Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2021 – 12:45 PM EDT

PDB ID	:	1Z1G
Title	:	Crystal structure of a lambda integrase tetramer bound to a Holliday junction
Authors	:	Biswas, T.; Aihara, H.; Radman-Livaja, M.; Filman, D.; Landy, A.; Ellenberger, T.
Deposited on	:	2005-03-03
Resolution	:	4.40 Å(reported)

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

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

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

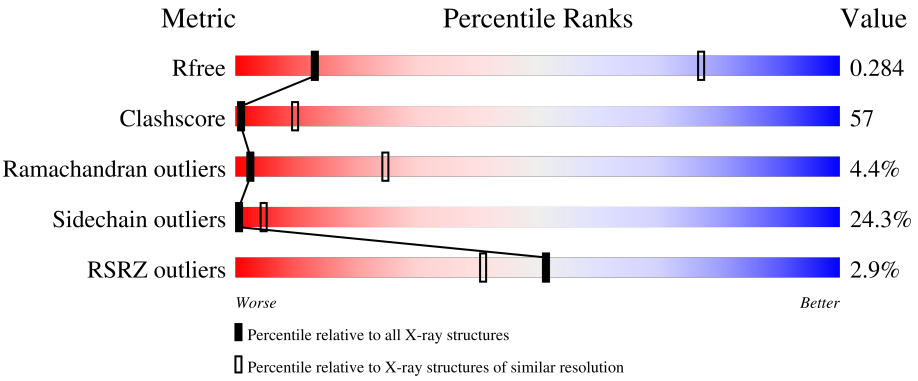
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 4.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1043 (5.00-3.80)
Clashscore	141614	1111 (5.00-3.80)
Ramachandran outliers	138981	1059 (5.00-3.80)
Sidechain outliers	138945	1041 (5.00-3.80)
RSRZ outliers	127900	1095 (5.08-3.70)

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	I	29	7% 24% 69%
2	J	29	24% 76%
3	K	29	3% 28% 72%
4	L	29	7% 45% 55%
5	E	25	20% 76% .

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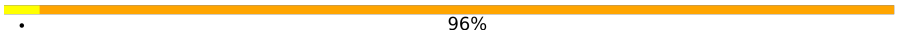
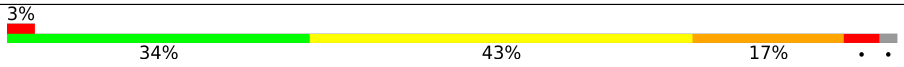
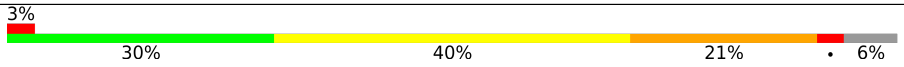
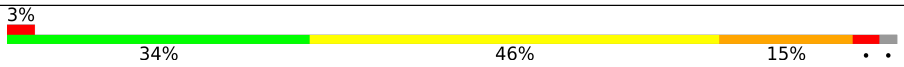
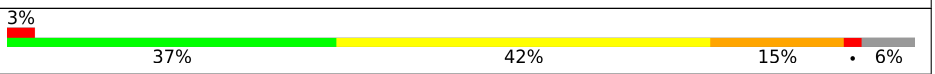
Mol	Chain	Length	Quality of chain
5	G	25	
6	F	25	
6	H	25	
7	A	356	
7	B	356	
7	C	356	
7	D	356	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 15156 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 DNA chain called 29-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	I	29	588	284	103	173	28	0	0	0

- Molecule 2 is a DNA chain called 29-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	J	29	594	286	110	170	28	0	0	0

- Molecule 3 is a DNA chain called 29-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	K	29	590	285	102	175	28	0	0	0

- Molecule 4 is a DNA chain called 29-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	L	29	594	285	111	170	28	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	E	24	487	234	93	137	23	0	0	0
5	G	24	Total 487	C 234	N 93	O 137	P 23	0	0	0

- Molecule 6 is a DNA chain called 25-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	25	Total	C	N	O	P	0	0	0
			513	247	89	153	24			
6	H	25	Total	C	N	O	P	0	0	0
			513	247	89	153	24			

- Molecule 7 is a protein called Integrase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	A	349	Total	C	N	O	S	Se	0	0	0
			2763	1730	505	517	4	7			
7	B	336	Total	C	N	O	S	Se	0	0	0
			2630	1652	474	494	4	6			
7	C	349	Total	C	N	O	S	Se	0	0	0
			2767	1732	506	518	4	7			
7	D	336	Total	C	N	O	S	Se	0	0	0
			2630	1652	474	494	4	6			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P03700
A	101	MSE	MET	modified residue	UNP P03700
A	127	MSE	MET	modified residue	UNP P03700
A	203	MSE	MET	modified residue	UNP P03700
A	219	MSE	MET	modified residue	UNP P03700
A	255	MSE	MET	modified residue	UNP P03700
A	290	MSE	MET	modified residue	UNP P03700
A	338	MSE	MET	modified residue	UNP P03700
A	342	PHE	TYR	engineered mutation	UNP P03700
B	1	MSE	MET	modified residue	UNP P03700
B	101	MSE	MET	modified residue	UNP P03700
B	127	MSE	MET	modified residue	UNP P03700
B	203	MSE	MET	modified residue	UNP P03700
B	219	MSE	MET	modified residue	UNP P03700
B	255	MSE	MET	modified residue	UNP P03700
B	290	MSE	MET	modified residue	UNP P03700
B	338	MSE	MET	modified residue	UNP P03700
B	342	PHE	TYR	engineered mutation	UNP P03700
C	1	MSE	MET	modified residue	UNP P03700
C	101	MSE	MET	modified residue	UNP P03700
C	127	MSE	MET	modified residue	UNP P03700
C	203	MSE	MET	modified residue	UNP P03700
C	219	MSE	MET	modified residue	UNP P03700

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Chain	Residue	Modelled	Actual	Comment	Reference
C	255	MSE	MET	modified residue	UNP P03700
C	290	MSE	MET	modified residue	UNP P03700
C	338	MSE	MET	modified residue	UNP P03700
C	342	PHE	TYR	engineered mutation	UNP P03700
D	1	MSE	MET	modified residue	UNP P03700
D	101	MSE	MET	modified residue	UNP P03700
D	127	MSE	MET	modified residue	UNP P03700
D	203	MSE	MET	modified residue	UNP P03700
D	219	MSE	MET	modified residue	UNP P03700
D	255	MSE	MET	modified residue	UNP P03700
D	290	MSE	MET	modified residue	UNP P03700
D	338	MSE	MET	modified residue	UNP P03700
D	342	PHE	TYR	engineered mutation	UNP P03700

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: 29-MER

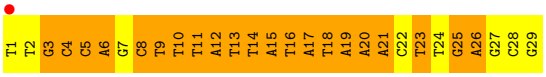
Chain I:

• Molecule 2: 29-MER

Chain J:

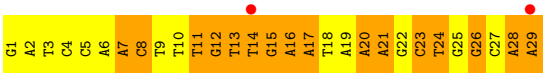
• Molecule 3: 29-MER

Chain K:



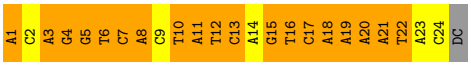
• Molecule 4: 29-MER

Chain L:



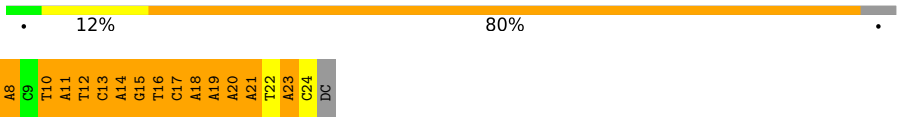
• Molecule 5: 5'-D(*AP*CP*AP*GP*GP*TP*CP*AP*CP*TP*AP*TP*CP*AP*GP*TP*CP*AP*AP*AP*AP*TP*AP*CP*C)-3'

Chain E:



• Molecule 5: 5'-D(*AP*CP*AP*GP*GP*TP*CP*AP*CP*TP*AP*TP*CP*AP*GP*TP*CP*AP*AP*AP*AP*TP*AP*CP*C)-3'

Chain G:

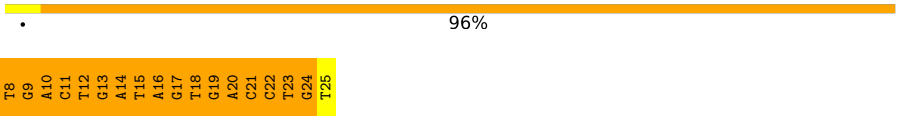


• Molecule 6: 25-MER

Chain F:

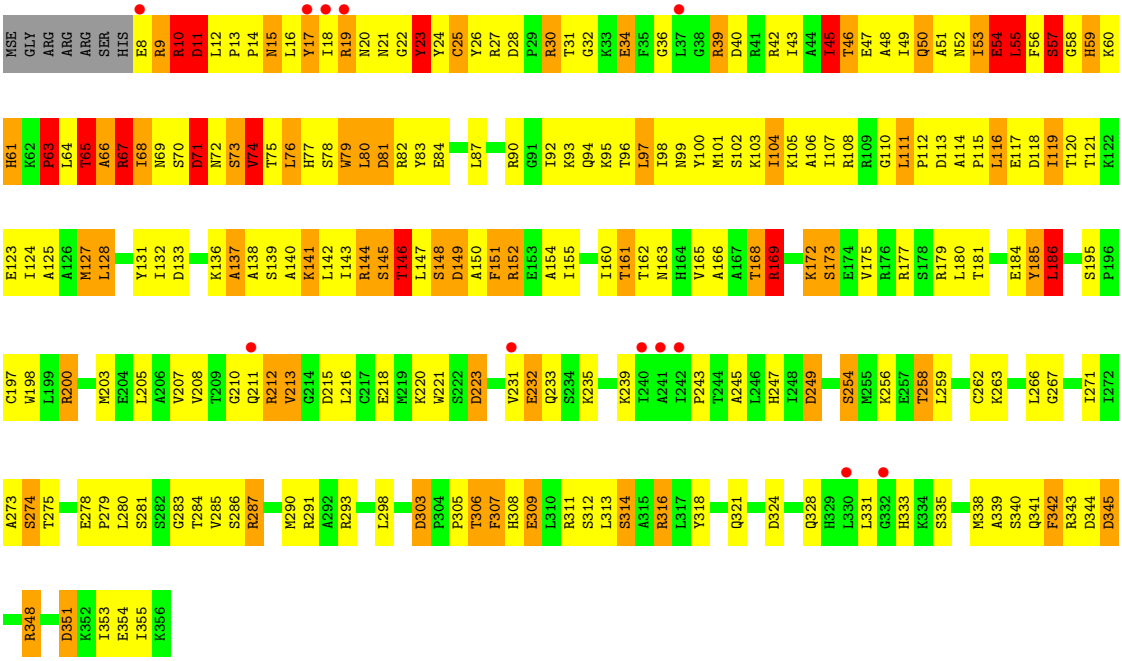
• Molecule 6: 25-MER

Chain H:



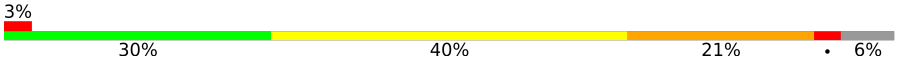
• Molecule 7: Integrase

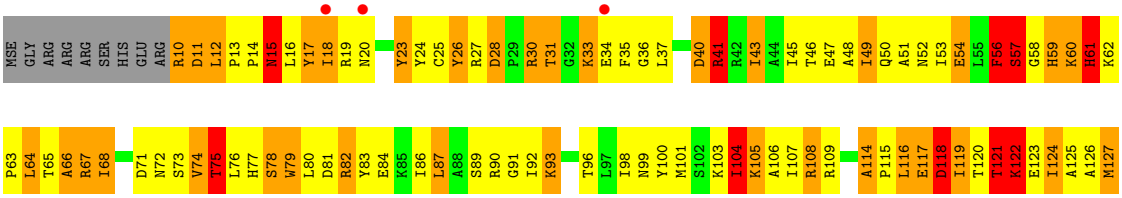
Chain A:



• Molecule 7: Integrase

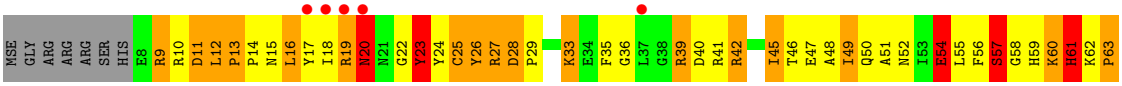
Chain B:

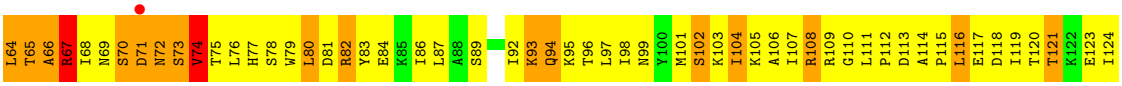


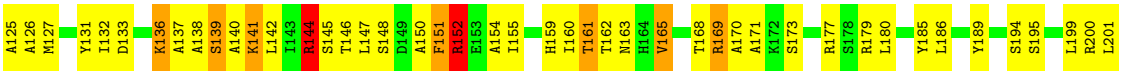


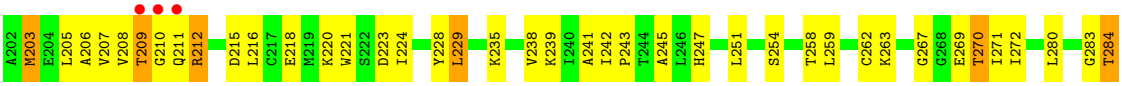
• Molecule 7: Integrase

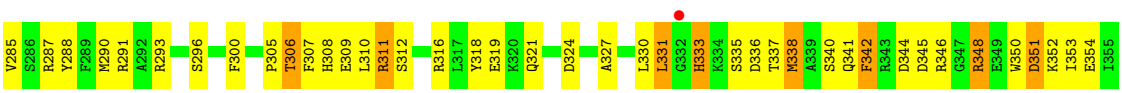
Chain C:

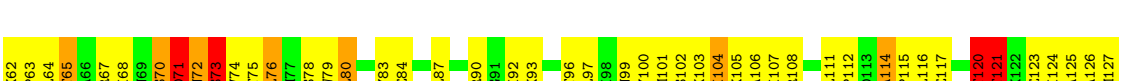


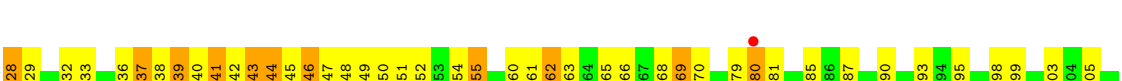






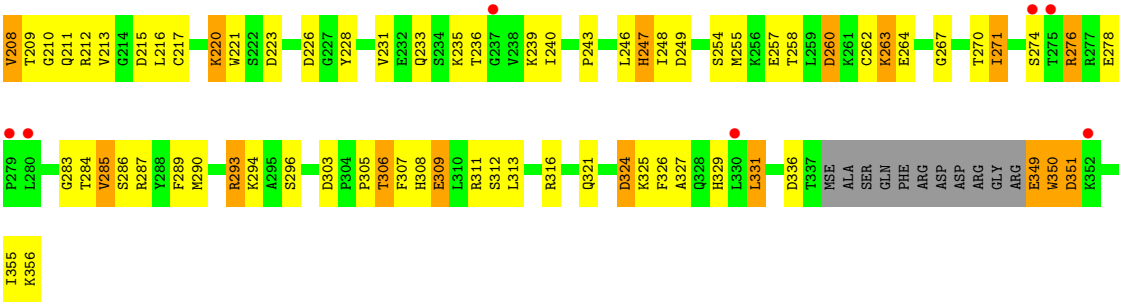






• Molecule 7: Integrase

Chain D:


V208 T209 G210 Q211 R212 V213 G214 D215 L216 C217 K220 W221 S222 D223 D226 G227 Y228 V231 E232 Q233 S234 K235 T236 G237 V238 K239 I240 P243 L246 H247 I248 D249 S254 M255 K256 E257 T258 L259 D260 K261 C262 K263 E264 G267 T270 I271 S274 T275 R276 R277 E278
P279 L280 G283 T284 V285 S286 R287 Y288 F289 M290 R293 K294 A295 S296 D303 P304 P305 T306 F307 H308 E309 L310 R311 S312 L313 R316 Q321 D324 K325 F326 A327 Q328 H329 L330 L331 D336 T337 MSE ALA SER GLN PHE ARG ASP ASP ARG GLY ARG E349 W350 D351 K352
I355 K356

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	109.76Å 109.76Å 265.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 4.40 44.75 – 4.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-4.40) 99.7 (44.75-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 4.45Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.244 , 0.292 0.248 , 0.284	Depositor DCC
R_{free} test set	1158 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	241.9	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.18 , 176.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l 0.066 for h,-h-k,-l 0.044 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15156	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[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
1	I	1.74	11/658 (1.7%)	2.96	78/1013 (7.7%)
2	J	1.89	15/667 (2.2%)	2.88	93/1028 (9.0%)
3	K	2.05	19/660 (2.9%)	3.19	110/1017 (10.8%)
4	L	1.84	8/667 (1.2%)	2.80	81/1028 (7.9%)
5	E	1.75	7/547 (1.3%)	3.17	87/841 (10.3%)
5	G	2.19	17/547 (3.1%)	3.59	107/841 (12.7%)
6	F	1.96	10/574 (1.7%)	3.24	93/886 (10.5%)
6	H	2.16	20/574 (3.5%)	3.67	124/886 (14.0%)
7	A	1.18	15/2804 (0.5%)	1.35	31/3762 (0.8%)
7	B	1.35	26/2670 (1.0%)	1.37	24/3589 (0.7%)
7	C	1.11	8/2808 (0.3%)	1.25	25/3767 (0.7%)
7	D	1.09	12/2670 (0.4%)	1.27	26/3589 (0.7%)
All	All	1.47	168/15846 (1.1%)	2.14	879/22247 (4.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	A	0	1
7	C	0	1
All	All	0	2

All (168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	15	DT	P-O5'	16.54	1.76	1.59
1	I	15	DC	C1'-N1	13.79	1.67	1.49
4	L	27	DC	C1'-N1	13.64	1.67	1.49
3	K	16	DT	C1'-N1	12.60	1.65	1.49
6	F	11	DC	C1'-N1	12.47	1.65	1.49
7	A	71	ASP	CB-CG	11.09	1.75	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	23	DA	N9-C4	9.82	1.43	1.37
2	J	15	DT	C3'-O3'	9.65	1.56	1.44
6	H	11	DC	C1'-N1	9.16	1.61	1.49
3	K	16	DT	P-O5'	8.84	1.68	1.59
5	G	10	DT	C1'-N1	8.59	1.60	1.49
7	D	35	PHE	CB-CG	-8.53	1.36	1.51
7	C	71	ASP	CB-CG	8.41	1.69	1.51
7	A	79	TRP	CB-CG	-8.14	1.35	1.50
7	D	56	PHE	CD1-CE1	8.04	1.55	1.39
6	H	15	DT	C1'-N1	7.97	1.59	1.49
4	L	15	DG	C3'-O3'	7.89	1.54	1.44
6	F	4	DA	C3'-O3'	-7.84	1.33	1.44
3	K	4	DC	C1'-N1	7.80	1.59	1.49
5	G	1	DA	C3'-O3'	7.79	1.54	1.44
6	F	11	DC	C2-N3	7.79	1.42	1.35
6	H	15	DT	C4'-O4'	7.72	1.52	1.45
2	J	17	DA	C6-N6	-7.71	1.27	1.33
2	J	4	DT	C1'-N1	7.58	1.59	1.49
3	K	20	DA	C3'-O3'	7.57	1.53	1.44
6	H	11	DC	C2-N3	7.41	1.41	1.35
7	C	152	ARG	NE-CZ	7.39	1.42	1.33
2	J	10	DT	C2-N3	-7.37	1.31	1.37
7	D	26	TYR	CB-CG	-7.37	1.40	1.51
7	B	124	ILE	CA-CB	-7.36	1.38	1.54
7	B	165	VAL	CA-CB	-7.27	1.39	1.54
2	J	10	DT	N3-C4	-7.27	1.32	1.38
7	D	72	ASN	CB-CG	7.24	1.67	1.51
7	D	11	ASP	CB-CG	7.21	1.66	1.51
7	A	152	ARG	NE-CZ	7.18	1.42	1.33
6	H	4	DA	C3'-O3'	-7.17	1.34	1.44
6	F	6	DT	N1-C2	7.16	1.43	1.38
5	G	24	DC	C1'-N1	7.15	1.58	1.49
7	B	119	ILE	CA-CB	-7.15	1.38	1.54
1	I	29	DC	C1'-N1	7.08	1.58	1.49
1	I	4	DT	C1'-N1	7.05	1.58	1.49
7	B	150	ALA	CA-CB	-7.04	1.37	1.52
7	D	54	GLU	CD-OE1	6.94	1.33	1.25
1	I	15	DC	P-O5'	6.93	1.66	1.59
6	F	25	DT	C1'-N1	6.93	1.58	1.49
7	B	33	LYS	CD-CE	6.92	1.68	1.51
4	L	3	DT	C1'-N1	6.86	1.58	1.49
1	I	6	DT	C1'-N1	6.82	1.58	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1	DT	C1'-N1	6.81	1.58	1.49
2	J	11	DT	N3-C4	-6.80	1.33	1.38
7	A	53	ILE	CB-CG2	6.77	1.73	1.52
5	E	10	DT	C1'-N1	6.75	1.58	1.49
7	A	23	TYR	CE1-CZ	6.74	1.47	1.38
5	E	20	DA	N9-C4	6.63	1.41	1.37
5	G	6	DT	C4-C5	-6.60	1.39	1.45
3	K	5	DC	P-O5'	6.59	1.66	1.59
6	F	6	DT	C1'-N1	6.55	1.57	1.49
7	A	31	THR	CA-CB	6.51	1.70	1.53
5	G	20	DA	N9-C4	6.47	1.41	1.37
5	E	9	DC	C1'-N1	6.30	1.57	1.49
3	K	21	DA	C3'-O3'	6.29	1.52	1.44
3	K	15	DA	C5'-C4'	6.28	1.58	1.51
7	B	350	TRP	CB-CG	6.23	1.61	1.50
2	J	11	DT	C4-C5	-6.21	1.39	1.45
7	A	8	GLU	N-CA	6.19	1.58	1.46
1	I	20	DA	C3'-O3'	6.16	1.51	1.44
6	F	17	DG	C3'-O3'	6.10	1.51	1.44
5	G	23	DA	C5-C4	6.10	1.43	1.38
6	H	22	DC	C1'-N1	6.07	1.57	1.49
2	J	9	DT	P-O5'	-6.04	1.53	1.59
6	H	6	DT	N1-C2	6.02	1.42	1.38
7	A	54	GLU	CD-OE2	6.02	1.32	1.25
7	B	72	ASN	CB-CG	6.01	1.64	1.51
7	D	155	ILE	CA-CB	-6.01	1.41	1.54
7	B	56	PHE	CB-CG	-5.99	1.41	1.51
7	A	54	GLU	CD-OE1	5.99	1.32	1.25
5	G	8	DA	N9-C4	5.97	1.41	1.37
7	A	168	THR	CA-CB	-5.96	1.37	1.53
7	B	174	GLU	CG-CD	5.95	1.60	1.51
7	B	143	ILE	CA-CB	-5.95	1.41	1.54
7	B	26	TYR	CB-CG	-5.93	1.42	1.51
2	J	9	DT	C3'-O3'	-5.92	1.36	1.44
7	A	151	PHE	CB-CG	-5.91	1.41	1.51
7	A	34	GLU	CD-OE1	5.88	1.32	1.25
2	J	20	DA	N9-C4	-5.88	1.34	1.37
7	C	54	GLU	CD-OE2	5.88	1.32	1.25
7	B	122	LYS	CB-CG	5.87	1.68	1.52
7	B	152	ARG	NE-CZ	5.85	1.40	1.33
5	E	8	DA	N9-C4	5.85	1.41	1.37
5	E	23	DA	N9-C4	5.83	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	11	DC	N1-C6	5.82	1.40	1.37
3	K	5	DC	C5'-C4'	5.81	1.57	1.51
6	H	9	DG	N9-C4	5.78	1.42	1.38
7	C	20	ASN	CB-CG	5.78	1.64	1.51
7	D	73	SER	CB-OG	5.75	1.49	1.42
4	L	4	DC	C1'-N1	5.73	1.56	1.49
1	I	15	DC	N1-C2	5.73	1.45	1.40
7	B	64	LEU	CA-C	5.72	1.67	1.52
7	D	17	TYR	CD1-CE1	5.71	1.48	1.39
7	D	56	PHE	CE2-CZ	5.71	1.48	1.37
7	B	17	TYR	CD1-CE1	5.69	1.47	1.39
3	K	17	DA	N7-C5	-5.68	1.35	1.39
6	H	25	DT	C1'-N1	5.65	1.56	1.49
1	I	28	DT	P-O5'	5.63	1.65	1.59
7	D	143	ILE	CA-CB	-5.62	1.42	1.54
5	G	12	DT	C1'-N1	5.62	1.56	1.49
5	G	15	DG	P-O5'	-5.59	1.54	1.59
6	H	24	DG	P-O5'	5.53	1.65	1.59
4	L	29	DA	N9-C4	5.53	1.41	1.37
6	H	17	DG	N7-C5	-5.53	1.35	1.39
3	K	17	DA	C5-C6	-5.51	1.36	1.41
6	F	2	DG	N9-C4	-5.50	1.33	1.38
4	L	15	DG	C6-N1	5.48	1.43	1.39
2	J	6	DA	C3'-O3'	-5.46	1.36	1.44
6	H	18	DT	C3'-O3'	-5.46	1.36	1.44
1	I	9	DT	C1'-N1	-5.42	1.39	1.47
3	K	2	DT	C1'-N1	5.41	1.56	1.49
7	B	105	LYS	CD-CE	5.40	1.64	1.51
7	A	11	ASP	CA-CB	-5.38	1.42	1.53
6	H	8	DT	N1-C2	5.38	1.42	1.38
5	G	6	DT	C3'-O3'	-5.37	1.36	1.44
3	K	6	DA	C3'-O3'	5.36	1.50	1.44
7	A	119	ILE	CA-CB	-5.32	1.42	1.54
4	L	18	DT	C5-C6	-5.32	1.30	1.34
7	B	117	GLU	CG-CD	5.31	1.59	1.51
7	B	134	GLU	CD-OE1	5.30	1.31	1.25
1	I	28	DT	C1'-N1	5.30	1.56	1.49
2	J	12	DA	N9-C4	-5.29	1.34	1.37
5	G	5	DG	C5-C4	-5.29	1.34	1.38
6	H	20	DA	C5-C6	-5.29	1.36	1.41
5	G	11	DA	C5-C6	5.28	1.45	1.41
6	H	8	DT	C1'-N1	5.27	1.56	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	28	DA	P-O5'	5.27	1.65	1.59
5	E	7	DC	N3-C4	-5.25	1.30	1.33
6	H	15	DT	C3'-O3'	-5.24	1.37	1.44
1	I	5	DC	C3'-O3'	-5.24	1.37	1.44
5	E	14	DA	C3'-O3'	5.23	1.50	1.44
5	G	2	DC	C3'-O3'	5.23	1.50	1.44
2	J	24	DA	N9-C4	-5.21	1.34	1.37
7	C	33	LYS	CB-CG	5.21	1.66	1.52
3	K	28	DC	P-O5'	5.20	1.65	1.59
7	B	155	ILE	CA-CB	-5.19	1.43	1.54
3	K	17	DA	C3'-O3'	-5.16	1.37	1.44
3	K	14	DT	C5-C6	-5.13	1.30	1.34
3	K	18	DT	N3-C4	-5.13	1.34	1.38
7	B	168	THR	CA-CB	-5.12	1.40	1.53
6	F	15	DT	P-O5'	5.11	1.64	1.59
7	B	71	ASP	CB-CG	5.10	1.62	1.51
2	J	1	DC	C3'-O3'	-5.09	1.37	1.44
7	B	104	ILE	CA-CB	-5.09	1.43	1.54
5	G	10	DT	N1-C6	5.08	1.41	1.38
7	B	15	ASN	CB-CG	-5.07	1.39	1.51
6	H	6	DT	C1'-N1	5.06	1.55	1.49
7	D	11	ASP	CA-CB	5.06	1.65	1.53
3	K	28	DC	C5'-C4'	5.05	1.56	1.51
7	B	57	SER	C-O	5.05	1.32	1.23
7	C	33	LYS	CD-CE	5.05	1.63	1.51
7	C	151	PHE	CB-CG	-5.04	1.42	1.51
7	B	17	TYR	CD2-CE2	5.04	1.47	1.39
6	H	4	DA	N9-C4	5.03	1.40	1.37
7	A	146	THR	CA-CB	-5.03	1.40	1.53
5	G	3	DA	N3-C4	-5.03	1.31	1.34
2	J	5	DC	N3-C4	-5.02	1.30	1.33
7	B	79	TRP	CG-CD1	-5.02	1.29	1.36
7	C	117	GLU	CD-OE1	5.02	1.31	1.25
5	G	12	DT	C5'-C4'	5.02	1.56	1.51
6	H	5	DT	C3'-O3'	-5.01	1.37	1.44
3	K	18	DT	C2-O2	-5.01	1.18	1.22

