



Full wwPDB X-ray Structure Validation Report i

Aug 20, 2023 – 04:24 AM EDT

PDB ID : 2H8R
Title : Hepatocyte Nuclear Factor 1b bound to DNA: MODY5 Gene Product
Authors : Lu, P.; Rha, G.B.; Chi, Y.I.
Deposited on : 2006-06-07
Resolution : 3.20 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 types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
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)	:	2.35

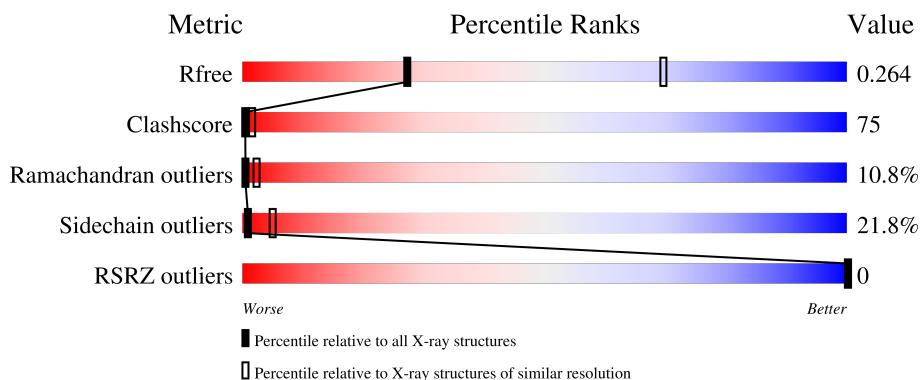
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.



2 Entry composition [\(i\)](#)

There are 4 unique types of molecules in this entry. The entry contains 3736 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 5'-D(*CP*TP*TP*GP*GP*TP*TP*AP*AP*TP*AP*A P*TP*TP*CP*AP*CP*CP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	20	Total	C	N	O	P	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	20	Total	C	N	O	P	0	0	0

- Molecule 3 is a protein called Hepatocyte nuclear factor 1-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	176	Total	C	N	O	S	0	0	0
3	B	176	Total	C	N	O	S	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	SER	-	cloning artifact	UNP P35680
B	90	SER	-	cloning artifact	UNP P35680

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	O	0	0
4	F	2	Total	O	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	B	3	Total O 3 3	0	0

3 Residue-property plots

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.

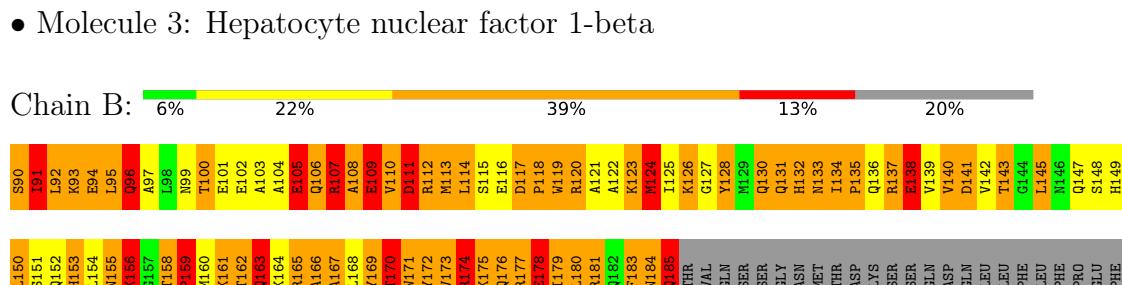
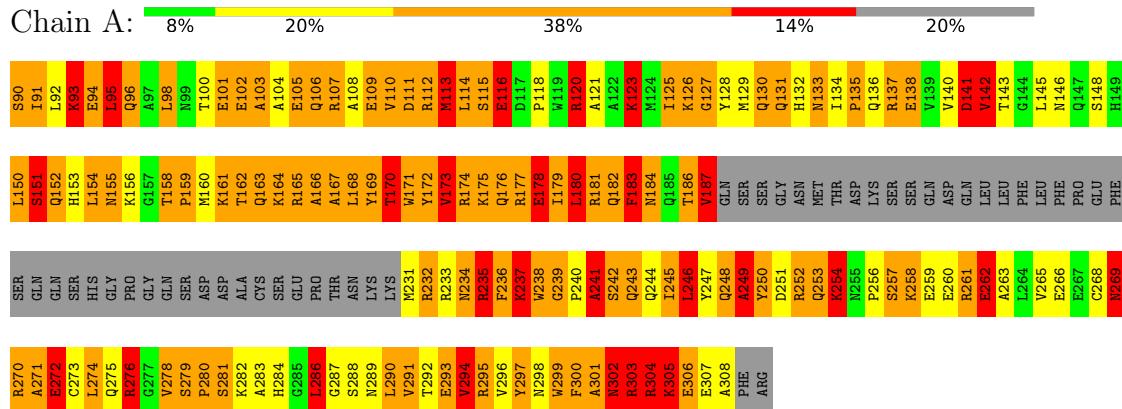
- Molecule 1: 5'-D(*CP*TP*TP*GP*GP*TP*TP*AP*AP*TP*AP*AP*TP*TP*CP*AP*CP*C P*AP*G)-3'



- Molecule 2: 5'-D(*GP*CP*TP*GP*GP*TP*GP*AP*AP*TP*TP*AP*TP*AP*TP*AP*CP*C P*AP*A)-3'



- Molecule 3: Hepatocyte nuclear factor 1-beta



SER	R270	A271	E272	C273	L274	Q275	R276	G277	V278	SER	GLN	GLN	SER	HIS	GLY	PRO	GLY	GLN	SER	ASP	ASP	S281	K282	A283	H284	GLU	GLU	PRO	ASP	P280	S288	R289	L290	LYS	LYS	R291	M231	R292	R232	R233	R234	R235	F236	F236	R297	R237	R292	E293	V294	R295	V296	V297	V298	W299	F300	A301	N302	R303	Q243	R304	Q244	Q245	E305	E306	E307	A308	F309	A249	R310	D250	D251	I252	Q253	K254	N255	P256	K256	E259	E260	R261	E262	A263	L264	V265	E266	E267	C268	M269
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4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	174.69Å 174.69Å 72.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.20 27.92 – 3.01	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-3.20) 83.8 (27.92-3.01)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ ¹	2.09 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R , R_{free}	0.223 , 0.290 0.195 , 0.264	Depositor DCC
R_{free} test set	691 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	79.5	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 20.3	EDS
L-test for twinning ²	$< L > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3736	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	E	6.56	188/453 (41.5%)	7.51	278/697 (39.9%)
2	F	6.32	183/459 (39.9%)	7.05	270/707 (38.2%)
3	A	3.51	211/1478 (14.3%)	2.43	81/1986 (4.1%)
3	B	3.73	232/1488 (15.6%)	2.41	90/1996 (4.5%)
All	All	4.45	814/3878 (21.0%)	4.26	719/5386 (13.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	2

