	219	ARG	2.6
1	g	228	ARG	2.6
2	6	13	DA	2.6
3	H	20	DT	2.6
1	E	128	VAL	2.6
1	l	137	LEU	2.6
2	O	25	DA	2.6
3	D	6	DT	2.6
1	9	133	GLU	2.6
1	d	137	LEU	2.6
1	d	216	GLN	2.6
3	Y	26	DC	2.6
2	O	13	DA	2.6
1	A	166	PHE	2.5
1	c	138	SER	2.5
1	k	166	PHE	2.5
1	c	136	GLY	2.5
1	5	133	GLU	2.5
1	N	167	MET	2.5
4	q	544	THR	2.5
1	J	211	HIS	2.5
1	5	153	LEU	2.5
1	I	156	GLY	2.5
1	R	195	VAL	2.5
1	W	174	TYR	2.5
2	T	1	DT	2.5
3	7	16	DT	2.5
3	b	4	DT	2.5
1	A	137	LEU	2.5
1	N	163	LEU	2.5
4	q	607	LEU	2.5
1	9	146	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
3	L	26	DC	2.5
4	q	584	ARG	2.5
3	3	10	DG	2.5
3	b	25	DG	2.5
3	U	5	DT	2.5
2	2	22	DA	2.5
3	Y	13	DA	2.5
1	A	172	ARG	2.5
3	j	15	DC	2.5
4	o	596	ARG	2.5
1	c	165	PHE	2.5
2	i	7	DT	2.5
1	I	193	ARG	2.5
1	I	228	ARG	2.5
1	c	190	VAL	2.5
2	T	12	DA	2.5
3	f	14	DA	2.5
2	m	19	DC	2.5
2	e	10	DT	2.5
1	Z	146	VAL	2.5
2	2	11	DA	2.5
3	L	24	DA	2.5
1	d	150	GLU	2.5
2	i	14	DG	2.5
2	a	18	DT	2.5
3	L	17	DT	2.5
3	P	9	DT	2.5
3	7	6	DT	2.5
1	S	224	ARG	2.5
3	f	12	DC	2.5
1	8	198	HIS	2.5
1	R	165	PHE	2.4
2	6	3	DG	2.4
2	C	16	DT	2.4
3	n	5	DT	2.4
1	E	195	VAL	2.4
1	5	218	VAL	2.4
2	G	14	DG	2.4
2	C	1	DT	2.4
2	6	7	DT	2.4
3	H	5	DT	2.4
3	U	4	DT	2.4

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Mol	Chain	Res	Type	RSRZ
3	P	22	DA	2.4
3	j	13	DA	2.4
1	h	198	HIS	2.4
3	3	4	DT	2.4
3	f	18	DT	2.4
1	W	145	ARG	2.4
1	d	167	MET	2.4
1	R	153	LEU	2.4
2	O	20	DA	2.4
2	m	3	DG	2.4
3	U	20	DT	2.4
1	F	167	MET	2.4
1	9	138	SER	2.4
1	S	198	HIS	2.4
1	R	193	ARG	2.4
1	h	146	VAL	2.4
2	2	2	DG	2.4
1	8	221	THR	2.4
3	3	15	DC	2.4
3	b	12	DC	2.4
1	M	162	LEU	2.4
1	V	166	PHE	2.4
1	h	190	VAL	2.4
3	j	9	DT	2.4
1	d	144	HIS	2.4
2	G	3	DG	2.4
2	T	2	DG	2.4
2	e	13	DA	2.4
3	3	2	DA	2.4
1	8	202	LEU	2.4
2	C	10	DT	2.4
3	7	7	DT	2.4
3	f	4	DT	2.4
2	T	14	DG	2.4
1	h	187	ASN	2.4
3	P	24	DA	2.4
1	d	145	ARG	2.3
2	T	15	DT	2.3
2	e	18	DT	2.3
2	K	17	DG	2.3
2	e	21	DC	2.3
1	S	135	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	195	VAL	2.3
3	Y	16	DT	2.3
1	8	162	LEU	2.3
1	g	202	LEU	2.3
1	R	192	ASP	2.3
1	4	196	ASP	2.3
2	6	17	DG	2.3
1	F	169	HIS	2.3
1	k	209	GLY	2.3
3	U	19	DA	2.3
2	a	7	DT	2.3
3	b	17	DT	2.3
3	3	3	DC	2.3
3	7	12	DC	2.3
1	W	198	HIS	2.3
1	d	132	ILE	2.3
1	g	133	GLU	2.3
2	C	7	DT	2.3
3	H	9	DT	2.3