All (879) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	27	DA	O4'-C1'-N9	22.20	123.54	108.00
1	I	12	DT	O4'-C1'-N1	-21.48	92.97	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	5	DG	O4'-C1'-N9	19.77	121.84	108.00
6	F	11	DC	O4'-C1'-N1	19.04	121.33	108.00
6	F	6	DT	O4'-C1'-N1	18.36	120.86	108.00
6	H	6	DT	O4'-C1'-N1	17.18	120.03	108.00
5	G	23	DA	O4'-C1'-N9	16.64	119.64	108.00
5	E	5	DG	O4'-C1'-N9	16.22	119.36	108.00
3	K	14	DT	O4'-C1'-N1	16.13	119.29	108.00
3	K	16	DT	O4'-C4'-C3'	-16.04	96.38	106.00
5	G	14	DA	O4'-C1'-N9	15.62	118.93	108.00
6	H	3	DT	O4'-C4'-C3'	-15.41	96.76	106.00
5	G	10	DT	O4'-C1'-N1	15.31	118.72	108.00
5	E	19	DA	O4'-C1'-N9	15.27	118.69	108.00
6	H	11	DC	O4'-C1'-N1	14.66	118.26	108.00
5	G	6	DT	N3-C4-O4	14.20	128.42	119.90
6	H	4	DA	O4'-C1'-N9	14.09	117.86	108.00
2	J	17	DA	C5-C6-N1	13.71	124.56	117.70
3	K	1	DT	O4'-C1'-N1	13.71	117.59	108.00
3	K	16	DT	C6-N1-C2	-13.44	114.58	121.30
5	G	5	DG	O4'-C1'-C2'	-13.39	95.18	105.90
6	F	11	DC	C6-N1-C2	-13.06	115.08	120.30
6	H	2	DG	O4'-C4'-C3'	-13.02	98.19	106.00
6	H	14	DA	O3'-P-O5'	13.00	128.70	104.00
1	I	12	DT	P-O3'-C3'	12.93	135.21	119.70
2	J	14	DA	O4'-C1'-N9	12.85	117.00	108.00
2	J	15	DT	C4'-C3'-C2'	-12.76	91.62	103.10
5	E	4	DG	O4'-C1'-N9	12.75	116.93	108.00
5	G	10	DT	N3-C4-O4	12.72	127.53	119.90
6	H	11	DC	N3-C4-C5	-12.55	116.88	121.90
5	G	6	DT	C4-C5-C7	-12.52	111.49	119.00
7	A	116	LEU	CA-CB-CG	-12.40	86.77	115.30
5	G	6	DT	O4'-C1'-N1	12.38	116.67	108.00
6	F	23	DT	O4'-C1'-N1	12.25	116.58	108.00
6	H	13	DG	O4'-C1'-N9	12.18	116.53	108.00
2	J	2	DG	O4'-C1'-N9	12.11	116.47	108.00
1	I	3	DC	O4'-C1'-N1	12.09	116.46	108.00
4	L	27	DC	O4'-C1'-N1	12.07	116.45	108.00
5	E	5	DG	C8-N9-C4	-12.07	101.57	106.40
5	G	15	DG	O4'-C4'-C3'	-12.02	98.79	106.00
6	F	14	DA	O4'-C1'-N9	11.89	116.33	108.00
5	E	14	DA	O4'-C1'-N9	11.88	116.31	108.00
2	J	10	DT	N3-C2-O2	-11.83	115.20	122.30
6	H	15	DT	O4'-C1'-N1	11.83	116.28	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	28	DA	O4'-C1'-N9	11.80	116.26	108.00
1	I	16	DA	C8-N9-C4	-11.78	101.09	105.80
6	H	11	DC	C6-N1-C2	-11.73	115.61	120.30
5	G	6	DT	C6-C5-C7	11.71	129.93	122.90
5	E	10	DT	O4'-C1'-N1	11.60	116.12	108.00
1	I	15	DC	C6-N1-C2	-11.47	115.71	120.30
4	L	27	DC	C6-N1-C2	-11.39	115.74	120.30
5	G	18	DA	O4'-C1'-C2'	-11.37	96.81	105.90
4	L	1	DG	O4'-C1'-N9	11.35	115.94	108.00
1	I	15	DC	N3-C2-O2	-11.29	114.00	121.90
6	F	3	DT	O4'-C4'-C3'	-11.26	99.24	106.00
2	J	17	DA	C4-C5-C6	-11.18	111.41	117.00
1	I	28	DT	O4'-C1'-N1	11.14	115.80	108.00
4	L	13	DT	O4'-C1'-N1	11.13	115.79	108.00
3	K	26	DA	O4'-C1'-N9	11.11	115.78	108.00
6	F	9	DG	O4'-C1'-N9	11.10	115.77	108.00
2	J	17	DA	O4'-C1'-N9	11.08	115.75	108.00
5	G	14	DA	C8-N9-C4	-11.08	101.37	105.80
4	L	14	DT	O4'-C1'-N1	11.06	115.74	108.00
5	G	1	DA	P-O3'-C3'	11.06	132.97	119.70
3	K	11	DT	N3-C4-O4	11.02	126.51	119.90
5	G	23	DA	C8-N9-C4	-10.95	101.42	105.80
3	K	27	DG	O4'-C1'-N9	10.85	115.60	108.00
5	E	11	DA	O4'-C1'-N9	10.82	115.58	108.00
6	H	7	DT	O4'-C4'-C3'	-10.79	99.52	106.00
1	I	15	DC	N1-C2-O2	10.72	125.33	118.90
3	K	21	DA	P-O3'-C3'	10.71	132.55	119.70
5	G	8	DA	O4'-C1'-N9	10.68	115.47	108.00
5	G	6	DT	C5-C4-O4	-10.66	117.44	124.90
6	H	25	DT	O5'-P-OP1	-10.65	96.11	105.70
6	H	17	DG	C8-N9-C4	-10.65	102.14	106.40
4	L	18	DT	O4'-C1'-N1	10.64	115.45	108.00
6	H	24	DG	O4'-C4'-C3'	-10.61	99.64	106.00
6	H	24	DG	P-O3'-C3'	10.58	132.40	119.70
6	H	14	DA	O4'-C1'-N9	10.54	115.38	108.00
6	F	17	DG	C8-N9-C4	-10.53	102.19	106.40
6	F	23	DT	C1'-O4'-C4'	-10.52	99.58	110.10
3	K	20	DA	P-O3'-C3'	10.51	132.31	119.70
3	K	14	DT	N1-C1'-C2'	-10.41	92.83	112.60
7	D	11	ASP	CB-CG-OD1	10.37	127.63	118.30
6	H	4	DA	C8-N9-C4	-10.36	101.66	105.80
3	K	16	DT	N1-C1'-C2'	10.34	132.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	21	DA	O4'-C4'-C3'	10.33	112.20	106.00
6	H	22	DC	O4'-C1'-N1	10.33	115.23	108.00
4	L	26	DG	O4'-C1'-N9	10.31	115.22	108.00
6	H	17	DG	N9-C4-C5	10.30	109.52	105.40
6	F	24	DG	O4'-C1'-N9	10.20	115.14	108.00
2	J	15	DT	N3-C4-O4	10.05	125.93	119.90
4	L	13	DT	N3-C2-O2	-10.01	116.29	122.30
5	E	15	DG	N9-C4-C5	10.01	109.40	105.40
3	K	14	DT	C4-C5-C7	10.01	125.00	119.00
4	L	15	DG	C4'-C3'-C2'	-10.00	94.10	103.10
6	H	9	DG	N3-C4-C5	-10.00	123.60	128.60
3	K	15	DA	O4'-C4'-C3'	-9.98	100.01	106.00
6	F	19	DG	P-O3'-C3'	9.90	131.59	119.70
6	H	21	DC	O4'-C1'-N1	9.87	114.91	108.00
6	F	11	DC	N3-C4-C5	-9.87	117.95	121.90
1	I	16	DA	N9-C4-C5	9.86	109.75	105.80
6	H	18	DT	O4'-C4'-C3'	-9.84	100.10	106.00
6	F	24	DG	O4'-C1'-C2'	-9.82	98.04	105.90
6	H	20	DA	N1-C6-N6	9.75	124.45	118.60
1	I	9	DT	O4'-C1'-N1	-9.72	101.19	108.00
5	G	15	DG	N3-C4-N9	-9.71	120.17	126.00
6	F	7	DT	P-O3'-C3'	9.68	131.32	119.70
5	G	14	DA	N7-C8-N9	9.67	118.63	113.80
1	I	16	DA	O4'-C1'-N9	-9.65	101.25	108.00
4	L	18	DT	C6-C5-C7	-9.64	117.12	122.90
3	K	6	DA	O4'-C1'-N9	9.54	114.68	108.00
3	K	16	DT	C6-C5-C7	-9.53	117.19	122.90
4	L	29	DA	O4'-C1'-N9	9.51	114.66	108.00
6	H	15	DT	N3-C4-O4	9.49	125.59	119.90
6	H	18	DT	C6-N1-C2	-9.45	116.57	121.30
5	E	6	DT	O4'-C1'-N1	9.44	114.61	108.00
3	K	16	DT	N1-C2-N3	9.44	120.26	114.60
7	C	142	LEU	CA-CB-CG	-9.42	93.64	115.30
6	F	2	DG	N3-C4-C5	9.41	133.30	128.60
6	F	8	DT	C4-C5-C7	9.40	124.64	119.00
6	H	14	DA	OP1-P-O3'	-9.39	84.53	105.20
5	G	10	DT	C5-C4-O4	-9.38	118.33	124.90
1	I	20	DA	P-O3'-C3'	9.36	130.94	119.70
7	A	133	ASP	CB-CG-OD2	9.35	126.71	118.30
6	F	1	DG	O4'-C1'-N9	-9.34	101.46	108.00
6	H	15	DT	P-O5'-C5'	9.34	135.84	120.90
3	K	9	DT	O4'-C1'-N1	-9.30	101.49	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	14	DT	N3-C4-O4	-9.26	114.34	119.90
5	E	18	DA	O4'-C4'-C3'	-9.26	100.44	106.00
4	L	14	DT	O4'-C4'-C3'	-9.25	100.45	106.00
5	G	19	DA	O4'-C1'-C2'	-9.20	98.54	105.90
5	G	12	DT	O4'-C1'-N1	9.19	114.43	108.00
3	K	20	DA	O4'-C1'-N9	9.18	114.43	108.00
1	I	14	DA	C8-N9-C4	9.18	109.47	105.80
2	J	14	DA	O4'-C1'-C2'	-9.15	98.58	105.90
6	H	18	DT	N3-C4-O4	9.08	125.35	119.90
3	K	19	DA	C8-N9-C4	-9.07	102.17	105.80
5	G	11	DA	N9-C4-C5	9.04	109.42	105.80
1	I	12	DT	C1'-O4'-C4'	-9.04	101.06	110.10
5	G	11	DA	N1-C6-N6	-9.03	113.18	118.60
6	F	2	DG	C4-N9-C1'	-9.00	114.80	126.50
5	G	22	DT	P-O3'-C3'	8.99	130.49	119.70
1	I	13	DT	N3-C4-O4	-8.96	114.52	119.90
6	H	6	DT	O4'-C1'-C2'	-8.94	98.75	105.90
6	H	2	DG	O4'-C1'-N9	-8.91	101.76	108.00
6	H	10	DA	O4'-C4'-C3'	-8.90	100.66	106.00
4	L	8	DC	O4'-C1'-N1	8.86	114.20	108.00
1	I	23	DT	O4'-C4'-C3'	-8.84	100.70	106.00
6	F	17	DG	P-O3'-C3'	8.84	130.30	119.70
4	L	17	DA	O4'-C4'-C3'	8.83	111.30	106.00
5	G	18	DA	O4'-C4'-C3'	-8.82	100.71	106.00
2	J	15	DT	P-O3'-C3'	8.80	130.26	119.70
5	G	18	DA	O5'-P-OP2	-8.79	97.79	105.70
6	H	15	DT	O4'-C1'-C2'	-8.78	98.88	105.90
2	J	4	DT	O4'-C1'-N1	8.77	114.14	108.00
5	E	16	DT	C5-C4-O4	-8.77	118.76	124.90
6	H	15	DT	C3'-C2'-C1'	8.77	113.02	102.50
4	L	20	DA	O4'-C1'-N9	8.77	114.14	108.00
6	F	2	DG	O4'-C1'-N9	-8.77	101.86	108.00
6	F	8	DT	C6-C5-C7	-8.76	117.64	122.90
6	H	19	DG	N3-C4-C5	-8.76	124.22	128.60
7	B	11	ASP	CB-CG-OD2	8.76	126.19	118.30
6	H	21	DC	O4'-C1'-C2'	-8.72	98.92	105.90
5	E	23	DA	C8-N9-C4	-8.71	102.31	105.80
6	F	4	DA	C8-N9-C4	-8.71	102.32	105.80
6	F	2	DG	C8-N9-C1'	8.70	138.30	127.00
5	E	15	DG	C8-N9-C4	-8.69	102.93	106.40
7	A	30	ARG	N-CA-CB	-8.68	94.97	110.60
6	F	2	DG	N3-C4-N9	-8.67	120.80	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	12	DA	P-O3'-C3'	8.66	130.09	119.70
7	A	74	VAL	N-CA-C	8.64	134.34	111.00
6	H	23	DT	O4'-C1'-C2'	-8.62	99.01	105.90
3	K	21	DA	O5'-P-OP2	-8.61	97.95	105.70
3	K	18	DT	N1-C2-N3	8.58	119.75	114.60
2	J	15	DT	C1'-O4'-C4'	-8.56	101.54	110.10
5	E	8	DA	O4'-C1'-N9	8.56	113.99	108.00
6	H	7	DT	P-O3'-C3'	8.54	129.95	119.70
6	H	9	DG	C2-N3-C4	8.54	116.17	111.90
3	K	28	DC	O4'-C1'-N1	8.54	113.98	108.00
1	I	14	DA	O4'-C1'-C2'	8.54	112.73	105.90
3	K	7	DG	O4'-C1'-N9	8.53	113.97	108.00
4	L	11	DT	P-O3'-C3'	8.52	129.92	119.70
6	H	15	DT	C6-N1-C2	-8.51	117.05	121.30
6	F	11	DC	C5-C6-N1	8.51	125.25	121.00
7	C	9	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	I	20	DA	O4'-C1'-N9	8.47	113.93	108.00
6	F	6	DT	O4'-C1'-C2'	-8.46	99.13	105.90
6	H	19	DG	C8-N9-C4	-8.44	103.03	106.40
6	H	13	DG	C8-N9-C4	-8.44	103.03	106.40
7	C	9	ARG	NE-CZ-NH2	-8.43	116.08	120.30
6	F	9	DG	O4'-C1'-C2'	-8.43	99.16	105.90
5	G	16	DT	O5'-P-OP2	8.42	120.80	110.70
3	K	27	DG	P-O3'-C3'	8.40	129.78	119.70
7	B	74	VAL	N-CA-C	-8.39	88.33	111.00
6	H	1	DG	O4'-C4'-C3'	-8.39	100.97	106.00
7	A	71	ASP	CB-CG-OD1	8.39	125.85	118.30
7	A	169	ARG	NE-CZ-NH1	8.38	124.49	120.30
7	A	118	ASP	CB-CG-OD2	8.36	125.82	118.30
5	E	5	DG	N9-C4-C5	8.34	108.73	105.40
6	F	4	DA	O4'-C1'-N9	8.31	113.82	108.00
6	F	23	DT	N3-C2-O2	-8.31	117.31	122.30
5	G	15	DG	O5'-P-OP2	-8.31	98.22	105.70
1	I	15	DC	O4'-C1'-N1	8.29	113.80	108.00
6	H	5	DT	C4-C5-C7	8.24	123.94	119.00
4	L	27	DC	P-O3'-C3'	8.21	129.56	119.70
2	J	9	DT	O5'-P-OP2	-8.21	98.31	105.70
6	F	20	DA	O4'-C1'-N9	8.20	113.74	108.00
1	I	12	DT	N1-C1'-C2'	8.20	128.18	112.60
7	D	55	LEU	CA-CB-CG	-8.20	96.44	115.30
7	A	76	LEU	CA-CB-CG	-8.19	96.45	115.30
4	L	15	DG	P-O3'-C3'	8.19	129.52	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	13	DC	C6-N1-C2	-8.17	117.03	120.30
5	E	20	DA	O4'-C1'-C2'	-8.17	99.37	105.90
1	I	15	DC	O4'-C1'-C2'	-8.15	99.38	105.90
1	I	5	DC	O4'-C4'-C3'	-8.11	101.13	106.00
2	J	10	DT	N3-C4-C5	8.10	120.06	115.20
3	K	6	DA	P-O3'-C3'	8.10	129.42	119.70
2	J	8	DG	O4'-C1'-N9	8.09	113.67	108.00
2	J	15	DT	C5-C4-O4	-8.09	119.24	124.90
1	I	6	DT	N3-C4-O4	8.08	124.75	119.90
2	J	16	DT	O4'-C4'-C3'	-8.08	101.15	106.00
3	K	20	DA	C1'-O4'-C4'	-8.08	102.02	110.10
2	J	17	DA	C8-N9-C1'	8.08	142.25	127.70
3	K	13	DT	N3-C2-O2	-8.06	117.46	122.30
1	I	12	DT	O4'-C1'-C2'	-8.05	99.46	105.90
6	H	24	DG	OP1-P-O3'	-8.05	87.50	105.20
4	L	18	DT	C4-C5-C7	8.04	123.82	119.00
1	I	19	DA	O4'-C4'-C3'	8.04	110.82	106.00
4	L	15	DG	N1-C6-O6	8.04	124.72	119.90
6	F	15	DT	N3-C4-O4	8.03	124.72	119.90
1	I	21	DA	O4'-C1'-N9	8.03	113.62	108.00
6	H	25	DT	O4'-C1'-N1	8.01	113.61	108.00
6	F	17	DG	N9-C4-C5	8.01	108.60	105.40
1	I	13	DT	C1'-O4'-C4'	-7.99	102.11	110.10
7	C	74	VAL	N-CA-C	7.94	132.44	111.00
3	K	14	DT	C6-N1-C2	7.89	125.24	121.30
5	G	23	DA	N7-C8-N9	7.88	117.74	113.80
4	L	18	DT	N3-C2-O2	-7.88	117.57	122.30
6	H	11	DC	C5-C6-N1	7.87	124.94	121.00
3	K	17	DA	C4'-C3'-C2'	-7.86	96.02	103.10
7	B	336	ASP	CB-CG-OD2	7.86	125.38	118.30
3	K	16	DT	C4-C5-C6	7.86	122.72	118.00
5	E	19	DA	C2-N3-C4	7.86	114.53	110.60
5	E	23	DA	O4'-C1'-N9	7.85	113.50	108.00
3	K	14	DT	C6-C5-C7	-7.84	118.19	122.90
7	B	161	THR	N-CA-CB	-7.84	95.40	110.30
6	F	12	DT	O4'-C4'-C3'	-7.83	101.30	106.00
3	K	24	DT	O4'-C1'-C2'	-7.81	99.65	105.90
3	K	14	DT	N1-C2-O2	7.81	129.34	123.10
7	B	87	LEU	CA-CB-CG	-7.80	97.35	115.30
2	J	17	DA	C8-N9-C4	-7.80	102.68	105.80
5	E	3	DA	P-O3'-C3'	7.78	129.03	119.70
1	I	11	DT	C4-C5-C7	-7.77	114.34	119.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	169	ARG	NE-CZ-NH2	-7.77	116.41	120.30
6	H	4	DA	O4'-C4'-C3'	-7.74	101.35	106.00
6	H	5	DT	C6-C5-C7	-7.73	118.26	122.90
2	J	17	DA	O5'-P-OP1	-7.72	98.75	105.70
6	F	17	DG	C4-C5-C6	7.69	123.42	118.80
5	E	15	DG	C4-C5-N7	-7.68	107.73	110.80
1	I	16	DA	N9-C1'-C2'	7.68	127.19	112.60
4	L	18	DT	C4'-C3'-C2'	-7.67	96.20	103.10
5	E	6	DT	C1'-O4'-C4'	-7.67	102.43	110.10
5	G	17	DC	O4'-C4'-C3'	-7.67	101.40	106.00
6	H	17	DG	C4-C5-N7	-7.67	107.73	110.80
7	B	28	ASP	CB-CG-OD2	7.66	125.20	118.30
3	K	4	DC	O4'-C1'-N1	7.66	113.36	108.00
2	J	12	DA	O4'-C4'-C3'	-7.66	101.41	106.00
3	K	16	DT	O4'-C1'-C2'	-7.65	99.78	105.90
6	F	25	DT	O4'-C1'-N1	7.64	113.35	108.00
6	F	18	DT	N3-C2-O2	-7.62	117.73	122.30
5	E	8	DA	O4'-C1'-C2'	-7.61	99.81	105.90
6	H	15	DT	N3-C4-C5	-7.60	110.64	115.20
3	K	23	DT	N3-C4-O4	7.59	124.45	119.90
6	F	15	DT	O4'-C1'-N1	7.58	113.31	108.00
6	H	10	DA	C3'-C2'-C1'	-7.58	93.40	102.50
6	F	2	DG	N9-C1'-C2'	7.58	127.00	112.60
5	G	18	DA	C3'-C2'-C1'	-7.57	93.42	102.50
3	K	26	DA	P-O5'-C5'	-7.55	108.82	120.90
6	H	11	DC	C2-N3-C4	7.54	123.67	119.90
5	G	18	DA	O5'-P-OP1	7.53	119.73	110.70
2	J	16	DT	O4'-C1'-C2'	-7.53	99.88	105.90
4	L	16	DA	C5-C6-N6	-7.53	117.68	123.70
1	I	15	DC	O5'-P-OP2	7.52	119.72	110.70
5	E	19	DA	O4'-C1'-C2'	-7.51	99.89	105.90
6	F	6	DT	N3-C4-O4	7.51	124.41	119.90
2	J	14	DA	N9-C4-C5	7.50	108.80	105.80
6	H	17	DG	O4'-C1'-N9	7.50	113.25	108.00
2	J	5	DC	N3-C2-O2	-7.49	116.66	121.90
6	H	15	DT	C1'-O4'-C4'	7.48	117.58	110.10
2	J	16	DT	O5'-P-OP1	-7.47	98.98	105.70
6	F	5	DT	O3'-P-O5'	-7.46	89.83	104.00
3	K	16	DT	P-O3'-C3'	7.46	128.65	119.70
2	J	9	DT	O4'-C1'-N1	-7.45	102.79	108.00
6	F	24	DG	OP2-P-O3'	7.44	121.57	105.20
4	L	15	DG	C1'-O4'-C4'	-7.44	102.66	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	15	DG	C1'-O4'-C4'	-7.43	102.67	110.10
6	H	17	DG	N3-C2-N2	-7.43	114.70	119.90
2	J	27	DG	C8-N9-C4	-7.43	103.43	106.40
1	I	11	DT	N3-C4-O4	7.43	124.36	119.90
2	J	11	DT	P-O3'-C3'	7.42	128.60	119.70
6	H	11	DC	N3-C4-N4	7.41	123.18	118.00
3	K	11	DT	C4-C5-C7	-7.39	114.56	119.00
6	H	8	DT	N3-C2-O2	-7.38	117.87	122.30
2	J	17	DA	N9-C1'-C2'	7.38	126.62	112.60
6	H	24	DG	P-O5'-C5'	7.38	132.70	120.90
3	K	17	DA	C8-N9-C4	-7.37	102.85	105.80
7	A	30	ARG	CA-CB-CG	7.37	129.62	113.40
5	E	17	DC	O5'-P-OP1	7.37	119.54	110.70
6	H	14	DA	C8-N9-C4	-7.37	102.85	105.80
1	I	28	DT	P-O5'-C5'	7.36	132.68	120.90
3	K	5	DC	P-O3'-C3'	7.35	128.52	119.70
6	F	11	DC	C2-N3-C4	7.34	123.57	119.90
7	C	28	ASP	CB-CG-OD2	7.33	124.90	118.30
6	H	9	DG	C5-C6-N1	7.29	115.14	111.50
5	G	19	DA	O3'-P-O5'	-7.28	90.16	104.00
5	G	7	DC	N3-C2-O2	-7.28	116.80	121.90
5	G	12	DT	O5'-P-OP2	-7.26	99.17	105.70
5	E	7	DC	C6-N1-C2	-7.25	117.40	120.30
5	G	13	DC	C5-C6-N1	7.25	124.62	121.00
6	H	4	DA	N9-C4-C5	7.24	108.69	105.80
6	F	16	DA	N9-C4-C5	-7.23	102.91	105.80
6	H	23	DT	C1'-O4'-C4'	-7.23	102.87	110.10
5	G	22	DT	C1'-O4'-C4'	-7.22	102.88	110.10
3	K	29	DG	C2-N3-C4	7.22	115.51	111.90
5	E	13	DC	O4'-C1'-N1	7.21	113.05	108.00
5	E	24	DC	O4'-C1'-N1	-7.21	102.95	108.00
3	K	11	DT	C5-C4-O4	-7.21	119.85	124.90
7	D	26	TYR	CA-CB-CG	-7.21	99.71	113.40
6	H	13	DG	N9-C4-C5	7.19	108.28	105.40
7	D	71	ASP	CB-CG-OD2	7.18	124.77	118.30
3	K	16	DT	C4'-C3'-C2'	-7.17	96.64	103.10
1	I	15	DC	P-O3'-C3'	7.17	128.31	119.70
5	E	16	DT	O5'-P-OP2	7.13	119.26	110.70
2	J	4	DT	C6-C5-C7	-7.12	118.63	122.90
6	F	18	DT	O4'-C4'-C3'	-7.11	101.66	104.50
5	G	15	DG	N3-C2-N2	-7.09	114.93	119.90
7	A	55	LEU	CB-CG-CD1	-7.08	98.97	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	14	DA	C5-N7-C8	-7.07	100.37	103.90
1	I	13	DT	C5-C4-O4	7.06	129.84	124.90
6	F	4	DA	O4'-C4'-C3'	-7.05	101.68	104.50
6	H	22	DC	C6-N1-C2	-7.05	117.48	120.30
1	I	6	DT	C6-N1-C2	-7.04	117.78	121.30
2	J	14	DA	C4-C5-N7	-7.04	107.18	110.70
5	G	15	DG	N3-C4-C5	7.04	132.12	128.60
3	K	23	DT	O4'-C4'-C3'	-7.03	101.69	104.50
2	J	9	DT	C5-C4-O4	-7.03	119.98	124.90
6	H	20	DA	C4-C5-N7	7.03	114.21	110.70
6	F	6	DT	C1'-O4'-C4'	-7.02	103.08	110.10
5	E	5	DG	N3-C4-C5	-7.01	125.10	128.60
6	H	17	DG	C4-C5-C6	7.01	123.00	118.80
6	H	4	DA	P-O3'-C3'	-7.00	111.30	119.70
4	L	16	DA	N7-C8-N9	6.99	117.29	113.80
5	G	7	DC	P-O3'-C3'	6.96	128.06	119.70
4	L	23	DC	O4'-C1'-N1	-6.96	103.13	108.00
5	G	20	DA	C8-N9-C4	-6.95	103.02	105.80
2	J	10	DT	N1-C2-O2	6.95	128.66	123.10
2	J	1	DC	O4'-C1'-N1	-6.95	103.14	108.00
5	E	7	DC	O4'-C4'-C3'	6.94	110.17	106.00
4	L	16	DA	N1-C6-N6	6.94	122.77	118.60
5	G	11	DA	P-O5'-C5'	6.94	132.00	120.90
6	F	8	DT	O5'-P-OP1	-6.93	99.46	105.70
1	I	15	DC	O4'-C4'-C3'	-6.93	101.73	104.50
1	I	15	DC	N1-C1'-C2'	6.92	125.75	112.60
5	E	3	DA	OP1-P-O3'	-6.92	89.97	105.20
5	G	5	DG	C1'-O4'-C4'	-6.92	103.18	110.10
5	E	19	DA	N1-C2-N3	-6.90	125.85	129.30
7	B	133	ASP	CB-CG-OD2	6.90	124.51	118.30
6	H	16	DA	O5'-P-OP1	-6.89	99.49	105.70
4	L	3	DT	C6-N1-C2	-6.88	117.86	121.30
5	E	1	DA	N9-C1'-C2'	6.88	125.67	112.60
5	G	8	DA	C8-N9-C4	-6.88	103.05	105.80
3	K	10	DT	N3-C2-O2	-6.88	118.17	122.30
6	H	6	DT	N3-C4-O4	6.86	124.01	119.90
2	J	4	DT	C4-C5-C7	6.85	123.11	119.00
6	F	5	DT	C1'-O4'-C4'	-6.85	103.25	110.10
2	J	17	DA	C5-N7-C8	-6.85	100.48	103.90
5	E	10	DT	N3-C4-O4	6.84	124.01	119.90
5	G	24	DC	OP1-P-OP2	6.84	129.86	119.60
6	F	24	DG	C8-N9-C4	-6.83	103.67	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	71	ASP	CB-CG-OD1	6.83	124.44	118.30
4	L	29	DA	C8-N9-C4	-6.82	103.07	105.80
3	K	16	DT	C4'-C3'-O3'	-6.82	92.66	109.70
5	G	22	DT	O4'-C1'-C2'	-6.81	100.45	105.90
4	L	13	DT	N1-C2-O2	6.80	128.54	123.10
4	L	17	DA	C4'-C3'-C2'	-6.79	96.99	103.10
6	F	17	DG	C4-C5-N7	-6.79	108.09	110.80
4	L	20	DA	N1-C6-N6	6.78	122.67	118.60
7	A	303	ASP	CB-CG-OD2	6.78	124.40	118.30
2	J	17	DA	C6-N1-C2	-6.77	114.54	118.60
5	E	17	DC	C6-N1-C1'	-6.77	112.67	120.80
2	J	24	DA	P-O3'-C3'	-6.75	111.59	119.70
4	L	12	DG	P-O3'-C3'	6.75	127.81	119.70
7	D	11	ASP	OD1-CG-OD2	-6.75	110.48	123.30
2	J	14	DA	N1-C6-N6	-6.74	114.56	118.60
6	H	20	DA	N9-C4-C5	-6.74	103.11	105.80
2	J	11	DT	C4-C5-C7	-6.73	114.96	119.00
2	J	9	DT	N3-C4-O4	6.73	123.94	119.90
3	K	17	DA	N1-C6-N6	6.73	122.64	118.60
3	K	14	DT	N3-C4-C5	6.71	119.22	115.20
3	K	20	DA	OP2-P-O3'	6.70	119.95	105.20
4	L	15	DG	N7-C8-N9	6.70	116.45	113.10
5	E	22	DT	P-O3'-C3'	6.70	127.74	119.70
2	J	11	DT	C6-C5-C7	6.68	126.91	122.90
2	J	21	DA	O4'-C4'-C3'	6.68	110.00	106.00
5	E	15	DG	C5-C6-O6	6.65	132.59	128.60
6	H	2	DG	N9-C1'-C2'	6.65	125.23	112.60
5	E	10	DT	C5-C4-O4	-6.64	120.25	124.90
7	B	118	ASP	CB-CG-OD2	6.63	124.26	118.30
1	I	12	DT	C5'-C4'-C3'	6.62	126.03	114.10
6	F	6	DT	P-O3'-C3'	6.62	127.64	119.70
5	G	7	DC	C6-N1-C2	-6.61	117.66	120.30
2	J	14	DA	C5-C6-N6	6.60	128.98	123.70
3	K	10	DT	N3-C4-O4	6.60	123.86	119.90
5	G	6	DT	O4'-C1'-C2'	-6.59	100.63	105.90
6	H	2	DG	C5'-C4'-C3'	6.59	125.96	114.10
1	I	28	DT	OP1-P-OP2	-6.58	109.73	119.60
6	H	20	DA	C6-C5-N7	-6.57	127.70	132.30
5	E	20	DA	P-O3'-C3'	6.57	127.58	119.70
2	J	6	DA	C8-N9-C4	-6.57	103.17	105.80
6	H	23	DT	N1-C2-N3	6.56	118.54	114.60
7	A	186	LEU	CA-CB-CG	6.54	130.35	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	9	DG	N9-C1'-C2'	6.54	125.03	112.60
6	H	9	DG	C8-N9-C4	-6.54	103.78	106.40
1	I	15	DC	P-O5'-C5'	6.53	131.34	120.90
5	E	23	DA	C4-C5-C6	6.52	120.26	117.00
5	G	6	DT	C6-N1-C2	-6.52	118.04	121.30
2	J	13	DT	N3-C2-O2	-6.51	118.39	122.30
5	E	12	DT	C4-C5-C7	6.51	122.91	119.00
4	L	4	DC	P-O3'-C3'	6.50	127.50	119.70
3	K	1	DT	P-O3'-C3'	6.49	127.49	119.70
3	K	13	DT	O4'-C1'-N1	-6.49	103.45	108.00
2	J	5	DC	C2-N3-C4	-6.49	116.65	119.90
3	K	11	DT	O4'-C4'-C3'	-6.49	101.90	104.50
4	L	16	DA	C5-N7-C8	-6.48	100.66	103.90
3	K	19	DA	O4'-C4'-C3'	6.48	109.89	106.00
1	I	15	DC	O5'-P-OP1	-6.47	99.87	105.70
5	G	23	DA	C3'-C2'-C1'	6.47	110.27	102.50