All (814) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	19	DA	N7-C5	23.41	1.53	1.39
2	F	2	DG	C5-C4	22.38	1.54	1.38
2	F	2	DG	N1-C2	21.66	1.55	1.37
1	E	19	DA	C5-C4	21.43	1.53	1.38
1	E	19	DA	N9-C4	20.63	1.50	1.37
1	E	2	DT	P-O5'	19.64	1.79	1.59
2	F	2	DG	C6-N1	19.43	1.53	1.39
1	E	9	DA	N3-C4	-19.25	1.23	1.34
1	E	2	DT	C2-O2	18.69	1.37	1.22
2	F	21	DA	C3'-O3'	18.45	1.68	1.44
3	B	156	LYS	CD-CE	18.17	1.96	1.51
1	E	11	DA	C6-N1	18.16	1.48	1.35
2	F	20	DA	C5-C4	17.52	1.51	1.38
2	F	3	DC	N3-C4	17.51	1.46	1.33
2	F	11	DT	C2-O2	-17.50	1.08	1.22
1	E	11	DA	N9-C4	-17.47	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	2	DT	O3'-P	17.28	1.81	1.61
1	E	1	DC	C2-N3	17.13	1.49	1.35
3	A	101	GLU	CD-OE2	16.76	1.44	1.25
1	E	2	DT	C2-N3	16.74	1.51	1.37
2	F	11	DT	N1-C2	-16.68	1.24	1.38
3	B	293	GLU	CD-OE1	16.68	1.44	1.25
2	F	6	DG	C6-N1	-16.65	1.27	1.39
1	E	2	DT	N1-C2	16.34	1.51	1.38
2	F	20	DA	P-O5'	16.23	1.75	1.59
1	E	4	DG	P-O5'	15.91	1.75	1.59
3	A	123	LYS	CD-CE	15.76	1.90	1.51
1	E	18	DC	P-O5'	15.74	1.75	1.59
2	F	2	DG	C2-N3	15.68	1.45	1.32
3	A	293	GLU	CD-OE2	15.33	1.42	1.25
2	F	2	DG	N9-C8	15.27	1.48	1.37
3	A	249	ALA	CA-CB	-15.17	1.20	1.52
1	E	19	DA	N3-C4	15.01	1.43	1.34
3	B	178	GLU	CD-OE1	14.81	1.42	1.25
2	F	20	DA	N7-C5	14.60	1.48	1.39
1	E	19	DA	C3'-O3'	14.51	1.62	1.44
3	B	109	GLU	CD-OE2	14.31	1.41	1.25
1	E	1	DC	C2-O2	14.28	1.37	1.24
1	E	14	DT	C2-O2	-14.24	1.11	1.22
3	A	166	ALA	CA-CB	-14.23	1.22	1.52
2	F	3	DC	P-O5'	14.06	1.73	1.59
2	F	5	DG	P-O5'	14.02	1.73	1.59
1	E	11	DA	N7-C5	-13.98	1.30	1.39
2	F	3	DC	C4-C5	13.95	1.54	1.43
2	F	3	DC	C2-N3	13.95	1.47	1.35
1	E	9	DA	C5-C4	-13.91	1.29	1.38
1	E	19	DA	C8-N7	13.86	1.41	1.31
2	F	12	DT	C3'-O3'	-13.85	1.25	1.44
1	E	20	DG	N1-C2	13.84	1.48	1.37
1	E	11	DA	C6-N6	13.79	1.45	1.33
3	A	94	GLU	CD-OE2	13.72	1.40	1.25
2	F	4	DT	C5-C6	13.62	1.43	1.34
1	E	18	DC	C3'-O3'	13.50	1.61	1.44
3	A	105	GLU	CD-OE2	13.38	1.40	1.25
3	B	138	GLU	CD-OE2	13.36	1.40	1.25
3	B	293	GLU	CD-OE2	13.35	1.40	1.25
3	B	178	GLU	CD-OE2	13.34	1.40	1.25
3	A	96	GLN	CG-CD	13.31	1.81	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	2	DT	N1-C6	13.28	1.47	1.38
1	E	18	DC	P-OP2	13.15	1.71	1.49
3	A	253	GLN	CG-CD	13.15	1.81	1.51
2	F	20	DA	C5-C6	13.12	1.52	1.41
2	F	2	DG	N7-C5	13.09	1.47	1.39
2	F	13	DA	N3-C4	-13.09	1.26	1.34
3	A	293	GLU	CG-CD	13.06	1.71	1.51
3	B	247	TYR	CD1-CE1	12.97	1.58	1.39
3	B	134	ILE	CG1-CD1	12.95	2.39	1.50
2	F	14	DT	P-OP2	12.92	1.71	1.49
1	E	11	DA	N3-C4	-12.88	1.27	1.34
2	F	4	DT	N3-C4	12.71	1.48	1.38
3	B	266	GLU	CD-OE1	12.70	1.39	1.25
3	A	178	GLU	CD-OE1	12.68	1.39	1.25
2	F	2	DG	N3-C4	12.67	1.44	1.35
2	F	18	DC	C3'-O3'	12.56	1.60	1.44
3	A	105	GLU	CD-OE1	12.43	1.39	1.25
2	F	3	DC	N1-C6	12.41	1.44	1.37
3	B	243	GLN	CD-OE1	12.38	1.51	1.24
2	F	15	DT	P-OP2	12.37	1.70	1.49
1	E	12	DA	N7-C5	-12.34	1.31	1.39
1	E	16	DA	N3-C4	12.29	1.42	1.34
3	A	102	GLU	CD-OE2	12.20	1.39	1.25
1	E	1	DC	O3'-P	12.18	1.75	1.61
1	E	20	DG	C6-O6	12.16	1.35	1.24
2	F	11	DT	C2-N3	-12.12	1.28	1.37
2	F	20	DA	N9-C4	12.12	1.45	1.37
3	A	101	GLU	CG-CD	11.91	1.69	1.51
1	E	1	DC	N3-C4	11.89	1.42	1.33
1	E	1	DC	N1-C2	11.88	1.52	1.40
1	E	20	DG	N9-C4	11.87	1.47	1.38
2	F	21	DA	C6-N1	11.85	1.43	1.35
3	A	93	LYS	CD-CE	11.84	1.80	1.51
1	E	20	DG	P-O5'	11.82	1.71	1.59
1	E	2	DT	C5-C6	11.80	1.42	1.34
3	B	272	GLU	CD-OE1	11.71	1.38	1.25
3	B	293	GLU	CG-CD	11.70	1.69	1.51
3	A	180	LEU	CG-CD2	11.69	1.95	1.51
2	F	2	DG	C4'-O4'	11.66	1.56	1.45
3	B	299	TRP	CD2-CE2	11.64	1.55	1.41
2	F	12	DT	C1'-N1	11.62	1.64	1.49
1	E	8	DA	N9-C8	-11.62	1.28	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	307	GLU	CD-OE1	11.57	1.38	1.25
3	B	296	VAL	CB-CG2	-11.57	1.28	1.52
3	A	300	PHE	CD1-CE1	11.49	1.62	1.39
3	B	152	GLN	CD-NE2	11.47	1.61	1.32
3	B	119	TRP	CE3-CZ3	-11.46	1.19	1.38
2	F	20	DA	C8-N7	11.44	1.39	1.31
3	B	291	VAL	CB-CG2	-11.35	1.29	1.52
3	B	293	GLU	CB-CG	11.34	1.73	1.52
3	A	250	TYR	CD2-CE2	11.24	1.56	1.39
3	A	300	PHE	CD2-CE2	11.24	1.61	1.39
2	F	14	DT	C4-O4	-11.18	1.13	1.23
1	E	17	DC	C3'-O3'	11.15	1.58	1.44
2	F	4	DT	P-O5'	11.05	1.70	1.59
2	F	15	DT	C4-C5	-11.05	1.35	1.45
3	B	274	LEU	CG-CD1	11.04	1.92	1.51
2	F	20	DA	N3-C4	11.02	1.41	1.34
3	B	140	VAL	CB-CG1	-11.01	1.29	1.52
2	F	2	DG	O4'-C1'	10.99	1.55	1.42
2	F	16	DA	C3'-O3'	-10.99	1.29	1.44
3	B	140	VAL	CB-CG2	-10.95	1.29	1.52
3	B	236	PHE	CE1-CZ	10.95	1.58	1.37
3	B	310	ARG	C-OXT	10.93	1.44	1.23
2	F	13	DA	N7-C5	-10.93	1.32	1.39
3	A	307	GLU	CD-OE2	10.93	1.37	1.25
3	B	267	GLU	CD-OE1	10.90	1.37	1.25
1	E	19	DA	C6-N1	10.86	1.43	1.35
1	E	1	DC	N1-C6	10.85	1.43	1.37
1	E	3	DT	N3-C4	10.83	1.47	1.38
3	B	299	TRP	CG-CD1	10.69	1.51	1.36
3	A	116	GLU	CD-OE2	10.69	1.37	1.25
1	E	3	DT	C2-N3	10.69	1.46	1.37
2	F	21	DA	C4'-C3'	10.67	1.64	1.53
3	B	276	ARG	CZ-NH1	10.66	1.47	1.33
3	A	138	GLU	CD-OE1	10.64	1.37	1.25
1	E	18	DC	N1-C2	10.59	1.50	1.40
3	B	174	ARG	NE-CZ	10.58	1.46	1.33
2	F	4	DT	N1-C6	10.56	1.45	1.38
2	F	5	DG	C3'-O3'	-10.54	1.30	1.44
2	F	10	DA	N9-C8	-10.52	1.29	1.37
1	E	17	DC	O3'-P	10.51	1.73	1.61
1	E	3	DT	C4-O4	10.48	1.32	1.23
2	F	2	DG	C2'-C1'	10.47	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	109	GLU	CD-OE1	10.43	1.37	1.25
2	F	20	DA	O3'-P	10.43	1.73	1.61
3	A	178	GLU	CG-CD	10.40	1.67	1.51
3	A	293	GLU	CD-OE1	10.39	1.37	1.25
1	E	1	DC	C5'-C4'	10.38	1.62	1.51
3	B	122	ALA	CA-CB	-10.38	1.30	1.52
2	F	10	DA	P-OP2	10.32	1.66	1.49
1	E	15	DC	C1'-N1	10.31	1.62	1.49
2	F	10	DA	C3'-O3'	-10.27	1.30	1.44
1	E	2	DT	P-OP1	10.26	1.66	1.49
1	E	10	DT	C2-O2	-10.25	1.14	1.22
2	F	15	DT	N1-C6	-10.25	1.31	1.38
3	A	237	LYS	CE-NZ	10.24	1.74	1.49
3	B	120	ARG	CG-CD	10.24	1.77	1.51
1	E	3	DT	P-O5'	10.22	1.70	1.59
1	E	16	DA	C5'-C4'	-10.22	1.40	1.51
1	E	18	DC	C1'-N1	10.19	1.62	1.49
2	F	2	DG	C6-O6	10.19	1.33	1.24
3	A	105	GLU	CG-CD	10.18	1.67	1.51
3	A	138	GLU	CD-OE2	10.18	1.36	1.25
3	B	108	ALA	CA-CB	-10.18	1.31	1.52
1	E	12	DA	N3-C4	-10.16	1.28	1.34
2	F	10	DA	C5-C4	-10.15	1.31	1.38
3	B	131	GLN	CG-CD	10.14	1.74	1.51
3	B	272	GLU	CD-OE2	10.13	1.36	1.25
1	E	10	DT	C2-N3	-10.10	1.29	1.37
3	B	96	GLN	CG-CD	10.07	1.74	1.51
2	F	21	DA	N3-C4	10.06	1.40	1.34
3	B	299	TRP	CZ3-CH2	10.06	1.56	1.40
1	E	3	DT	C4-C5	10.05	1.53	1.45
3	A	243	GLN	CG-CD	10.03	1.74	1.51
3	B	169	TYR	CD2-CE2	10.02	1.54	1.39
3	B	128	TYR	CD1-CE1	9.98	1.54	1.39
3	B	165	ARG	CZ-NH2	9.95	1.46	1.33
3	A	248	GLN	CG-CD	9.91	1.73	1.51
3	A	169	TYR	CB-CG	-9.89	1.36	1.51
1	E	19	DA	C5-C6	9.87	1.50	1.41
3	B	93	LYS	CD-CE	9.86	1.75	1.51
1	E	12	DA	C2-N3	9.84	1.42	1.33
2	F	3	DC	P-OP2	9.81	1.65	1.49
3	A	128	TYR	CG-CD2	-9.79	1.26	1.39
1	E	13	DT	C4-O4	-9.78	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	232	ARG	CG-CD	9.77	1.76	1.51
3	B	267	GLU	CD-OE2	9.71	1.36	1.25
3	B	247	TYR	CD2-CE2	9.71	1.53	1.39
1	E	20	DG	C3'-O3'	9.70	1.56	1.44
2	F	16	DA	N9-C4	-9.68	1.32	1.37
3	A	123	LYS	CE-NZ	9.67	1.73	1.49
3	B	119	TRP	CE2-CZ2	-9.67	1.23	1.39
1	E	19	DA	N9-C8	9.67	1.45	1.37
1	E	16	DA	P-OP1	9.66	1.65	1.49
3	A	299	TRP	CG-CD1	9.60	1.50	1.36
3	B	178	GLU	CG-CD	9.59	1.66	1.51
1	E	4	DG	O5'-C5'	9.57	1.66	1.42
3	B	243	GLN	CD-NE2	9.55	1.56	1.32
3	B	259	GLU	CD-OE1	9.54	1.36	1.25
1	E	15	DC	P-OP2	9.52	1.65	1.49