3	n	4	DT	2.3
1	V	160	PHE	2.3
3	H	19	DA	2.3
2	2	5	DT	2.3
1	M	223	TYR	2.3
2	X	19	DC	2.3
2	e	19	DC	2.3
3	b	3	DC	2.3
3	b	23	DC	2.3
3	n	12	DC	2.3
2	m	14	DG	2.3
3	3	25	DG	2.3
4	q	557	LYS	2.3
1	R	131	VAL	2.3
1	M	167	MET	2.3
1	W	193	ARG	2.3
2	e	7	DT	2.3
3	7	19	DA	2.3
1	A	217	THR	2.3
1	E	223	TYR	2.3
2	T	9	DA	2.2
3	j	22	DA	2.2
4	q	568	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	165	PHE	2.2
2	K	21	DC	2.2
3	3	23	DC	2.2
3	n	26	DC	2.2
1	F	139	LEU	2.2
1	J	136	GLY	2.2
1	M	134	MET	2.2
2	a	11	DA	2.2
2	e	23	DA	2.2
3	U	2	DA	2.2
1	M	170	PRO	2.2
1	k	218	VAL	2.2
3	H	26	DC	2.2
3	P	19	DA	2.2
2	m	2	DG	2.2
3	b	10	DG	2.2
2	G	15	DT	2.2
2	O	10	DT	2.2
3	D	17	DT	2.2
3	P	4	DT	2.2
3	3	20	DT	2.2
1	g	160	PHE	2.2
3	b	19	DA	2.2
1	R	218	VAL	2.2
1	B	167	MET	2.2
1	F	176	ARG	2.2
2	i	17	DG	2.2
3	j	7	DT	2.2
3	n	17	DT	2.2
1	N	216	GLN	2.2
1	c	139	LEU	2.2
1	W	192	ASP	2.2
3	L	22	DA	2.2
3	j	2	DA	2.2
1	W	172	ARG	2.2
3	H	16	DT	2.2
1	h	163	LEU	2.2
3	7	3	DC	2.2
1	V	193	ARG	2.2
2	C	25	DA	2.2
3	H	24	DA	2.2
3	j	11	DA	2.2

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Mol	Chain	Res	Type	RSRZ
3	n	11	DA	2.2
1	I	198	HIS	2.2
1	F	134	MET	2.2
2	e	6	DG	2.1
3	7	2	DA	2.1
3	3	7	DT	2.1
2	i	21	DC	2.1
3	D	12	DC	2.1
4	q	564	GLY	2.1
2	2	3	DG	2.1
2	a	26	DG	2.1
3	D	23	DC	2.1
4	o	560	ARG	2.1
3	L	25	DG	2.1
3	n	7	DT	2.1
3	L	11	DA	2.1
1	W	136	GLY	2.1
1	k	154	GLU	2.1
3	Y	7	DT	2.1
3	Y	9	DT	2.1
3	j	17	DT	2.1
2	X	4	DC	2.1
1	Z	209	GLY	2.1
3	f	7	DT	2.1
4	o	598	LEU	2.1
2	G	19	DC	2.1
3	U	15	DC	2.1
1	F	198	HIS	2.1
1	B	163	LEU	2.1
1	5	217	THR	2.1
3	H	4	DT	2.1
2	C	17	DG	2.1
1	h	195	VAL	2.1
3	f	15	DC	2.1
2	T	22	DA	2.1
3	f	19	DA	2.1
2	C	15	DT	2.1
3	L	6	DT	2.1
3	L	9	DT	2.1
3	n	18	DT	2.0
1	R	135	GLN	2.0
1	d	217	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	O	26	DG	2.0
3	H	10	DG	2.0
1	R	146	VAL	2.0
2	G	21	DC	2.0
1	9	147	MET	2.0
1	4	202	LEU	2.0
2	G	24	DA	2.0
2	X	13	DA	2.0
2	K	7	DT	2.0
2	K	18	DT	2.0
2	X	10	DT	2.0
1	4	215	VAL	2.0
3	Y	21	DG	2.0
3	H	23	DC	2.0
1	h	138	SER	2.0
1	S	156	GLY	2.0
2	C	13	DA	2.0
3	D	9	DT	2.0
3	b	18	DT	2.0
1	9	196	ASP	2.0
1	I	166	PHE	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 oligosaccharides 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.