6	H	15	DT	O5'-P-OP2	-6.46	99.88	105.70
3	K	21	DA	O4'-C1'-N9	6.46	112.52	108.00
7	D	16	LEU	CB-CG-CD1	-6.45	100.03	111.00
3	K	19	DA	O4'-C1'-N9	6.45	112.52	108.00
5	G	11	DA	C6-C5-N7	6.45	136.81	132.30
7	A	152	ARG	NE-CZ-NH1	6.45	123.52	120.30
5	G	4	DG	P-O3'-C3'	6.44	127.42	119.70
3	K	10	DT	O4'-C1'-N1	6.42	112.50	108.00
6	H	2	DG	C8-N9-C1'	6.42	135.35	127.00
1	I	4	DT	O4'-C1'-N1	6.42	112.49	108.00
6	H	11	DC	O4'-C1'-C2'	-6.42	100.77	105.90
5	E	16	DT	N3-C4-O4	6.40	123.74	119.90
5	G	24	DC	N3-C4-N4	-6.40	113.52	118.00
5	G	15	DG	C2-N3-C4	-6.39	108.70	111.90
3	K	8	DC	O4'-C1'-C2'	6.39	111.01	105.90
7	D	133	ASP	CB-CG-OD2	6.39	124.05	118.30
3	K	9	DT	N3-C4-O4	6.38	123.73	119.90
6	H	23	DT	C6-C5-C7	-6.38	119.07	122.90
1	I	14	DA	C4-C5-C6	-6.38	113.81	117.00
4	L	28	DA	P-O3'-C3'	6.38	127.35	119.70
7	C	16	LEU	CA-CB-CG	-6.37	100.64	115.30
5	G	11	DA	C4-C5-N7	-6.37	107.52	110.70
5	G	5	DG	C5-C6-N1	6.37	114.68	111.50
4	L	17	DA	N1-C6-N6	6.36	122.42	118.60
6	H	19	DG	P-O3'-C3'	6.35	127.32	119.70
2	J	21	DA	N9-C4-C5	6.35	108.34	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	9	DT	P-O5'-C5'	-6.34	110.75	120.90
7	C	152	ARG	NE-CZ-NH1	6.34	123.47	120.30
6	H	10	DA	C5-C6-N1	6.34	120.87	117.70
1	I	14	DA	N1-C2-N3	-6.34	126.13	129.30
5	G	23	DA	N3-C4-C5	-6.34	122.36	126.80
5	G	11	DA	C5-C6-N6	6.33	128.77	123.70
4	L	15	DG	C5-C6-O6	-6.33	124.80	128.60
7	B	109	ARG	NE-CZ-NH1	6.32	123.46	120.30
6	H	20	DA	C5-C6-N6	-6.32	118.64	123.70
1	I	16	DA	N7-C8-N9	6.32	116.96	113.80
3	K	3	DG	O4'-C4'-C3'	-6.32	101.97	104.50
5	G	12	DT	C4-C5-C7	6.32	122.79	119.00
1	I	29	DC	O4'-C1'-N1	6.32	112.42	108.00
6	H	15	DT	C5-C6-N1	6.31	127.49	123.70
7	C	61	HIS	N-CA-C	-6.31	93.96	111.00
4	L	14	DT	C6-N1-C2	-6.30	118.15	121.30
3	K	15	DA	P-O3'-C3'	6.29	127.25	119.70
5	E	6	DT	C5'-C4'-O4'	-6.28	97.36	109.30
7	B	223	ASP	CB-CG-OD2	6.28	123.95	118.30
5	E	17	DC	P-O5'-C5'	-6.27	110.87	120.90
6	H	25	DT	N3-C4-O4	6.27	123.66	119.90
7	B	26	TYR	CA-CB-CG	-6.27	101.49	113.40
6	F	3	DT	C6-N1-C2	-6.26	118.17	121.30
5	E	9	DC	C6-N1-C1'	6.26	128.31	120.80
6	H	9	DG	N3-C4-N9	6.26	129.75	126.00
6	H	23	DT	N1-C1'-C2'	6.25	124.48	112.60
7	C	118	ASP	CB-CG-OD2	6.25	123.92	118.30
6	F	10	DA	P-O3'-C3'	6.24	127.19	119.70
1	I	23	DT	O4'-C1'-N1	-6.24	103.63	108.00
2	J	17	DA	C4-N9-C1'	-6.24	115.07	126.30
7	C	133	ASP	CB-CG-OD2	6.23	123.91	118.30
3	K	15	DA	O5'-C5'-C4'	6.23	126.56	111.00
5	G	16	DT	C5-C4-O4	-6.22	120.54	124.90
5	E	17	DC	N1-C2-O2	6.22	122.63	118.90
6	F	4	DA	C1'-O4'-C4'	6.21	116.31	110.10
3	K	14	DT	N3-C2-O2	-6.21	118.58	122.30
7	D	33	LYS	CD-CE-NZ	6.21	125.97	111.70
6	H	14	DA	N9-C4-C5	6.20	108.28	105.80
1	I	15	DC	C2-N1-C1'	6.19	125.61	118.80
5	G	24	DC	N3-C4-C5	6.19	124.38	121.90
6	H	3	DT	N3-C2-O2	-6.19	118.59	122.30
4	L	3	DT	N1-C1'-C2'	6.18	124.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	10	DT	P-O3'-C3'	6.18	127.11	119.70
6	H	24	DG	OP2-P-O3'	6.16	118.76	105.20
1	I	23	DT	C4-C5-C7	6.16	122.70	119.00
3	K	21	DA	C3'-C2'-C1'	6.16	109.89	102.50
3	K	15	DA	OP1-P-O3'	-6.15	91.66	105.20
7	C	13	PRO	N-CD-CG	-6.15	93.97	103.20
2	J	16	DT	O5'-C5'-C4'	-6.15	95.63	111.00
5	G	17	DC	O5'-P-OP1	6.15	118.08	110.70
5	G	12	DT	N3-C4-O4	6.14	123.58	119.90
7	A	34	GLU	CB-CA-C	-6.14	98.13	110.40
7	B	121	THR	N-CA-CB	-6.13	98.65	110.30
5	E	11	DA	C6-C5-N7	6.13	136.59	132.30
4	L	19	DA	O4'-C1'-N9	6.12	112.28	108.00
1	I	1	DA	O4'-C1'-C2'	-6.11	101.01	105.90
4	L	24	DT	O4'-C1'-C2'	-6.10	101.02	105.90
6	F	17	DG	N3-C2-N2	-6.10	115.63	119.90
4	L	20	DA	O5'-P-OP1	6.08	118.00	110.70
4	L	23	DC	O4'-C1'-C2'	-6.08	101.04	105.90
6	F	21	DC	O4'-C1'-N1	6.07	112.25	108.00
5	G	11	DA	P-O3'-C3'	6.07	126.98	119.70
5	E	23	DA	N7-C8-N9	6.07	116.83	113.80
3	K	25	DG	P-O3'-C3'	6.06	126.97	119.70
6	H	13	DG	N7-C8-N9	6.06	116.13	113.10
7	A	15	ASN	CB-CA-C	-6.06	98.28	110.40
2	J	5	DC	N3-C4-C5	6.04	124.32	121.90
1	I	14	DA	P-O5'-C5'	-6.04	111.24	120.90
6	F	17	DG	N3-C4-C5	-6.04	125.58	128.60
5	E	18	DA	C3'-C2'-C1'	-6.03	95.27	102.50
6	F	16	DA	C8-N9-C4	6.02	108.21	105.80
5	G	10	DT	O4'-C1'-C2'	-6.02	101.08	105.90
7	A	71	ASP	OD1-CG-OD2	-6.01	111.88	123.30
5	E	23	DA	N3-C4-C5	-6.01	122.59	126.80
7	D	26	TYR	CB-CG-CD1	-6.00	117.40	121.00
5	G	8	DA	O4'-C1'-C2'	-6.00	101.10	105.90
6	H	12	DT	O4'-C1'-C2'	-6.00	101.10	105.90
3	K	29	DG	C8-N9-C4	-5.99	104.00	106.40
6	H	23	DT	N3-C2-O2	-5.99	118.71	122.30
6	H	4	DA	N7-C8-N9	5.98	116.79	113.80
1	I	8	DC	O4'-C1'-C2'	5.98	110.68	105.90
2	J	6	DA	N7-C8-N9	5.98	116.79	113.80
5	E	17	DC	C2-N1-C1'	5.97	125.37	118.80
4	L	16	DA	C4-C5-N7	5.97	113.68	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	149	ASP	CB-CG-OD2	5.97	123.67	118.30
3	K	16	DT	N3-C4-C5	-5.96	111.62	115.20
2	J	20	DA	C2-N3-C4	-5.96	107.62	110.60
3	K	19	DA	N9-C4-C5	5.95	108.18	105.80
3	K	29	DG	N3-C4-C5	-5.93	125.63	128.60
1	I	29	DC	C6-N1-C2	-5.93	117.93	120.30
6	F	17	DG	C5-C6-N1	-5.93	108.54	111.50
4	L	15	DG	C8-N9-C4	-5.92	104.03	106.40
7	C	351	ASP	CB-CG-OD2	5.92	123.63	118.30
2	J	17	DA	N9-C4-C5	5.92	108.17	105.80
2	J	9	DT	P-O5'-C5'	-5.91	111.45	120.90
6	F	21	DC	N3-C4-N4	-5.90	113.87	118.00
6	H	2	DG	C3'-C2'-C1'	-5.90	95.42	102.50
4	L	21	DA	O4'-C1'-N9	5.90	112.13	108.00
1	I	27	DA	C4'-C3'-C2'	-5.90	97.79	103.10
5	E	7	DC	C4-C5-C6	5.88	120.34	117.40
5	G	10	DT	C2-N3-C4	5.88	130.73	127.20
7	C	165	VAL	CB-CA-C	-5.87	100.25	111.40
1	I	17	DA	N1-C6-N6	5.87	122.12	118.60
4	L	20	DA	C8-N9-C4	-5.85	103.46	105.80
7	D	21	ASN	N-CA-CB	-5.85	100.07	110.60
3	K	15	DA	O3'-P-O5'	5.85	115.11	104.00
5	G	23	DA	O5'-P-OP1	-5.85	100.44	105.70
5	G	21	DA	N1-C6-N6	-5.84	115.09	118.60
5	E	11	DA	C4-C5-C6	-5.84	114.08	117.00
4	L	24	DT	N3-C4-O4	5.83	123.40	119.90
6	H	13	DG	N3-C4-N9	-5.83	122.50	126.00
3	K	29	DG	N9-C1'-C2'	5.82	123.66	112.60
5	E	18	DA	O4'-C1'-C2'	-5.82	101.24	105.90
7	C	324	ASP	CB-CG-OD2	5.82	123.54	118.30
5	G	4	DG	N9-C4-C5	5.82	107.73	105.40
4	L	20	DA	C5-N7-C8	-5.81	101.00	103.90
6	F	6	DT	N1-C2-O2	5.81	127.75	123.10
7	A	324	ASP	CB-CG-OD2	5.81	123.53	118.30
5	G	11	DA	OP2-P-O3'	5.81	117.97	105.20
6	H	12	DT	N1-C1'-C2'	5.81	123.63	112.60
4	L	29	DA	N9-C4-C5	5.80	108.12	105.80
6	H	15	DT	C2-N3-C4	5.80	130.68	127.20
2	J	10	DT	C2-N3-C4	-5.79	123.72	127.20
4	L	1	DG	N3-C4-C5	-5.79	125.70	128.60
1	I	13	DT	N1-C1'-C2'	5.79	123.60	112.60
2	J	18	DA	P-O3'-C3'	5.78	126.63	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	24	DG	P-O3'-C3'	5.78	126.63	119.70
5	E	9	DC	N1-C1'-C2'	5.77	123.57	112.60
5	G	15	DG	N9-C4-C5	5.77	107.71	105.40
5	G	10	DT	C1'-O4'-C4'	-5.77	104.33	110.10
1	I	15	DC	C5-C6-N1	5.77	123.88	121.00
1	I	15	DC	C1'-O4'-C4'	5.76	115.86	110.10
2	J	13	DT	N1-C1'-C2'	5.76	123.55	112.60
5	E	11	DA	N1-C6-N6	-5.76	115.14	118.60
7	A	9	ARG	NE-CZ-NH1	5.76	123.18	120.30
7	A	249	ASP	CB-CG-OD2	5.76	123.48	118.30
6	F	25	DT	O5'-P-OP2	-5.75	100.52	105.70
2	J	5	DC	OP1-P-O3'	5.75	117.84	105.20
5	G	23	DA	C5'-C4'-C3'	-5.74	103.77	114.10
7	B	61	HIS	N-CA-C	-5.74	95.52	111.00
7	B	10	ARG	NE-CZ-NH1	5.72	123.16	120.30
2	J	5	DC	P-O3'-C3'	-5.72	112.83	119.70
2	J	14	DA	OP2-P-O3'	5.71	117.76	105.20
7	B	75	THR	CB-CA-C	-5.69	96.23	111.60
5	E	21	DA	O4'-C4'-C3'	-5.69	102.22	104.50
2	J	18	DA	O4'-C1'-C2'	-5.68	101.36	105.90
2	J	16	DT	O5'-P-OP2	-5.68	100.59	105.70
6	F	16	DA	N9-C1'-C2'	-5.68	101.81	112.60
3	K	10	DT	C5-C4-O4	-5.68	120.92	124.90
5	E	7	DC	N1-C2-N3	5.68	123.18	119.20
1	I	14	DA	C1'-O4'-C4'	-5.68	104.42	110.10
5	E	6	DT	OP2-P-O3'	5.67	117.68	105.20
5	G	7	DC	O4'-C4'-C3'	5.67	109.41	106.00
4	L	27	DC	N1-C1'-C2'	5.67	123.38	112.60
6	H	7	DT	N1-C1'-C2'	5.67	123.38	112.60
5	E	11	DA	N9-C4-C5	5.67	108.07	105.80
7	C	152	ARG	CB-CA-C	-5.66	99.07	110.40
1	I	5	DC	O4'-C1'-N1	-5.66	104.04	108.00
5	G	6	DT	C6-N1-C1'	5.65	128.88	120.40
6	H	7	DT	C4'-C3'-C2'	-5.64	98.02	103.10
5	E	15	DG	P-O3'-C3'	5.64	126.47	119.70
4	L	23	DC	N1-C1'-C2'	5.64	123.31	112.60
6	F	1	DG	P-O3'-C3'	5.64	126.46	119.70
6	H	19	DG	O4'-C1'-N9	5.64	111.95	108.00
7	D	59	HIS	N-CA-CB	5.64	120.75	110.60
6	F	16	DA	P-O3'-C3'	5.63	126.46	119.70
5	G	10	DT	C5-C6-N1	5.63	127.08	123.70
4	L	22	DG	N1-C6-O6	-5.62	116.53	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	14	DA	N7-C8-N9	-5.62	110.99	113.80
3	K	5	DC	P-O5'-C5'	5.62	129.90	120.90
5	G	14	DA	N9-C4-C5	5.62	108.05	105.80
6	H	18	DT	P-O5'-C5'	5.62	129.90	120.90
6	H	19	DG	C6-N1-C2	-5.62	121.73	125.10
7	D	73	SER	CA-C-N	-5.62	104.83	117.20
5	E	5	DG	N7-C8-N9	5.62	115.91	113.10
6	F	16	DA	O4'-C4'-C3'	5.62	109.37	106.00
7	D	324	ASP	CB-CG-OD2	5.61	123.35	118.30
1	I	19	DA	N1-C6-N6	-5.60	115.24	118.60
2	J	27	DG	O4'-C1'-N9	5.60	111.92	108.00
7	D	180	LEU	CA-CB-CG	5.60	128.18	115.30
4	L	14	DT	N1-C2-O2	-5.60	118.62	123.10
2	J	15	DT	C6-C5-C7	5.59	126.26	122.90
6	F	16	DA	C1'-O4'-C4'	-5.59	104.51	110.10
6	F	4	DA	N9-C4-C5	5.59	108.04	105.80
7	C	80	LEU	CA-CB-CG	-5.59	102.44	115.30
7	A	54	GLU	N-CA-CB	-5.59	100.54	110.60
6	F	12	DT	O4'-C1'-C2'	-5.59	101.43	105.90
5	G	16	DT	OP2-P-O3'	5.59	117.49	105.20
2	J	17	DA	P-O5'-C5'	-5.59	111.96	120.90
2	J	3	DC	O4'-C1'-N1	5.58	111.91	108.00
5	G	23	DA	C5'-C4'-O4'	5.57	119.88	109.30
3	K	18	DT	C4-C5-C6	5.57	121.34	118.00
3	K	8	DC	O4'-C1'-N1	5.57	111.90	108.00
7	D	121	THR	N-CA-CB	-5.56	99.73	110.30
4	L	23	DC	N3-C4-C5	-5.56	119.68	121.90
7	D	260	ASP	CB-CG-OD2	5.55	123.30	118.30
4	L	18	DT	N1-C2-O2	5.55	127.54	123.10
5	G	7	DC	N1-C2-N3	5.55	123.08	119.20
5	G	6	DT	N1-C2-O2	-5.55	118.66	123.10
6	F	21	DC	N3-C4-C5	5.54	124.12	121.90
2	J	7	DA	O3'-P-O5'	-5.54	93.47	104.00
4	L	3	DT	P-O3'-C3'	5.54	126.35	119.70
4	L	28	DA	P-O5'-C5'	5.54	129.76	120.90
2	J	17	DA	C5'-C4'-O4'	-5.53	98.80	109.30
4	L	26	DG	P-O3'-C3'	5.53	126.33	119.70
5	G	18	DA	O4'-C1'-N9	5.53	111.87	108.00
3	K	10	DT	C4-C5-C7	-5.52	115.69	119.00
3	K	5	DC	OP1-P-OP2	-5.52	111.33	119.60
4	L	14	DT	P-O5'-C5'	5.51	129.72	120.90
6	F	19	DG	C8-N9-C4	-5.50	104.20	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	11	DT	C6-C5-C7	5.50	126.20	122.90
3	K	4	DC	C6-N1-C2	-5.50	118.10	120.30
7	A	30	ARG	CB-CA-C	5.50	121.39	110.40
5	E	13	DC	C6-N1-C2	-5.49	118.11	120.30
5	G	2	DC	O4'-C1'-C2'	-5.49	101.51	105.90
3	K	2	DT	N3-C4-O4	5.49	123.19	119.90
2	J	16	DT	C3'-C2'-C1'	5.47	109.07	102.50
5	E	19	DA	C5-C6-N1	5.47	120.44	117.70
2	J	21	DA	O4'-C1'-C2'	5.47	110.28	105.90
5	E	15	DG	N3-C4-N9	-5.47	122.72	126.00
7	C	116	LEU	CA-CB-CG	-5.47	102.72	115.30
6	F	19	DG	N1-C6-O6	-5.46	116.62	119.90
5	G	8	DA	C2-N3-C4	5.46	113.33	110.60
5	E	6	DT	N3-C4-O4	5.46	123.17	119.90
5	E	1	DA	O4'-C1'-N9	-5.46	104.18	108.00
2	J	17	DA	OP1-P-OP2	5.45	127.78	119.60
7	A	351	ASP	CB-CG-OD2	5.44	123.20	118.30
6	H	15	DT	C5'-C4'-O4'	5.44	119.64	109.30
7	B	165	VAL	CB-CA-C	-5.44	101.07	111.40
7	C	336	ASP	CB-CG-OD2	5.43	123.19	118.30
1	I	6	DT	C5-C4-O4	-5.43	121.10	124.90
7	B	56	PHE	CB-CG-CD2	-5.42	117.00	120.80
2	J	17	DA	N3-C4-N9	-5.42	123.06	127.40
3	K	12	DA	P-O3'-C3'	5.42	126.20	119.70
3	K	2	DT	N1-C1'-C2'	5.42	122.89	112.60
2	J	22	DG	O4'-C1'-N9	-5.41	104.21	108.00
5	E	11	DA	P-O3'-C3'	5.41	126.19	119.70
5	G	4	DG	C1'-O4'-C4'	-5.41	104.69	110.10
3	K	9	DT	C5-C4-O4	-5.41	121.11	124.90
7	C	20	ASN	C-N-CA	-5.41	108.18	121.70
2	J	15	DT	C5'-C4'-C3'	5.40	123.82	114.10
6	H	18	DT	N1-C1'-C2'	5.40	122.86	112.60
5	G	10	DT	C6-C5-C7	5.40	126.14	122.90
6	F	24	DG	C4-C5-C6	5.40	122.04	118.80
7	D	59	HIS	CA-C-N	-5.39	105.33	117.20
5	E	13	DC	C5-C6-N1	5.39	123.70	121.00
6	H	9	DG	O4'-C1'-C2'	-5.39	101.58	105.90
6	H	25	DT	C6-N1-C2	-5.39	118.60	121.30
5	G	8	DA	N3-C4-C5	-5.39	123.03	126.80
6	F	15	DT	N3-C2-O2	5.38	125.53	122.30
5	E	4	DG	C2-N3-C4	5.38	114.59	111.90
2	J	9	DT	O5'-C5'-C4'	-5.38	97.55	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	2	DG	C4-N9-C1'	-5.38	119.51	126.50
7	A	116	LEU	CB-CG-CD2	-5.38	101.86	111.00
5	G	10	DT	C4'-C3'-O3'	-5.38	96.26	109.70
5	G	20	DA	O4'-C1'-C2'	-5.38	101.60	105.90
6	F	2	DG	C3'-C2'-C1'	-5.37	96.05	102.50
4	L	13	DT	C4-C5-C7	5.37	122.22	119.00
7	D	336	ASP	CB-CG-OD2	5.37	123.13	118.30
3	K	24	DT	C1'-O4'-C4'	-5.37	104.73	110.10
4	L	19	DA	O3'-P-O5'	-5.36	93.81	104.00
5	E	7	DC	O4'-C1'-N1	5.36	111.75	108.00
7	D	120	THR	CB-CA-C	-5.36	97.13	111.60
5	E	20	DA	O4'-C1'-N9	5.36	111.75	108.00
5	E	17	DC	C4'-C3'-C2'	-5.35	98.28	103.10
6	H	15	DT	O5'-P-OP1	5.35	117.12	110.70
6	H	18	DT	C4-C5-C7	-5.35	115.79	119.00
1	I	28	DT	C4-C5-C7	5.35	122.21	119.00
7	B	303	ASP	CB-CG-OD2	5.35	123.11	118.30
4	L	15	DG	C5-N7-C8	-5.35	101.63	104.30
2	J	12	DA	C8-N9-C4	-5.34	103.66	105.80
6	F	3	DT	N1-C2-N3	5.34	117.81	114.60
5	E	12	DT	C5-C6-N1	5.34	126.90	123.70
6	F	24	DG	N9-C4-C5	5.33	107.53	105.40
7	B	41	ARG	NE-CZ-NH1	5.33	122.97	120.30
7	C	41	ARG	NE-CZ-NH1	5.33	122.97	120.30
3	K	7	DG	N9-C4-C5	5.33	107.53	105.40
4	L	28	DA	N1-C6-N6	-5.33	115.40	118.60
5	G	15	DG	C5-C6-N1	-5.33	108.84	111.50
5	E	15	DG	O4'-C1'-C2'	-5.32	101.64	105.90
5	E	17	DC	O5'-P-OP2	-5.32	100.91	105.70
7	D	351	ASP	CB-CG-OD2	5.32	123.09	118.30
6	H	3	DT	O4'-C1'-C2'	-5.32	101.64	105.90
3	K	11	DT	O4'-C1'-N1	-5.32	104.28	108.00
5	E	7	DC	O5'-P-OP2	-5.31	100.92	105.70
1	I	7	DG	O5'-P-OP1	5.31	117.07	110.70
3	K	18	DT	P-O5'-C5'	-5.31	112.40	120.90
3	K	2	DT	C4'-C3'-O3'	-5.31	96.43	109.70
1	I	5	DC	C4'-C3'-O3'	-5.30	96.44	109.70
1	I	8	DC	O4'-C4'-C3'	5.30	109.18	106.00
2	J	1	DC	C4'-C3'-O3'	-5.30	96.45	109.70
6	F	3	DT	C3'-C2'-C1'	-5.30	96.14	102.50
2	J	15	DT	O5'-P-OP2	-5.30	100.93	105.70
3	K	23	DT	C5-C4-O4	-5.29	121.19	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	19	DG	C6-N1-C2	-5.29	121.92	125.10
6	H	18	DT	N1-C2-N3	5.29	117.78	114.60
6	F	6	DT	N3-C2-O2	-5.29	119.13	122.30
1	I	4	DT	C6-N1-C2	-5.28	118.66	121.30
2	J	19	DA	C8-N9-C4	-5.28	103.69	105.80
6	F	3	DT	N3-C2-O2	-5.28	119.13	122.30
6	F	17	DG	N9-C1'-C2'	5.28	122.63	112.60
6	H	14	DA	C4'-C3'-C2'	5.28	107.85	103.10
1	I	14	DA	C3'-C2'-C1'	-5.28	96.17	102.50
7	C	33	LYS	CD-CE-NZ	5.28	123.83	111.70
2	J	24	DA	C1'-O4'-C4'	-5.27	104.83	110.10
6	F	25	DT	C5-C4-O4	-5.27	121.21	124.90
6	F	4	DA	N7-C8-N9	5.27	116.43	113.80
6	H	4	DA	C5'-C4'-O4'	5.27	119.31	109.30
6	F	3	DT	P-O3'-C3'	5.26	126.02	119.70
6	H	16	DA	C5-C6-N1	-5.26	115.07	117.70
6	F	2	DG	C4-C5-C6	-5.25	115.65	118.80
7	A	57	SER	N-CA-C	5.25	125.17	111.00
5	G	14	DA	O4'-C4'-C3'	5.24	109.15	106.00
7	D	73	SER	CB-CA-C	5.24	120.06	110.10
1	I	11	DT	C5-C4-O4	-5.24	121.23	124.90
6	F	4	DA	P-O3'-C3'	-5.24	113.41	119.70
3	K	11	DT	C6-C5-C7	5.24	126.04	122.90
6	H	17	DG	C5'-C4'-O4'	-5.24	99.35	109.30
6	F	6	DT	C5-C4-O4	-5.23	121.24	124.90
3	K	8	DC	O4'-C4'-C3'	5.22	109.13	106.00
5	E	18	DA	P-O5'-C5'	5.21	129.24	120.90
3	K	26	DA	OP1-P-OP2	5.21	127.41	119.60
5	E	7	DC	N3-C2-O2	-5.21	118.26	121.90
3	K	7	DG	N1-C6-O6	-5.20	116.78	119.90
7	A	223	ASP	CB-CG-OD2	5.20	122.98	118.30
4	L	15	DG	C6-C5-N7	-5.19	127.28	130.40
7	B	66	ALA	N-CA-C	-5.19	96.98	111.00
7	B	174	GLU	OE1-CD-OE2	-5.19	117.07	123.30
3	K	6	DA	P-O5'-C5'	5.18	129.20	120.90
3	K	17	DA	N7-C8-N9	5.18	116.39	113.80
4	L	16	DA	P-O5'-C5'	-5.18	112.61	120.90
6	F	23	DT	C5'-C4'-O4'	5.18	119.14	109.30
2	J	24	DA	C3'-C2'-C1'	-5.18	96.29	102.50
4	L	15	DG	C4-C5-N7	5.18	112.87	110.80
5	E	9	DC	C2-N1-C1'	-5.17	113.11	118.80
2	J	17	DA	C5-C6-N6	-5.17	119.56	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	16	DA	O5'-P-OP1	-5.16	101.06	105.70
5	G	4	DG	P-O5'-C5'	-5.16	112.65	120.90
5	G	5	DG	C8-N9-C1'	5.15	133.70	127.00
5	G	11	DA	C8-N9-C4	-5.15	103.74	105.80
7	D	303	ASP	CB-CG-OD2	5.15	122.94	118.30
4	L	17	DA	C4-C5-N7	5.15	113.28	110.70
3	K	27	DG	C5-C6-N1	5.15	114.08	111.50
5	G	2	DC	N1-C1'-C2'	5.15	122.39	112.60
7	D	162	THR	N-CA-CB	-5.15	100.52	110.30
4	L	16	DA	C8-N9-C4	-5.15	103.74	105.80
5	E	14	DA	C8-N9-C4	-5.15	103.74	105.80
6	H	16	DA	N1-C6-N6	5.14	121.69	118.60
5	G	19	DA	C2-N3-C4	5.14	113.17	110.60
5	E	15	DG	N1-C6-O6	-5.14	116.82	119.90
7	A	111	LEU	CB-CG-CD1	-5.13	102.27	111.00
4	L	1	DG	C8-N9-C4	-5.13	104.35	106.40
6	H	16	DA	C2-N3-C4	-5.13	108.03	110.60
6	H	18	DT	C5-C4-O4	-5.13	121.31	124.90
7	D	226	ASP	CB-CG-OD2	5.13	122.92	118.30
7	D	23	TYR	CB-CA-C	-5.13	100.14	110.40
5	G	17	DC	P-O3'-C3'	-5.13	113.55	119.70
2	J	17	DA	O4'-C1'-C2'	5.12	110.00	105.90
5	G	20	DA	N7-C8-N9	5.12	116.36	113.80
7	A	10	ARG	N-CA-C	5.12	124.81	111.00
7	B	12	LEU	CB-CG-CD1	5.11	119.69	111.00
3	K	17	DA	C5-C6-N6	-5.11	119.61	123.70
5	E	6	DT	O4'-C4'-C3'	-5.11	102.46	104.50
7	B	82	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	I	16	DA	C5-C6-N6	5.11	127.79	123.70
7	D	40	ASP	CB-CG-OD1	5.11	122.90	118.30
6	F	19	DG	N3-C4-C5	-5.11	126.05	128.60
4	L	20	DA	N7-C8-N9	5.10	116.35	113.80
3	K	9	DT	N3-C2-O2	5.10	125.36	122.30
3	K	15	DA	O4'-C1'-N9	-5.10	104.43	108.00
5	E	24	DC	O5'-P-OP2	-5.10	101.11	105.70
6	H	2	DG	C5-C6-O6	-5.09	125.54	128.60
2	J	9	DT	O4'-C1'-C2'	-5.09	101.83	105.90
2	J	17	DA	C6-C5-N7	5.09	135.87	132.30
1	I	18	DC	P-O5'-C5'	-5.09	112.75	120.90
4	L	2	DA	O4'-C4'-C3'	-5.09	102.46	104.50
6	H	5	DT	C1'-O4'-C4'	-5.09	105.01	110.10
6	F	25	DT	OP1-P-OP2	5.08	127.23	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	10	DT	C6-N1-C2	-5.08	118.76	121.30
2	J	14	DA	N1-C2-N3	5.08	131.84	129.30
1	I	13	DT	C2-N1-C1'	-5.08	110.08	118.20
1	I	23	DT	C6-C5-C7	-5.08	119.85	122.90
3	K	20	DA	N9-C1'-C2'	-5.08	102.96	112.60
3	K	17	DA	C6-C5-N7	-5.07	128.75	132.30
5	G	20	DA	P-O3'-C3'	5.07	125.79	119.70
2	J	15	DT	P-O5'-C5'	-5.07	112.78	120.90
5	E	24	DC	N1-C1'-C2'	5.07	122.24	112.60
4	L	7	DA	O4'-C1'-N9	5.07	111.55	108.00
2	J	29	DT	O4'-C1'-N1	5.07	111.55	108.00
2	J	19	DA	O4'-C4'-C3'	-5.07	102.47	104.50
7	A	132	ILE	CB-CA-C	-5.07	101.47	111.60
4	L	17	DA	C5-C6-N6	-5.06	119.65	123.70
7	C	57	SER	N-CA-C	5.06	124.66	111.00
7	B	152	ARG	NE-CZ-NH1	5.06	122.83	120.30
4	L	24	DT	C5-C4-O4	-5.05	121.36	124.90
1	I	13	DT	P-O3'-C3'	5.05	125.76	119.70
2	J	10	DT	N3-C4-O4	-5.05	116.87	119.90
6	F	19	DG	N9-C4-C5	5.05	107.42	105.40
3	K	16	DT	C5-C4-O4	5.04	128.43	124.90
3	K	16	DT	OP1-P-O3'	5.03	116.27	105.20
6	H	2	DG	C5-N7-C8	-5.03	101.78	104.30
5	G	16	DT	O4'-C4'-C3'	-5.03	102.49	104.50
7	C	73	SER	CB-CA-C	5.03	119.65	110.10
6	H	19	DG	N1-C2-N3	5.02	126.91	123.90
5	G	20	DA	N1-C6-N6	5.02	121.61	118.60
1	I	7	DG	O3'-P-O5'	-5.02	94.47	104.00
6	H	2	DG	N3-C4-C5	5.01	131.11	128.60
3	K	14	DT	C3'-C2'-C1'	5.01	108.51	102.50
5	G	6	DT	O5'-C5'-C4'	-5.01	98.47	111.00
7	A	80	LEU	CA-CB-CG	-5.01	103.78	115.30
3	K	5	DC	C5'-C4'-C3'	5.01	123.11	114.10
4	L	28	DA	C2-N3-C4	5.01	113.10	110.60
5	E	5	DG	C6-N1-C2	-5.00	122.10	125.10
2	J	16	DT	N1-C2-N3	5.00	117.60	114.60
7	C	23	TYR	CB-CA-C	5.00	120.40	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A	73	SER	Peptide
7	C	73	SER	Peptide