3	B	128	TYR	CD2-CE2	9.51	1.53	1.39
3	B	233	ARG	CG-CD	9.50	1.75	1.51
3	B	166	ALA	CA-CB	-9.48	1.32	1.52
2	F	20	DA	P-OP2	9.48	1.65	1.49
3	A	251	ASP	CB-CG	9.43	1.71	1.51
3	A	138	GLU	CG-CD	9.42	1.66	1.51
1	E	14	DT	P-OP2	9.41	1.65	1.49
3	B	93	LYS	CE-NZ	9.41	1.72	1.49
2	F	8	DG	C8-N7	9.38	1.36	1.30
1	E	20	DG	C2'-C1'	9.37	1.61	1.52
2	F	19	DC	P-OP2	9.34	1.64	1.49
3	B	231	MET	CG-SD	9.32	2.05	1.81
2	F	3	DC	N1-C2	9.31	1.49	1.40
3	B	180	LEU	CG-CD1	9.28	1.86	1.51
1	E	14	DT	N1-C2	-9.26	1.30	1.38
3	A	250	TYR	CD1-CE1	9.25	1.53	1.39
2	F	21	DA	C2'-C1'	9.24	1.61	1.52
2	F	2	DG	C2-N2	9.24	1.43	1.34
3	B	250	TYR	CD2-CE2	9.23	1.53	1.39
1	E	20	DG	P-OP2	9.21	1.64	1.49
3	B	105	GLU	CD-OE2	9.20	1.35	1.25
3	B	185	GLN	CB-CG	9.17	1.77	1.52
1	E	17	DC	N1-C6	-9.13	1.31	1.37
2	F	19	DC	P-OP1	9.13	1.64	1.49
1	E	15	DC	P-O5'	9.12	1.68	1.59
3	B	120	ARG	CZ-NH2	9.11	1.44	1.33
3	B	123	LYS	CD-CE	9.10	1.74	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4	DT	P-OP1	9.09	1.64	1.49
2	F	2	DG	C5-C6	9.07	1.51	1.42
3	B	172	TYR	CG-CD1	9.05	1.50	1.39
1	E	11	DA	C2-N3	9.04	1.41	1.33
2	F	16	DA	N7-C5	-9.03	1.33	1.39
3	A	254	LYS	CB-CG	9.03	1.76	1.52
1	E	7	DT	P-OP2	8.99	1.64	1.49
3	B	148	SER	CB-OG	8.99	1.53	1.42
1	E	9	DA	N1-C2	-8.97	1.26	1.34
3	A	93	LYS	CG-CD	8.94	1.82	1.52
3	A	126	LYS	CD-CE	8.92	1.73	1.51
2	F	9	DA	P-OP2	8.90	1.64	1.49
2	F	5	DG	C5'-C4'	8.90	1.61	1.51
3	B	161	LYS	CG-CD	8.90	1.82	1.52
1	E	3	DT	P-OP2	8.88	1.64	1.49
3	B	250	TYR	CD1-CE1	8.85	1.52	1.39
1	E	5	DG	N7-C5	-8.84	1.33	1.39
2	F	3	DC	P-OP1	8.84	1.64	1.49
3	A	272	GLU	CD-OE1	8.84	1.35	1.25
3	B	121	ALA	CA-CB	-8.84	1.33	1.52
3	B	163	GLN	CD-NE2	8.83	1.54	1.32
1	E	10	DT	C5-C6	8.82	1.40	1.34
1	E	10	DT	C4'-O4'	-8.82	1.36	1.45
2	F	10	DA	N9-C4	8.81	1.43	1.37
1	E	16	DA	N1-C2	8.81	1.42	1.34
2	F	3	DC	C4-N4	8.80	1.41	1.33
2	F	18	DC	N1-C6	-8.76	1.31	1.37
1	E	20	DG	C6-N1	8.75	1.45	1.39
2	F	21	DA	C4'-O4'	8.73	1.53	1.45
3	B	169	TYR	CB-CG	-8.73	1.38	1.51
2	F	18	DC	P-O5'	8.72	1.68	1.59
1	E	17	DC	C2-N3	8.68	1.42	1.35
1	E	5	DG	C3'-O3'	-8.66	1.32	1.44
3	A	241	ALA	CA-CB	-8.64	1.34	1.52
3	B	94	GLU	CD-OE2	8.64	1.35	1.25
2	F	17	DA	P-O5'	-8.64	1.51	1.59
3	A	110	VAL	CA-CB	-8.64	1.36	1.54
3	B	126	LYS	CE-NZ	8.63	1.70	1.49
2	F	4	DT	C2-N3	8.62	1.44	1.37
1	E	1	DC	O5'-C5'	8.60	1.63	1.42
1	E	12	DA	C3'-C2'	-8.60	1.42	1.52
1	E	3	DT	C2-O2	8.60	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	13	DT	C5-C6	8.60	1.40	1.34
3	B	165	ARG	C-O	8.56	1.39	1.23
3	A	303	ARG	CZ-NH1	8.55	1.44	1.33
1	E	20	DG	C5'-C4'	8.55	1.60	1.51
2	F	3	DC	C5-C6	8.54	1.41	1.34
1	E	18	DC	P-OP1	8.54	1.63	1.49
2	F	10	DA	N7-C5	-8.54	1.34	1.39
2	F	11	DT	C3'-O3'	-8.51	1.32	1.44
1	E	20	DG	O5'-C5'	8.51	1.63	1.42
1	E	7	DT	C4'-O4'	8.50	1.53	1.45
3	A	93	LYS	CE-NZ	8.48	1.70	1.49
1	E	15	DC	N3-C4	8.47	1.39	1.33
2	F	20	DA	N9-C8	8.45	1.44	1.37
3	B	278	VAL	C-O	8.44	1.39	1.23
1	E	14	DT	C2'-C1'	-8.43	1.43	1.52
3	B	90	SER	CB-OG	8.41	1.53	1.42
3	A	232	ARG	NE-CZ	8.40	1.44	1.33
3	B	232	ARG	NE-CZ	8.40	1.44	1.33
3	A	121	ALA	CA-CB	-8.39	1.34	1.52
1	E	20	DG	C4'-C3'	8.38	1.61	1.53
1	E	19	DA	P-O5'	8.36	1.68	1.59
2	F	13	DA	N9-C4	-8.34	1.32	1.37
3	B	120	ARG	CZ-NH1	8.34	1.43	1.33
1	E	1	DC	C4'-O4'	8.31	1.53	1.45
2	F	21	DA	C5'-C4'	8.30	1.60	1.51
3	B	137	ARG	CA-CB	-8.29	1.35	1.53
3	B	297	TYR	CE2-CZ	8.29	1.49	1.38
3	B	250	TYR	CE1-CZ	8.26	1.49	1.38
3	A	132	HIS	C-O	8.24	1.39	1.23
3	B	174	ARG	CZ-NH1	8.24	1.43	1.33
2	F	19	DC	C3'-O3'	8.20	1.54	1.44
3	B	283	ALA	CA-CB	-8.20	1.35	1.52
3	B	120	ARG	CB-CG	8.20	1.74	1.52
2	F	18	DC	C5'-C4'	8.17	1.60	1.51
1	E	1	DC	C1'-N1	8.16	1.59	1.49
3	A	120	ARG	NE-CZ	8.15	1.43	1.33
1	E	8	DA	N3-C4	8.15	1.39	1.34
2	F	21	DA	P-O5'	8.14	1.67	1.59
3	A	302	ASN	C-O	8.14	1.38	1.23
3	B	231	MET	SD-CE	8.11	2.23	1.77
3	B	171	TRP	CE3-CZ3	-8.09	1.24	1.38
1	E	4	DG	C6-N1	-8.08	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	14	DT	C2-N3	-8.07	1.31	1.37
1	E	1	DC	C3'-O3'	8.07	1.54	1.44
1	E	15	DC	C2-O2	-8.07	1.17	1.24
2	F	8	DG	O3'-P	8.07	1.70	1.61
2	F	5	DG	C4'-O4'	8.04	1.53	1.45
2	F	16	DA	C4'-O4'	8.04	1.53	1.45
3	A	150	LEU	N-CA	-8.04	1.30	1.46
1	E	9	DA	P-O5'	8.03	1.67	1.59
3	B	259	GLU	CG-CD	8.03	1.64	1.51
3	B	247	TYR	CE2-CZ	-8.02	1.28	1.38
2	F	3	DC	O3'-P	8.01	1.70	1.61
3	B	270	ARG	NE-CZ	8.00	1.43	1.33
2	F	19	DC	C4-C5	7.99	1.49	1.43
3	B	169	TYR	CD1-CE1	7.99	1.51	1.39
2	F	20	DA	C4'-O4'	7.98	1.53	1.45
3	B	172	TYR	CG-CD2	7.97	1.49	1.39
3	B	266	GLU	CD-OE2	7.97	1.34	1.25
3	B	130	GLN	C-O	7.97	1.38	1.23
1	E	20	DG	C5-C6	7.97	1.50	1.42
3	A	101	GLU	CB-CG	7.97	1.67	1.52
3	A	169	TYR	CG-CD1	-7.97	1.28	1.39
1	E	4	DG	C5-C4	7.94	1.44	1.38
3	B	176	GLN	CG-CD	7.92	1.69	1.51
2	F	6	DG	C3'-O3'	-7.91	1.33	1.44
3	A	307	GLU	CG-CD	7.91	1.63	1.51
3	A	272	GLU	CD-OE2	7.89	1.34	1.25
2	F	13	DA	O3'-P	7.86	1.70	1.61
1	E	3	DT	C5-C6	7.86	1.39	1.34
3	B	272	GLU	CG-CD	7.86	1.63	1.51
2	F	15	DT	N1-C2	-7.86	1.31	1.38
3	A	156	LYS	CD-CE	7.85	1.70	1.51
3	A	248	GLN	CD-OE1	7.85	1.41	1.24
2	F	7	DT	C2-N3	-7.84	1.31	1.37
3	A	101	GLU	CD-OE1	7.84	1.34	1.25
3	B	130	GLN	CD-OE1	7.84	1.41	1.24
2	F	18	DC	N1-C2	-7.83	1.32	1.40
2	F	20	DA	C6-N1	7.79	1.41	1.35
2	F	4	DT	C4-C5	7.76	1.51	1.45
3	A	100	THR	CA-CB	7.75	1.73	1.53
3	B	235	ARG	CZ-NH1	7.75	1.43	1.33
3	A	294	VAL	CB-CG1	-7.74	1.36	1.52
3	A	271	ALA	CA-CB	-7.74	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	282	LYS	CB-CG	7.74	1.73	1.52
3	A	244	GLN	CG-CD	7.73	1.68	1.51
1	E	8	DA	N7-C5	-7.72	1.34	1.39
1	E	2	DT	N3-C4	7.72	1.44	1.38
2	F	20	DA	C2-N3	7.72	1.40	1.33
3	B	294	VAL	CB-CG1	-7.69	1.36	1.52
3	A	116	GLU	CD-OE1	7.69	1.34	1.25
1	E	9	DA	C5-C6	7.69	1.48	1.41
1	E	19	DA	N1-C2	7.64	1.41	1.34
1	E	2	DT	C1'-N1	7.58	1.59	1.49
1	E	18	DC	C4'-O4'	7.58	1.52	1.45
1	E	17	DC	C4-N4	7.57	1.40	1.33
1	E	20	DG	C1'-N9	7.56	1.59	1.49
2	F	12	DT	C5-C6	-7.56	1.29	1.34
3	B	150	LEU	C-O	7.56	1.37	1.23
3	B	128	TYR	CE2-CZ	-7.56	1.28	1.38
3	A	238	TRP	CA-CB	-7.56	1.37	1.53
1	E	8	DA	C5'-C4'	7.53	1.59	1.51
1	E	11	DA	C5-C6	7.53	1.47	1.41
1	E	11	DA	C3'-O3'	-7.52	1.34	1.44
3	A	96	GLN	CD-OE1	7.50	1.40	1.24
2	F	11	DT	P-O5'	7.49	1.67	1.59
1	E	1	DC	C4'-C3'	7.49	1.60	1.53
3	B	235	ARG	CZ-NH2	7.48	1.42	1.33
3	A	103	ALA	CA-CB	-7.48	1.36	1.52
3	B	173	VAL	CB-CG2	-7.47	1.37	1.52
2	F	16	DA	N9-C8	-7.46	1.31	1.37
3	A	303	ARG	CZ-NH2	7.45	1.42	1.33
3	A	174	ARG	CG-CD	7.44	1.70	1.51
3	B	270	ARG	CZ-NH2	7.44	1.42	1.33
3	A	176	GLN	CD-NE2	7.43	1.51	1.32
3	A	128	TYR	CE1-CZ	-7.43	1.28	1.38
2	F	12	DT	N1-C6	-7.41	1.33	1.38
3	A	94	GLU	CG-CD	7.40	1.63	1.51
1	E	8	DA	C5-C4	-7.40	1.33	1.38
3	B	265	VAL	CA-CB	-7.40	1.39	1.54
3	A	159	PRO	C-O	7.39	1.38	1.23
3	A	306	GLU	CD-OE2	7.39	1.33	1.25
3	B	158	THR	CA-CB	-7.38	1.34	1.53
3	B	184	ASN	CB-CG	7.37	1.68	1.51
2	F	18	DC	O3'-P	7.36	1.70	1.61
3	A	133	ASN	CB-CG	-7.35	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	288	SER	CB-OG	7.32	1.51	1.42
1	E	19	DA	O3'-P	7.31	1.70	1.61
3	A	305	LYS	C-O	-7.29	1.09	1.23
2	F	21	DA	C3'-C2'	7.28	1.60	1.52
3	A	236	PHE	CE1-CZ	7.28	1.51	1.37
3	A	129	MET	CG-SD	7.26	2.00	1.81
1	E	10	DT	O5'-C5'	-7.26	1.24	1.42
1	E	20	DG	P-OP1	7.25	1.61	1.49
2	F	5	DG	C5-C4	-7.25	1.33	1.38
2	F	16	DA	P-O5'	-7.25	1.52	1.59
3	A	153	HIS	CA-CB	-7.24	1.38	1.53
1	E	16	DA	N7-C5	-7.21	1.34	1.39
1	E	20	DG	C8-N7	7.20	1.35	1.30
3	B	238	TRP	C-O	-7.20	1.09	1.23
2	F	6	DG	N3-C4	-7.20	1.30	1.35
2	F	11	DT	C1'-N1	7.19	1.58	1.49
1	E	13	DT	C2'-C1'	-7.17	1.45	1.52
3	A	270	ARG	CG-CD	7.17	1.69	1.51
1	E	4	DG	C5'-C4'	7.16	1.59	1.51
3	A	134	ILE	CA-CB	-7.16	1.38	1.54
2	F	11	DT	C5-C6	7.16	1.39	1.34
3	A	123	LYS	CB-CG	7.15	1.71	1.52
2	F	6	DG	N1-C2	-7.15	1.32	1.37
3	A	299	TRP	CD2-CE2	7.15	1.50	1.41
1	E	2	DT	C3'-O3'	7.13	1.53	1.44
3	B	106	GLN	C-O	-7.13	1.09	1.23
1	E	10	DT	C1'-N1	7.11	1.58	1.49
3	B	141	ASP	N-CA	-7.10	1.32	1.46
3	A	142	VAL	CA-CB	-7.10	1.39	1.54
3	B	120	ARG	NE-CZ	7.10	1.42	1.33
3	B	152	GLN	CD-OE1	7.08	1.39	1.24
3	B	237	LYS	CG-CD	7.04	1.76	1.52
2	F	5	DG	O5'-C5'	7.04	1.59	1.42
1	E	14	DT	P-O5'	7.02	1.66	1.59
3	B	112	ARG	CG-CD	7.02	1.69	1.51
2	F	13	DA	P-O5'	-7.01	1.52	1.59
3	A	102	GLU	CG-CD	7.00	1.62	1.51
2	F	11	DT	C4'-C3'	-7.00	1.45	1.52
2	F	2	DG	O5'-C5'	6.99	1.59	1.42
1	E	4	DG	P-OP2	6.96	1.60	1.49
1	E	15	DC	P-OP1	6.95	1.60	1.49
2	F	18	DC	C4-N4	6.95	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	115	SER	CB-OG	6.94	1.51	1.42
2	F	15	DT	P-OP1	6.93	1.60	1.49
3	A	238	TRP	CB-CG	-6.93	1.37	1.50
3	B	138	GLU	C-O	-6.92	1.10	1.23
2	F	17	DA	N9-C8	-6.92	1.32	1.37
3	A	177	ARG	NE-CZ	6.91	1.42	1.33
3	B	113	MET	CG-SD	6.89	1.99	1.81
3	A	291	VAL	CB-CG2	-6.88	1.38	1.52
3	A	128	TYR	CZ-OH	6.88	1.49	1.37
3	B	260	GLU	CD-OE1	6.88	1.33	1.25
3	B	238	TRP	CG-CD1	-6.87	1.27	1.36
3	A	116	GLU	CG-CD	6.87	1.62	1.51
3	B	278	VAL	CA-CB	-6.87	1.40	1.54
3	B	171	TRP	CG-CD1	6.85	1.46	1.36
2	F	20	DA	C3'-O3'	6.84	1.52	1.44
3	B	238	TRP	CB-CG	-6.84	1.38	1.50
1	E	17	DC	C4'-O4'	6.83	1.51	1.45
3	A	91	ILE	CA-CB	-6.83	1.39	1.54
3	B	248	GLN	CD-OE1	6.83	1.39	1.24
3	B	250	TYR	CZ-OH	6.83	1.49	1.37
3	A	127	GLY	CA-C	-6.82	1.41	1.51
2	F	8	DG	N3-C4	-6.82	1.30	1.35
3	B	113	MET	SD-CE	-6.78	1.40	1.77
3	B	123	LYS	CE-NZ	6.77	1.66	1.49
3	B	233	ARG	NE-CZ	6.76	1.41	1.33
1	E	12	DA	C5-C6	6.75	1.47	1.41
2	F	6	DG	C5-C4	-6.75	1.33	1.38
1	E	14	DT	C3'-O3'	-6.75	1.35	1.44
2	F	13	DA	C6-N6	-6.74	1.28	1.33
1	E	13	DT	P-OP2	6.74	1.60	1.49
3	A	126	LYS	CE-NZ	6.73	1.65	1.49
2	F	7	DT	C3'-O3'	-6.72	1.35	1.44
1	E	10	DT	C4-O4	-6.72	1.17	1.23
1	E	16	DA	N9-C4	6.71	1.41	1.37
3	B	248	GLN	CD-NE2	6.70	1.49	1.32
2	F	20	DA	C5'-C4'	6.69	1.58	1.51
1	E	9	DA	P-OP2	6.69	1.60	1.49
3	B	297	TYR	CZ-OH	6.69	1.49	1.37
1	E	17	DC	P-OP2	6.68	1.60	1.49
1	E	10	DT	C5'-C4'	6.68	1.58	1.51
3	A	151	SER	CA-C	-6.68	1.35	1.52
3	A	299	TRP	CA-CB	-6.68	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	18	DC	C4-C5	6.68	1.48	1.43
3	A	164	LYS	CD-CE	6.67	1.68	1.51
3	B	126	LYS	CD-CE	6.66	1.68	1.51
3	A	132	HIS	CA-CB	-6.65	1.39	1.53
3	A	137	ARG	CA-CB	-6.65	1.39	1.53
3	A	129	MET	CA-C	-6.65	1.35	1.52
2	F	20	DA	N1-C2	6.65	1.40	1.34
3	B	278	VAL	CB-CG1	-6.64	1.38	1.52
2	F	19	DC	C5'-C4'	6.64	1.58	1.51
3	B	238	TRP	CE2-CZ2	-6.63	1.28	1.39
3	A	257	SER	CB-OG	6.63	1.50	1.42
3	A	295	ARG	CZ-NH1	6.63	1.41	1.33
3	B	116	GLU	N-CA	-6.63	1.33	1.46
3	B	291	VAL	CB-CG1	-6.63	1.39	1.52
2	F	20	DA	O5'-C5'	6.62	1.58	1.42
1	E	2	DT	C4-C5	6.62	1.50	1.45
1	E	14	DT	C5-C6	6.62	1.39	1.34
3	A	243	GLN	CD-NE2	6.61	1.49	1.32
2	F	10	DA	N3-C4	-6.61	1.30	1.34
3	B	159	PRO	C-O	6.61	1.36	1.23
3	A	135	PRO	N-CD	-6.60	1.38	1.47
2	F	5	DG	P-OP1	6.60	1.60	1.49
1	E	14	DT	C4-O4	-6.59	1.17	1.23
2	F	20	DA	C6-N6	6.58	1.39	1.33
2	F	2	DG	C5'-C4'	6.58	1.58	1.51
3	B	283	ALA	N-CA	-6.57	1.33	1.46
3	A	184	ASN	CB-CG	6.57	1.66	1.51
2	F	5	DG	P-OP2	6.56	1.60	1.49
3	A	131	GLN	CG-CD	6.55	1.66	1.51
2	F	21	DA	N9-C4	6.54	1.41	1.37
3	B	237	LYS	CD-CE	6.49	1.67	1.51
3	A	245	ILE	CB-CG2	6.49	1.73	1.52
3	B	299	TRP	CA-CB	-6.49	1.39	1.53
3	B	262	GLU	CD-OE2	6.47	1.32	1.25
2	F	14	DT	N1-C6	6.45	1.42	1.38
1	E	20	DG	C2-N2	6.44	1.41	1.34
3	B	301	ALA	CA-CB	-6.44	1.39	1.52
3	B	116	GLU	CD-OE1	6.44	1.32	1.25
3	A	106	GLN	C-O	-6.43	1.11	1.23
3	A	138	GLU	CB-CG	-6.43	1.40	1.52
3	B	118	PRO	CB-CG	-6.42	1.17	1.50
2	F	20	DA	C3'-C2'	6.41	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	282	LYS	CG-CD	6.41	1.74	1.52
2	F	17	DA	N7-C5	-6.40	1.35	1.39
2	F	5	DG	N3-C4	-6.40	1.30	1.35
3	B	112	ARG	NE-CZ	6.38	1.41	1.33
1	E	5	DG	N9-C8	-6.38	1.33	1.37
2	F	15	DT	P-O5'	6.37	1.66	1.59
3	B	177	ARG	NE-CZ	6.37	1.41	1.33
3	A	181	ARG	CG-CD	6.36	1.67	1.51
3	B	127	GLY	CA-C	-6.36	1.41	1.51
1	E	8	DA	N9-C4	6.34	1.41	1.37
3	B	115	SER	CB-OG	6.34	1.50	1.42
1	E	4	DG	P-OP1	6.33	1.59	1.49
1	E	19	DA	C4'-O4'	6.33	1.51	1.45
3	B	270	ARG	CZ-NH1	6.33	1.41	1.33
1	E	10	DT	C2'-C1'	-6.32	1.46	1.52
1	E	1	DC	C5-C6	6.31	1.39	1.34
3	B	270	ARG	CG-CD	6.30	1.67	1.51
3	A	173	VAL	CB-CG1	-6.28	1.39	1.52
2	F	20	DA	P-OP1	6.28	1.59	1.49
3	A	98	LEU	CG-CD1	6.28	1.75	1.51
3	A	242	SER	CB-OG	6.27	1.50	1.42
3	B	131	GLN	C-O	6.27	1.35	1.23
3	B	114	LEU	CA-C	-6.26	1.36	1.52
3	B	142	VAL	CB-CG1	-6.25	1.39	1.52
3	A	239	GLY	C-O	6.25	1.33	1.23
2	F	3	DC	C2-O2	6.24	1.30	1.24
1	E	5	DG	C6-N1	-6.24	1.35	1.39
2	F	7	DT	O3'-P	-6.21	1.53	1.61
3	A	138	GLU	CA-CB	-6.21	1.40	1.53
1	E	18	DC	O3'-P	6.20	1.68	1.61
3	A	169	TYR	CA-CB	-6.19	1.40	1.53
3	B	236	PHE	CB-CG	-6.18	1.40	1.51
2	F	3	DC	O4'-C1'	6.17	1.49	1.42
3	A	177	ARG	CG-CD	6.17	1.67	1.51
3	B	261	ARG	CD-NE	6.16	1.56	1.46
3	A	112	ARG	NE-CZ	6.15	1.41	1.33
3	A	272	GLU	CG-CD	6.15	1.61	1.51
3	B	167	ALA	CA-CB	-6.14	1.39	1.52
1	E	16	DA	O5'-C5'	-6.11	1.26	1.42
3	B	237	LYS	CA-CB	-6.09	1.40	1.53
3	A	100	THR	CB-CG2	6.08	1.72	1.52
3	A	297	TYR	CD2-CE2	6.08	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4	DT	N1-C2	6.08	1.43	1.38
3	B	96	GLN	CD-NE2	6.07	1.48	1.32
3	B	154	LEU	CG-CD2	-6.07	1.29	1.51
3	A	232	ARG	CZ-NH1	6.06	1.41	1.33
2	F	16	DA	C8-N7	6.06	1.35	1.31
2	F	19	DC	N1-C2	6.06	1.46	1.40
3	B	266	GLU	CG-CD	6.05	1.61	1.51
3	B	172	TYR	N-CA	-6.04	1.34	1.46
3	B	119	TRP	CZ3-CH2	6.04	1.49	1.40
3	A	151	SER	N-CA	6.03	1.58	1.46
3	A	172	TYR	C-O	6.02	1.34	1.23
3	A	231	MET	CA-C	6.02	1.68	1.52
3	A	174	ARG	CZ-NH1	-6.01	1.25	1.33
1	E	20	DG	N3-C4	6.01	1.39	1.35
3	B	132	HIS	CA-CB	-6.00	1.40	1.53
3	A	270	ARG	NE-CZ	5.99	1.40	1.33
3	A	180	LEU	CG-CD1	5.98	1.74	1.51
3	A	165	ARG	CG-CD	-5.97	1.37	1.51
3	A	181	ARG	NE-CZ	5.97	1.40	1.33
3	B	181	ARG	NE-CZ	5.97	1.40	1.33
3	B	297	TYR	CG-CD1	5.97	1.47	1.39
3	A	115	SER	CA-CB	5.96	1.61	1.52
3	B	119	TRP	CD2-CE2	5.96	1.48	1.41
3	B	234	ASN	CB-CG	5.95	1.64	1.51
2	F	17	DA	C3'-O3'	-5.94	1.36	1.44
3	B	298	ASN	C-O	-5.94	1.12	1.23
3	A	250	TYR	C-O	5.93	1.34	1.23
3	B	172	TYR	CA-CB	-5.93	1.41	1.53
3	A	155	ASN	CG-ND2	5.92	1.47	1.32
2	F	8	DG	C4'-O4'	5.92	1.50	1.45
3	B	134	ILE	C-O	5.92	1.34	1.23
3	A	232	ARG	CZ-NH2	5.90	1.40	1.33
1	E	14	DT	O3'-P	5.89	1.68	1.61
1	E	10	DT	C4-C5	-5.89	1.39	1.45
3	B	235	ARG	NE-CZ	5.88	1.40	1.33
2	F	13	DA	O5'-C5'	-5.86	1.27	1.42
3	A	295	ARG	CZ-NH2	5.86	1.40	1.33
1	E	18	DC	C5'-C4'	5.85	1.57	1.51
3	A	164	LYS	CE-NZ	5.85	1.63	1.49
1	E	18	DC	O4'-C1'	5.85	1.49	1.42
1	E	7	DT	C5-C6	-5.84	1.30	1.34
3	B	175	LYS	CA-CB	-5.84	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	21	DA	N1-C2	5.84	1.39	1.34
1	E	5	DG	P-OP1	5.83	1.58	1.49
3	B	95	LEU	C-O	-5.83	1.12	1.23
3	B	178	GLU	N-CA	-5.82	1.34	1.46
1	E	3	DT	O3'-P	5.82	1.68	1.61