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	I	588	0	331	75	0
2	J	594	0	328	70	1
3	K	590	0	332	54	0
4	L	594	0	329	39	0
5	E	487	0	271	56	1
5	G	487	0	271	46	0
6	F	513	0	287	62	0
6	H	513	0	287	63	0
7	A	2763	0	2795	342	0
7	B	2630	0	2628	350	0
7	C	2767	0	2801	322	0
7	D	2630	0	2628	293	0
All	All	15156	0	13288	1615	1

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 57.

All (1615) 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)
7:A:71:ASP:CB	7:A:71:ASP:CG	1.75	1.55
7:C:101:MSE:SE	7:C:101:MSE:CE	2.18	1.41
7:D:101:MSE:SE	7:D:101:MSE:CE	2.18	1.40
1:I:13:DT:N3	2:J:17:DA:N6	1.69	1.39
1:I:13:DT:H3	2:J:17:DA:N6	1.12	1.39
7:A:338:MSE:SE	7:A:338:MSE:CE	2.23	1.36
7:B:101:MSE:SE	7:B:101:MSE:CE	2.24	1.34
7:D:169:ARG:HD2	7:D:169:ARG:C	1.43	1.28
7:D:165:VAL:O	7:D:168:THR:HG22	1.31	1.24
5:E:12:DT:H2"	5:E:13:DC:C5'	1.67	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:74:VAL:CG1	7:C:75:THR:H	1.49	1.22
1:I:12:DT:OP1	7:A:212:ARG:NH2	1.76	1.19
7:C:75:THR:CG2	7:C:78:SER:HB3	1.73	1.18
6:H:6:DT:H2"	6:H:7:DT:H5"	1.27	1.17
7:A:50:GLN:O	7:A:53:ILE:HG22	1.39	1.17
7:C:47:GLU:OE2	7:D:63:PRO:HD2	1.42	1.16
1:I:13:DT:C4	2:J:17:DA:N6	2.13	1.16
7:B:23:TYR:HD2	7:B:24:TYR:N	1.42	1.16
7:C:75:THR:HG23	7:C:78:SER:CB	1.74	1.16
7:A:61:HIS:NE2	7:D:47:GLU:OE1	1.77	1.16
3:K:14:DT:H4'	3:K:15:DA:OP1	1.46	1.14
7:C:148:SER:OG	7:C:152:ARG:NH2	1.80	1.13
7:B:120:THR:HG22	7:B:122:LYS:N	1.62	1.13
7:C:74:VAL:HG12	7:C:75:THR:N	1.47	1.13
7:D:306:THR:O	7:D:309:GLU:HB2	1.46	1.13
2:J:9:DT:H2"	2:J:10:DT:H5'	1.23	1.13
7:B:195:SER:HB3	7:B:199:LEU:CD2	1.78	1.12
2:J:16:DT:H2'	2:J:17:DA:H5"	1.24	1.12
7:C:47:GLU:HB3	7:D:63:PRO:HG2	1.32	1.11
7:D:101:MSE:HA	7:D:104:ILE:HD12	1.32	1.10
7:D:52:ASN:O	7:D:56:PHE:O	1.68	1.10
5:E:12:DT:C2'	5:E:13:DC:H5"	1.81	1.10
7:D:169:ARG:HD2	7:D:169:ARG:O	1.48	1.09
7:A:23:TYR:OH	7:A:36:GLY:HA2	1.52	1.09
7:C:19:ARG:HG2	7:C:19:ARG:HH11	0.98	1.09
7:B:76:LEU:O	7:B:80:LEU:HD12	1.51	1.08
3:K:23:DT:OP1	7:B:306:THR:OG1	1.71	1.08
7:A:75:THR:HG23	7:A:78:SER:HB2	1.33	1.07
7:B:195:SER:CB	7:B:199:LEU:HD22	1.85	1.07
7:D:104:ILE:HA	7:D:107:ILE:HD12	1.30	1.06
6:F:2:DG:H2"	6:F:3:DT:H71	1.33	1.05
7:B:27:ARG:CD	7:B:34:GLU:HG2	1.86	1.05
7:C:101:MSE:HA	7:C:104:ILE:HD12	1.37	1.05
7:A:28:ASP:OD2	7:A:30:ARG:HB3	1.57	1.05
7:D:211:GLN:C	7:D:311:ARG:HD2	1.77	1.04
7:B:76:LEU:HG	7:B:80:LEU:HD11	1.33	1.04
7:A:163:ASN:OD1	7:A:165:VAL:HB	1.57	1.03
1:I:18:DC:H2"	1:I:19:DA:H5"	1.06	1.03
5:E:12:DT:H2"	5:E:13:DC:H5"	1.04	1.03
7:C:14:PRO:O	7:C:15:ASN:HB2	1.57	1.03
2:J:19:DA:H2'	7:A:96:THR:CG2	1.90	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:6:DT:H2"	6:F:7:DT:H5"	1.36	1.02
7:D:144:ARG:NH2	7:D:168:THR:O	1.92	1.02
7:D:33:LYS:HA	7:D:33:LYS:HE3	1.38	1.02
2:J:16:DT:H2'	2:J:16:DT:O2	1.56	1.01
7:D:144:ARG:HE	7:D:168:THR:HG23	1.26	1.01
7:B:306:THR:O	7:B:309:GLU:HB2	1.58	1.01
7:A:309:GLU:O	7:A:309:GLU:OE1	1.77	1.01
7:B:129:ASN:HA	7:B:132:ILE:HD12	1.38	1.01
7:D:154:ALA:HB3	7:D:160:ILE:HD11	1.43	1.00
5:G:6:DT:H2"	5:G:7:DC:H6	1.20	1.00
5:G:6:DT:H2"	5:G:7:DC:C6	1.96	1.00
7:D:31:THR:OG1	7:D:33:LYS:HG2	1.61	1.00
7:D:79:TRP:CZ2	7:D:154:ALA:HA	1.97	0.99
7:D:221:TRP:CH2	7:D:263:LYS:HB3	1.97	0.99
7:A:160:ILE:HG22	7:A:161:THR:N	1.74	0.98
7:B:195:SER:HB3	7:B:199:LEU:HD22	1.42	0.98
7:B:270:THR:OG1	7:B:272:ILE:O	1.80	0.98
6:F:9:DG:H2"	7:A:20:ASN:HD21	1.28	0.98
7:A:116:LEU:O	7:A:119:ILE:HD12	1.64	0.98
7:A:114:ALA:HB1	7:A:115:PRO:HD3	1.43	0.98
7:A:114:ALA:HB1	7:A:115:PRO:CD	1.93	0.97
7:B:155:ILE:HG13	7:B:160:ILE:HG12	1.42	0.97
3:K:9:DT:H2"	3:K:10:DT:H5"	1.45	0.97
7:C:23:TYR:HD2	7:C:24:TYR:N	1.63	0.97
1:I:13:DT:O4	2:J:17:DA:N6	1.98	0.97
7:C:19:ARG:HG2	7:C:19:ARG:NH1	1.64	0.96
7:D:169:ARG:C	7:D:169:ARG:CD	2.32	0.96
2:J:19:DA:H2'	7:A:96:THR:HG21	1.47	0.96
7:B:60:LYS:O	7:B:61:HIS:HB3	1.63	0.96
7:B:205:LEU:O	7:B:208:VAL:HG12	1.65	0.96
1:I:5:DC:H1'	1:I:6:DT:H5'	1.47	0.96
3:K:12:DA:OP1	7:C:212:ARG:NH2	1.98	0.96
7:B:23:TYR:CD2	7:B:24:TYR:N	2.33	0.95
7:B:31:THR:OG1	7:B:33:LYS:HG2	1.66	0.95
7:D:76:LEU:O	7:D:76:LEU:HD12	1.65	0.95
7:C:26:TYR:CE1	7:C:51:ALA:HB3	2.01	0.95
6:F:6:DT:C2'	6:F:7:DT:H5"	1.96	0.94
2:J:16:DT:C2'	2:J:17:DA:H5"	1.97	0.94
7:B:213:VAL:HA	7:B:216:LEU:HD12	1.49	0.94
7:C:57:SER:O	7:C:59:HIS:N	1.99	0.94
7:C:160:ILE:HG22	7:C:161:THR:N	1.78	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:249:ASP:OD2	7:D:321:GLN:NE2	2.01	0.94
7:B:114:ALA:HB1	7:B:115:PRO:HD3	1.50	0.94
7:C:54:GLU:OE2	7:C:55:LEU:HD23	1.67	0.94
4:L:8:DC:H2'	4:L:9:DT:H71	1.48	0.94
1:I:8:DC:OP1	7:A:136:LYS:NZ	2.01	0.93
7:B:196:PRO:O	7:B:199:LEU:HD13	1.68	0.93
6:H:17:DG:C8	6:H:18:DT:H71	2.03	0.93
6:F:10:DA:N6	7:A:19:ARG:HH21	1.67	0.93
7:B:27:ARG:NH1	7:B:34:GLU:OE1	2.01	0.93
7:C:23:TYR:OH	7:C:36:GLY:HA2	1.68	0.92
7:B:120:THR:HG22	7:B:122:LYS:H	1.34	0.92
7:C:307:PHE:O	7:C:310:LEU:HG	1.69	0.92
7:A:57:SER:O	7:A:59:HIS:N	2.01	0.92
1:I:8:DC:P	7:A:136:LYS:HZ3	1.91	0.92
1:I:8:DC:P	7:A:136:LYS:NZ	2.42	0.92
7:B:84:GLU:HA	7:B:87:LEU:HD12	1.52	0.92
7:C:205:LEU:O	7:C:209:THR:HG23	1.71	0.91
7:C:111:LEU:HD22	7:C:112:PRO:HD2	1.52	0.91
7:B:149:ASP:HA	7:B:152:ARG:HD2	1.52	0.91
7:C:23:TYR:CD2	7:C:24:TYR:N	2.38	0.91
7:A:120:THR:HG22	7:A:123:GLU:HG3	1.52	0.91
7:D:27:ARG:HG3	7:D:34:GLU:HG2	1.51	0.91
7:B:205:LEU:HD23	7:B:272:ILE:HD11	1.53	0.91
7:A:116:LEU:HA	7:A:119:ILE:HD11	1.51	0.90
6:F:9:DG:C2'	7:A:20:ASN:HD21	1.85	0.90
7:C:23:TYR:OH	7:C:36:GLY:CA	2.19	0.90
7:B:50:GLN:HA	7:B:53:ILE:HD12	1.51	0.90
3:K:12:DA:H2'	3:K:13:DT:H72	1.52	0.90
7:D:70:SER:O	7:D:73:SER:N	2.05	0.90
7:D:80:LEU:CD2	7:D:104:ILE:HG23	2.01	0.90
7:B:155:ILE:CG1	7:B:160:ILE:HG12	2.01	0.89
1:I:18:DC:C2'	1:I:19:DA:H5"	1.99	0.89
7:C:354:GLU:HB2	7:C:356:LYS:HB2	1.53	0.89
7:B:79:TRP:CH2	7:B:154:ALA:HA	2.08	0.89
7:C:47:GLU:CB	7:D:63:PRO:HG2	2.03	0.89
7:B:155:ILE:HG13	7:B:160:ILE:CG1	2.01	0.89
7:D:19:ARG:HD3	7:D:20:ASN:H	1.36	0.88
4:L:13:DT:H5"	7:D:236:THR:HG21	1.53	0.88
7:A:23:TYR:C	7:A:23:TYR:CD2	2.42	0.88
7:C:74:VAL:CG1	7:C:75:THR:N	2.20	0.88
7:D:80:LEU:HD21	7:D:104:ILE:HG23	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:154:ALA:CB	7:D:160:ILE:HD11	2.02	0.88
7:D:169:ARG:O	7:D:169:ARG:CD	2.22	0.88
7:B:305:PRO:HB3	7:B:309:GLU:HG3	1.55	0.88
7:B:52:ASN:O	7:B:56:PHE:O	1.92	0.88
7:B:195:SER:CB	7:B:199:LEU:CD2	2.46	0.88
6:H:1:DG:H2"	6:H:2:DG:OP2	1.74	0.88
7:A:293:ARG:NH1	7:A:305:PRO:O	2.06	0.88
7:C:19:ARG:HH11	7:C:19:ARG:CG	1.87	0.88
7:B:27:ARG:HD3	7:B:34:GLU:HG2	1.54	0.87
7:B:76:LEU:C	7:B:80:LEU:HD12	1.94	0.87
7:B:114:ALA:HB1	7:B:115:PRO:CD	2.02	0.87
5:G:7:DC:H2'	5:G:8:DA:C8	2.08	0.87
7:A:76:LEU:N	7:A:76:LEU:HD12	1.87	0.87
7:B:155:ILE:HG22	7:B:155:ILE:O	1.71	0.87
7:B:195:SER:HB3	7:B:199:LEU:HD21	1.57	0.87
7:D:19:ARG:CD	7:D:20:ASN:N	2.38	0.87
6:H:17:DG:OP2	7:D:17:TYR:CE2	2.26	0.87
7:A:152:ARG:O	7:A:155:ILE:HB	1.74	0.87
7:D:19:ARG:CD	7:D:20:ASN:H	1.87	0.87
7:D:211:GLN:HA	7:D:311:ARG:HH11	1.40	0.87
7:C:145:SER:O	7:C:148:SER:HB3	1.73	0.86
2:J:8:DG:O5'	7:B:136:LYS:HD3	1.75	0.86
7:B:195:SER:HB2	7:B:199:LEU:HD22	1.56	0.86
7:D:75:THR:HG23	7:D:78:SER:HB2	1.57	0.86
7:C:26:TYR:HE1	7:C:51:ALA:HB3	1.40	0.86
7:C:116:LEU:N	7:C:116:LEU:HD12	1.90	0.86
7:B:350:TRP:CZ3	7:C:239:LYS:HB3	2.10	0.86
6:H:13:DG:H2"	6:H:14:DA:O5'	1.75	0.86
7:A:160:ILE:CG2	7:A:161:THR:N	2.36	0.86
5:E:16:DT:O4	7:A:19:ARG:NH2	2.08	0.86
6:F:2:DG:H2"	6:F:3:DT:C7	2.04	0.86
7:C:114:ALA:HB1	7:C:115:PRO:CD	2.06	0.86
7:C:9:ARG:HD2	7:C:10:ARG:HE	1.41	0.86
7:A:211:GLN:C	7:A:311:ARG:HD2	1.96	0.86
7:B:47:GLU:OE1	7:C:61:HIS:NE2	2.08	0.86
7:D:23:TYR:CD2	7:D:24:TYR:N	2.43	0.86
6:H:8:DT:OP2	7:C:12:LEU:HD21	1.74	0.86
7:C:160:ILE:CG2	7:C:161:THR:N	2.36	0.86
7:C:224:ILE:HD11	7:C:271:ILE:HD11	1.57	0.86
7:A:110:GLY:O	7:A:111:LEU:HD23	1.75	0.85
7:A:165:VAL:HG12	7:A:166:ALA:N	1.89	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:45:ILE:O	7:B:48:ALA:HB3	1.75	0.85
7:C:40:ASP:OD2	7:C:42:ARG:HG3	1.77	0.85
7:A:210:GLY:O	7:A:311:ARG:NH1	2.10	0.85
5:E:10:DT:H2"	5:E:11:DA:N7	1.92	0.85
7:B:54:GLU:OE2	7:B:54:GLU:HA	1.74	0.85
7:A:75:THR:CG2	7:A:78:SER:HB2	2.06	0.84
7:A:76:LEU:O	7:A:80:LEU:HD12	1.76	0.84
7:A:179:ARG:NH1	7:A:312:SER:OG	2.09	0.84
7:D:84:GLU:HA	7:D:87:LEU:HD12	1.57	0.84
6:F:17:DG:OP2	7:B:17:TYR:CE2	2.30	0.84
7:B:155:ILE:HG13	7:B:160:ILE:CD1	2.08	0.84
1:I:8:DC:O5'	7:A:136:LYS:NZ	2.10	0.83
7:A:10:ARG:NH2	7:A:12:LEU:HD22	1.91	0.83
1:I:23:DT:OP1	7:D:306:THR:OG1	1.96	0.83
7:A:18:ILE:HG13	7:A:24:TYR:CE2	2.13	0.83
7:C:221:TRP:CH2	7:C:263:LYS:HB2	2.13	0.83
7:C:23:TYR:HD2	7:C:24:TYR:H	1.22	0.83
7:C:45:ILE:O	7:C:48:ALA:HB3	1.78	0.83
7:D:76:LEU:HD12	7:D:76:LEU:C	1.94	0.83
7:B:27:ARG:HD3	7:B:34:GLU:CG	2.08	0.83
1:I:16:DA:C6	4:L:15:DG:N2	2.47	0.83
7:A:18:ILE:HD11	7:A:22:GLY:HA2	1.61	0.83
7:D:19:ARG:HD3	7:D:20:ASN:N	1.92	0.83
7:A:169:ARG:HH21	7:B:152:ARG:HD3	1.44	0.83
7:B:49:ILE:O	7:B:53:ILE:HG13	1.79	0.82
1:I:12:DT:P	7:A:212:ARG:NH2	2.51	0.82
7:A:75:THR:HG23	7:A:78:SER:CB	2.09	0.82
5:G:2:DC:H2"	5:G:3:DA:N7	1.93	0.82
7:A:103:LYS:O	7:A:106:ALA:HB3	1.78	0.82
7:A:117:GLU:OE1	7:A:117:GLU:N	2.09	0.82
7:C:74:VAL:HG12	7:C:75:THR:H	0.68	0.82
5:G:15:DG:N7	7:C:19:ARG:HD2	1.93	0.82
7:B:27:ARG:HD3	7:B:34:GLU:CD	1.99	0.82
7:D:50:GLN:HA	7:D:53:ILE:HD11	1.59	0.82
2:J:7:DA:H2"	2:J:8:DG:H5"	1.60	0.82
7:D:212:ARG:NE	7:D:233:GLN:OE1	2.13	0.82
7:A:165:VAL:O	7:A:168:THR:HG22	1.79	0.82
7:A:111:LEU:HD22	7:A:112:PRO:HD2	1.62	0.81
7:A:169:ARG:HG2	7:A:169:ARG:HH11	1.42	0.81
7:A:254:SER:O	7:A:258:THR:OG1	1.97	0.81
7:B:23:TYR:HD2	7:B:24:TYR:H	1.26	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:306:THR:O	7:C:309:GLU:HB2	1.81	0.81
1:I:24:DT:OP2	7:D:293:ARG:NH2	2.13	0.81
7:A:116:LEU:O	7:A:119:ILE:CD1	2.27	0.81
7:A:169:ARG:HG2	7:A:169:ARG:NH1	1.95	0.81
7:B:155:ILE:O	7:B:155:ILE:CG2	2.26	0.81
7:A:160:ILE:CG2	7:A:161:THR:H	1.94	0.81
7:A:309:GLU:OE1	7:A:312:SER:HB3	1.81	0.81
7:B:27:ARG:CD	7:B:34:GLU:CG	2.59	0.81
7:C:18:ILE:HD11	7:C:22:GLY:HA2	1.63	0.81
6:F:23:DT:H2"	6:F:24:DG:C8	2.16	0.80
7:D:15:ASN:HB2	7:D:26:TYR:HE1	1.46	0.80
2:J:9:DT:H2"	2:J:10:DT:C5'	2.10	0.80
5:G:6:DT:C2'	5:G:7:DC:H6	1.92	0.80
7:B:76:LEU:O	7:B:80:LEU:CD1	2.30	0.80
7:A:144:ARG:HE	7:A:168:THR:HG23	1.47	0.80
6:H:19:DG:H2'	6:H:20:DA:C8	2.16	0.80
6:H:2:DG:OP2	6:H:2:DG:H8	1.64	0.80
7:B:62:LYS:O	7:B:65:THR:N	2.14	0.80
7:B:123:GLU:O	7:B:126:ALA:HB3	1.82	0.80
6:H:8:DT:H2"	6:H:9:DG:C8	2.17	0.79
7:B:203:MSE:O	7:B:207:VAL:HG23	1.82	0.79
7:A:77:HIS:HB2	7:A:113:ASP:OD1	1.83	0.79
7:B:19:ARG:HG2	7:B:20:ASN:H	1.47	0.79
7:B:101:MSE:HA	7:B:104:ILE:HD12	1.64	0.79
4:L:20:DA:H2"	4:L:21:DA:O4'	1.82	0.79
7:A:14:PRO:O	7:A:15:ASN:ND2	2.16	0.79
7:A:333:HIS:NE2	7:A:338:MSE:HB2	1.98	0.79
7:A:148:SER:HB2	7:A:165:VAL:HG11	1.64	0.79
7:D:180:LEU:O	7:D:316:ARG:NH2	2.16	0.78
3:K:8:DC:H2'	3:K:9:DT:H71	1.66	0.78
7:C:160:ILE:CG2	7:C:161:THR:H	1.95	0.78
7:A:54:GLU:OE2	7:A:55:LEU:N	2.16	0.78
2:J:16:DT:C2'	2:J:17:DA:C5'	2.62	0.78
6:H:6:DT:C6	6:H:7:DT:H72	2.18	0.78
7:A:57:SER:OG	7:A:59:HIS:CB	2.32	0.78
7:B:50:GLN:HA	7:B:53:ILE:CD1	2.13	0.78
7:C:354:GLU:C	7:C:356:LYS:H	1.83	0.78
7:A:69:ASN:O	7:A:73:SER:HB2	1.82	0.78
7:D:114:ALA:HB1	7:D:115:PRO:HD3	1.66	0.78
7:D:104:ILE:CA	7:D:107:ILE:HD12	2.12	0.77
6:H:15:DT:H2"	6:H:16:DA:O5'	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:163:ASN:OD1	7:B:165:VAL:HB	1.82	0.77
7:C:23:TYR:CE2	7:C:24:TYR:O	2.38	0.77
3:K:16:DT:H1'	3:K:17:DA:C8	2.20	0.77
7:A:76:LEU:C	7:A:80:LEU:HD12	2.05	0.77
1:I:13:DT:H2"	1:I:14:DA:H8	1.49	0.77
6:H:17:DG:C8	6:H:18:DT:C7	2.67	0.77
7:C:165:VAL:O	7:C:168:THR:HG22	1.84	0.77
7:C:120:THR:HG22	7:C:123:GLU:HG3	1.67	0.77
1:I:7:DG:H2"	1:I:8:DC:H5"	1.66	0.76
7:B:16:LEU:HD23	7:B:16:LEU:C	2.05	0.76
7:C:92:ILE:CG2	7:C:96:THR:HB	2.15	0.76
7:B:19:ARG:HG2	7:B:20:ASN:N	2.01	0.76
2:J:18:DA:H2"	7:A:100:TYR:OH	1.86	0.76
7:C:79:TRP:CE2	7:C:154:ALA:HB2	2.19	0.76
2:J:19:DA:H2'	7:A:96:THR:HG23	1.66	0.76
5:G:6:DT:C2'	5:G:7:DC:C6	2.66	0.76
7:B:74:VAL:HG12	7:B:75:THR:N	2.00	0.76
2:J:14:DA:H1'	2:J:15:DT:H5'	1.66	0.76
7:B:77:HIS:HA	7:B:80:LEU:HD12	1.67	0.76
7:A:101:MSE:HA	7:A:104:ILE:CD1	2.15	0.76
4:L:23:DC:H5"	7:C:306:THR:HG21	1.68	0.75
7:B:40:ASP:OD1	7:B:40:ASP:N	2.12	0.75
7:A:232:GLU:O	7:A:232:GLU:HG2	1.86	0.75
7:B:54:GLU:CG	7:C:65:THR:HG23	2.17	0.75
2:J:2:DG:H4'	7:B:276:ARG:NH2	2.01	0.75
7:A:57:SER:OG	7:A:59:HIS:HB2	1.85	0.75
1:I:10:DT:H5'	7:A:175:VAL:HG13	1.67	0.75
7:C:57:SER:C	7:C:59:HIS:H	1.88	0.75
5:E:6:DT:H2'	5:E:7:DC:C6	2.21	0.75
7:B:41:ARG:O	7:B:45:ILE:HG13	1.86	0.75
1:I:10:DT:H2'	1:I:11:DT:H71	1.68	0.75
7:B:290:MSE:O	7:B:293:ARG:HB2	1.87	0.75
1:I:27:DA:H1'	1:I:28:DT:H5'	1.68	0.75
2:J:14:DA:H2"	2:J:15:DT:OP2	1.86	0.75
6:F:10:DA:N6	7:A:19:ARG:NH2	2.33	0.75
7:A:101:MSE:HA	7:A:104:ILE:HD12	1.68	0.75
7:C:186:LEU:CD1	7:C:251:LEU:HD22	2.17	0.75
6:F:10:DA:H61	7:A:19:ARG:NH2	1.84	0.74
7:D:23:TYR:CE2	7:D:24:TYR:O	2.40	0.74
2:J:20:DA:H2"	2:J:21:DA:H5"	1.68	0.74
5:E:2:DC:H2"	5:E:3:DA:N7	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:12:DT:H2"	5:E:13:DC:H5'	1.66	0.74
7:B:212:ARG:HG3	7:B:215:ASP:OD2	1.86	0.74
7:D:15:ASN:HB2	7:D:26:TYR:CE1	2.22	0.74
7:C:56:PHE:O	7:C:57:SER:HB3	1.88	0.74
2:J:21:DA:H2'	2:J:22:DG:H8	1.52	0.74
7:A:104:ILE:O	7:A:107:ILE:N	2.20	0.74
7:A:306:THR:O	7:A:309:GLU:HB2	1.87	0.74
7:B:36:GLY:O	7:C:67:ARG:NH2	2.20	0.74
7:C:87:LEU:N	7:C:87:LEU:HD12	2.03	0.74
7:A:211:GLN:HA	7:A:311:ARG:HH11	1.49	0.74
7:D:211:GLN:HA	7:D:311:ARG:NH1	2.02	0.74
7:A:9:ARG:HB2	7:A:10:ARG:HG3	1.70	0.74
7:C:47:GLU:HB3	7:D:63:PRO:CG	2.14	0.74
7:C:75:THR:CG2	7:C:78:SER:CB	2.49	0.74
7:A:144:ARG:NH2	7:A:168:THR:O	2.20	0.74
7:C:64:LEU:HD13	7:C:67:ARG:HD3	1.70	0.74
6:H:17:DG:OP2	7:D:17:TYR:HE2	1.68	0.74
7:B:37:LEU:HD12	7:B:37:LEU:N	2.01	0.74
7:B:205:LEU:CD2	7:B:272:ILE:HD11	2.18	0.73
6:H:19:DG:H2'	6:H:20:DA:H8	1.54	0.73
7:D:24:TYR:HE1	7:D:41:ARG:N	1.86	0.73
2:J:21:DA:H2'	2:J:22:DG:C8	2.24	0.73
7:C:14:PRO:O	7:C:15:ASN:CB	2.32	0.73
7:D:15:ASN:HA	7:D:17:TYR:CZ	2.24	0.73
7:B:104:ILE:O	7:B:107:ILE:N	2.21	0.73
7:C:242:ILE:HG23	7:C:330:LEU:HD11	1.70	0.73
3:K:26:DA:N6	7:B:287:ARG:NH2	2.37	0.73
6:F:9:DG:C2'	7:A:20:ASN:ND2	2.52	0.73
7:D:104:ILE:HA	7:D:107:ILE:CD1	2.12	0.73
5:G:12:DT:H2"	5:G:13:DC:H5'	1.71	0.73
7:A:45:ILE:HG22	7:A:46:THR:N	2.04	0.73
7:B:77:HIS:HA	7:B:80:LEU:CD1	2.19	0.73
7:B:207:VAL:O	7:B:314:SER:OG	2.06	0.73
7:C:23:TYR:HE2	7:C:24:TYR:O	1.72	0.73
7:D:45:ILE:O	7:D:48:ALA:HB3	1.88	0.73
7:B:28:ASP:OD2	7:B:30:ARG:HB2	1.89	0.73
7:B:84:GLU:CA	7:B:87:LEU:HD12	2.18	0.72
7:A:120:THR:CG2	7:A:123:GLU:HG3	2.18	0.72
7:C:72:ASN:H	7:C:72:ASN:ND2	1.84	0.72
7:D:23:TYR:HD2	7:D:24:TYR:N	1.86	0.72
7:A:104:ILE:HA	7:A:107:ILE:HD12	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:163:ASN:OD1	7:A:165:VAL:N	2.23	0.72
3:K:19:DA:H2"	3:K:20:DA:O4'	1.88	0.72
6:F:9:DG:H2"	6:F:10:DA:N7	2.04	0.72
6:H:2:DG:OP2	6:H:2:DG:C8	2.41	0.72
7:C:77:HIS:HA	7:C:80:LEU:HD12	1.71	0.72
7:C:306:THR:OG1	7:C:307:PHE:N	2.21	0.72
7:A:309:GLU:OE1	7:A:309:GLU:CA	2.38	0.72
7:A:338:MSE:C	7:A:340:SER:H	1.93	0.72
7:D:83:TYR:CE1	7:D:150:ALA:HA	2.25	0.72
7:D:33:LYS:HA	7:D:33:LYS:CE	2.19	0.72
7:C:224:ILE:CD1	7:C:271:ILE:HD11	2.20	0.72
7:C:103:LYS:O	7:C:106:ALA:HB3	1.90	0.71
7:A:47:GLU:HB3	7:B:63:PRO:HG2	1.70	0.71
7:B:27:ARG:CG	7:B:34:GLU:HG2	2.19	0.71
7:D:24:TYR:OH	7:D:41:ARG:HB2	1.89	0.71
5:G:14:DA:H8	7:C:23:TYR:CE1	2.08	0.71
7:A:160:ILE:HG22	7:A:162:THR:H	1.53	0.71
1:I:24:DT:P	7:D:293:ARG:HH22	2.13	0.71
7:C:101:MSE:HA	7:C:104:ILE:CD1	2.17	0.71
7:D:141:LYS:C	7:D:141:LYS:CD	2.59	0.71
2:J:2:DG:H2"	2:J:3:DC:OP2	1.90	0.71
7:C:212:ARG:HB2	7:C:215:ASP:OD2	1.90	0.71
7:C:79:TRP:CZ2	7:C:154:ALA:HB2	2.26	0.71
7:C:163:ASN:OD1	7:C:165:VAL:N	2.24	0.71
6:F:23:DT:C2'	6:F:24:DG:C8	2.73	0.71
7:D:306:THR:O	7:D:309:GLU:CB	2.33	0.71
3:K:12:DA:H2'	3:K:13:DT:C7	2.19	0.71
7:A:197:CYS:O	7:A:200:ARG:HG3	1.91	0.71
7:A:221:TRP:CH2	7:A:263:LYS:HB2	2.26	0.71
7:A:84:GLU:CA	7:A:87:LEU:HD12	2.20	0.70
7:B:77:HIS:CA	7:B:80:LEU:HD12	2.21	0.70
7:C:76:LEU:HG	7:C:80:LEU:HD11	1.71	0.70
7:A:148:SER:HA	7:A:165:VAL:HG21	1.74	0.70
7:A:168:THR:OG1	7:A:169:ARG:N	2.22	0.70
7:A:293:ARG:HH12	7:A:306:THR:HG22	1.56	0.70
7:D:258:THR:O	7:D:262:CYS:SG	2.48	0.70
7:A:68:ILE:HG22	7:A:69:ASN:N	2.06	0.70
7:B:54:GLU:HG3	7:C:65:THR:HG23	1.74	0.70
7:C:116:LEU:HB3	7:C:160:ILE:HD11	1.72	0.70
7:C:208:VAL:O	7:C:318:TYR:OH	2.09	0.70
7:D:144:ARG:HE	7:D:168:THR:CG2	2.03	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:17:TYR:HE1	7:D:27:ARG:HB3	1.57	0.70
7:A:84:GLU:HA	7:A:87:LEU:HD12	1.73	0.70
7:D:24:TYR:CE1	7:D:41:ARG:HA	2.27	0.70
1:I:27:DA:H2"	1:I:28:DT:OP2	1.91	0.70
5:E:15:DG:N7	7:A:19:ARG:HD2	2.06	0.70
7:A:9:ARG:CB	7:A:10:ARG:HG3	2.21	0.70
7:B:176:ARG:HG3	7:B:303:ASP:OD2	1.91	0.70
3:K:20:DA:H2"	3:K:21:DA:O4'	1.92	0.70
7:B:198:TRP:CE3	7:B:199:LEU:HD12	2.27	0.70
2:J:15:DT:H73	2:J:16:DT:H71	1.74	0.69
7:A:12:LEU:HD11	7:A:16:LEU:HD23	1.73	0.69
7:D:114:ALA:HB1	7:D:115:PRO:CD	2.22	0.69