3	A	142	VAL	C-O	5.81	1.34	1.23
3	B	232	ARG	CD-NE	5.81	1.56	1.46
3	B	264	LEU	CA-C	-5.80	1.37	1.52
3	A	130	GLN	CD-OE1	5.80	1.36	1.24
3	A	254	LYS	CE-NZ	5.80	1.63	1.49
3	B	119	TRP	CG-CD2	-5.80	1.33	1.43
3	B	159	PRO	CB-CG	5.79	1.78	1.50
3	A	120	ARG	CZ-NH1	5.79	1.40	1.33
3	A	290	LEU	CG-CD1	5.79	1.73	1.51
2	F	21	DA	N7-C5	-5.78	1.35	1.39
2	F	18	DC	C4'-O4'	5.78	1.50	1.45
3	A	130	GLN	C-O	5.78	1.34	1.23
3	B	116	GLU	C-O	5.77	1.34	1.23
3	B	163	GLN	CG-CD	5.77	1.64	1.51
2	F	5	DG	N1-C2	-5.77	1.33	1.37
3	A	248	GLN	CD-NE2	5.75	1.47	1.32
3	A	289	ASN	N-CA	-5.74	1.34	1.46
1	E	5	DG	P-OP2	5.74	1.58	1.49
3	A	163	GLN	CD-OE1	5.74	1.36	1.24
2	F	10	DA	P-OP1	5.71	1.58	1.49
2	F	19	DC	O3'-P	5.71	1.68	1.61
3	A	170	THR	CA-CB	-5.71	1.38	1.53
3	B	249	ALA	CA-CB	-5.70	1.40	1.52
1	E	19	DA	C2-N3	5.70	1.38	1.33
3	A	184	ASN	CG-ND2	5.70	1.47	1.32
3	A	298	ASN	C-O	-5.69	1.12	1.23
3	A	293	GLU	CA-CB	5.68	1.66	1.53
3	B	282	LYS	CA-C	-5.68	1.38	1.52
1	E	1	DC	C4-N4	5.67	1.39	1.33
1	E	9	DA	C6-N1	-5.67	1.31	1.35
3	A	130	GLN	CB-CG	5.67	1.67	1.52
3	A	237	LYS	CD-CE	5.67	1.65	1.51
3	B	270	ARG	CB-CG	5.67	1.67	1.52
3	A	276	ARG	CZ-NH1	5.66	1.40	1.33
1	E	9	DA	N9-C8	-5.66	1.33	1.37
3	A	242	SER	C-O	-5.64	1.12	1.23
3	B	172	TYR	CB-CG	5.64	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	181	ARG	CZ-NH2	5.64	1.40	1.33
3	B	231	MET	CA-CB	5.64	1.66	1.53
1	E	12	DA	C1'-N9	5.63	1.56	1.49
1	E	13	DT	O3'-P	5.63	1.68	1.61
1	E	10	DT	N1-C6	5.62	1.42	1.38
2	F	18	DC	C3'-C2'	5.61	1.58	1.52
3	A	274	LEU	C-O	5.60	1.33	1.23
3	A	179	ILE	CG1-CD1	5.60	1.89	1.50
3	B	105	GLU	CD-OE1	5.60	1.31	1.25
3	B	172	TYR	CD1-CE1	5.59	1.47	1.39
3	A	233	ARG	CG-CD	5.58	1.66	1.51
3	B	133	ASN	CA-C	-5.58	1.38	1.52
3	A	120	ARG	C-O	-5.58	1.12	1.23
3	B	238	TRP	CA-CB	-5.57	1.41	1.53
3	B	301	ALA	N-CA	-5.57	1.35	1.46
1	E	15	DC	N1-C2	5.57	1.45	1.40
3	A	232	ARG	CG-CD	5.57	1.65	1.51
3	A	150	LEU	CA-CB	-5.56	1.41	1.53
3	B	174	ARG	CB-CG	-5.56	1.37	1.52
1	E	13	DT	N1-C2	5.55	1.42	1.38
2	F	21	DA	P-OP2	5.55	1.58	1.49
3	B	233	ARG	CZ-NH1	5.55	1.40	1.33
2	F	11	DT	C4'-O4'	-5.54	1.39	1.45
3	A	295	ARG	N-CA	-5.54	1.35	1.46
2	F	3	DC	C4'-C3'	5.53	1.58	1.53
3	B	174	ARG	CG-CD	5.52	1.65	1.51
3	A	272	GLU	C-O	5.52	1.33	1.23
2	F	9	DA	O4'-C1'	5.51	1.48	1.42
3	B	175	LYS	CD-CE	5.51	1.65	1.51
3	A	304	ARG	CA-C	-5.50	1.38	1.52
3	B	297	TYR	N-CA	-5.50	1.35	1.46
3	A	102	GLU	CD-OE1	5.50	1.31	1.25
3	B	238	TRP	NE1-CE2	-5.50	1.30	1.37
3	A	288	SER	CA-CB	-5.49	1.44	1.52
3	B	279	SER	C-O	5.49	1.33	1.23
2	F	9	DA	C5'-C4'	5.48	1.57	1.51
3	A	233	ARG	CD-NE	5.48	1.55	1.46
2	F	15	DT	C2-N3	-5.46	1.33	1.37
3	A	297	TYR	CD1-CE1	5.46	1.47	1.39
3	B	112	ARG	CZ-NH2	5.46	1.40	1.33
3	B	179	ILE	CA-C	-5.46	1.38	1.52
3	B	249	ALA	C-O	-5.46	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	254	LYS	CD-CE	5.46	1.64	1.51
3	B	299	TRP	CG-CD2	-5.46	1.34	1.43
1	E	15	DC	N1-C6	5.45	1.40	1.37
3	B	183	PHE	CB-CG	5.44	1.60	1.51
3	A	254	LYS	CG-CD	5.43	1.71	1.52
3	A	171	TRP	CD2-CE3	-5.43	1.32	1.40
2	F	14	DT	C3'-O3'	5.42	1.50	1.44
3	B	280	PRO	CA-C	-5.42	1.42	1.52
3	B	276	ARG	NE-CZ	-5.42	1.26	1.33
1	E	11	DA	O4'-C1'	5.41	1.48	1.42
3	B	172	TYR	CD2-CE2	-5.41	1.31	1.39
3	B	259	GLU	CD-OE2	5.41	1.31	1.25
1	E	1	DC	C4-C5	5.40	1.47	1.43
3	A	112	ARG	CA-CB	-5.40	1.42	1.53
2	F	6	DG	O3'-P	-5.39	1.54	1.61
3	A	137	ARG	CB-CG	-5.39	1.38	1.52
3	B	163	GLN	CD-OE1	5.38	1.35	1.24
3	A	294	VAL	CA-CB	-5.38	1.43	1.54
3	B	143	THR	CA-CB	5.37	1.67	1.53
1	E	17	DC	N3-C4	5.37	1.37	1.33
3	B	150	LEU	N-CA	-5.37	1.35	1.46
2	F	2	DG	C8-N7	5.37	1.34	1.30
3	B	135	PRO	CA-CB	-5.36	1.42	1.53
3	A	111	ASP	CG-OD2	5.35	1.37	1.25
3	A	180	LEU	C-O	-5.35	1.13	1.23
3	A	233	ARG	NE-CZ	5.35	1.40	1.33
2	F	14	DT	O5'-C5'	-5.34	1.28	1.42
2	F	9	DA	C6-N6	5.34	1.38	1.33
3	A	297	TYR	CG-CD1	5.34	1.46	1.39
3	B	298	ASN	CA-C	-5.34	1.39	1.52
2	F	20	DA	C4'-C3'	-5.33	1.47	1.52
3	B	294	VAL	CA-CB	-5.33	1.43	1.54
1	E	6	DT	N3-C4	5.32	1.43	1.38
3	A	172	TYR	CE2-CZ	-5.32	1.31	1.38
3	A	237	LYS	CA-CB	-5.32	1.42	1.53
3	B	171	TRP	CA-CB	-5.32	1.42	1.53
1	E	8	DA	C2-N3	5.31	1.38	1.33
3	A	169	TYR	CD2-CE2	5.31	1.47	1.39
2	F	16	DA	P-OP2	5.31	1.57	1.49
1	E	19	DA	C6-N6	5.31	1.38	1.33
2	F	21	DA	P-OP1	5.31	1.57	1.49
2	F	21	DA	O4'-C1'	5.31	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	137	ARG	CB-CG	-5.30	1.38	1.52
2	F	9	DA	O3'-P	5.29	1.67	1.61
3	A	137	ARG	C-O	5.29	1.33	1.23
1	E	8	DA	P-OP2	5.28	1.57	1.49
2	F	4	DT	O5'-C5'	5.28	1.55	1.42
3	A	182	GLN	CB-CG	-5.28	1.38	1.52
3	B	91	ILE	C-O	-5.27	1.13	1.23
3	B	244	GLN	CG-CD	5.27	1.63	1.51
3	A	187	VAL	CB-CG1	5.26	1.64	1.52
1	E	20	DG	C2-N3	5.26	1.36	1.32
3	A	301	ALA	CA-CB	-5.26	1.41	1.52
1	E	1	DC	O4'-C1'	5.26	1.48	1.42
2	F	2	DG	C1'-N9	5.26	1.56	1.49
1	E	18	DC	C2-O2	5.25	1.29	1.24
2	F	19	DC	C3'-C2'	5.25	1.58	1.52
1	E	19	DA	C3'-C2'	5.25	1.58	1.52
3	B	172	TYR	CE1-CZ	5.25	1.45	1.38
3	B	176	GLN	C-O	-5.24	1.13	1.23
3	A	128	TYR	CE2-CZ	-5.24	1.31	1.38
3	B	150	LEU	CA-CB	-5.23	1.41	1.53
3	B	247	TYR	CE1-CZ	5.22	1.45	1.38
3	A	275	GLN	CG-CD	5.22	1.63	1.51
3	A	290	LEU	CB-CG	5.22	1.67	1.52
3	A	297	TYR	C-O	5.22	1.33	1.23
1	E	10	DT	O4'-C1'	-5.21	1.35	1.42
3	B	109	GLU	C-O	-5.21	1.13	1.23
3	A	236	PHE	CD2-CE2	-5.21	1.28	1.39
3	B	90	SER	C-O	-5.21	1.13	1.23
3	B	155	ASN	C-O	5.21	1.33	1.23
3	B	161	LYS	CD-CE	5.20	1.64	1.51
3	A	161	LYS	CD-CE	5.20	1.64	1.51
3	A	303	ARG	NE-CZ	5.20	1.39	1.33
3	B	170	THR	CA-CB	-5.20	1.39	1.53
3	A	235	ARG	NE-CZ	5.20	1.39	1.33
2	F	15	DT	C2-O2	-5.19	1.18	1.22
3	A	183	PHE	CD2-CE2	-5.19	1.28	1.39
3	A	95	LEU	C-O	-5.19	1.13	1.23
3	B	124	MET	N-CA	-5.19	1.35	1.46
3	A	183	PHE	CD1-CE1	-5.18	1.28	1.39
3	B	260	GLU	C-O	5.18	1.33	1.23
1	E	2	DT	O5'-C5'	5.18	1.55	1.42
3	A	297	TYR	N-CA	-5.18	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	252	ARG	CG-CD	5.17	1.64	1.51
2	F	2	DG	C4'-C3'	5.16	1.58	1.53
3	B	91	ILE	CB-CG2	-5.15	1.36	1.52
2	F	8	DG	P-O5'	-5.15	1.54	1.59
3	A	180	LEU	N-CA	-5.14	1.36	1.46
3	A	303	ARG	CA-C	-5.14	1.39	1.52
3	A	305	LYS	CG-CD	5.13	1.70	1.52
1	E	13	DT	C3'-O3'	5.13	1.50	1.44
3	A	245	ILE	C-O	-5.13	1.13	1.23
3	A	234	ASN	CG-OD1	-5.13	1.12	1.24
3	A	297	TYR	CA-CB	-5.13	1.42	1.53
2	F	17	DA	O5'-C5'	-5.12	1.29	1.42
3	B	130	GLN	CD-NE2	5.12	1.45	1.32
1	E	12	DA	C4'-O4'	-5.12	1.40	1.45
3	A	286	LEU	N-CA	-5.11	1.36	1.46
2	F	16	DA	C6-N1	5.11	1.39	1.35
2	F	8	DG	C5-C6	-5.11	1.37	1.42
3	B	232	ARG	N-CA	5.11	1.56	1.46
1	E	19	DA	P-OP1	5.10	1.57	1.49
3	A	300	PHE	CA-C	-5.10	1.39	1.52
3	B	243	GLN	CA-CB	-5.10	1.42	1.53
3	B	174	ARG	CZ-NH2	5.09	1.39	1.33
1	E	15	DC	C4-C5	5.09	1.47	1.43
2	F	11	DT	C5'-C4'	-5.09	1.45	1.51
1	E	20	DG	C5-C4	5.09	1.42	1.38
3	B	177	ARG	CZ-NH1	5.07	1.39	1.33
3	B	107	ARG	CG-CD	5.06	1.64	1.51
3	A	175	LYS	CA-CB	-5.05	1.42	1.53
3	A	163	GLN	CG-CD	5.05	1.62	1.51
3	B	137	ARG	CA-C	-5.05	1.39	1.52
3	B	185	GLN	CD-OE1	5.05	1.35	1.24
3	A	253	GLN	CD-NE2	5.04	1.45	1.32
3	B	178	GLU	C-O	-5.04	1.13	1.23
3	A	232	ARG	CA-CB	5.04	1.65	1.53
3	A	270	ARG	CZ-NH2	5.03	1.39	1.33
2	F	16	DA	C5'-C4'	5.03	1.56	1.51
3	A	236	PHE	C-O	-5.03	1.13	1.23
2	F	10	DA	P-O5'	5.01	1.64	1.59
3	B	94	GLU	CG-CD	5.01	1.59	1.51
3	A	169	TYR	CE2-CZ	5.01	1.45	1.38
2	F	5	DG	N9-C4	-5.00	1.33	1.38
3	B	184	ASN	CG-OD1	5.00	1.34	1.24

All (719) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	9	DA	N9-C4-C5	31.43	118.37	105.80
2	F	10	DA	C5-N7-C8	30.70	119.25	103.90
1	E	9	DA	C6-N1-C2	-27.61	102.04	118.60
1	E	17	DC	N3-C4-C5	-26.25	111.40	121.90
1	E	4	DG	C2-N3-C4	-25.37	99.22	111.90
1	E	11	DA	C8-N9-C4	-25.25	95.70	105.80
2	F	8	DG	C5-C6-O6	-24.93	113.64	128.60
1	E	12	DA	C8-N9-C4	-24.84	95.86	105.80
1	E	9	DA	O4'-C1'-N9	-24.70	90.71	108.00
2	F	18	DC	N3-C4-C5	-24.20	112.22	121.90
2	F	18	DC	N1-C2-O2	-23.61	104.73	118.90
2	F	16	DA	C5-N7-C8	-23.57	92.12	103.90
1	E	10	DT	C4-C5-C6	-23.17	104.10	118.00
1	E	12	DA	C6-N1-C2	-22.81	104.92	118.60
1	E	9	DA	C2-N3-C4	22.80	122.00	110.60
1	E	12	DA	N1-C2-N3	22.75	140.67	129.30
2	F	18	DC	N3-C4-N4	22.71	133.90	118.00
2	F	10	DA	C4-C5-N7	-22.64	99.38	110.70
2	F	19	DC	C5-C6-N1	-22.02	109.99	121.00
3	B	276	ARG	NE-CZ-NH2	-21.99	109.31	120.30
1	E	15	DC	O4'-C1'-N1	21.89	123.32	108.00
2	F	8	DG	C5-N7-C8	-21.83	93.39	104.30
1	E	9	DA	N1-C6-N6	-21.82	105.51	118.60
1	E	12	DA	N9-C4-C5	21.79	114.51	105.80
2	F	10	DA	N7-C8-N9	-21.73	102.93	113.80
2	F	13	DA	N9-C4-C5	21.54	114.42	105.80
2	F	14	DT	N3-C4-C5	21.53	128.12	115.20
2	F	11	DT	O4'-C4'-C3'	-20.89	93.47	106.00
1	E	20	DG	C4-C5-N7	-20.85	102.46	110.80
1	E	9	DA	C4-C5-N7	-20.70	100.35	110.70
2	F	16	DA	N7-C8-N9	20.37	123.98	113.80
2	F	8	DG	C6-N1-C2	-20.30	112.92	125.10
1	E	13	DT	N3-C4-O4	-20.23	107.76	119.90
1	E	9	DA	N3-C4-C5	-20.09	112.73	126.80
1	E	20	DG	C5-N7-C8	19.78	114.19	104.30
1	E	4	DG	N1-C2-N3	19.32	135.49	123.90
1	E	11	DA	N7-C8-N9	18.86	123.23	113.80
1	E	20	DG	C5-C6-N1	-18.81	102.09	111.50
2	F	11	DT	C4-C5-C6	-18.55	106.87	118.00
1	E	15	DC	N3-C4-C5	17.97	129.09	121.90
1	E	14	DT	N1-C2-N3	17.89	125.33	114.60
2	F	13	DA	N1-C2-N3	17.64	138.12	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	6	DG	O5'-P-OP1	-17.60	89.58	110.70
1	E	11	DA	N9-C4-C5	17.55	112.82	105.80
2	F	4	DT	O4'-C1'-N1	17.53	120.27	108.00
1	E	9	DA	C5-C6-N1	17.46	126.43	117.70
1	E	7	DT	N3-C2-O2	-17.43	111.84	122.30
1	E	18	DC	O5'-P-OP2	17.37	131.54	110.70
2	F	19	DC	OP1-P-OP2	17.27	145.51	119.60
2	F	19	DC	C4-C5-C6	17.27	126.03	117.40
2	F	8	DG	N7-C8-N9	17.18	121.69	113.10
1	E	8	DA	C5-N7-C8	17.08	112.44	103.90
2	F	11	DT	O4'-C1'-C2'	-17.01	92.29	105.90
2	F	5	DG	O5'-P-OP2	-16.86	90.47	110.70
1	E	10	DT	N3-C4-C5	16.83	125.30	115.20
2	F	8	DG	C4-C5-N7	16.81	117.52	110.80
1	E	20	DG	O4'-C1'-N9	16.73	119.71	108.00
1	E	15	DC	C2-N3-C4	-16.72	111.54	119.90
1	E	5	DG	C4-C5-C6	16.55	128.73	118.80
2	F	13	DA	C6-N1-C2	-16.54	108.68	118.60
2	F	18	DC	C6-N1-C2	-16.52	113.69	120.30
2	F	18	DC	O4'-C4'-C3'	-16.50	96.10	106.00
1	E	4	DG	N1-C2-N2	-16.45	101.40	116.20
1	E	5	DG	O4'-C1'-N9	16.34	119.44	108.00
2	F	7	DT	N3-C2-O2	-16.05	112.67	122.30
1	E	19	DA	C8-N9-C4	15.95	112.18	105.80
2	F	8	DG	N1-C2-N3	15.92	133.45	123.90
1	E	10	DT	C5-C6-N1	15.88	133.23	123.70
1	E	11	DA	N1-C2-N3	15.73	137.16	129.30
3	A	174	ARG	NE-CZ-NH2	15.69	128.15	120.30
2	F	6	DG	C5-C6-O6	15.65	137.99	128.60
2	F	21	DA	O5'-P-OP2	-15.65	91.61	105.70
2	F	5	DG	N1-C2-N2	-15.60	102.16	116.20
2	F	8	DG	C6-C5-N7	-15.54	121.08	130.40
1	E	8	DA	O4'-C1'-C2'	15.53	118.32	105.90
1	E	5	DG	C6-C5-N7	-15.42	121.15	130.40
2	F	7	DT	N3-C4-C5	15.33	124.40	115.20
3	A	137	ARG	NE-CZ-NH2	-15.21	112.69	120.30
1	E	18	DC	O4'-C4'-C3'	-15.16	96.90	106.00
1	E	15	DC	O5'-P-OP1	15.09	128.81	110.70
2	F	2	DG	N1-C6-O6	15.06	128.94	119.90
1	E	3	DT	N3-C2-O2	15.05	131.33	122.30
2	F	8	DG	N1-C6-O6	14.93	128.86	119.90
1	E	16	DA	P-O5'-C5'	-14.90	97.05	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	6	DG	N1-C6-O6	-14.86	110.99	119.90
2	F	8	DG	C8-N9-C4	-14.74	100.50	106.40
2	F	7	DT	C4-C5-C6	-14.74	109.16	118.00
2	F	14	DT	N3-C4-O4	-14.74	111.06	119.90
1	E	8	DA	C4-C5-N7	-14.72	103.34	110.70
2	F	18	DC	O5'-P-OP2	-14.67	92.50	105.70
2	F	10	DA	O5'-P-OP2	-14.67	92.50	105.70
2	F	13	DA	N1-C6-N6	-14.65	109.81	118.60
1	E	18	DC	N3-C4-C5	14.63	127.75	121.90
1	E	3	DT	O4'-C1'-N1	-14.55	97.81	108.00
1	E	13	DT	N3-C4-C5	14.51	123.91	115.20
1	E	9	DA	C8-N9-C4	-14.44	100.03	105.80
2	F	19	DC	N3-C2-O2	-14.43	111.80	121.90
1	E	14	DT	C6-N1-C2	-14.30	114.15	121.30
1	E	4	DG	C5-C6-O6	14.30	137.18	128.60
1	E	17	DC	C4-C5-C6	14.26	124.53	117.40
1	E	8	DA	N1-C6-N6	-14.26	110.05	118.60
1	E	4	DG	O5'-P-OP1	-14.23	92.89	105.70
2	F	13	DA	C8-N9-C4	-14.13	100.15	105.80
2	F	16	DA	C5-C6-N1	14.13	124.76	117.70
2	F	16	DA	C8-N9-C4	-13.98	100.21	105.80
1	E	5	DG	O5'-P-OP1	-13.89	93.20	105.70
2	F	14	DT	C2-N3-C4	-13.80	118.92	127.20
2	F	17	DA	O5'-P-OP2	-13.79	93.29	105.70
1	E	13	DT	C6-N1-C2	-13.73	114.43	121.30
1	E	11	DA	N1-C6-N6	13.69	126.81	118.60
1	E	10	DT	C6-N1-C2	-13.68	114.46	121.30
2	F	3	DC	O4'-C1'-C2'	13.61	116.79	105.90
1	E	1	DC	C2-N3-C4	13.60	126.70	119.90
1	E	13	DT	C2-N3-C4	-13.54	119.08	127.20
2	F	14	DT	C4-C5-C6	-13.44	109.94	118.00
1	E	16	DA	OP1-P-OP2	13.35	139.62	119.60
2	F	5	DG	N3-C2-N2	13.33	129.23	119.90
1	E	13	DT	N1-C2-N3	13.27	122.56	114.60
2	F	16	DA	C4-C5-N7	13.23	117.32	110.70
2	F	2	DG	N7-C8-N9	13.20	119.70	113.10
1	E	14	DT	N3-C2-O2	-13.18	114.39	122.30
1	E	20	DG	C4-C5-C6	13.15	126.69	118.80
1	E	12	DA	C4-C5-C6	13.12	123.56	117.00
1	E	5	DG	C8-N9-C4	-13.06	101.18	106.40
1	E	6	DT	C5-C6-N1	13.06	131.53	123.70
2	F	10	DA	C4-C5-C6	13.04	123.52	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	4	DG	C5-C6-N1	-13.04	104.98	111.50
1	E	14	DT	C4-C5-C6	-13.02	110.19	118.00
1	E	17	DC	N3-C4-N4	13.01	127.11	118.00
2	F	5	DG	C6-N1-C2	-12.95	117.33	125.10
2	F	19	DC	OP1-P-O3'	-12.90	76.83	105.20
2	F	13	DA	C4'-C3'-C2'	-12.68	91.68	103.10
2	F	7	DT	P-O3'-C3'	-12.57	104.61	119.70
1	E	5	DG	C5-C6-N1	-12.56	105.22	111.50
2	F	13	DA	C4-C5-N7	-12.53	104.44	110.70
1	E	15	DC	C5-C4-N4	-12.44	111.49	120.20
1	E	9	DA	C5-N7-C8	12.43	110.11	103.90
1	E	18	DC	O4'-C1'-N1	12.42	116.69	108.00
2	F	21	DA	N1-C6-N6	12.37	126.02	118.60
1	E	18	DC	C2-N3-C4	-12.35	113.72	119.90
1	E	7	DT	O4'-C1'-C2'	-12.35	96.02	105.90
1	E	20	DG	N9-C4-C5	12.35	110.34	105.40
2	F	3	DC	C4'-C3'-C2'	12.33	114.20	103.10
2	F	12	DT	N1-C2-N3	12.30	121.98	114.60
1	E	20	DG	C5-C6-O6	12.29	135.97	128.60
2	F	21	DA	O4'-C1'-N9	12.23	116.56	108.00
2	F	11	DT	C5-C6-N1	12.21	131.03	123.70
2	F	5	DG	P-O3'-C3'	-12.14	105.13	119.70
1	E	9	DA	N1-C2-N3	12.14	135.37	129.30
1	E	10	DT	C5'-C4'-C3'	12.12	135.91	114.10
2	F	18	DC	O4'-C1'-N1	12.09	116.46	108.00
2	F	12	DT	C2-N3-C4	-12.03	119.98	127.20
2	F	18	DC	N3-C2-O2	12.03	130.32	121.90
2	F	19	DC	O5'-P-OP1	-12.00	94.90	105.70
1	E	11	DA	C5-N7-C8	-12.00	97.90	103.90
1	E	16	DA	C2-N3-C4	-11.98	104.61	110.60
2	F	11	DT	C1'-O4'-C4'	11.95	122.05	110.10
1	E	10	DT	C4-C5-C7	11.94	126.16	119.00
2	F	8	DG	C5-C6-N1	11.91	117.46	111.50
1	E	6	DT	C4-C5-C6	-11.83	110.90	118.00
2	F	10	DA	N9-C4-C5	11.77	110.51	105.80
2	F	6	DG	O4'-C4'-C3'	11.74	113.05	106.00
1	E	6	DT	P-O3'-C3'	-11.74	105.61	119.70
3	A	175	LYS	CD-CE-NZ	11.74	138.70	111.70
2	F	10	DA	O4'-C1'-N9	-11.68	99.82	108.00
1	E	5	DG	C2-N3-C4	-11.59	106.10	111.90
3	A	276	ARG	NE-CZ-NH2	-11.58	114.51	120.30
1	E	19	DA	C6-N1-C2	11.54	125.52	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	21	DA	N1-C2-N3	-11.48	123.56	129.30
2	F	4	DT	N1-C2-O2	-11.47	113.92	123.10
2	F	3	DC	C6-N1-C2	11.41	124.86	120.30
1	E	10	DT	C6-C5-C7	11.40	129.74	122.90
1	E	3	DT	O5'-P-OP1	-11.37	95.47	105.70
2	F	2	DG	C5-C6-N1	-11.37	105.82	111.50
1	E	19	DA	C5-C6-N1	-11.36	112.02	117.70
1	E	11	DA	C6-N1-C2	-11.34	111.80	118.60
3	A	128	TYR	CZ-CE2-CD2	11.33	130.00	119.80
1	E	1	DC	C5-C6-N1	11.26	126.63	121.00
2	F	18	DC	O5'-P-OP1	11.23	124.17	110.70
1	E	7	DT	N1-C2-O2	11.18	132.04	123.10
1	E	7	DT	C3'-C2'-C1'	11.15	115.88	102.50
1	E	6	DT	O4'-C1'-N1	11.08	115.75	108.00
2	F	7	DT	O5'-P-OP1	-10.97	95.83	105.70
2	F	17	DA	C2-N3-C4	10.92	116.06	110.60
2	F	6	DG	N1-C2-N2	-10.88	106.41	116.20
1	E	10	DT	P-O3'-C3'	-10.86	106.67	119.70
2	F	7	DT	N3-C4-O4	-10.79	113.42	119.90
3	B	281	SER	C-N-CA	-10.78	94.75	121.70
1	E	14	DT	C2-N3-C4	-10.77	120.74	127.20
1	E	3	DT	N3-C4-C5	-10.76	108.74	115.20
2	F	21	DA	O5'-P-OP1	10.74	123.59	110.70
2	F	6	DG	C1'-O4'-C4'	-10.71	99.39	110.10
1	E	3	DT	N1-C2-O2	-10.70	114.54	123.10
2	F	19	DC	C2-N3-C4	-10.70	114.55	119.90
2	F	10	DA	OP1-P-OP2	10.66	135.59	119.60
3	A	165	ARG	NE-CZ-NH2	-10.63	114.99	120.30
1	E	1	DC	O4'-C4'-C3'	-10.62	99.63	106.00
3	B	235	ARG	NE-CZ-NH1	-10.55	115.03	120.30
1	E	16	DA	N9-C4-C5	-10.51	101.60	105.80
2	F	2	DG	O4'-C1'-N9	10.50	115.35	108.00
1	E	5	DG	OP1-P-OP2	10.47	135.30	119.60
2	F	2	DG	C5-N7-C8	-10.46	99.07	104.30