4:L:6:DA:H2"	4:L:7:DA:OP2	1.92	0.69
5:E:5:DG:OP2	7:B:36:GLY:N	2.25	0.69
7:D:36:GLY:C	7:D:37:LEU:HD23	2.12	0.69
7:D:141:LYS:O	7:D:144:ARG:HB3	1.92	0.69
3:K:9:DT:C2'	3:K:10:DT:H5"	2.21	0.69
7:D:76:LEU:HD11	7:D:80:LEU:HD13	1.74	0.69
7:A:215:ASP:OD2	7:A:233:GLN:HG3	1.93	0.69
6:F:10:DA:H2"	6:F:11:DC:OP2	1.93	0.69
7:A:103:LYS:O	7:A:104:ILE:C	2.29	0.69
7:C:45:ILE:HG22	7:C:46:THR:N	2.07	0.69
7:C:101:MSE:CA	7:C:104:ILE:HD12	2.18	0.69
7:D:23:TYR:HE2	7:D:24:TYR:O	1.76	0.69
7:A:94:GLN:O	7:A:98:ILE:HD12	1.93	0.68
7:B:120:THR:O	7:B:121:THR:C	2.32	0.68
7:C:92:ILE:HG22	7:C:93:LYS:N	2.06	0.68
7:D:144:ARG:NE	7:D:168:THR:HG23	2.05	0.68
7:D:313:LEU:HA	7:D:316:ARG:NH2	2.09	0.68
5:G:2:DC:H2"	5:G:3:DA:C8	2.28	0.68
7:C:23:TYR:CD2	7:C:23:TYR:C	2.66	0.68
7:C:160:ILE:HG22	7:C:162:THR:N	2.08	0.68
7:A:76:LEU:N	7:A:76:LEU:CD1	2.55	0.68
7:C:75:THR:HG23	7:C:78:SER:HB3	0.84	0.68
7:D:76:LEU:C	7:D:76:LEU:CD1	2.61	0.68
1:I:7:DG:C2	1:I:8:DC:C2	2.82	0.68
4:L:9:DT:H2"	4:L:10:DT:H5"	1.75	0.68
2:J:16:DT:H2'	2:J:17:DA:C5'	2.11	0.68
7:B:99:ASN:O	7:B:103:LYS:HG2	1.93	0.68
6:F:9:DG:H2'	7:A:20:ASN:ND2	2.10	0.67
7:B:121:THR:OG1	7:B:164:HIS:ND1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:6:DT:H2"	5:E:7:DC:O4'	1.95	0.67
7:C:45:ILE:O	7:C:49:ILE:HG12	1.93	0.67
7:D:15:ASN:HA	7:D:17:TYR:OH	1.94	0.67
7:D:50:GLN:O	7:D:53:ILE:HG13	1.94	0.67
1:I:13:DT:H2"	1:I:14:DA:C8	2.29	0.67
5:E:6:DT:H2'	5:E:7:DC:H6	1.58	0.67
7:B:300:PHE:HE1	7:B:304:PRO:HB3	1.57	0.67
7:D:139:SER:O	7:D:143:ILE:HG13	1.94	0.67
7:B:213:VAL:CA	7:B:216:LEU:HD12	2.23	0.67
6:F:10:DA:N7	7:A:20:ASN:ND2	2.43	0.67
7:D:293:ARG:NH1	7:D:305:PRO:O	2.27	0.67
3:K:15:DA:C8	3:K:16:DT:H73	2.30	0.67
7:C:94:GLN:O	7:C:98:ILE:HD12	1.95	0.67
7:A:163:ASN:OD1	7:A:165:VAL:CB	2.41	0.67
7:B:103:LYS:O	7:B:104:ILE:C	2.31	0.67
7:A:114:ALA:CB	7:A:115:PRO:CD	2.66	0.67
7:C:186:LEU:CD1	7:C:251:LEU:CD2	2.73	0.67
6:F:7:DT:H5'	6:F:7:DT:H6	1.59	0.67
7:A:305:PRO:HB3	7:A:309:GLU:HG3	1.77	0.67
7:D:17:TYR:HE1	7:D:27:ARG:CB	2.08	0.67
7:A:67:ARG:NH1	7:D:36:GLY:O	2.27	0.66
7:C:270:THR:HB	7:C:272:ILE:O	1.94	0.66
7:D:23:TYR:CD2	7:D:23:TYR:C	2.66	0.66
2:J:19:DA:C2'	7:A:96:THR:HG21	2.23	0.66
7:C:51:ALA:O	7:C:54:GLU:HG3	1.96	0.66
2:J:11:DT:H4'	2:J:12:DA:OP1	1.95	0.66
7:A:55:LEU:HB3	7:A:56:PHE:HD1	1.58	0.66
7:C:104:ILE:O	7:C:107:ILE:N	2.28	0.66
7:D:19:ARG:CG	7:D:20:ASN:H	2.08	0.66
7:A:18:ILE:HG13	7:A:24:TYR:HE2	1.60	0.66
7:B:120:THR:HG21	7:B:122:LYS:HB3	1.78	0.66
7:B:84:GLU:HA	7:B:87:LEU:CD1	2.24	0.66
3:K:15:DA:N9	3:K:16:DT:H71	2.11	0.66
7:A:64:LEU:HD21	7:D:26:TYR:CD2	2.31	0.66
7:A:309:GLU:OE1	7:A:309:GLU:HA	1.95	0.66
7:C:26:TYR:HD2	7:C:27:ARG:N	1.94	0.66
1:I:12:DT:H5"	7:A:235:LYS:NZ	2.11	0.66
3:K:3:DG:H2"	3:K:4:DC:OP2	1.96	0.66
3:K:15:DA:C8	3:K:16:DT:C7	2.78	0.66
7:A:23:TYR:C	7:A:23:TYR:HD2	1.95	0.66
7:A:45:ILE:O	7:A:48:ALA:HB3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:148:SER:O	7:C:151:PHE:HB2	1.96	0.66
7:C:160:ILE:HG22	7:C:162:THR:H	1.59	0.66
7:A:111:LEU:HD22	7:A:112:PRO:CD	2.26	0.66
7:B:83:TYR:O	7:B:86:ILE:HB	1.96	0.66
7:C:114:ALA:HB1	7:C:115:PRO:HD3	1.78	0.66
7:D:31:THR:OG1	7:D:33:LYS:CG	2.42	0.66
7:A:104:ILE:HG22	7:A:105:LYS:N	2.09	0.65
5:E:21:DA:C8	5:E:22:DT:H71	2.31	0.65
7:B:293:ARG:O	7:B:296:SER:OG	2.12	0.65
6:F:18:DT:H2'	6:F:19:DG:C8	2.31	0.65
7:D:221:TRP:CZ2	7:D:263:LYS:HB3	2.30	0.65
7:B:129:ASN:HA	7:B:132:ILE:CD1	2.22	0.65
2:J:7:DA:C4	2:J:8:DG:C8	2.84	0.65
7:B:151:PHE:O	7:B:154:ALA:HB3	1.96	0.65
7:D:33:LYS:HE3	7:D:33:LYS:CA	2.21	0.65
6:F:19:DG:H2'	6:F:20:DA:C8	2.32	0.65
7:A:163:ASN:OD1	7:A:163:ASN:C	2.31	0.65
7:B:160:ILE:N	7:B:160:ILE:HD13	2.12	0.65
7:D:141:LYS:C	7:D:141:LYS:HD2	2.16	0.65
7:A:23:TYR:OH	7:A:36:GLY:CA	2.40	0.65
7:A:309:GLU:OE1	7:A:309:GLU:C	2.34	0.65
7:C:23:TYR:OH	7:C:36:GLY:HA3	1.95	0.65
3:K:9:DT:H2"	3:K:10:DT:C5'	2.23	0.65
7:A:169:ARG:NH2	7:B:152:ARG:HD3	2.12	0.65
7:B:36:GLY:C	7:B:37:LEU:HD12	2.16	0.65
7:B:353:ILE:HD13	7:C:330:LEU:HD12	1.79	0.65
7:C:259:LEU:HD11	7:C:271:ILE:HD13	1.78	0.65
7:A:28:ASP:CG	7:A:30:ARG:HB3	2.16	0.65
7:A:67:ARG:NH2	7:D:36:GLY:O	2.30	0.65
7:C:105:LYS:HA	7:C:108:ARG:HG3	1.79	0.64
7:C:258:THR:O	7:C:262:CYS:SG	2.54	0.64
7:A:40:ASP:OD1	7:A:43:ILE:HG12	1.96	0.64
5:E:21:DA:C5	5:E:22:DT:H73	2.31	0.64
1:I:7:DG:C4	1:I:8:DC:C6	2.85	0.64
7:C:185:TYR:HD1	7:C:186:LEU:HD12	1.62	0.64
7:A:142:LEU:O	7:A:146:THR:OG1	2.16	0.64
7:A:160:ILE:HG22	7:A:162:THR:N	2.12	0.64
7:D:79:TRP:CZ2	7:D:154:ALA:CA	2.77	0.64
7:A:57:SER:OG	7:A:59:HIS:HB3	1.96	0.64
7:A:76:LEU:HD12	7:A:76:LEU:H	1.62	0.64
7:A:290:MSE:O	7:A:293:ARG:HB3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:159:HIS:O	7:B:160:ILE:HG22	1.98	0.64
7:C:17:TYR:CE1	7:C:27:ARG:HB2	2.32	0.64
5:G:12:DT:H2'	5:G:13:DC:C6	2.33	0.64
7:A:26:TYR:CE2	7:A:51:ALA:HB1	2.33	0.64
7:B:105:LYS:O	7:B:106:ALA:C	2.35	0.64
7:B:61:HIS:CE1	7:B:63:PRO:HA	2.33	0.64
7:C:353:ILE:HD11	7:D:240:ILE:HB	1.79	0.64
7:A:28:ASP:OD2	7:A:30:ARG:CB	2.41	0.64
7:B:74:VAL:CG1	7:B:75:THR:N	2.61	0.64
7:C:111:LEU:HD22	7:C:112:PRO:CD	2.26	0.64
2:J:15:DT:C7	2:J:16:DT:H71	2.27	0.63
4:L:5:DC:H2"	4:L:6:DA:C8	2.34	0.63
7:C:114:ALA:HB1	7:C:115:PRO:HD2	1.79	0.63
7:C:350:TRP:CE3	7:D:239:LYS:HB3	2.34	0.63
4:L:7:DA:C5	4:L:8:DC:C4	2.86	0.63
4:L:13:DT:H5"	7:D:236:THR:CG2	2.28	0.63
7:C:83:TYR:CE1	7:C:150:ALA:HA	2.33	0.63
3:K:16:DT:H1'	3:K:17:DA:H8	1.63	0.63
7:B:300:PHE:CE1	7:B:304:PRO:HB3	2.32	0.63
7:D:74:VAL:CG1	7:D:75:THR:N	2.61	0.63
6:H:17:DG:N7	6:H:18:DT:H73	2.13	0.63
7:C:92:ILE:CG2	7:C:93:LYS:N	2.60	0.63
7:C:144:ARG:HG2	7:C:145:SER:N	2.14	0.63
7:C:146:THR:O	7:C:147:LEU:C	2.34	0.63
3:K:21:DA:H2'	3:K:22:DC:C6	2.34	0.63
5:E:11:DA:C8	5:E:12:DT:H73	2.33	0.63
7:A:146:THR:O	7:A:147:LEU:C	2.37	0.63
1:I:19:DA:H2'	1:I:20:DA:C8	2.34	0.63
7:A:185:TYR:CD1	7:A:185:TYR:C	2.72	0.63
7:B:163:ASN:OD1	7:B:165:VAL:CB	2.45	0.63
7:A:10:ARG:HH22	7:A:12:LEU:HD22	1.63	0.63
7:D:80:LEU:HD23	7:D:104:ILE:HG23	1.80	0.63
6:H:20:DA:C2	6:H:21:DC:C2	2.87	0.63
1:I:21:DA:H62	7:D:99:ASN:ND2	1.98	0.62
7:B:84:GLU:O	7:B:87:LEU:HD12	1.99	0.62
5:E:10:DT:H2"	5:E:11:DA:C8	2.33	0.62
7:C:92:ILE:HG21	7:C:96:THR:HB	1.81	0.62
7:D:100:TYR:O	7:D:103:LYS:HG2	1.98	0.62
7:D:313:LEU:HA	7:D:316:ARG:CZ	2.29	0.62
7:A:16:LEU:C	7:A:17:TYR:CD2	2.73	0.62
1:I:7:DG:C6	1:I:8:DC:C4	2.87	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:19:DA:C6	1:I:20:DA:C6	2.88	0.62
2:J:20:DA:H2"	2:J:21:DA:O4'	1.99	0.62
6:H:17:DG:N7	6:H:18:DT:C7	2.61	0.62
7:B:103:LYS:O	7:B:106:ALA:HB3	2.00	0.62
7:C:18:ILE:HG12	7:C:19:ARG:N	2.13	0.62
7:C:97:LEU:HD23	7:C:98:ILE:HG13	1.81	0.62
1:I:12:DT:P	7:A:212:ARG:HH21	2.14	0.62
6:F:9:DG:H2"	6:F:10:DA:C8	2.33	0.62
7:B:121:THR:O	7:B:124:ILE:HB	1.99	0.62
7:B:270:THR:HG21	7:B:279:PRO:HB3	1.81	0.62
7:C:186:LEU:HD12	7:C:251:LEU:HD22	1.80	0.62
1:I:12:DT:O5'	7:A:212:ARG:NH2	2.31	0.62
5:E:2:DC:H2"	5:E:3:DA:C8	2.33	0.62
7:A:151:PHE:O	7:A:152:ARG:C	2.38	0.62
7:D:111:LEU:HD22	7:D:112:PRO:HD2	1.82	0.62
7:B:25:CYS:SG	7:B:34:GLU:HB3	2.40	0.62
7:C:114:ALA:CB	7:C:115:PRO:CD	2.78	0.62
7:C:116:LEU:N	7:C:116:LEU:CD1	2.61	0.62
5:G:14:DA:H8	7:C:23:TYR:HE1	1.47	0.62
7:C:77:HIS:HB2	7:C:113:ASP:OD2	2.00	0.61
2:J:23:DC:H2"	2:J:24:DA:C8	2.35	0.61
7:C:136:LYS:O	7:C:139:SER:HB2	1.99	0.61
7:C:147:LEU:HG	7:C:151:PHE:HE2	1.65	0.61
7:C:221:TRP:HH2	7:C:263:LYS:HB2	1.65	0.61
7:D:142:LEU:O	7:D:146:THR:OG1	2.17	0.61
7:D:211:GLN:CA	7:D:311:ARG:HH11	2.12	0.61
2:J:16:DT:H2"	2:J:17:DA:O5'	1.99	0.61
7:D:151:PHE:O	7:D:154:ALA:HB3	1.99	0.61
3:K:19:DA:H2'	3:K:20:DA:H8	1.65	0.61
6:F:17:DG:OP2	7:B:17:TYR:CZ	2.53	0.61
7:C:87:LEU:HD12	7:C:87:LEU:H	1.64	0.61
7:C:287:ARG:O	7:C:290:MSE:HB3	2.01	0.61
5:E:21:DA:C5	5:E:22:DT:C7	2.84	0.61
7:A:10:ARG:HH21	7:A:12:LEU:HB2	1.65	0.61
7:B:59:HIS:O	7:B:60:LYS:O	2.17	0.61
7:D:212:ARG:NH2	7:D:233:GLN:OE1	2.33	0.61
7:A:18:ILE:HG13	7:A:24:TYR:CD2	2.35	0.61
7:A:98:ILE:HA	7:A:101:MSE:HB2	1.81	0.61
7:A:198:TRP:HB3	7:A:266:LEU:HD11	1.81	0.61
1:I:17:DA:C2	1:I:18:DC:C2	2.88	0.61
7:B:23:TYR:HD2	7:B:23:TYR:C	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:139:SER:O	7:B:140:ALA:C	2.37	0.61
7:B:160:ILE:HD13	7:B:160:ILE:H	1.65	0.61
4:L:23:DC:H5"	7:C:306:THR:CG2	2.31	0.61
7:A:213:VAL:O	7:A:216:LEU:HB3	2.00	0.61
7:B:61:HIS:ND1	7:B:62:LYS:O	2.33	0.61
7:C:47:GLU:OE2	7:D:63:PRO:CD	2.34	0.61
7:C:120:THR:CG2	7:C:123:GLU:HG3	2.31	0.61
7:C:199:LEU:O	7:C:203:MSE:CG	2.48	0.61
7:D:212:ARG:HE	7:D:233:GLN:CD	2.04	0.61
6:H:13:DG:C2'	6:H:14:DA:H8	2.13	0.60
7:A:103:LYS:O	7:A:106:ALA:N	2.34	0.60
7:B:76:LEU:C	7:B:80:LEU:CD1	2.67	0.60
7:C:83:TYR:O	7:C:87:LEU:CD1	2.49	0.60
6:H:9:DG:H2'	7:C:20:ASN:ND2	2.16	0.60
7:B:58:GLY:O	7:B:59:HIS:HB2	2.01	0.60
7:B:229:LEU:HD22	7:B:255:MSE:HE1	1.83	0.60
7:C:211:GLN:C	7:C:311:ARG:HD2	2.21	0.60
1:I:7:DG:C5	1:I:8:DC:C5	2.89	0.60
1:I:22:DG:H2"	1:I:23:DT:H5'	1.82	0.60
7:A:74:VAL:HG12	7:A:75:THR:HG22	1.83	0.60
7:B:26:TYR:C	7:B:26:TYR:CD2	2.72	0.60
7:B:146:THR:O	7:B:147:LEU:C	2.38	0.60
7:D:290:MSE:O	7:D:293:ARG:HB2	2.01	0.60
1:I:9:DT:O2	1:I:10:DT:C6	2.54	0.60
3:K:25:DG:H1'	3:K:26:DA:H5"	1.83	0.60
6:H:23:DT:H2"	6:H:24:DG:N7	2.15	0.60
7:A:64:LEU:HB2	7:D:47:GLU:OE2	2.01	0.60
7:B:289:PHE:C	7:B:289:PHE:CD2	2.74	0.60
3:K:9:DT:C2	3:K:10:DT:C6	2.89	0.60
6:F:2:DG:C2'	6:F:3:DT:H71	2.19	0.60
7:D:83:TYR:CD2	7:D:87:LEU:HD11	2.36	0.60
7:D:97:LEU:O	7:D:100:TYR:HB2	2.01	0.60
6:H:14:DA:H2"	6:H:15:DT:C6	2.36	0.60
7:A:12:LEU:HD11	7:A:16:LEU:CD2	2.31	0.60
7:A:345:ASP:N	7:A:345:ASP:OD1	2.34	0.60
7:B:159:HIS:O	7:B:160:ILE:CG2	2.49	0.60
7:B:212:ARG:NH1	7:B:233:GLN:OE1	2.35	0.60
7:C:11:ASP:O	7:C:13:PRO:HD3	2.02	0.60
7:C:305:PRO:HB3	7:C:309:GLU:HG3	1.84	0.60
7:D:221:TRP:CE2	7:D:271:ILE:HG12	2.35	0.60
2:J:15:DT:C7	2:J:16:DT:C7	2.79	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:153:GLU:O	7:B:156:ALA:HB3	2.02	0.60
7:C:54:GLU:HG3	7:C:55:LEU:N	2.17	0.60
7:D:198:TRP:CE3	7:D:199:LEU:N	2.70	0.60
7:A:61:HIS:HE2	7:D:47:GLU:CD	1.98	0.60
7:D:120:THR:O	7:D:121:THR:C	2.40	0.60
5:G:10:DT:H2"	5:G:11:DA:N7	2.17	0.60
7:A:55:LEU:HD22	7:A:56:PHE:HE1	1.65	0.60
7:A:307:PHE:CD1	7:A:307:PHE:C	2.75	0.59
6:F:7:DT:OP2	7:A:14:PRO:HA	2.02	0.59
7:B:283:GLY:O	7:B:287:ARG:HB2	2.01	0.59
7:D:162:THR:O	7:D:162:THR:HG22	2.02	0.59
4:L:20:DA:H2"	4:L:21:DA:H5"	1.84	0.59
6:F:11:DC:C5	6:F:12:DT:H73	2.37	0.59
7:A:76:LEU:CD1	7:A:76:LEU:H	2.14	0.59
4:L:7:DA:C5	4:L:8:DC:C5	2.90	0.59
7:A:83:TYR:CE1	7:A:150:ALA:HA	2.37	0.59
7:A:120:THR:HG22	7:A:123:GLU:CG	2.29	0.59
7:B:267:GLY:O	7:B:277:ARG:HG3	2.03	0.59
7:B:350:TRP:CE3	7:C:239:LYS:HB3	2.37	0.59
7:D:213:VAL:HB	7:D:307:PHE:CE1	2.37	0.59
3:K:26:DA:N6	7:B:287:ARG:HH22	2.01	0.59
7:A:57:SER:C	7:A:59:HIS:N	2.55	0.59
7:B:25:CYS:HA	7:B:37:LEU:HD13	1.85	0.59
7:B:137:ALA:O	7:B:138:ALA:C	2.37	0.59
7:C:152:ARG:O	7:C:155:ILE:HB	2.02	0.59
7:C:160:ILE:CG2	7:C:162:THR:H	2.15	0.59
7:A:45:ILE:CG2	7:A:46:THR:N	2.66	0.59
7:A:203:MSE:O	7:A:207:VAL:HG23	2.02	0.59
7:C:151:PHE:O	7:C:154:ALA:N	2.36	0.59
7:C:186:LEU:HD11	7:C:251:LEU:CD2	2.33	0.59
7:C:103:LYS:O	7:C:104:ILE:C	2.41	0.59
7:B:60:LYS:O	7:B:61:HIS:CB	2.45	0.59
7:B:159:HIS:C	7:B:160:ILE:CG2	2.71	0.59
7:C:79:TRP:CZ2	7:C:154:ALA:CA	2.86	0.59
2:J:16:DT:O2	2:J:17:DA:H5"	2.03	0.59
7:C:338:MSE:C	7:C:340:SER:N	2.56	0.59
7:D:55:LEU:N	7:D:55:LEU:HD12	2.18	0.59
7:D:212:ARG:N	7:D:311:ARG:HD2	2.18	0.59
4:L:14:DT:H2"	4:L:15:DG:OP2	2.04	0.58
7:A:333:HIS:CE1	7:A:338:MSE:HB2	2.38	0.58
7:B:26:TYR:CD2	7:B:27:ARG:N	2.71	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:79:TRP:CZ2	7:B:154:ALA:CA	2.86	0.58
7:C:180:LEU:HD13	7:C:305:PRO:HB2	1.84	0.58
6:F:14:DA:H2"	6:F:15:DT:C6	2.38	0.58
7:A:160:ILE:HG22	7:A:161:THR:H	1.51	0.58
7:A:19:ARG:NH1	7:A:19:ARG:HG2	2.18	0.58
7:A:23:TYR:CD2	7:A:24:TYR:N	2.71	0.58
7:A:306:THR:O	7:A:309:GLU:CB	2.50	0.58
7:B:60:LYS:HE3	7:D:46:THR:CG2	2.34	0.58
2:J:24:DA:C2	2:J:25:DG:C6	2.92	0.58
4:L:7:DA:C4	4:L:8:DC:C6	2.92	0.58
7:B:75:THR:HA	7:B:115:PRO:HA	1.86	0.58
7:B:79:TRP:CZ2	7:B:154:ALA:HA	2.39	0.58
7:D:129:ASN:OD1	7:D:132:ILE:HD12	2.04	0.58
3:K:17:DA:H8	3:K:17:DA:H5'	1.69	0.58
6:H:13:DG:C2'	6:H:14:DA:C8	2.87	0.58
7:B:104:ILE:O	7:B:105:LYS:C	2.41	0.58
7:C:199:LEU:O	7:C:203:MSE:HG3	2.03	0.58
7:C:83:TYR:O	7:C:87:LEU:HD13	2.03	0.58
7:D:37:LEU:HD23	7:D:37:LEU:N	2.19	0.58
7:A:116:LEU:HA	7:A:119:ILE:CD1	2.30	0.58
7:D:17:TYR:CE1	7:D:27:ARG:HB2	2.39	0.58
7:D:19:ARG:HD2	7:D:21:ASN:H	1.69	0.58
7:D:54:GLU:OE2	7:D:54:GLU:HA	2.04	0.58
5:G:5:DG:N2	5:G:6:DT:C2	2.71	0.57
5:G:12:DT:H2'	5:G:13:DC:H6	1.68	0.57
7:A:75:THR:CG2	7:A:78:SER:CB	2.77	0.57
7:C:64:LEU:O	7:C:65:THR:C	2.42	0.57
7:A:76:LEU:O	7:A:80:LEU:CD1	2.51	0.57
7:D:169:ARG:O	7:D:169:ARG:NE	2.36	0.57
4:L:7:DA:C8	4:L:8:DC:C5	2.92	0.57
7:B:74:VAL:CG1	7:B:75:THR:H	2.17	0.57
7:D:155:ILE:HG22	7:D:155:ILE:O	2.04	0.57
7:A:55:LEU:HB3	7:A:56:PHE:CD1	2.39	0.57
7:B:145:SER:O	7:B:148:SER:HB3	2.04	0.57
7:B:220:LYS:O	7:B:223:ASP:HB2	2.04	0.57
7:D:47:GLU:O	7:D:50:GLN:HB2	2.05	0.57
1:I:20:DA:C2	1:I:21:DA:C4	2.93	0.57
3:K:12:DA:C2'	3:K:13:DT:H72	2.29	0.57
5:E:4:DG:C4	5:E:5:DG:C8	2.92	0.57
6:F:13:DG:C4	6:F:14:DA:C8	2.92	0.57
7:D:45:ILE:HG22	7:D:46:THR:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:16:DA:C5	4:L:15:DG:N2	2.73	0.57
7:A:27:ARG:HE	7:A:32:GLY:HA2	1.70	0.57
7:B:75:THR:OG1	7:B:78:SER:OG	2.03	0.57
7:C:79:TRP:O	7:C:83:TYR:N	2.34	0.57
7:D:146:THR:O	7:D:147:LEU:C	2.42	0.57
7:D:215:ASP:OD2	7:D:233:GLN:HA	2.04	0.57
6:H:17:DG:C4	6:H:18:DT:C5	2.93	0.57
7:D:212:ARG:CZ	7:D:233:GLN:OE1	2.53	0.57
7:D:305:PRO:HB3	7:D:309:GLU:HG3	1.87	0.57
6:H:9:DG:O6	7:C:19:ARG:NH2	2.38	0.57
7:A:60:LYS:HZ2	7:B:67:ARG:CB	2.18	0.57
7:A:64:LEU:HD23	7:D:51:ALA:HB2	1.86	0.57
7:A:160:ILE:CG2	7:A:162:THR:H	2.17	0.57
7:A:311:ARG:NH2	7:A:331:LEU:HG	2.19	0.57
7:B:23:TYR:CD2	7:B:23:TYR:C	2.71	0.57
7:C:144:ARG:HE	7:C:168:THR:HG23	1.70	0.57
6:F:17:DG:OP2	7:B:17:TYR:HE2	1.84	0.57
7:A:103:LYS:O	7:A:106:ALA:CB	2.49	0.57
7:A:144:ARG:O	7:A:145:SER:C	2.43	0.56
7:B:27:ARG:HD3	7:B:34:GLU:OE1	2.05	0.56
7:D:211:GLN:O	7:D:311:ARG:HD2	2.05	0.56
4:L:7:DA:H2"	4:L:8:DC:H5"	1.88	0.56
7:A:116:LEU:HB3	7:A:160:ILE:HD11	1.85	0.56
7:A:211:GLN:CA	7:A:311:ARG:HH11	2.18	0.56
7:D:121:THR:HA	7:D:124:ILE:HD12	1.87	0.56
2:J:8:DG:C5'	7:B:136:LYS:HD3	2.33	0.56
3:K:10:DT:H4'	7:C:177:ARG:NH1	2.19	0.56
3:K:12:DA:P	7:C:212:ARG:HH21	2.25	0.56
3:K:19:DA:H2'	3:K:20:DA:C8	2.40	0.56
3:K:21:DA:OP2	7:B:93:LYS:HD3	2.05	0.56
7:B:146:THR:O	7:B:149:ASP:N	2.37	0.56
7:B:181:THR:O	7:B:184:GLU:HG3	2.05	0.56
7:C:144:ARG:CG	7:C:145:SER:N	2.68	0.56
7:C:180:LEU:HD13	7:C:305:PRO:CB	2.35	0.56
7:C:220:LYS:O	7:C:223:ASP:HB2	2.06	0.56
7:C:354:GLU:C	7:C:356:LYS:N	2.54	0.56
5:E:11:DA:C2	5:E:12:DT:C4	2.93	0.56
7:A:101:MSE:CA	7:A:104:ILE:HD12	2.35	0.56
7:B:287:ARG:O	7:B:290:MSE:HB3	2.06	0.56
7:B:34:GLU:O	7:B:35:PHE:CD2	2.59	0.56
7:B:144:ARG:NH1	7:B:170:ALA:HB2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:285:VAL:HG12	7:C:307:PHE:CE2	2.41	0.56
7:D:27:ARG:HG3	7:D:34:GLU:CG	2.31	0.56
7:D:124:ILE:HG22	7:D:128:LEU:HD12	1.88	0.56
7:D:290:MSE:CG	7:D:293:ARG:HH21	2.18	0.56
7:D:327:ALA:O	7:D:331:LEU:HG	2.05	0.56
2:J:20:DA:C2	2:J:21:DA:C4	2.93	0.56
7:A:60:LYS:NZ	7:B:67:ARG:CB	2.68	0.56
7:A:105:LYS:O	7:A:106:ALA:C	2.43	0.56
6:H:6:DT:C5	6:H:7:DT:H72	2.41	0.56
7:A:55:LEU:HD22	7:A:56:PHE:CE1	2.40	0.56
7:B:198:TRP:CE3	7:B:199:LEU:N	2.74	0.56
7:D:123:GLU:O	7:D:126:ALA:HB3	2.06	0.56
2:J:15:DT:H73	2:J:16:DT:C7	2.36	0.56
7:A:148:SER:O	7:A:151:PHE:HB2	2.06	0.56
7:B:151:PHE:O	7:B:152:ARG:C	2.41	0.56
7:B:181:THR:HG23	7:B:184:GLU:CD	2.26	0.56
7:B:199:LEU:O	7:B:203:MSE:HG2	2.06	0.56
7:C:203:MSE:O	7:C:207:VAL:HG23	2.06	0.56
7:D:283:GLY:O	7:D:287:ARG:HB2	2.05	0.56
1:I:10:DT:H4'	7:A:177:ARG:NH1	2.21	0.56
3:K:9:DT:O2	3:K:10:DT:C6	2.59	0.56
6:H:17:DG:C5	6:H:18:DT:C5	2.94	0.56
6:H:23:DT:H2"	6:H:24:DG:C8	2.40	0.56
7:D:15:ASN:ND2	7:D:52:ASN:HD21	2.04	0.56
7:B:159:HIS:C	7:B:160:ILE:HG23	2.26	0.56
7:C:144:ARG:NH1	7:C:170:ALA:HB2	2.20	0.56
7:C:189:TYR:CZ	7:C:200:ARG:NH2	2.74	0.56
7:D:305:PRO:HB3	7:D:309:GLU:CG	2.35	0.56
5:E:7:DC:H2'	5:E:8:DA:C8	2.41	0.55
7:A:19:ARG:HG2	7:A:19:ARG:HH11	1.72	0.55
1:I:17:DA:H5'	1:I:17:DA:H8	1.71	0.55
4:L:28:DA:H2"	4:L:29:DA:OP2	2.05	0.55
7:B:27:ARG:HG3	7:B:34:GLU:HG2	1.86	0.55
7:C:151:PHE:O	7:C:152:ARG:C	2.42	0.55
7:C:307:PHE:O	7:C:308:HIS:C	2.41	0.55
6:H:9:DG:H2"	6:H:10:DA:C8	2.41	0.55
7:C:224:ILE:HD13	7:C:259:LEU:HD21	1.89	0.55
7:D:212:ARG:N	7:D:311:ARG:HH11	2.05	0.55
7:B:114:ALA:CB	7:B:115:PRO:CD	2.76	0.55
7:D:15:ASN:HD21	7:D:52:ASN:ND2	2.04	0.55
7:D:27:ARG:CD	7:D:34:GLU:OE1	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:19:ARG:CG	7:B:20:ASN:H	2.19	0.55
7:C:57:SER:O	7:C:59:HIS:HB2	2.06	0.55
7:D:17:TYR:CE1	7:D:27:ARG:CB	2.89	0.55
3:K:12:DA:OP2	7:C:342:PHE:CE2	2.59	0.55
6:H:6:DT:C2'	6:H:7:DT:H5"	2.17	0.55
7:A:211:GLN:HA	7:A:311:ARG:NH1	2.18	0.55
7:B:27:ARG:HD2	7:B:34:GLU:HG2	1.82	0.55
7:B:124:ILE:HG22	7:B:125:ALA:N	2.19	0.55