2	F	6	DG	N1-C2-N3	10.45	130.17	123.90
1	E	11	DA	N3-C4-N9	-10.42	119.06	127.40
1	E	1	DC	N1-C2-N3	-10.39	111.93	119.20
1	E	12	DA	C4-C5-N7	-10.37	105.51	110.70
3	B	283	ALA	N-CA-CB	-10.29	95.70	110.10
2	F	12	DT	C6-N1-C2	-10.26	116.17	121.30
3	B	156	LYS	CD-CE-NZ	10.26	135.29	111.70
3	A	113	MET	CG-SD-CE	10.21	116.54	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	7	DT	N1-C2-O2	10.20	131.26	123.10
2	F	16	DA	O5'-P-OP2	-10.19	96.53	105.70
2	F	20	DA	P-O3'-C3'	-10.17	107.49	119.70
1	E	8	DA	N7-C8-N9	-10.17	108.72	113.80
3	A	308	ALA	CA-C-O	-10.12	98.86	120.10
1	E	1	DC	N1-C2-O2	10.10	124.96	118.90
2	F	20	DA	C5'-C4'-C3'	-10.09	95.95	114.10
1	E	9	DA	C5'-C4'-C3'	10.05	132.20	114.10
1	E	19	DA	O4'-C4'-C3'	-10.04	99.97	106.00
1	E	17	DC	N3-C2-O2	10.03	128.92	121.90
1	E	5	DG	N1-C2-N2	-10.01	107.19	116.20
1	E	1	DC	O4'-C1'-N1	-9.98	101.01	108.00
2	F	4	DT	N1-C2-N3	9.97	120.58	114.60
1	E	10	DT	O4'-C4'-C3'	-9.88	100.07	106.00
1	E	3	DT	C2-N1-C1'	-9.83	102.47	118.20
2	F	10	DA	C6-N1-C2	-9.82	112.71	118.60
2	F	19	DC	O4'-C4'-C3'	-9.80	100.12	106.00
1	E	19	DA	N1-C6-N6	9.79	124.47	118.60
1	E	17	DC	O3'-P-O5'	-9.78	85.43	104.00
3	B	91	ILE	CB-CA-C	-9.77	92.06	111.60
1	E	5	DG	N1-C6-O6	9.73	125.74	119.90
1	E	13	DT	O4'-C4'-C3'	-9.72	100.17	106.00
2	F	10	DA	N1-C2-N3	9.69	134.15	129.30
1	E	15	DC	C6-N1-C2	-9.69	116.42	120.30
2	F	8	DG	O4'-C1'-C2'	-9.69	98.15	105.90
3	B	120	ARG	NE-CZ-NH1	-9.67	115.47	120.30
1	E	8	DA	O5'-P-OP1	-9.63	97.03	105.70
1	E	5	DG	N1-C2-N3	9.60	129.66	123.90
2	F	15	DT	C5-C6-N1	9.58	129.45	123.70
1	E	15	DC	C4-C5-C6	-9.52	112.64	117.40
2	F	17	DA	O4'-C1'-C2'	9.49	113.49	105.90
1	E	17	DC	C2-N3-C4	9.47	124.64	119.90
2	F	15	DT	C6-N1-C2	-9.46	116.57	121.30
2	F	11	DT	C6-C5-C7	9.42	128.55	122.90
1	E	15	DC	N1-C2-N3	9.41	125.79	119.20
2	F	4	DT	N3-C4-O4	9.40	125.54	119.90
1	E	19	DA	N9-C4-C5	-9.36	102.06	105.80
2	F	6	DG	C4-C5-N7	-9.36	107.06	110.80
1	E	10	DT	N3-C4-O4	-9.36	114.28	119.90
1	E	12	DA	N3-C4-C5	-9.33	120.27	126.80
1	E	1	DC	C5'-C4'-C3'	9.31	130.87	114.10
1	E	13	DT	C4-C5-C6	-9.31	112.41	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	8	DA	C1'-O4'-C4'	-9.31	100.79	110.10
2	F	7	DT	C2-N3-C4	-9.30	121.62	127.20
2	F	11	DT	C4-C5-C7	9.29	124.58	119.00
2	F	16	DA	C5-C6-N6	-9.25	116.30	123.70
2	F	2	DG	C2-N3-C4	-9.25	107.28	111.90
2	F	16	DA	O4'-C1'-C2'	-9.22	98.52	105.90
2	F	9	DA	C1'-O4'-C4'	-9.19	100.91	110.10
2	F	4	DT	C1'-O4'-C4'	-9.16	100.94	110.10
2	F	5	DG	O4'-C1'-N9	9.14	114.40	108.00
3	B	264	LEU	CB-CG-CD1	9.14	126.53	111.00
2	F	6	DG	N9-C4-C5	9.10	109.04	105.40
3	A	137	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	E	8	DA	OP2-P-O3'	9.07	125.15	105.20
1	E	6	DT	O3'-P-O5'	-9.05	86.81	104.00
2	F	15	DT	C5-C4-O4	-9.05	118.57	124.90
2	F	18	DC	C5-C4-N4	-9.04	113.87	120.20
2	F	6	DG	O4'-C1'-N9	9.02	114.31	108.00
2	F	4	DT	C5-C4-O4	-8.98	118.61	124.90
3	B	91	ILE	CG1-CB-CG2	-8.96	91.68	111.40
3	A	154	LEU	CA-CB-CG	8.96	135.90	115.30
2	F	16	DA	C6-N1-C2	-8.95	113.23	118.60
3	B	137	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	E	18	DC	P-O3'-C3'	8.93	130.42	119.70
2	F	8	DG	C4'-C3'-C2'	-8.93	95.06	103.10
1	E	16	DA	C5-N7-C8	8.91	108.35	103.90
1	E	14	DT	N3-C4-C5	8.90	120.54	115.20
3	A	123	LYS	CD-CE-NZ	8.89	132.15	111.70
3	B	276	ARG	NH1-CZ-NH2	8.89	129.17	119.40
1	E	12	DA	O4'-C1'-C2'	-8.88	98.80	105.90
3	B	170	THR	CA-CB-CG2	-8.87	99.98	112.40
2	F	15	DT	N3-C4-O4	8.87	125.22	119.90
2	F	2	DG	N3-C4-C5	8.86	133.03	128.60
2	F	19	DC	C6-N1-C2	8.85	123.84	120.30
2	F	17	DA	P-O5'-C5'	-8.82	106.78	120.90
2	F	10	DA	N3-C4-C5	-8.81	120.64	126.80
2	F	5	DG	C5-C6-O6	-8.80	123.32	128.60
2	F	18	DC	C5-C6-N1	8.77	125.38	121.00
1	E	9	DA	C6-C5-N7	8.72	138.41	132.30
2	F	3	DC	N3-C4-C5	-8.72	118.41	121.90
1	E	8	DA	C6-N1-C2	-8.72	113.37	118.60
2	F	20	DA	O4'-C1'-C2'	-8.72	98.92	105.90
1	E	1	DC	N3-C4-C5	-8.71	118.42	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	18	DC	C4-C5-C6	8.71	121.75	117.40
1	E	20	DG	N7-C8-N9	-8.69	108.75	113.10
1	E	14	DT	C5-C6-N1	8.69	128.91	123.70
1	E	8	DA	N9-C4-C5	8.68	109.27	105.80
1	E	19	DA	N7-C8-N9	-8.67	109.47	113.80
1	E	5	DG	N7-C8-N9	8.60	117.40	113.10
1	E	14	DT	O3'-P-O5'	-8.59	87.68	104.00
2	F	10	DA	N1-C6-N6	-8.59	113.45	118.60
3	A	303	ARG	NE-CZ-NH2	-8.57	116.01	120.30
3	B	280	PRO	N-CD-CG	-8.56	90.36	103.20
2	F	4	DT	O3'-P-O5'	8.56	120.26	104.00
2	F	21	DA	C5-C6-N6	-8.51	116.89	123.70
1	E	10	DT	OP2-P-O3'	8.51	123.92	105.20
1	E	15	DC	P-O3'-C3'	8.49	129.89	119.70
2	F	17	DA	OP1-P-OP2	8.49	132.33	119.60
1	E	14	DT	O4'-C1'-N1	8.48	113.94	108.00
1	E	9	DA	C4-C5-C6	8.48	121.24	117.00
2	F	12	DT	O4'-C4'-C3'	8.46	111.08	106.00
2	F	16	DA	C2-N3-C4	8.45	114.82	110.60
3	B	247	TYR	CB-CG-CD1	8.42	126.05	121.00
2	F	13	DA	O5'-P-OP2	-8.36	98.17	105.70
1	E	6	DT	OP1-P-O3'	-8.36	86.81	105.20
1	E	3	DT	C6-N1-C1'	8.33	132.89	120.40
1	E	6	DT	N1-C2-O2	8.33	129.76	123.10
1	E	5	DG	C4'-C3'-C2'	-8.29	95.64	103.10
1	E	17	DC	N1-C2-O2	-8.29	113.93	118.90
2	F	2	DG	C6-C5-N7	-8.28	125.43	130.40
2	F	4	DT	O5'-P-OP1	8.28	120.64	110.70
3	A	252	ARG	NE-CZ-NH1	-8.28	116.16	120.30
2	F	13	DA	C5-C6-N6	8.25	130.30	123.70
2	F	9	DA	P-O3'-C3'	-8.23	109.83	119.70
1	E	9	DA	O4'-C1'-C2'	-8.21	99.33	105.90
3	A	112	ARG	NE-CZ-NH1	8.20	124.40	120.30
3	B	288	SER	N-CA-CB	-8.19	98.21	110.50
3	B	179	ILE	CG1-CB-CG2	-8.19	93.38	111.40
2	F	17	DA	N1-C6-N6	-8.19	113.69	118.60
1	E	5	DG	N3-C4-C5	-8.18	124.51	128.60
1	E	13	DT	N3-C2-O2	-8.18	117.39	122.30
2	F	18	DC	N1-C2-N3	8.16	124.92	119.20
2	F	10	DA	C5-C6-N6	8.16	130.23	123.70
2	F	10	DA	C5'-C4'-O4'	-8.16	93.80	109.30
3	A	98	LEU	CB-CG-CD1	8.13	124.82	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1	DC	OP1-P-O3'	8.13	123.08	105.20
2	F	19	DC	N1-C2-N3	8.12	124.89	119.20
1	E	7	DT	OP2-P-O3'	8.11	123.04	105.20
1	E	12	DA	C4'-C3'-C2'	-8.11	95.80	103.10
1	E	8	DA	C3'-C2'-C1'	-8.09	92.79	102.50
2	F	5	DG	C5'-C4'-O4'	8.09	124.67	109.30
1	E	4	DG	P-O3'-C3'	-8.05	110.04	119.70
2	F	3	DC	N3-C2-O2	8.03	127.52	121.90
1	E	15	DC	OP1-P-OP2	-8.01	107.58	119.60
2	F	9	DA	N1-C6-N6	8.00	123.40	118.60
1	E	19	DA	C5'-C4'-C3'	-7.99	99.72	114.10
2	F	2	DG	C5'-C4'-O4'	7.98	124.45	109.30
2	F	3	DC	C4-C5-C6	7.97	121.39	117.40
1	E	7	DT	C5-C4-O4	-7.94	119.34	124.90
1	E	7	DT	O4'-C1'-N1	7.92	113.54	108.00
2	F	6	DG	C2-N3-C4	-7.91	107.94	111.90
3	A	107	ARG	NE-CZ-NH2	-7.90	116.35	120.30
2	F	17	DA	N1-C2-N3	-7.89	125.36	129.30
2	F	11	DT	C4'-C3'-C2'	7.86	110.17	103.10
2	F	11	DT	C5'-C4'-C3'	7.86	128.24	114.10
3	A	181	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	E	16	DA	O4'-C1'-N9	7.84	113.49	108.00
1	E	11	DA	O4'-C1'-C2'	-7.79	99.67	105.90
2	F	5	DG	N1-C2-N3	7.79	128.57	123.90
2	F	14	DT	O4'-C1'-N1	7.76	113.43	108.00
1	E	11	DA	C4-C5-C6	7.75	120.88	117.00
2	F	17	DA	O4'-C1'-N9	7.71	113.40	108.00
1	E	20	DG	P-O5'-C5'	7.71	133.23	120.90
1	E	8	DA	C5-C6-N1	7.69	121.55	117.70
1	E	20	DG	N3-C4-N9	-7.68	121.39	126.00
2	F	4	DT	O4'-C4'-C3'	7.68	110.61	106.00
1	E	3	DT	N3-C4-O4	7.67	124.50	119.90
1	E	7	DT	C1'-O4'-C4'	7.66	117.76	110.10
2	F	11	DT	C6-N1-C2	-7.66	117.47	121.30
1	E	14	DT	C5-C4-O4	-7.66	119.54	124.90
1	E	18	DC	P-O5'-C5'	7.62	133.10	120.90
3	B	111	ASP	CB-CG-OD1	-7.61	111.45	118.30
2	F	2	DG	OP2-P-O3'	-7.60	88.48	105.20
2	F	20	DA	C5'-C4'-O4'	7.59	123.72	109.30
1	E	1	DC	C4'-C3'-C2'	7.55	109.90	103.10
1	E	10	DT	OP1-P-OP2	7.55	130.93	119.60
2	F	4	DT	C4'-C3'-C2'	-7.55	96.31	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	169	TYR	CB-CG-CD1	-7.54	116.48	121.00
2	F	20	DA	C5-C6-N6	7.51	129.71	123.70
1	E	1	DC	OP2-P-O3'	-7.51	88.69	105.20
1	E	18	DC	C5'-C4'-O4'	7.50	123.56	109.30
2	F	4	DT	C2-N3-C4	-7.50	122.70	127.20
2	F	11	DT	N3-C4-O4	-7.50	115.40	119.90
1	E	7	DT	C2-N3-C4	-7.47	122.72	127.20
2	F	7	DT	C6-C5-C7	7.47	127.38	122.90
1	E	19	DA	C5-N7-C8	7.46	107.63	103.90
2	F	7	DT	C4-C5-C7	7.44	123.46	119.00
2	F	11	DT	C5'-C4'-O4'	-7.43	95.18	109.30
1	E	16	DA	C5-C6-N1	-7.42	113.99	117.70
1	E	2	DT	P-O5'-C5'	7.42	132.77	120.90
3	B	281	SER	N-CA-CB	7.41	121.62	110.50
1	E	6	DT	N3-C2-O2	-7.41	117.85	122.30
2	F	18	DC	C5'-C4'-O4'	7.41	123.38	109.30
2	F	8	DG	OP2-P-O3'	7.40	121.47	105.20
1	E	1	DC	N1-C1'-C2'	7.37	126.59	112.60
1	E	16	DA	C8-N9-C4	7.33	108.73	105.80
1	E	4	DG	OP1-P-OP2	7.33	130.60	119.60
2	F	4	DT	O5'-P-OP2	-7.32	99.11	105.70
3	B	110	VAL	CB-CA-C	-7.32	97.49	111.40
1	E	16	DA	C5-C6-N6	7.31	129.55	123.70
3	A	270	ARG	NE-CZ-NH2	7.30	123.95	120.30
3	A	251	ASP	CB-CG-OD1	7.30	124.87	118.30
2	F	4	DT	O4'-C1'-C2'	7.29	111.73	105.90
2	F	19	DC	N1-C2-O2	7.29	123.28	118.90