7:C:131:TYR:HD1	7:C:131:TYR:N	2.03	0.55
7:C:307:PHE:O	7:C:310:LEU:CG	2.50	0.55
7:D:50:GLN:HA	7:D:53:ILE:CD1	2.32	0.55
7:D:53:ILE:HG22	7:D:57:SER:HB2	1.89	0.55
7:A:51:ALA:O	7:A:54:GLU:HB3	2.06	0.55
7:A:104:ILE:O	7:A:105:LYS:C	2.45	0.55
7:B:153:GLU:HA	7:B:156:ALA:HB2	1.89	0.55
7:B:200:ARG:HA	7:B:203:MSE:HG3	1.89	0.55
7:C:201:LEU:HD22	7:C:262:CYS:SG	2.46	0.55
2:J:9:DT:C2'	2:J:10:DT:H5'	2.17	0.55
3:K:23:DT:H4'	7:B:306:THR:HG21	1.87	0.55
6:F:2:DG:OP2	6:F:2:DG:H2'	2.07	0.55
7:B:312:SER:HB2	7:B:316:ARG:HH21	1.70	0.55
7:C:147:LEU:HG	7:C:151:PHE:CE2	2.42	0.55
7:D:34:GLU:C	7:D:35:PHE:CD1	2.80	0.55
4:L:10:DT:H2'	4:L:11:DT:C6	2.42	0.55
7:A:145:SER:O	7:A:148:SER:HB3	2.07	0.55
7:D:141:LYS:NZ	7:D:145:SER:HB2	2.22	0.55
2:J:20:DA:H2"	2:J:21:DA:C5'	2.37	0.55
6:H:9:DG:C6	6:H:10:DA:N6	2.75	0.55
7:A:212:ARG:N	7:A:311:ARG:HD2	2.20	0.55
1:I:19:DA:H2'	1:I:20:DA:H8	1.72	0.54
5:E:1:DA:C2	5:E:2:DC:C2	2.95	0.54
7:A:169:ARG:HH21	7:B:152:ARG:CD	2.17	0.54
7:B:232:GLU:O	7:B:232:GLU:CG	2.54	0.54
7:B:281:SER:O	7:B:284:THR:OG1	2.18	0.54
7:D:24:TYR:CE1	7:D:41:ARG:CA	2.89	0.54
7:A:125:ALA:O	7:A:128:LEU:N	2.40	0.54
7:B:144:ARG:O	7:B:145:SER:C	2.45	0.54
7:B:120:THR:CG2	7:B:122:LYS:H	2.12	0.54
7:B:144:ARG:HH11	7:B:170:ALA:HB2	1.72	0.54
3:K:12:DA:P	7:C:212:ARG:NH2	2.80	0.54
4:L:21:DA:H62	7:C:99:ASN:ND2	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:17:DG:OP2	7:D:17:TYR:CZ	2.60	0.54
7:A:180:LEU:N	7:A:309:GLU:OE2	2.37	0.54
7:B:15:ASN:HB2	7:B:26:TYR:CZ	2.43	0.54
7:B:255:MSE:HE3	7:B:259:LEU:HD11	1.89	0.54
7:C:9:ARG:HD2	7:C:10:ARG:NE	2.18	0.54
7:C:18:ILE:HG13	7:C:24:TYR:CE2	2.42	0.54
7:C:120:THR:O	7:C:121:THR:C	2.46	0.54
7:C:221:TRP:CH2	7:C:263:LYS:CB	2.89	0.54
7:C:338:MSE:C	7:C:340:SER:H	2.11	0.54
7:D:105:LYS:HA	7:D:108:ARG:HD2	1.88	0.54
2:J:4:DT:H2"	2:J:5:DC:OP2	2.07	0.54
3:K:15:DA:C1'	3:K:16:DT:H71	2.38	0.54
5:E:4:DG:C6	5:E:5:DG:C5	2.95	0.54
7:A:25:CYS:HB2	7:A:34:GLU:OE2	2.07	0.54
7:B:293:ARG:NH1	7:B:305:PRO:O	2.38	0.54
7:B:205:LEU:O	7:B:209:THR:OG1	2.25	0.54
7:C:54:GLU:HG3	7:C:55:LEU:H	1.70	0.54
4:L:8:DC:C5'	7:D:136:LYS:HD3	2.38	0.54
7:B:25:CYS:SG	7:B:35:PHE:N	2.80	0.54
7:D:14:PRO:HG2	7:D:52:ASN:HD22	1.73	0.54
7:D:19:ARG:CG	7:D:20:ASN:N	2.69	0.54
3:K:17:DA:C8	3:K:17:DA:H5'	2.42	0.54
5:E:7:DC:C2'	5:E:8:DA:C8	2.90	0.54
7:A:11:ASP:O	7:A:13:PRO:HD3	2.07	0.54
7:A:114:ALA:CB	7:A:115:PRO:HD3	2.20	0.54
7:B:62:LYS:C	7:B:64:LEU:N	2.58	0.54
7:D:220:LYS:O	7:D:223:ASP:HB2	2.07	0.54
2:J:16:DT:C2'	2:J:17:DA:O5'	2.55	0.54
7:A:144:ARG:HE	7:A:168:THR:CG2	2.18	0.54
7:B:62:LYS:O	7:B:64:LEU:C	2.46	0.54
7:C:224:ILE:HD11	7:C:271:ILE:CD1	2.35	0.54
6:F:6:DT:C6	6:F:7:DT:H72	2.42	0.54
6:H:13:DG:H2'	6:H:14:DA:C8	2.43	0.54
7:A:92:ILE:CG2	7:A:93:LYS:N	2.70	0.54
7:B:15:ASN:HA	7:B:17:TYR:CZ	2.43	0.54
7:C:131:TYR:N	7:C:131:TYR:CD1	2.73	0.54
2:J:2:DG:C4'	7:B:276:ARG:NH2	2.69	0.53
6:F:9:DG:H2"	7:A:20:ASN:ND2	2.09	0.53
6:H:13:DG:C2	6:H:14:DA:C4	2.96	0.53
7:A:205:LEU:O	7:A:208:VAL:HG12	2.09	0.53
7:B:262:CYS:O	7:B:266:LEU:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:285:VAL:HG12	7:D:286:SER:N	2.22	0.53
5:E:21:DA:C4	5:E:22:DT:C5	2.96	0.53
7:A:239:LYS:HB3	7:D:350:TRP:CE3	2.43	0.53
7:B:155:ILE:HG13	7:B:160:ILE:HD11	1.86	0.53
7:A:18:ILE:HG12	7:A:19:ARG:N	2.23	0.53
7:C:120:THR:HG23	7:C:123:GLU:H	1.73	0.53
7:D:74:VAL:HG12	7:D:75:THR:N	2.23	0.53
3:K:10:DT:H2"	3:K:11:DT:O5'	2.08	0.53
7:C:327:ALA:O	7:C:331:LEU:HD22	2.08	0.53
7:D:198:TRP:HE3	7:D:199:LEU:N	2.07	0.53
4:L:7:DA:N7	4:L:8:DC:C5	2.76	0.53
7:B:75:THR:HG22	7:B:114:ALA:C	2.29	0.53
7:C:83:TYR:CE2	7:C:87:LEU:HD21	2.43	0.53
7:D:18:ILE:HD11	7:D:22:GLY:HA2	1.91	0.53
7:A:63:PRO:O	7:A:67:ARG:HB2	2.09	0.53
7:A:102:SER:OG	7:A:103:LYS:NZ	2.39	0.53
7:B:142:LEU:N	7:B:142:LEU:HD12	2.24	0.53
7:A:338:MSE:C	7:A:340:SER:N	2.61	0.53
7:C:68:ILE:HG22	7:C:69:ASN:N	2.21	0.53
7:B:27:ARG:CD	7:B:34:GLU:OE1	2.56	0.53
7:C:60:LYS:HB2	7:C:60:LYS:NZ	2.23	0.53
1:I:9:DT:C2	1:I:10:DT:C5	2.97	0.53
1:I:21:DA:H62	7:D:99:ASN:HD21	1.57	0.53
7:C:79:TRP:CH2	7:C:154:ALA:HA	2.44	0.53
7:C:120:THR:HG22	7:C:123:GLU:CG	2.38	0.53
2:J:8:DG:H2'	2:J:9:DT:H71	1.90	0.53
7:B:45:ILE:O	7:B:48:ALA:CB	2.54	0.53
7:B:74:VAL:HG12	7:B:75:THR:H	1.69	0.53
7:B:100:TYR:HA	7:B:103:LYS:HG3	1.91	0.53
7:C:76:LEU:O	7:C:80:LEU:HG	2.09	0.53
4:L:8:DC:OP1	7:D:136:LYS:NZ	2.40	0.52
7:C:18:ILE:HG13	7:C:24:TYR:CD2	2.44	0.52
7:C:26:TYR:CE1	7:C:51:ALA:CB	2.86	0.52
7:D:18:ILE:HG12	7:D:19:ARG:N	2.24	0.52
7:D:169:ARG:HD2	7:D:170:ALA:N	2.16	0.52
1:I:13:DT:C7	7:A:338:MSE:HE3	2.39	0.52
2:J:15:DT:C5	2:J:16:DT:H73	2.44	0.52
3:K:15:DA:C8	3:K:16:DT:H71	2.43	0.52
5:E:16:DT:C4	5:E:17:DC:N4	2.77	0.52
7:B:31:THR:HG1	7:B:33:LYS:HG2	1.73	0.52
7:C:307:PHE:CE1	7:C:310:LEU:HD12	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:11:DT:H1'	3:K:12:DA:H5"	1.91	0.52
6:F:8:DT:H2"	6:F:9:DG:C8	2.44	0.52
7:A:184:GLU:OE2	7:A:298:LEU:HD23	2.10	0.52
7:B:61:HIS:HE1	7:B:63:PRO:HA	1.72	0.52
7:B:285:VAL:CG1	7:B:307:PHE:CE2	2.92	0.52
1:I:9:DT:C2	1:I:10:DT:C6	2.97	0.52
6:F:13:DG:OP2	6:F:13:DG:H8	1.91	0.52
7:D:24:TYR:CE1	7:D:41:ARG:N	2.74	0.52
5:E:3:DA:H2'	5:E:4:DG:H8	1.74	0.52
7:A:184:GLU:OE2	7:A:298:LEU:CD2	2.57	0.52
7:B:185:TYR:CE2	7:B:203:MSE:HE2	2.45	0.52
7:C:74:VAL:HB	7:C:116:LEU:HD13	1.92	0.52
3:K:14:DT:C4'	3:K:15:DA:OP1	2.37	0.52
5:E:16:DT:C5	5:E:17:DC:N4	2.78	0.52
7:A:83:TYR:CD2	7:A:87:LEU:HD11	2.44	0.52
7:C:77:HIS:HB2	7:C:113:ASP:CG	2.30	0.52
7:C:87:LEU:H	7:C:87:LEU:CD1	2.22	0.52
1:I:19:DA:N6	1:I:20:DA:N6	2.58	0.52
7:B:125:ALA:O	7:B:128:LEU:N	2.43	0.52
7:C:98:ILE:O	7:C:102:SER:OG	2.28	0.52
7:D:180:LEU:HB2	7:D:309:GLU:HG3	1.92	0.52
1:I:18:DC:H5'	1:I:18:DC:H6	1.74	0.52
4:L:12:DG:C8	4:L:13:DT:H72	2.45	0.52
7:B:35:PHE:O	7:B:37:LEU:HD12	2.10	0.52
7:D:141:LYS:O	7:D:141:LYS:HD3	2.10	0.52
1:I:17:DA:C2	1:I:18:DC:N3	2.78	0.52
7:C:147:LEU:CG	7:C:151:PHE:HE2	2.23	0.52
7:C:199:LEU:O	7:C:203:MSE:HG2	2.08	0.52
7:D:152:ARG:HA	7:D:155:ILE:HD12	1.91	0.52
7:B:48:ALA:O	7:B:51:ALA:HB3	2.09	0.51
7:B:115:PRO:O	7:B:118:ASP:HB2	2.10	0.51
7:B:216:LEU:HA	7:B:219:MSE:SE	2.60	0.51
7:B:293:ARG:NH1	7:B:304:PRO:HB2	2.25	0.51
7:C:79:TRP:CZ2	7:C:154:ALA:CB	2.93	0.51
5:E:4:DG:C2	5:E:5:DG:C4	2.99	0.51
7:A:12:LEU:CD1	7:A:16:LEU:CD2	2.88	0.51
7:C:144:ARG:HG2	7:C:145:SER:H	1.75	0.51
6:H:13:DG:H2'	6:H:14:DA:H8	1.74	0.51
7:B:293:ARG:CZ	7:B:304:PRO:HB2	2.39	0.51
7:C:228:TYR:HD2	7:C:241:ALA:HB1	1.75	0.51
6:F:23:DT:H2'	6:F:24:DG:C8	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:26:TYR:CE2	7:A:51:ALA:CB	2.93	0.51
7:A:143:ILE:O	7:A:144:ARG:C	2.46	0.51
7:A:169:ARG:HH11	7:A:169:ARG:CG	2.21	0.51
7:A:307:PHE:O	7:A:308:HIS:C	2.47	0.51
7:B:66:ALA:O	7:B:68:ILE:N	2.34	0.51
7:B:309:GLU:HA	7:B:312:SER:HG	1.76	0.51
6:H:1:DG:C2'	6:H:2:DG:OP2	2.48	0.51
7:B:96:THR:O	7:B:99:ASN:HB2	2.11	0.51
7:D:101:MSE:O	7:D:104:ILE:HB	2.10	0.51
4:L:20:DA:C2	4:L:21:DA:C4	2.99	0.51
7:C:63:PRO:O	7:C:66:ALA:HB3	2.10	0.51
7:C:116:LEU:HA	7:C:119:ILE:HD12	1.92	0.51
7:D:48:ALA:O	7:D:51:ALA:HB3	2.10	0.51
5:E:5:DG:H2"	5:E:6:DT:H6	1.76	0.51
5:E:21:DA:N7	5:E:22:DT:H73	2.25	0.51
7:B:18:ILE:HG12	7:B:19:ARG:N	2.26	0.51
7:B:79:TRP:CH2	7:B:154:ALA:CA	2.88	0.51
1:I:7:DG:C5	1:I:8:DC:C4	2.99	0.51
3:K:15:DA:N9	3:K:16:DT:C7	2.73	0.51
5:E:1:DA:C4	5:E:2:DC:C6	2.99	0.51
5:G:23:DA:C2	6:H:4:DA:C2	2.99	0.51
7:A:120:THR:O	7:A:121:THR:C	2.48	0.51
7:B:79:TRP:O	7:B:83:TYR:N	2.42	0.51
7:B:255:MSE:CE	7:B:259:LEU:HD11	2.41	0.51
7:D:148:SER:HA	7:D:165:VAL:HG21	1.93	0.51
7:C:40:ASP:CG	7:C:42:ARG:HG3	2.32	0.51
7:D:23:TYR:CD2	7:D:24:TYR:O	2.63	0.51
2:J:2:DG:H4'	7:B:276:ARG:CZ	2.41	0.50
7:B:137:ALA:O	7:B:140:ALA:N	2.44	0.50
7:B:208:VAL:HG13	7:B:209:THR:HG23	1.92	0.50
7:C:76:LEU:HD22	7:C:119:ILE:CD1	2.40	0.50
7:C:107:ILE:O	7:C:108:ARG:C	2.49	0.50
7:C:229:LEU:O	7:C:229:LEU:HG	2.01	0.50
7:D:28:ASP:OD2	7:D:30:ARG:HB2	2.11	0.50
7:D:154:ALA:HB1	7:D:160:ILE:HD11	1.91	0.50
5:G:4:DG:H2"	5:G:5:DG:O4'	2.10	0.50
7:B:199:LEU:HD12	7:B:199:LEU:H	1.76	0.50
7:B:208:VAL:HA	7:B:318:TYR:OH	2.12	0.50
7:D:163:ASN:OD1	7:D:166:ALA:N	2.35	0.50
7:D:205:LEU:O	7:D:208:VAL:HG12	2.11	0.50
6:H:5:DT:H2"	6:H:6:DT:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:67:ARG:CZ	7:D:36:GLY:O	2.59	0.50
7:B:61:HIS:HD1	7:B:62:LYS:C	2.13	0.50
7:B:306:THR:O	7:B:309:GLU:N	2.44	0.50
2:J:19:DA:P	7:A:90:ARG:HH21	2.35	0.50
6:F:19:DG:C2'	6:F:20:DA:C8	2.95	0.50
5:G:15:DG:OP2	7:C:36:GLY:N	2.45	0.50
7:C:79:TRP:NE1	7:C:154:ALA:HB2	2.26	0.50
3:K:9:DT:C2	3:K:10:DT:C5	3.00	0.50
6:F:14:DA:C2'	6:F:15:DT:C6	2.95	0.50
7:A:23:TYR:HD2	7:A:23:TYR:O	1.94	0.50
7:A:83:TYR:O	7:A:84:GLU:C	2.50	0.50
7:B:77:HIS:O	7:B:81:ASP:OD2	2.29	0.50
7:B:138:ALA:O	7:B:139:SER:C	2.48	0.50
5:E:6:DT:C2'	5:E:7:DC:O4'	2.60	0.50
6:F:16:DA:H3'	7:B:17:TYR:OH	2.12	0.50
7:A:64:LEU:HD21	7:D:26:TYR:HD2	1.74	0.50
7:B:153:GLU:HA	7:B:156:ALA:CB	2.42	0.50
7:B:208:VAL:HG13	7:B:209:THR:N	2.27	0.50
7:C:116:LEU:HD12	7:C:116:LEU:H	1.69	0.50
7:D:155:ILE:HG23	7:D:160:ILE:O	2.11	0.50
7:D:203:MSE:HE3	7:D:289:PHE:HE1	1.76	0.50
7:A:138:ALA:O	7:A:141:LYS:HB3	2.11	0.50
7:C:120:THR:N	7:C:123:GLU:OE1	2.29	0.50
7:C:179:ARG:NH1	7:C:344:ASP:O	2.44	0.50
7:D:141:LYS:CD	7:D:141:LYS:O	2.60	0.50
1:I:18:DC:OP1	7:C:169:ARG:NH2	2.45	0.50
5:G:2:DC:C2	5:G:3:DA:C6	3.00	0.50
6:H:21:DC:C2	6:H:22:DC:C6	3.00	0.50
7:D:221:TRP:HZ3	7:D:263:LYS:HZ1	1.57	0.50
1:I:16:DA:H1'	1:I:17:DA:C8	2.47	0.49
7:A:185:TYR:HD1	7:A:186:LEU:N	2.10	0.49
7:B:208:VAL:CG1	7:B:209:THR:N	2.74	0.49
7:B:274:SER:OG	7:B:275:THR:N	2.45	0.49
7:C:17:TYR:CE1	7:C:27:ARG:CB	2.95	0.49
7:D:18:ILE:HG12	7:D:19:ARG:H	1.77	0.49
7:C:116:LEU:CD1	7:C:116:LEU:H	2.23	0.49
7:C:350:TRP:O	7:C:352:LYS:N	2.44	0.49
7:D:92:ILE:HD11	7:D:97:LEU:HD13	1.92	0.49
7:A:15:ASN:HB2	7:A:26:TYR:CE1	2.46	0.49
7:B:124:ILE:O	7:B:127:MSE:HE2	2.12	0.49
7:C:76:LEU:CD1	7:C:80:LEU:HD11	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:148:SER:HG	7:C:152:ARG:NH2	2.02	0.49
7:D:15:ASN:O	7:D:17:TYR:CE1	2.64	0.49
7:D:103:LYS:O	7:D:104:ILE:C	2.50	0.49
7:D:210:GLY:C	7:D:311:ARG:HG2	2.32	0.49
1:I:10:DT:H2"	1:I:11:DT:O5'	2.12	0.49
2:J:16:DT:O2	2:J:17:DA:C8	2.65	0.49
5:G:10:DT:H2"	5:G:11:DA:C8	2.47	0.49
6:H:8:DT:OP2	7:C:12:LEU:CD2	2.54	0.49
7:D:105:LYS:O	7:D:106:ALA:C	2.50	0.49
7:A:84:GLU:HA	7:A:87:LEU:CD1	2.41	0.49
7:A:344:ASP:OD1	7:B:334:LYS:HD3	2.13	0.49
7:B:314:SER:O	7:B:318:TYR:CD2	2.65	0.49
7:A:163:ASN:CG	7:A:165:VAL:HB	2.29	0.49
7:A:180:LEU:O	7:A:313:LEU:HD13	2.12	0.49
7:B:61:HIS:ND1	7:B:62:LYS:C	2.66	0.49
7:B:84:GLU:C	7:B:87:LEU:HD12	2.33	0.49
7:C:11:ASP:O	7:C:13:PRO:CD	2.59	0.49
7:C:199:LEU:HD22	7:C:288:TYR:HB3	1.95	0.49
7:D:276:ARG:HH22	7:D:278:GLU:CD	2.14	0.49
5:E:11:DA:C6	5:E:12:DT:O4	2.65	0.49
7:A:114:ALA:HB1	7:A:115:PRO:HD2	1.90	0.49
7:B:140:ALA:O	7:B:141:LYS:C	2.50	0.49
1:I:27:DA:H1'	1:I:28:DT:C5'	2.42	0.49
4:L:7:DA:C6	4:L:8:DC:C4	3.00	0.49
5:G:5:DG:C2	5:G:6:DT:C6	3.01	0.49
6:H:19:DG:H2"	6:H:20:DA:O5'	2.13	0.49
7:B:198:TRP:CD2	7:B:199:LEU:HD12	2.48	0.49
7:B:229:LEU:HD23	7:B:242:ILE:HB	1.95	0.49
6:F:16:DA:H3'	7:B:17:TYR:HH	1.78	0.49
7:A:77:HIS:CB	7:A:113:ASP:OD1	2.58	0.49
7:C:79:TRP:CZ2	7:C:154:ALA:HA	2.47	0.49
7:D:254:SER:HB3	7:D:257:GLU:HB2	1.95	0.49
3:K:12:DA:C2'	3:K:13:DT:C7	2.87	0.49
5:E:18:DA:H4'	5:E:19:DA:OP1	2.12	0.49
6:H:17:DG:C4	6:H:18:DT:C6	3.01	0.49
7:C:64:LEU:CD1	7:C:67:ARG:HD3	2.40	0.49
7:D:83:TYR:CZ	7:D:87:LEU:HD21	2.48	0.49
2:J:7:DA:C6	2:J:8:DG:C5	3.01	0.48
2:J:20:DA:C2'	2:J:21:DA:H5"	2.40	0.48
7:B:49:ILE:O	7:B:50:GLN:C	2.52	0.48
7:B:286:SER:O	7:B:289:PHE:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:76:LEU:HD22	7:C:119:ILE:HD11	1.93	0.48
5:G:3:DA:H2'	5:G:4:DG:H8	1.78	0.48
7:A:10:ARG:HH21	7:A:12:LEU:HD22	1.77	0.48
7:B:37:LEU:N	7:B:37:LEU:CD1	2.71	0.48
7:B:163:ASN:OD1	7:B:165:VAL:CG2	2.61	0.48
7:C:144:ARG:O	7:C:145:SER:C	2.51	0.48
7:C:350:TRP:HE3	7:D:239:LYS:HB3	1.76	0.48
7:D:146:THR:O	7:D:149:ASP:N	2.46	0.48
6:H:9:DG:H2"	6:H:10:DA:H8	1.78	0.48
7:A:120:THR:HG23	7:A:123:GLU:H	1.78	0.48
7:C:205:LEU:O	7:C:208:VAL:HG12	2.14	0.48
7:D:144:ARG:O	7:D:145:SER:C	2.52	0.48
7:D:313:LEU:HD12	7:D:316:ARG:HH12	1.78	0.48
7:B:199:LEU:H	7:B:199:LEU:CD1	2.26	0.48
7:C:49:ILE:O	7:C:52:ASN:HB2	2.14	0.48
2:J:26:DA:H2'	2:J:27:DG:C8	2.48	0.48
5:E:4:DG:C2	5:E:5:DG:N9	2.81	0.48
7:A:26:TYR:CZ	7:A:51:ALA:HB3	2.47	0.48
7:B:160:ILE:CD1	7:B:160:ILE:N	2.76	0.48
7:C:82:ARG:O	7:C:83:TYR:C	2.49	0.48
2:J:16:DT:O2	2:J:16:DT:C2'	2.38	0.48
6:F:19:DG:H2'	6:F:20:DA:N7	2.28	0.48
5:G:3:DA:C2'	5:G:4:DG:H8	2.26	0.48
6:H:2:DG:H4'	6:H:3:DT:OP1	2.12	0.48
7:B:15:ASN:HA	7:B:17:TYR:OH	2.14	0.48
7:B:198:TRP:CZ3	7:B:199:LEU:HD12	2.48	0.48
7:C:210:GLY:C	7:C:311:ARG:HG2	2.34	0.48
7:D:96:THR:O	7:D:99:ASN:HB2	2.14	0.48
7:B:155:ILE:HG12	7:B:160:ILE:O	2.13	0.48
7:D:42:ARG:HB3	7:D:42:ARG:CZ	2.43	0.48
7:D:307:PHE:O	7:D:308:HIS:C	2.49	0.48
1:I:21:DA:N6	7:D:99:ASN:HD21	2.12	0.48
7:D:19:ARG:HG2	7:D:20:ASN:H	1.79	0.48
7:A:306:THR:OG1	7:A:307:PHE:N	2.44	0.48
7:B:35:PHE:O	7:B:37:LEU:CD1	2.61	0.48
7:B:290:MSE:O	7:B:293:ARG:CB	2.61	0.48
7:D:79:TRP:CH2	7:D:154:ALA:HA	2.44	0.48
5:G:5:DG:OP2	7:D:36:GLY:N	2.43	0.48
7:A:83:TYR:CZ	7:A:87:LEU:HD21	2.48	0.48
7:B:27:ARG:HD2	7:B:34:GLU:CG	2.38	0.48
7:B:101:MSE:O	7:B:104:ILE:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:285:VAL:HG12	7:B:307:PHE:CE2	2.49	0.48
7:C:81:ASP:OD2	7:C:108:ARG:NH2	2.47	0.48
7:C:98:ILE:HA	7:C:101:MSE:HB2	1.94	0.48
7:D:287:ARG:O	7:D:290:MSE:HB3	2.14	0.48
7:A:207:VAL:O	7:A:314:SER:HB2	2.14	0.47
7:B:83:TYR:CZ	7:B:87:LEU:HD21	2.49	0.47
7:B:307:PHE:O	7:B:308:HIS:C	2.50	0.47
7:C:103:LYS:O	7:C:106:ALA:N	2.47	0.47
6:F:17:DG:OP2	7:B:17:TYR:OH	2.31	0.47
7:A:15:ASN:ND2	7:A:52:ASN:OD1	2.47	0.47
7:A:211:GLN:O	7:A:311:ARG:HD2	2.15	0.47
7:A:283:GLY:O	7:A:287:ARG:HB2	2.14	0.47
7:B:27:ARG:CD	7:B:34:GLU:CD	2.77	0.47
7:B:309:GLU:HA	7:B:312:SER:OG	2.13	0.47
7:C:16:LEU:HD22	7:C:48:ALA:HB2	1.96	0.47
6:F:17:DG:C8	6:F:18:DT:C7	2.97	0.47
6:H:6:DT:H2"	6:H:7:DT:C5'	2.19	0.47
7:A:121:THR:O	7:A:124:ILE:HB	2.14	0.47
7:B:285:VAL:HG12	7:B:307:PHE:CD2	2.49	0.47
6:H:10:DA:N6	7:C:19:ARG:HH21	2.12	0.47
6:H:17:DG:OP2	7:D:15:ASN:HA	2.14	0.47
7:A:14:PRO:O	7:A:15:ASN:CG	2.52	0.47
7:D:15:ASN:HD21	7:D:52:ASN:HD21	1.62	0.47
2:J:23:DC:H5"	7:A:306:THR:OG1	2.15	0.47
3:K:20:DA:C2	3:K:21:DA:C4	3.02	0.47
6:F:6:DT:OP2	7:A:27:ARG:NH1	2.47	0.47
6:F:7:DT:H5'	6:F:7:DT:C6	2.44	0.47
6:F:20:DA:C2	6:F:21:DC:C2	3.02	0.47
7:B:61:HIS:CE1	7:B:62:LYS:O	2.67	0.47
7:B:103:LYS:HG2	7:B:103:LYS:H	1.25	0.47
7:B:351:ASP:OD1	7:B:352:LYS:N	2.47	0.47
7:C:72:ASN:ND2	7:C:72:ASN:N	2.56	0.47
6:F:11:DC:C4	6:F:12:DT:H73	2.49	0.47
7:A:67:ARG:HH22	7:D:36:GLY:N	2.13	0.47
7:A:116:LEU:O	7:A:119:ILE:CG1	2.62	0.47
7:B:77:HIS:N	7:B:80:LEU:HD12	2.30	0.47
7:B:116:LEU:HA	7:B:119:ILE:HD12	1.97	0.47
7:B:229:LEU:O	7:B:241:ALA:HA	2.15	0.47
7:B:331:LEU:HB3	7:B:333:HIS:HD2	1.79	0.47
7:D:49:ILE:O	7:D:50:GLN:C	2.53	0.47
1:I:2:DA:H2"	1:I:3:DC:OP2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:8:DC:H2'	3:K:9:DT:C6	2.49	0.47
5:E:7:DC:H2"	5:E:8:DA:C8	2.50	0.47
6:F:10:DA:H61	7:A:19:ARG:HH21	1.38	0.47
6:F:17:DG:P	7:B:17:TYR:HE2	2.38	0.47
6:H:1:DG:H2"	6:H:2:DG:C8	2.49	0.47
7:A:13:PRO:O	7:A:16:LEU:HB3	2.15	0.47
7:A:16:LEU:O	7:A:17:TYR:HD2	1.98	0.47
7:B:43:ILE:HD12	7:B:46:THR:OG1	2.15	0.47
2:J:11:DT:C4'	2:J:12:DA:OP1	2.62	0.47
7:A:26:TYR:CZ	7:A:51:ALA:CB	2.98	0.47
7:A:61:HIS:C	7:A:61:HIS:CD2	2.88	0.47
7:A:81:ASP:O	7:A:84:GLU:HB2	2.15	0.47
7:A:239:LYS:HD2	7:D:349:GLU:HA	1.95	0.47
7:C:105:LYS:O	7:C:106:ALA:C	2.53	0.47
7:D:34:GLU:O	7:D:35:PHE:CD2	2.68	0.47
5:G:6:DT:C2	5:G:7:DC:C6	3.03	0.47
7:A:77:HIS:CE1	7:A:108:ARG:HG3	2.50	0.47
7:C:283:GLY:O	7:C:287:ARG:HB2	2.14	0.47
1:I:14:DA:H8	1:I:14:DA:H5'	1.80	0.46
2:J:2:DG:H4'	7:B:276:ARG:HH22	1.78	0.46
5:G:17:DC:H2"	5:G:18:DA:C8	2.50	0.46
6:H:14:DA:H2'	6:H:15:DT:H72	1.96	0.46
7:A:101:MSE:O	7:A:104:ILE:HB	2.15	0.46
7:C:310:LEU:HD23	7:C:310:LEU:N	2.30	0.46
1:I:12:DT:C5'	7:A:235:LYS:HZ3	2.28	0.46
5:E:3:DA:H2"	5:E:4:DG:O5'	2.14	0.46
5:G:11:DA:H2"	5:G:12:DT:O5'	2.14	0.46
7:A:152:ARG:O	7:A:155:ILE:N	2.48	0.46
7:C:60:LYS:HB2	7:C:60:LYS:HZ3	1.78	0.46
7:D:104:ILE:O	7:D:107:ILE:N	2.48	0.46
5:G:16:DT:O4	7:C:19:ARG:NH2	2.48	0.46
7:B:82:ARG:O	7:B:86:ILE:HG13	2.15	0.46
7:C:10:ARG:HB3	7:C:12:LEU:CD1	2.45	0.46
7:C:160:ILE:HG23	7:C:161:THR:H	1.76	0.46
7:C:186:LEU:HD11	7:C:251:LEU:HD23	1.96	0.46
7:D:75:THR:CG2	7:D:78:SER:HB2	2.36	0.46
7:D:151:PHE:O	7:D:154:ALA:N	2.49	0.46
7:D:165:VAL:O	7:D:168:THR:CG2	2.27	0.46
5:E:11:DA:C4	5:E:12:DT:C5	3.04	0.46
5:G:7:DC:C2'	5:G:8:DA:C8	2.89	0.46
7:A:92:ILE:CG2	7:A:96:THR:HB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:285:VAL:HG12	7:A:286:SER:N	2.31	0.46
7:A:307:PHE:C	7:A:307:PHE:HD1	2.16	0.46
7:B:105:LYS:O	7:B:108:ARG:HB2	2.16	0.46
7:B:313:LEU:HD13	7:B:316:ARG:NH1	2.31	0.46
7:C:54:GLU:CG	7:C:55:LEU:N	2.78	0.46
7:C:83:TYR:O	7:C:84:GLU:C	2.54	0.46
7:C:138:ALA:O	7:C:141:LYS:HB2	2.15	0.46
3:K:11:DT:C2	3:K:12:DA:C8	3.03	0.46
7:B:116:LEU:HB3	7:B:160:ILE:HG21	1.97	0.46
7:B:307:PHE:CD1	7:B:307:PHE:C	2.88	0.46
7:C:163:ASN:OD1	7:C:163:ASN:C	2.53	0.46
7:C:212:ARG:CB	7:C:215:ASP:OD2	2.62	0.46
2:J:24:DA:C2	2:J:25:DG:C5	3.04	0.46
3:K:8:DC:C2'	3:K:9:DT:H71	2.42	0.46
4:L:16:DA:C2'	4:L:17:DA:H5"	2.45	0.46
5:G:2:DC:C2'	5:G:3:DA:N7	2.72	0.46
7:A:16:LEU:HG	7:A:17:TYR:N	2.31	0.46
7:B:100:TYR:O	7:B:103:LYS:N	2.48	0.46
7:D:17:TYR:CD1	7:D:27:ARG:HB2	2.51	0.46
6:F:2:DG:C2'	6:F:3:DT:C7	2.86	0.46
7:B:103:LYS:O	7:B:106:ALA:N	2.48	0.46
7:B:199:LEU:O	7:B:203:MSE:CG	2.63	0.46
7:A:147:LEU:HD12	7:A:147:LEU:O	2.16	0.46
7:A:338:MSE:O	7:A:342:PHE:HB2	2.16	0.46
7:B:306:THR:O	7:B:309:GLU:CB	2.47	0.46
7:B:350:TRP:HZ3	7:C:239:LYS:HB3	1.72	0.46
7:D:34:GLU:C	7:D:35:PHE:CG	2.88	0.46
5:E:12:DT:C2'	5:E:13:DC:H6	2.28	0.46
7:A:137:ALA:O	7:A:138:ALA:C	2.54	0.46
7:A:313:LEU:HA	7:A:316:ARG:HH21	1.80	0.46
7:B:211:GLN:NE2	7:B:330:LEU:O	2.42	0.46
7:D:107:ILE:O	7:D:108:ARG:C	2.55	0.46
5:G:6:DT:C2	5:G:7:DC:C5	3.04	0.46
7:A:67:ARG:NH2	7:D:36:GLY:N	2.63	0.46
7:A:79:TRP:O	7:A:83:TYR:N	2.42	0.46
7:B:215:ASP:O	7:B:218:GLU:HB2	2.16	0.46
7:C:306:THR:O	7:C:309:GLU:N	2.47	0.46
7:D:163:ASN:OD1	7:D:165:VAL:N	2.49	0.46
5:E:1:DA:H1'	5:E:2:DC:O4'	2.16	0.45
5:G:11:DA:C4	5:G:12:DT:C5	3.04	0.45
7:A:92:ILE:HG23	7:A:96:THR:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:76:LEU:CG	7:C:80:LEU:HD11	2.42	0.45
7:C:99:ASN:O	7:C:103:LYS:HG2	2.16	0.45
3:K:4:DC:H2"	3:K:5:DC:OP2	2.17	0.45
7:B:15:ASN:HB2	7:B:26:TYR:CE1	2.51	0.45
7:B:120:THR:HG22	7:B:121:THR:C	2.32	0.45
7:B:125:ALA:O	7:B:126:ALA:C	2.55	0.45
7:B:189:TYR:O	7:B:192:ALA:HB3	2.15	0.45
7:C:72:ASN:H	7:C:72:ASN:HD22	1.63	0.45
7:C:280:LEU:HD23	7:C:280:LEU:HA	1.49	0.45
7:D:121:THR:O	7:D:124:ILE:HB	2.16	0.45
7:D:129:ASN:O	7:D:132:ILE:HB	2.17	0.45
1:I:10:DT:C2	1:I:11:DT:C5	3.04	0.45
5:E:11:DA:C4	5:E:12:DT:C4	3.04	0.45
7:A:82:ARG:O	7:A:83:TYR:C	2.53	0.45
7:A:274:SER:N	7:A:280:LEU:HD11	2.31	0.45
7:B:11:ASP:O	7:B:13:PRO:HD3	2.17	0.45
7:D:62:LYS:O	7:D:65:THR:N	2.49	0.45
7:D:121:THR:CA	7:D:124:ILE:HD12	2.47	0.45
1:I:21:DA:N6	7:D:99:ASN:ND2	2.63	0.45
2:J:20:DA:H8	7:A:96:THR:HG23	1.81	0.45
4:L:16:DA:H2'	4:L:17:DA:H5"	1.97	0.45
5:E:17:DC:H6	5:E:17:DC:H2'	1.49	0.45
7:A:104:ILE:CG2	7:A:105:LYS:N	2.70	0.45
7:A:221:TRP:NE1	7:A:271:ILE:HA	2.32	0.45
7:B:66:ALA:C	7:B:68:ILE:H	2.18	0.45
7:D:290:MSE:HG3	7:D:293:ARG:HH21	1.81	0.45
3:K:20:DA:C4	3:K:21:DA:C8	3.05	0.45
4:L:20:DA:O3'	7:C:235:LYS:HG3	2.16	0.45
7:C:13:PRO:HA	7:C:14:PRO:HD3	1.78	0.45
1:I:12:DT:C5'	7:A:235:LYS:NZ	2.79	0.45
1:I:21:DA:H2'	1:I:22:DG:C8	2.52	0.45
7:C:111:LEU:CD2	7:C:112:PRO:HD2	2.35	0.45
4:L:5:DC:H2"	4:L:6:DA:H8	1.81	0.45
5:G:19:DA:H2"	5:G:20:DA:H8	1.81	0.45
5:G:19:DA:C5	5:G:20:DA:N7	2.85	0.45
7:A:17:TYR:CD2	7:A:17:TYR:N	2.79	0.45
7:A:50:GLN:HE22	7:A:61:HIS:CB	2.30	0.45
7:C:103:LYS:O	7:C:106:ALA:CB	2.63	0.45
7:D:100:TYR:C	7:D:103:LYS:HG2	2.37	0.45
3:K:5:DC:H2"	3:K:6:DA:OP2	2.16	0.45
7:A:127:MSE:HE3	7:A:128:LEU:CA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:54:GLU:OE2	7:B:54:GLU:CA	2.56	0.45
7:B:60:LYS:HE3	7:D:46:THR:HG22	1.97	0.45
7:B:79:TRP:CZ2	7:B:154:ALA:HB2	2.52	0.45
7:B:83:TYR:O	7:B:84:GLU:C	2.53	0.45
7:C:186:LEU:HD11	7:C:251:LEU:HD22	1.92	0.45
5:G:4:DG:C4	5:G:5:DG:C8	3.05	0.45
7:A:124:ILE:O	7:A:127:MSE:HE2	2.16	0.45
7:A:138:ALA:O	7:A:139:SER:C	2.54	0.45
7:B:47:GLU:OE2	7:C:64:LEU:HB2	2.16	0.45
7:C:49:ILE:HG12	7:C:49:ILE:H	1.26	0.45
7:A:139:SER:O	7:A:140:ALA:C	2.56	0.44
7:A:355:ILE:HG22	7:A:355:ILE:O	2.17	0.44
7:C:16:LEU:N	7:C:16:LEU:HD12	2.31	0.44
7:C:97:LEU:HD22	7:C:98:ILE:CD1	2.48	0.44
7:D:75:THR:HA	7:D:115:PRO:HA	1.99	0.44
5:E:21:DA:N7	5:E:22:DT:C7	2.80	0.44
7:A:9:ARG:HB3	7:A:10:ARG:HG3	1.99	0.44
7:A:14:PRO:O	7:A:15:ASN:CB	2.64	0.44
7:B:12:LEU:HA	7:B:13:PRO:HD2	1.71	0.44
7:B:77:HIS:HA	7:B:80:LEU:HD13	1.96	0.44
7:B:138:ALA:O	7:B:141:LYS:HB2	2.17	0.44
7:D:163:ASN:OD1	7:D:165:VAL:HB	2.16	0.44
1:I:5:DC:C1'	1:I:6:DT:H5'	2.33	0.44
6:H:10:DA:H61	7:C:19:ARG:HH21	1.66	0.44
7:C:92:ILE:CG2	7:C:96:THR:CB	2.92	0.44
7:C:242:ILE:CG2	7:C:330:LEU:HD11	2.44	0.44
2:J:20:DA:C8	7:A:96:THR:HG23	2.53	0.44
6:F:12:DT:H1'	6:F:13:DG:C8	2.52	0.44
7:B:100:TYR:O	7:B:103:LYS:CG	2.66	0.44
7:C:10:ARG:HB3	7:C:12:LEU:HD12	1.98	0.44
7:C:18:ILE:HG12	7:C:19:ARG:H	1.81	0.44
7:D:37:LEU:N	7:D:37:LEU:CD2	2.80	0.44
2:J:7:DA:C2	2:J:8:DG:C4	3.05	0.44
2:J:8:DG:H2'	2:J:9:DT:C6	2.52	0.44
5:E:21:DA:C8	5:E:22:DT:C7	2.99	0.44
7:A:131:TYR:N	7:A:131:TYR:CD1	2.86	0.44
7:A:212:ARG:NH1	7:A:233:GLN:OE1	2.50	0.44
7:C:345:ASP:OD1	7:C:348:ARG:HB2	2.18	0.44
7:D:151:PHE:O	7:D:152:ARG:C	2.53	0.44
1:I:7:DG:C4	1:I:8:DC:C5	3.05	0.44
2:J:10:DT:C2	2:J:11:DT:C5	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:165:VAL:HG12	7:A:166:ALA:CA	2.46	0.44
7:B:82:ARG:O	7:B:83:TYR:C	2.55	0.44
7:D:50:GLN:NE2	7:D:53:ILE:HD11	2.33	0.44
6:F:18:DT:OP1	7:B:10:ARG:NH2	2.51	0.44
7:B:100:TYR:O	7:B:103:LYS:HG2	2.17	0.44
7:B:151:PHE:O	7:B:154:ALA:N	2.51	0.44
7:C:10:ARG:HB2	7:C:12:LEU:HD13	1.99	0.44
7:D:137:ALA:O	7:D:138:ALA:C	2.54	0.44
7:D:243:PRO:HG2	7:D:246:LEU:CD1	2.47	0.44
2:J:26:DA:C2'	2:J:27:DG:C8	3.01	0.44
3:K:19:DA:C6	3:K:20:DA:C6	3.06	0.44
6:H:13:DG:N3	6:H:14:DA:C4	2.86	0.44
7:A:216:LEU:HD23	7:A:216:LEU:C	2.38	0.44
7:B:144:ARG:NH2	7:B:168:THR:O	2.51	0.44
7:C:121:THR:O	7:C:124:ILE:HB	2.17	0.44
7:C:331:LEU:HD23	7:C:333:HIS:HD2	1.83	0.44
7:D:116:LEU:HA	7:D:116:LEU:HD23	1.67	0.44
2:J:27:DG:C2	2:J:28:DT:C2	3.06	0.43
7:B:25:CYS:HG	7:B:35:PHE:C	2.21	0.43
7:B:155:ILE:HA	7:B:160:ILE:HD13	2.00	0.43
7:C:123:GLU:O	7:C:126:ALA:HB3	2.17	0.43
7:C:205:LEU:HD23	7:C:216:LEU:HD11	1.99	0.43
1:I:1:DA:C4	1:I:2:DA:N7	2.86	0.43
1:I:14:DA:C8	1:I:14:DA:H5'	2.52	0.43
7:A:10:ARG:HH21	7:A:12:LEU:CB	2.31	0.43
7:A:64:LEU:HD12	7:A:64:LEU:HA	1.61	0.43
7:A:120:THR:N	7:A:123:GLU:OE1	2.34	0.43
7:A:314:SER:O	7:A:318:TYR:CD2	2.71	0.43
7:B:53:ILE:O	7:B:57:SER:N	2.51	0.43
7:B:278:GLU:HB3	7:B:279:PRO:CD	2.48	0.43
7:C:104:ILE:O	7:C:105:LYS:C	2.56	0.43
7:C:284:THR:HA	7:C:287:ARG:HB2	2.00	0.43
7:D:49:ILE:O	7:D:52:ASN:N	2.51	0.43
1:I:1:DA:H2"	1:I:2:DA:O5'	2.18	0.43
6:F:12:DT:H2"	6:F:13:DG:OP2	2.18	0.43
7:A:16:LEU:HD23	7:A:16:LEU:C	2.39	0.43
7:A:111:LEU:CD2	7:A:112:PRO:HD2	2.40	0.43
7:B:47:GLU:O	7:B:50:GLN:HB2	2.19	0.43
7:B:155:ILE:N	7:B:160:ILE:HD11	2.32	0.43
7:B:199:LEU:HD12	7:B:199:LEU:N	2.32	0.43
7:C:64:LEU:HA	7:C:67:ARG:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:208:VAL:HG13	7:C:209:THR:HG22	2.00	0.43
7:D:13:PRO:HG3	7:D:45:ILE:HG13	1.99	0.43
7:D:27:ARG:HD2	7:D:34:GLU:OE1	2.18	0.43
4:L:7:DA:C6	4:L:8:DC:N3	2.86	0.43
5:E:19:DA:C6	5:E:20:DA:C6	3.06	0.43
6:F:6:DT:C2'	6:F:7:DT:C5'	2.83	0.43
7:A:256:LYS:HD2	7:A:256:LYS:HA	1.73	0.43
7:B:61:HIS:CE1	7:B:63:PRO:CA	3.01	0.43
7:D:104:ILE:O	7:D:105:LYS:C	2.56	0.43
1:I:12:DT:H5"	7:A:235:LYS:HZ3	1.82	0.43
2:J:10:DT:H4'	7:B:177:ARG:NH1	2.33	0.43
6:F:17:DG:C8	6:F:18:DT:H71	2.53	0.43
7:B:98:ILE:O	7:B:99:ASN:C	2.57	0.43
7:C:74:VAL:HG21	7:C:159:HIS:CD2	2.53	0.43
7:C:103:LYS:HG2	7:C:103:LYS:H	1.50	0.43
7:C:308:HIS:O	7:C:310:LEU:N	2.52	0.43
7:D:18:ILE:HG13	7:D:24:TYR:CD2	2.53	0.43
7:D:71:ASP:OD1	7:D:71:ASP:N	2.52	0.43
3:K:8:DC:C2	3:K:9:DT:C7	3.01	0.43
7:A:67:ARG:NH2	7:D:36:GLY:H	2.17	0.43
7:B:205:LEU:C	7:B:208:VAL:HG12	2.36	0.43
7:C:45:ILE:CG2	7:C:46:THR:N	2.74	0.43
7:D:128:LEU:HD21	7:D:144:ARG:HB2	2.00	0.43
7:D:180:LEU:HD22	7:D:309:GLU:HB3	2.01	0.43
7:D:260:ASP:HA	7:D:263:LYS:HG2	2.00	0.43
7:D:293:ARG:HH12	7:D:306:THR:HG22	1.83	0.43
5:G:3:DA:H2"	5:G:4:DG:O5'	2.18	0.43
7:A:141:LYS:O	7:A:144:ARG:HB3	2.17	0.43
7:B:13:PRO:HA	7:B:14:PRO:HD2	1.53	0.43
7:D:83:TYR:CE2	7:D:87:LEU:HD11	2.54	0.43
7:D:145:SER:O	7:D:148:SER:HB3	2.18	0.43
7:D:247:HIS:HB3	7:D:254:SER:HA	2.01	0.43
6:H:19:DG:H5"	7:D:20:ASN:ND2	2.34	0.43
7:A:12:LEU:HA	7:A:13:PRO:HD2	1.88	0.43
7:A:306:THR:O	7:A:309:GLU:N	2.49	0.43
7:B:47:GLU:OE1	7:C:61:HIS:CE1	2.69	0.43
7:B:124:ILE:O	7:B:125:ALA:C	2.55	0.43
7:B:125:ALA:C	7:B:129:ASN:HD22	2.22	0.43
7:B:209:THR:O	7:B:211:GLN:HG2	2.19	0.43
7:C:16:LEU:C	7:C:17:TYR:CD2	2.92	0.43
7:D:306:THR:O	7:D:309:GLU:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:76:LEU:HD11	7:A:119:ILE:HD11	2.01	0.43
7:A:77:HIS:ND1	7:A:108:ARG:HG3	2.34	0.43
7:C:84:GLU:O	7:C:87:LEU:HB2	2.19	0.43
5:E:11:DA:N9	5:E:12:DT:C7	2.82	0.43
6:F:13:DG:C2	6:F:14:DA:C4	3.07	0.43
7:A:107:ILE:O	7:A:108:ARG:C	2.55	0.43
7:D:26:TYR:CD1	7:D:27:ARG:N	2.87	0.43
7:D:185:TYR:CD1	7:D:185:TYR:C	2.92	0.43
7:C:45:ILE:O	7:C:49:ILE:CG1	2.64	0.42
7:C:59:HIS:C	7:C:60:LYS:HD3	2.39	0.42
7:C:80:LEU:O	7:C:83:TYR:HB3	2.19	0.42
5:G:14:DA:H2"	5:G:15:DG:O5'	2.20	0.42
7:A:79:TRP:CZ2	7:A:154:ALA:HA	2.54	0.42
7:D:313:LEU:CA	7:D:316:ARG:NH2	2.81	0.42
5:E:4:DG:N1	5:E:5:DG:C4	2.87	0.42
6:H:11:DC:H2"	6:H:12:DT:O5'	2.16	0.42
7:A:39:ARG:HD2	7:A:39:ARG:HA	1.47	0.42
7:A:76:LEU:HD13	7:A:114:ALA:O	2.19	0.42
7:B:56:PHE:HD2	7:B:56:PHE:HA	1.34	0.42
7:B:100:TYR:O	7:B:103:LYS:CB	2.66	0.42
7:C:51:ALA:O	7:C:54:GLU:CG	2.66	0.42
7:C:185:TYR:CD1	7:C:186:LEU:HD12	2.49	0.42
3:K:18:DT:H6	3:K:18:DT:H5'	1.84	0.42
4:L:8:DC:O5'	7:D:136:LYS:HD3	2.19	0.42
6:F:22:DC:H2"	6:F:23:DT:O4'	2.19	0.42
7:B:100:TYR:O	7:B:103:LYS:HB2	2.19	0.42
7:B:180:LEU:O	7:B:313:LEU:HD13	2.19	0.42
7:B:212:ARG:O	7:B:216:LEU:HG	2.18	0.42
7:C:139:SER:O	7:C:140:ALA:C	2.57	0.42
7:D:168:THR:OG1	7:D:169:ARG:N	2.52	0.42
7:D:311:ARG:NH2	7:D:331:LEU:HB3	2.35	0.42
5:G:5:DG:N3	5:G:6:DT:C6	2.88	0.42
7:A:262:CYS:O	7:A:266:LEU:HB2	2.20	0.42
7:B:63:PRO:C	7:B:65:THR:H	2.23	0.42
7:B:198:TRP:HA	7:B:201:LEU:HD12	2.02	0.42
7:C:42:ARG:O	7:C:45:ILE:HB	2.19	0.42
7:D:74:VAL:O	7:D:115:PRO:HA	2.19	0.42
7:D:228:TYR:HD2	7:D:243:PRO:HA	1.85	0.42
1:I:17:DA:H5'	1:I:17:DA:C8	2.51	0.42
1:I:23:DT:H2"	1:I:24:DT:H5"	2.01	0.42
4:L:24:DT:H2"	4:L:25:DG:OP2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:8:DT:P	7:A:10:ARG:HH22	2.42	0.42
7:A:66:ALA:O	7:A:68:ILE:N	2.53	0.42
7:A:77:HIS:CD2	7:A:113:ASP:HA	2.54	0.42
7:B:15:ASN:ND2	7:B:26:TYR:OH	2.50	0.42
7:B:107:ILE:HD13	7:B:147:LEU:HD13	2.02	0.42
7:B:127:MSE:HE3	7:B:128:LEU:HD12	2.02	0.42
7:C:120:THR:O	7:C:123:GLU:N	2.52	0.42
7:C:205:LEU:HB3	7:C:216:LEU:HD11	2.02	0.42
7:D:12:LEU:HA	7:D:13:PRO:HD2	1.85	0.42
7:D:141:LYS:C	7:D:141:LYS:HD3	2.36	0.42
1:I:19:DA:H2"	1:I:20:DA:O4'	2.19	0.42
2:J:4:DT:H1'	2:J:5:DC:H5'	2.01	0.42
2:J:16:DT:H2"	2:J:17:DA:C5'	2.45	0.42
3:K:12:DA:OP2	7:C:342:PHE:CZ	2.73	0.42
5:E:5:DG:C2'	5:E:6:DT:H6	2.33	0.42
6:H:2:DG:H2'	6:H:2:DG:P	2.59	0.42
6:H:9:DG:C5	6:H:10:DA:N6	2.88	0.42
7:C:68:ILE:O	7:C:69:ASN:C	2.58	0.42
7:D:26:TYR:HD1	7:D:26:TYR:HA	1.59	0.42
6:H:8:DT:H2"	6:H:9:DG:N7	2.33	0.42
7:A:11:ASP:O	7:A:13:PRO:CD	2.67	0.42
7:A:121:THR:O	7:A:124:ILE:N	2.53	0.42
7:B:136:LYS:O	7:B:137:ALA:C	2.58	0.42
7:C:94:GLN:O	7:C:97:LEU:HB3	2.20	0.42
7:D:293:ARG:HD3	7:D:305:PRO:O	2.20	0.42
4:L:25:DG:H2"	4:L:26:DG:O4'	2.20	0.42
5:E:12:DT:H2'	5:E:13:DC:C6	2.54	0.42
6:F:19:DG:C2'	6:F:20:DA:H8	2.33	0.42
5:G:14:DA:C8	7:C:23:TYR:CE1	2.99	0.42
7:A:287:ARG:O	7:A:290:MSE:HB3	2.20	0.42
7:B:204:GLU:O	7:B:205:LEU:C	2.58	0.42
7:C:306:THR:HG1	7:C:307:PHE:N	2.18	0.42
7:D:15:ASN:HA	7:D:17:TYR:HH	1.85	0.42
7:D:53:ILE:HG13	7:D:53:ILE:H	1.57	0.42
7:D:211:GLN:C	7:D:311:ARG:HH11	2.23	0.42
5:E:12:DT:C1'	5:E:13:DC:H5"	2.47	0.42
7:A:144:ARG:HG2	7:A:145:SER:N	2.35	0.42
7:A:147:LEU:HD11	7:A:151:PHE:CE1	2.55	0.42
7:C:12:LEU:HA	7:C:13:PRO:HD2	1.89	0.42
7:D:100:TYR:HA	7:D:103:LYS:HG2	2.02	0.42
4:L:8:DC:H2'	4:L:9:DT:C7	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:13:DG:H1'	6:F:14:DA:O4'	2.20	0.41
6:H:4:DA:H2"	6:H:5:DT:O5'	2.20	0.41
7:A:65:THR:O	7:A:66:ALA:C	2.58	0.41
7:C:25:CYS:HB3	7:C:35:PHE:O	2.19	0.41
7:C:243:PRO:C	7:C:245:ALA:H	2.23	0.41
2:J:27:DG:H2"	2:J:28:DT:OP2	2.19	0.41
3:K:16:DT:O2	3:K:17:DA:C8	2.73	0.41
5:G:3:DA:C2'	5:G:4:DG:C8	3.04	0.41
7:A:266:LEU:HD13	7:A:273:ALA:H	1.85	0.41
7:B:185:TYR:CD1	7:B:185:TYR:C	2.92	0.41
7:B:211:GLN:C	7:B:311:ARG:HD2	2.40	0.41
7:C:61:HIS:CD2	7:C:61:HIS:C	2.93	0.41
7:D:23:TYR:HD2	7:D:23:TYR:C	2.11	0.41
7:D:155:ILE:HG13	7:D:160:ILE:CD1	2.50	0.41
4:L:16:DA:C2'	4:L:17:DA:C5'	2.98	0.41
6:H:17:DG:C5	6:H:18:DT:C4	3.08	0.41
7:A:95:LYS:O	7:A:96:THR:C	2.58	0.41
7:A:146:THR:O	7:A:149:ASP:N	2.53	0.41
7:A:172:LYS:HD2	7:A:173:SER:H	1.85	0.41
7:B:79:TRP:CZ2	7:B:154:ALA:N	2.87	0.41
7:B:83:TYR:HA	7:B:86:ILE:HD12	2.03	0.41
7:B:120:THR:CG2	7:B:122:LYS:N	2.54	0.41
7:B:127:MSE:HE3	7:B:128:LEU:CA	2.50	0.41
7:C:97:LEU:CD2	7:C:98:ILE:HG13	2.50	0.41
7:C:203:MSE:HE3	7:C:203:MSE:HB3	1.90	0.41
6:F:17:DG:C4	6:F:18:DT:C5	3.08	0.41
7:B:104:ILE:H	7:B:104:ILE:HG13	1.44	0.41
7:B:165:VAL:H	7:B:165:VAL:HG23	1.16	0.41
7:C:79:TRP:CZ2	7:C:154:ALA:N	2.88	0.41
7:C:132:ILE:HD11	7:C:171:ALA:HB2	2.01	0.41
7:D:246:LEU:HD21	7:D:326:PHE:HZ	1.86	0.41
4:L:23:DC:H5"	7:C:306:THR:OG1	2.21	0.41
6:F:11:DC:C5	6:F:12:DT:C7	3.02	0.41
7:A:220:LYS:O	7:A:223:ASP:HB2	2.20	0.41
7:D:35:PHE:O	7:D:37:LEU:HD23	2.20	0.41
7:D:41:ARG:HG2	7:D:45:ILE:HD13	2.02	0.41
7:D:139:SER:O	7:D:140:ALA:C	2.57	0.41
7:D:305:PRO:HB3	7:D:309:GLU:HG2	2.00	0.41
5:E:4:DG:C6	5:E:5:DG:N7	2.89	0.41
6:F:17:DG:C5	6:F:18:DT:C4	3.08	0.41
6:F:19:DG:C2	6:F:20:DA:C5	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:17:DG:H5'	7:D:17:TYR:HE2	1.86	0.41
7:C:82:ARG:O	7:C:86:ILE:HD12	2.19	0.41
7:C:165:VAL:HG13	7:C:168:THR:HG21	2.03	0.41
7:C:308:HIS:O	7:C:311:ARG:N	2.46	0.41
7:D:125:ALA:O	7:D:128:LEU:N	2.54	0.41
7:D:307:PHE:CD1	7:D:307:PHE:C	2.94	0.41
7:A:84:GLU:O	7:A:87:LEU:HB2	2.20	0.41
7:A:98:ILE:O	7:A:99:ASN:C	2.59	0.41
7:B:23:TYR:CE2	7:B:24:TYR:O	2.73	0.41
7:C:39:ARG:HD3	7:C:39:ARG:HA	1.80	0.41
7:C:203:MSE:O	7:C:206:ALA:HB3	2.21	0.41
7:D:75:THR:HG23	7:D:78:SER:CB	2.39	0.41
1:I:8:DC:C6	1:I:9:DT:H72	2.56	0.41
1:I:18:DC:H5'	1:I:18:DC:C6	2.55	0.41
5:G:20:DA:H1'	5:G:21:DA:O5'	2.20	0.41
7:A:65:THR:HG23	7:D:54:GLU:CD	2.41	0.41
7:A:94:GLN:O	7:A:98:ILE:CD1	2.65	0.41
7:A:168:THR:HG23	7:A:168:THR:O	2.19	0.41
7:A:314:SER:O	7:A:318:TYR:HD2	2.04	0.41
7:C:28:ASP:OD2	7:C:29:PRO:HD2	2.20	0.41
7:D:79:TRP:O	7:D:83:TYR:N	2.44	0.41
7:D:190:GLN:O	7:D:193:GLU:HG2	2.20	0.41
7:D:209:THR:HG22	7:D:255:MSE:HE3	2.03	0.41
7:D:243:PRO:HG2	7:D:246:LEU:HD11	2.03	0.41
1:I:11:DT:H1'	7:A:235:LYS:HZ3	1.85	0.41
5:E:11:DA:N3	5:E:12:DT:C4	2.89	0.41
5:E:12:DT:H2'	5:E:13:DC:H6	1.86	0.41
5:G:17:DC:H6	5:G:17:DC:H2'	1.66	0.41
7:A:97:LEU:O	7:A:100:TYR:HB2	2.20	0.41
7:A:127:MSE:HE3	7:A:128:LEU:N	2.36	0.41
7:A:131:TYR:N	7:A:131:TYR:HD1	2.19	0.41
7:A:149:ASP:O	7:A:150:ALA:C	2.58	0.41
7:A:243:PRO:C	7:A:245:ALA:H	2.21	0.41
7:A:259:LEU:O	7:A:262:CYS:HB2	2.21	0.41
7:A:278:GLU:HB3	7:A:279:PRO:HD2	2.03	0.41
7:A:313:LEU:HA	7:A:316:ARG:NH2	2.36	0.41
7:B:15:ASN:ND2	7:B:52:ASN:ND2	2.68	0.41
7:B:127:MSE:O	7:B:128:LEU:C	2.58	0.41
7:B:163:ASN:OD1	7:B:165:VAL:HG23	2.20	0.41
7:B:243:PRO:C	7:B:245:ALA:H	2.24	0.41
7:C:308:HIS:C	7:C:310:LEU:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:138:ALA:O	7:D:139:SER:C	2.58	0.41
5:G:12:DT:H2"	5:G:13:DC:C5'	2.45	0.41
7:A:92:ILE:HG22	7:A:93:LYS:N	2.33	0.41
7:A:101:MSE:HA	7:A:104:ILE:HD13	1.99	0.41
7:A:221:TRP:CZ3	7:A:263:LYS:HD2	2.56	0.41
7:B:53:ILE:HA	7:B:56:PHE:O	2.20	0.41
7:B:100:TYR:HD1	7:B:100:TYR:H	1.67	0.41
7:B:201:LEU:HD12	7:B:266:LEU:HD11	2.03	0.41
7:B:307:PHE:C	7:B:307:PHE:HD1	2.25	0.41
7:C:124:ILE:HG22	7:C:125:ALA:N	2.36	0.41
7:D:228:TYR:HE2	7:D:243:PRO:HB3	1.85	0.41
5:G:23:DA:N3	6:H:4:DA:C2	2.89	0.40
6:H:17:DG:C6	6:H:18:DT:C4	3.09	0.40
6:H:19:DG:C2'	6:H:20:DA:O5'	2.69	0.40
7:A:12:LEU:CD1	7:A:16:LEU:HD23	2.47	0.40
7:A:127:MSE:O	7:A:128:LEU:C	2.58	0.40
7:B:120:THR:CG2	7:B:122:LYS:HB3	2.49	0.40
7:D:45:ILE:O	7:D:46:THR:C	2.58	0.40
7:D:74:VAL:HG13	7:D:75:THR:H	1.87	0.40
7:D:143:ILE:O	7:D:144:ARG:C	2.60	0.40
2:J:7:DA:C5	2:J:8:DG:N7	2.89	0.40
2:J:19:DA:H3'	7:A:96:THR:HG21	2.03	0.40
5:E:4:DG:H2"	5:E:5:DG:O5'	2.20	0.40
5:G:14:DA:H8	7:C:23:TYR:CD1	2.39	0.40
7:B:83:TYR:CD2	7:B:87:LEU:HD11	2.57	0.40
7:B:147:LEU:HD12	7:B:147:LEU:HA	1.85	0.40
7:B:205:LEU:HD12	7:B:205:LEU:HA	1.84	0.40
2:J:15:DT:C7	2:J:16:DT:H73	2.51	0.40
5:G:2:DC:C2'	5:G:3:DA:C8	3.03	0.40
7:A:74:VAL:O	7:A:75:THR:HB	2.22	0.40
7:C:95:LYS:O	7:C:96:THR:C	2.60	0.40
7:C:211:GLN:HA	7:C:311:ARG:HH11	1.85	0.40
7:A:75:THR:HA	7:A:114:ALA:O	2.21	0.40
7:A:147:LEU:C	7:A:147:LEU:HD12	2.42	0.40
7:B:163:ASN:OD1	7:B:165:VAL:N	2.55	0.40
7:C:110:GLY:O	7:C:111:LEU:HD23	2.22	0.40
7:C:144:ARG:NH2	7:C:168:THR:O	2.55	0.40
7:D:313:LEU:HD13	7:D:316:ARG:HH22	1.85	0.40
7:D:349:GLU:N	7:D:349:GLU:OE2	2.54	0.40
1:I:10:DT:N1	1:I:11:DT:H71	2.37	0.40
4:L:21:DA:OP2	7:C:93:LYS:HD3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:11:DA:C2'	5:E:12:DT:H71	2.51	0.40
6:H:14:DA:H2'	6:H:15:DT:C7	2.51	0.40
7:B:99:ASN:O	7:B:100:TYR:C	2.59	0.40
7:C:62:LYS:HA	7:C:63:PRO:HD2	1.95	0.40
7:C:229:LEU:HD23	7:C:242:ILE:HB	2.04	0.40
7:D:221:TRP:NE1	7:D:271:ILE:HG12	2.37	0.40

All (1) 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)
2:J:29:DT:OP2	5:E:1:DA:O5'[1_565]	1.99	0.21

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	A	347/356 (98%)	286 (82%)	45 (13%)	16 (5%)	2 24
7	B	332/356 (93%)	277 (83%)	42 (13%)	13 (4%)	3 26
7	C	347/356 (98%)	286 (82%)	44 (13%)	17 (5%)	2 23
7	D	332/356 (93%)	285 (86%)	33 (10%)	14 (4%)	3 25
All	All	1358/1424 (95%)	1134 (84%)	164 (12%)	60 (4%)	2 25

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	A	63	PRO
7	A	67	ARG
7	A	74	VAL
7	A	335	SER

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Mol	Chain	Res	Type
7	A	348	ARG
7	B	60	LYS
7	B	61	HIS
7	B	67	ARG
7	B	350	TRP
7	C	57	SER
7	C	58	GLY
7	C	70	SER
7	C	74	VAL
7	C	351	ASP
7	D	59	HIS
7	D	67	ARG
7	D	68	ILE
7	D	70	SER
7	A	58	GLY
7	A	104	ILE
7	A	267	GLY
7	B	68	ILE
7	B	104	ILE
7	B	121	THR
7	B	267	GLY
7	C	45	ILE
7	C	67	ARG
7	C	267	GLY
7	C	341	GLN
7	D	104	ILE
7	D	137	ALA
7	D	267	GLY
7	D	355	ILE
7	A	66	ALA
7	B	59	HIS
7	C	12	LEU
7	C	63	PRO
7	C	104	ILE
7	C	144	ARG
7	D	65	THR
7	D	71	ASP
7	D	121	THR
7	A	45	ILE
7	A	65	THR
7	A	137	ALA
7	A	144	ARG

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Mol	Chain	Res	Type
7	A	339	ALA
7	B	137	ALA
7	C	121	THR
7	C	137	ALA
7	D	144	ARG
7	A	351	ASP
7	B	144	ARG
7	C	66	ALA
7	D	64	LEU
7	A	59	HIS
7	C	65	THR
7	D	114	ALA
7	B	91	GLY
7	B	114	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	A	292/292 (100%)	220 (75%)	72 (25%)	0	4
7	B	273/292 (94%)	201 (74%)	72 (26%)	0	4
7	C	293/292 (100%)	226 (77%)	67 (23%)	1	5
7	D	273/292 (94%)	209 (77%)	64 (23%)	1	5
All	All	1131/1168 (97%)	856 (76%)	275 (24%)	0	5

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	A	10	ARG
7	A	11	ASP
7	A	17	TYR
7	A	19	ARG
7	A	21	ASN
7	A	23	TYR
7	A	25	CYS

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Mol	Chain	Res	Type
7	A	39	ARG
7	A	42	ARG
7	A	45	ILE
7	A	46	THR
7	A	49	ILE
7	A	50	GLN
7	A	54	GLU
7	A	55	LEU
7	A	57	SER
7	A	61	HIS
7	A	63	PRO
7	A	65	THR
7	A	67	ARG
7	A	68	ILE
7	A	70	SER
7	A	71	ASP
7	A	72	ASN
7	A	74	VAL
7	A	81	ASP
7	A	97	LEU
7	A	127	MSE
7	A	128	LEU
7	A	141	LYS
7	A	145	SER
7	A	146	THR
7	A	148	SER
7	A	161	THR
7	A	169	ARG
7	A	172	LYS
7	A	173	SER
7	A	181	THR
7	A	185	TYR
7	A	186	LEU
7	A	195	SER
7	A	200	ARG
7	A	212	ARG
7	A	213	VAL
7	A	218	GLU
7	A	231	VAL
7	A	232	GLU
7	A	247	HIS
7	A	249	ASP

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Mol	Chain	Res	Type
7	A	254	SER
7	A	258	THR
7	A	274	SER
7	A	275	THR
7	A	281	SER
7	A	284	THR
7	A	287	ARG
7	A	291	ARG
7	A	303	ASP
7	A	306	THR
7	A	307	PHE
7	A	309	GLU
7	A	314	SER
7	A	316	ARG
7	A	321	GLN
7	A	328	GLN
7	A	341	GLN
7	A	342	PHE
7	A	343	ARG
7	A	345	ASP
7	A	348	ARG
7	A	353	ILE
7	A	354	GLU
7	B	15	ASN
7	B	18	ILE
7	B	23	TYR
7	B	30	ARG
7	B	31	THR
7	B	40	ASP
7	B	41	ARG
7	B	43	ILE
7	B	49	ILE
7	B	54	GLU
7	B	56	PHE
7	B	57	SER
7	B	61	HIS
7	B	73	SER
7	B	75	THR
7	B	78	SER
7	B	89	SER
7	B	90	ARG
7	B	92	ILE

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Mol	Chain	Res	Type
7	B	93	LYS
7	B	108	ARG
7	B	116	LEU
7	B	117	GLU
7	B	118	ASP
7	B	122	LYS
7	B	127	MSE
7	B	128	LEU
7	B	139	SER
7	B	146	THR
7	B	160	ILE
7	B	161	THR
7	B	162	THR
7	B	164	HIS
7	B	176	ARG
7	B	181	THR
7	B	184	GLU
7	B	187	LYS
7	B	203	MSE
7	B	209	THR
7	B	212	ARG
7	B	213	VAL
7	B	215	ASP
7	B	220	LYS
7	B	231	VAL
7	B	232	GLU
7	B	235	LYS
7	B	247	HIS
7	B	249	ASP
7	B	255	MSE
7	B	263	LYS
7	B	264	GLU
7	B	276	ARG
7	B	282	SER
7	B	284	THR
7	B	286	SER
7	B	287	ARG
7	B	293	ARG
7	B	296	SER
7	B	299	SER
7	B	300	PHE
7	B	303	ASP

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Mol	Chain	Res	Type
7	B	306	THR
7	B	307	PHE
7	B	312	SER
7	B	316	ARG
7	B	321	GLN
7	B	324	ASP
7	B	331	LEU
7	B	335	SER
7	B	336	ASP
7	B	350	TRP
7	B	354	GLU
7	C	11	ASP
7	C	19	ARG
7	C	20	ASN
7	C	23	TYR
7	C	25	CYS
7	C	26	TYR
7	C	27	ARG
7	C	33	LYS
7	C	39	ARG
7	C	42	ARG
7	C	49	ILE
7	C	50	GLN
7	C	54	GLU
7	C	60	LYS
7	C	61	HIS
7	C	64	LEU
7	C	67	ARG
7	C	70	SER
7	C	71	ASP
7	C	72	ASN
7	C	82	ARG
7	C	89	SER
7	C	93	LYS
7	C	94	GLN
7	C	102	SER
7	C	108	ARG
7	C	109	ARG
7	C	127	MSE
7	C	136	LYS
7	C	139	SER
7	C	141	LYS

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Mol	Chain	Res	Type
7	C	144	ARG
7	C	152	ARG
7	C	161	THR
7	C	169	ARG
7	C	173	SER
7	C	194	SER
7	C	195	SER
7	C	203	MSE
7	C	209	THR
7	C	212	ARG
7	C	218	GLU
7	C	229	LEU
7	C	238	VAL
7	C	247	HIS
7	C	254	SER
7	C	269	GLU
7	C	270	THR
7	C	284	THR
7	C	291	ARG
7	C	293	ARG
7	C	296	SER
7	C	300	PHE
7	C	306	THR
7	C	311	ARG
7	C	312	SER
7	C	316	ARG
7	C	319	GLU
7	C	321	GLN
7	C	331	LEU
7	C	333	HIS
7	C	335	SER
7	C	337	THR
7	C	338	MSE
7	C	342	PHE
7	C	346	ARG
7	C	348	ARG
7	D	11	ASP
7	D	15	ASN
7	D	19	ARG
7	D	20	ASN
7	D	37	LEU
7	D	42	ARG

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Mol	Chain	Res	Type
7	D	43	ILE
7	D	45	ILE
7	D	46	THR
7	D	47	GLU
7	D	53	ILE
7	D	56	PHE
7	D	59	HIS
7	D	61	HIS
7	D	72	ASN
7	D	73	SER
7	D	76	LEU
7	D	80	LEU
7	D	90	ARG
7	D	93	LYS
7	D	102	SER
7	D	117	GLU
7	D	120	THR
7	D	127	MSE
7	D	128	LEU
7	D	139	SER
7	D	141	LYS
7	D	146	THR
7	D	161	THR
7	D	169	ARG
7	D	179	ARG
7	D	181	THR
7	D	187	LYS
7	D	195	SER
7	D	208	VAL
7	D	216	LEU
7	D	217	CYS
7	D	220	LYS
7	D	231	VAL
7	D	235	LYS
7	D	247	HIS
7	D	248	ILE
7	D	263	LYS
7	D	264	GLU
7	D	270	THR
7	D	271	ILE
7	D	274	SER
7	D	276	ARG

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Mol	Chain	Res	Type
7	D	284	THR
7	D	285	VAL
7	D	293	ARG
7	D	294	LYS
7	D	296	SER
7	D	306	THR
7	D	309	GLU
7	D	312	SER
7	D	324	ASP
7	D	325	LYS
7	D	329	HIS
7	D	331	LEU
7	D	349	GLU
7	D	350	TRP
7	D	351	ASP
7	D	356	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
7	A	15	ASN
7	A	20	ASN
7	A	50	GLN
7	A	72	ASN
7	A	99	ASN
7	A	308	HIS
7	B	15	ASN
7	B	21	ASN
7	B	129	ASN
7	B	333	HIS
7	C	20	ASN
7	C	72	ASN
7	C	99	ASN
7	C	333	HIS
7	D	15	ASN
7	D	20	ASN
7	D	50	GLN
7	D	72	ASN
7	D	99	ASN
7	D	321	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides 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	I	29/29 (100%)	-0.57	0 100 100	108, 108, 108, 108	0
2	J	29/29 (100%)	-0.49	0 100 100	108, 108, 108, 108	0
3	K	29/29 (100%)	-0.31	1 (3%) 45 36	108, 108, 108, 108	0
4	L	29/29 (100%)	0.02	2 (6%) 16 13	108, 108, 108, 108	0
5	E	24/25 (96%)	-0.34	0 100 100	108, 108, 108, 108	0
5	G	24/25 (96%)	-0.62	0 100 100	108, 108, 108, 108	0
6	F	25/25 (100%)	-0.26	0 100 100	108, 108, 108, 108	0
6	H	25/25 (100%)	-0.64	0 100 100	108, 108, 108, 108	0
7	A	342/356 (96%)	-0.25	12 (3%) 44 35	108, 108, 108, 200	0
7	B	330/356 (92%)	-0.27	9 (2%) 54 45	108, 108, 108, 108	0
7	C	342/356 (96%)	-0.19	10 (2%) 51 41	108, 108, 108, 200	0
7	D	330/356 (92%)	-0.17	11 (3%) 46 37	103, 108, 108, 108	0
All	All	1558/1640 (95%)	-0.24	45 (2%) 51 41	103, 108, 108, 200	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	C	210	GLY	5.0
7	C	18	ILE	5.0
7	B	231	VAL	4.9
7	C	209	THR	4.8
7	C	17	TYR	4.1
7	C	332	GLY	3.9
7	B	355	ILE	3.8
7	D	280	LEU	3.7
7	B	232	GLU	3.5
7	A	8	GLU	3.4
3	K	1	DT	3.4

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Mol	Chain	Res	Type	RSRZ
7	C	19	ARG	3.3
7	A	330	LEU	3.2
7	B	352	LYS	3.1
7	D	279	PRO	3.1
7	D	25	CYS	3.1
7	B	18	ILE	2.9
7	B	240	ILE	2.9
7	D	34	GLU	2.8
7	A	231	VAL	2.7
7	D	352	LYS	2.6
7	D	274	SER	2.6
7	A	37	LEU	2.5
7	C	71	ASP	2.5
7	C	37	LEU	2.4
4	L	29	DA	2.4
7	A	17	TYR	2.4
7	B	34	GLU	2.4
7	C	20	ASN	2.4
7	C	211	GLN	2.4
7	D	330	LEU	2.4
7	A	241	ALA	2.3
7	D	180	LEU	2.3
7	D	18	ILE	2.3
7	D	275	THR	2.3
7	A	242	ILE	2.3
7	A	240	ILE	2.2
7	A	211	GLN	2.2
4	L	14	DT	2.2
7	D	237	GLY	2.2
7	A	19	ARG	2.1
7	B	211	GLN	2.1
7	A	18	ILE	2.1
7	B	20	ASN	2.0
7	A	332	GLY	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 monosaccharides 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.