1	E	11	DA	C5-C6-N1	-7.27	114.07	117.70
2	F	6	DG	OP1-P-OP2	7.26	130.50	119.60
2	F	16	DA	O5'-P-OP1	7.26	119.41	110.70
2	F	14	DT	P-O3'-C3'	7.25	128.40	119.70
1	E	12	DA	N7-C8-N9	7.24	117.42	113.80
2	F	19	DC	C5-C4-N4	7.23	125.26	120.20
1	E	20	DG	N3-C2-N2	-7.22	114.84	119.90
2	F	11	DT	N1-C2-O2	-7.21	117.33	123.10
1	E	15	DC	N3-C2-O2	-7.20	116.86	121.90
1	E	8	DA	N3-C4-C5	-7.20	121.76	126.80
3	B	169	TYR	CB-CG-CD2	7.16	125.29	121.00
2	F	20	DA	N1-C6-N6	-7.15	114.31	118.60
3	B	165	ARG	NE-CZ-NH2	-7.11	116.74	120.30
3	B	246	LEU	CB-CG-CD2	-7.11	98.92	111.00
1	E	6	DT	C4'-C3'-C2'	-7.10	96.71	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	4	DT	C5'-C4'-C3'	-7.09	101.35	114.10
1	E	18	DC	C5-C6-N1	-7.07	117.47	121.00
2	F	7	DT	OP1-P-OP2	7.04	130.15	119.60
2	F	3	DC	O4'-C1'-N1	7.03	112.92	108.00
2	F	5	DG	OP1-P-OP2	7.02	130.12	119.60
3	A	257	SER	N-CA-CB	7.01	121.02	110.50
1	E	10	DT	C5-C4-O4	-7.01	119.99	124.90
2	F	21	DA	C4-C5-N7	7.00	114.20	110.70
3	A	246	LEU	CA-CB-CG	-7.00	99.19	115.30
1	E	6	DT	OP2-P-O3'	7.00	120.59	105.20
3	A	165	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	E	15	DC	OP2-P-O3'	-6.95	89.92	105.20
2	F	2	DG	C6-N1-C2	6.94	129.26	125.10
3	B	140	VAL	CG1-CB-CG2	-6.93	99.81	110.90
1	E	14	DT	C4-C5-C7	6.92	123.15	119.00
2	F	14	DT	C4-C5-C7	6.91	123.14	119.00
2	F	20	DA	O4'-C4'-C3'	-6.90	101.74	104.50
3	B	172	TYR	N-CA-CB	-6.89	98.19	110.60
3	B	90	SER	N-CA-CB	6.88	120.83	110.50
1	E	16	DA	C6-N1-C2	6.88	122.73	118.60
2	F	12	DT	N1-C1'-C2'	6.87	125.66	112.60
3	B	232	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	E	12	DA	C3'-C2'-C1'	6.87	110.74	102.50
2	F	10	DA	C6-C5-N7	6.85	137.10	132.30
2	F	18	DC	P-O5'-C5'	-6.85	109.94	120.90
2	F	7	DT	N1-C1'-C2'	6.85	125.61	112.60
1	E	20	DG	C6-N1-C2	6.83	129.20	125.10
2	F	6	DG	O5'-P-OP2	6.83	118.90	110.70
3	B	177	ARG	CG-CD-NE	6.83	126.14	111.80
1	E	19	DA	O3'-P-O5'	-6.82	91.03	104.00
1	E	5	DG	C1'-O4'-C4'	-6.81	103.29	110.10
2	F	16	DA	P-O3'-C3'	6.80	127.86	119.70
3	B	126	LYS	CD-CE-NZ	6.79	127.32	111.70
3	B	150	LEU	CB-CG-CD1	-6.79	99.45	111.00
3	B	276	ARG	CG-CD-NE	-6.79	97.55	111.80
3	B	177	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	E	19	DA	C3'-C2'-C1'	-6.78	94.37	102.50
2	F	10	DA	O4'-C4'-C3'	6.77	110.06	106.00
3	A	232	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	E	8	DA	OP1-P-O3'	-6.75	90.35	105.20
1	E	19	DA	O5'-P-OP1	6.74	118.79	110.70
1	E	12	DA	C5-C6-N1	6.73	121.07	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	5	DG	N9-C4-C5	6.73	108.09	105.40
2	F	13	DA	N3-C4-N9	-6.72	122.03	127.40
1	E	3	DT	N1-C1'-C2'	6.71	125.35	112.60
3	A	257	SER	O-C-N	6.71	133.43	122.70
1	E	15	DC	C5-C6-N1	6.69	124.35	121.00
3	A	295	ARG	NE-CZ-NH2	-6.67	116.96	120.30
2	F	6	DG	C4-C5-C6	6.67	122.80	118.80
2	F	8	DG	C2-N3-C4	-6.66	108.57	111.90
3	A	180	LEU	CA-CB-CG	6.66	130.63	115.30
3	A	90	SER	N-CA-CB	6.63	120.45	110.50
3	A	125	ILE	CB-CA-C	-6.62	98.35	111.60
3	A	109	GLU	OE1-CD-OE2	-6.60	115.38	123.30
1	E	10	DT	N1-C2-N3	6.60	118.56	114.60
1	E	15	DC	C2-N1-C1'	6.59	126.05	118.80
1	E	6	DT	C6-N1-C2	-6.59	118.01	121.30
1	E	16	DA	N7-C8-N9	-6.58	110.51	113.80
3	A	278	VAL	CB-CA-C	-6.57	98.91	111.40
2	F	14	DT	C6-C5-C7	6.57	126.84	122.90
3	A	174	ARG	NE-CZ-NH1	-6.53	117.03	120.30
3	A	235	ARG	NE-CZ-NH1	6.53	123.56	120.30
3	B	117	ASP	CB-CG-OD1	6.53	124.17	118.30
2	F	11	DT	P-O3'-C3'	-6.51	111.89	119.70
1	E	8	DA	C4-C5-C6	6.49	120.25	117.00
3	A	130	GLN	N-CA-CB	-6.49	98.91	110.60
1	E	12	DA	OP1-P-O3'	6.48	119.45	105.20
3	B	284	HIS	N-CA-C	-6.48	93.52	111.00
3	B	173	VAL	CB-CA-C	-6.47	99.11	111.40
3	B	246	LEU	CB-CG-CD1	-6.44	100.06	111.00
3	A	130	GLN	CA-CB-CG	6.42	127.52	113.40
1	E	18	DC	O5'-P-OP1	-6.39	99.95	105.70
2	F	13	DA	P-O3'-C3'	-6.39	112.03	119.70
3	B	163	GLN	N-CA-CB	-6.39	99.10	110.60
2	F	13	DA	O4'-C1'-N9	-6.36	103.55	108.00
2	F	13	DA	C4-C5-C6	6.36	120.18	117.00
1	E	10	DT	O4'-C1'-N1	-6.36	103.55	108.00
3	B	165	ARG	NE-CZ-NH1	-6.36	117.12	120.30
2	F	5	DG	C5-C6-N1	6.34	114.67	111.50
2	F	3	DC	C5-C6-N1	-6.34	117.83	121.00
1	E	19	DA	O4'-C1'-C2'	-6.33	100.83	105.90
2	F	6	DG	N3-C4-C5	-6.33	125.44	128.60
2	F	12	DT	N1-C2-O2	-6.32	118.04	123.10
2	F	11	DT	O4'-C1'-N1	6.32	112.42	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	17	DC	P-O3'-C3'	6.32	127.28	119.70
1	E	19	DA	O4'-C1'-N9	-6.30	103.59	108.00
3	A	110	VAL	CA-CB-CG2	-6.30	101.45	110.90
2	F	2	DG	C4-C5-N7	6.29	113.31	110.80
3	B	159	PRO	N-CD-CG	6.27	112.61	103.20
1	E	11	DA	P-O3'-C3'	6.27	127.22	119.70
1	E	14	DT	C6-C5-C7	6.27	126.66	122.90
3	A	126	LYS	CB-CA-C	-6.27	97.86	110.40
3	B	137	ARG	CA-CB-CG	-6.26	99.62	113.40
1	E	2	DT	N3-C4-C5	6.26	118.95	115.20
2	F	6	DG	C4'-C3'-C2'	-6.25	97.48	103.10
1	E	12	DA	O4'-C1'-N9	-6.25	103.63	108.00
3	A	107	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	E	13	DT	C5-C6-N1	6.21	127.43	123.70
3	B	275	GLN	CA-CB-CG	6.20	127.05	113.40
2	F	3	DC	C5'-C4'-O4'	-6.20	97.53	109.30
1	E	2	DT	OP1-P-OP2	-6.19	110.31	119.60
2	F	20	DA	N1-C2-N3	6.19	132.40	129.30
1	E	17	DC	O5'-P-OP2	6.17	118.10	110.70
3	A	151	SER	N-CA-CB	6.17	119.75	110.50
1	E	11	DA	C5'-C4'-C3'	6.16	125.19	114.10
3	B	171	TRP	CA-CB-CG	-6.15	102.02	113.70
2	F	8	DG	N3-C2-N2	-6.14	115.60	119.90
3	A	112	ARG	CG-CD-NE	6.14	124.70	111.80
3	B	237	LYS	CB-CG-CD	6.14	127.58	111.60
3	A	305	LYS	N-CA-CB	6.13	121.64	110.60
3	B	116	GLU	N-CA-CB	-6.12	99.58	110.60
2	F	19	DC	O5'-P-OP2	-6.12	100.19	105.70
3	A	178	GLU	N-CA-CB	-6.12	99.59	110.60
3	A	168	LEU	N-CA-C	-6.09	94.56	111.00
3	B	145	LEU	CB-CG-CD1	6.09	121.35	111.00
2	F	4	DT	P-O3'-C3'	-6.08	112.40	119.70
2	F	14	DT	C5-C4-O4	-6.08	120.64	124.90
3	B	158	THR	CA-CB-CG2	-6.08	103.89	112.40
3	B	165	ARG	NH1-CZ-NH2	6.07	126.08	119.40
2	F	6	DG	O4'-C1'-C2'	6.07	110.75	105.90
3	A	246	LEU	CB-CG-CD1	-6.06	100.69	111.00
2	F	21	DA	O4'-C1'-C2'	6.05	110.74	105.90
3	B	159	PRO	CB-CG-CD	-6.05	82.91	106.50
1	E	14	DT	OP1-P-OP2	6.05	128.67	119.60
2	F	13	DA	O4'-C4'-C3'	6.04	109.62	106.00
3	B	145	LEU	CB-CG-CD2	-6.03	100.75	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	16	DA	OP2-P-O3'	6.03	118.46	105.20
1	E	18	DC	C6-N1-C1'	-6.03	113.57	120.80
3	A	280	PRO	CA-N-CD	-6.03	103.06	111.50
2	F	14	DT	C4'-C3'-C2'	-6.02	97.68	103.10
3	A	304	ARG	N-CA-C	-6.01	94.78	111.00
1	E	6	DT	C4-C5-C7	6.00	122.60	119.00
1	E	4	DG	N3-C4-C5	6.00	131.60	128.60
1	E	6	DT	C6-C5-C7	6.00	126.50	122.90
1	E	7	DT	O5'-P-OP1	5.99	117.89	110.70
3	A	173	VAL	CA-CB-CG1	-5.99	101.92	110.90
2	F	11	DT	O5'-P-OP2	-5.98	100.31	105.70
2	F	15	DT	C5'-C4'-C3'	-5.97	103.36	114.10
3	A	245	ILE	C-N-CA	-5.91	106.92	121.70
2	F	3	DC	N3-C4-N4	5.90	122.13	118.00
2	F	15	DT	O5'-P-OP2	5.89	117.77	110.70
3	B	153	HIS	C-N-CA	-5.88	107.00	121.70
3	A	135	PRO	C-N-CA	-5.88	107.00	121.70
3	B	92	LEU	CB-CG-CD2	5.88	120.99	111.00
3	A	111	ASP	CB-CG-OD1	-5.88	113.01	118.30
1	E	8	DA	C6-C5-N7	5.87	136.41	132.30
2	F	21	DA	C5'-C4'-C3'	5.87	124.67	114.10
2	F	7	DT	OP1-P-O3'	5.87	118.11	105.20
2	F	21	DA	C6-C5-N7	-5.84	128.21	132.30
2	F	8	DG	N1-C2-N2	-5.84	110.94	116.20
1	E	10	DT	C6-N1-C1'	5.83	129.15	120.40
3	B	296	VAL	CA-CB-CG2	-5.83	102.15	110.90
3	A	181	ARG	N-CA-C	-5.83	95.25	111.00
3	B	180	LEU	CB-CG-CD1	5.83	120.92	111.00
1	E	18	DC	N3-C2-O2	-5.81	117.83	121.90
1	E	3	DT	C6-N1-C2	5.81	124.20	121.30
3	B	297	TYR	CA-CB-CG	-5.80	102.38	113.40
1	E	8	DA	C5-C6-N6	5.79	128.33	123.70
1	E	2	DT	OP2-P-O3'	5.78	117.92	105.20
3	B	282	LYS	CA-C-N	-5.78	104.48	117.20
1	E	8	DA	O5'-P-OP2	5.77	117.63	110.70
1	E	2	DT	C5-C4-O4	-5.77	120.86	124.90
1	E	11	DA	C5-C6-N6	-5.77	119.08	123.70
2	F	4	DT	C6-N1-C2	-5.77	118.42	121.30
3	A	169	TYR	CB-CG-CD1	-5.76	117.54	121.00
2	F	5	DG	N3-C4-C5	-5.76	125.72	128.60
2	F	13	DA	OP2-P-O3'	5.76	117.88	105.20
3	A	302	ASN	CA-C-N	-5.76	104.53	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	233	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	E	18	DC	C5-C4-N4	-5.74	116.18	120.20
2	F	13	DA	C5-N7-C8	5.74	106.77	103.90
3	B	265	VAL	CB-CA-C	-5.72	100.53	111.40
3	B	117	ASP	OD1-CG-OD2	-5.72	112.44	123.30
2	F	13	DA	OP1-P-OP2	5.72	128.17	119.60
2	F	10	DA	N9-C1'-C2'	5.69	123.41	112.60
2	F	16	DA	C6-C5-N7	-5.69	128.32	132.30
3	A	167	ALA	C-N-CA	-5.68	107.49	121.70
3	A	252	ARG	CA-C-N	5.68	129.70	117.20
3	A	110	VAL	CB-CA-C	-5.67	100.63	111.40
2	F	2	DG	C5-C6-O6	-5.66	125.20	128.60
3	B	165	ARG	CA-C-N	-5.66	104.74	117.20
2	F	11	DT	N1-C2-N3	5.66	118.00	114.60
3	A	142	VAL	CA-CB-CG1	-5.66	102.41	110.90
1	E	12	DA	C4-N9-C1'	5.66	136.48	126.30
3	B	137	ARG	NH1-CZ-NH2	5.66	125.62	119.40
1	E	5	DG	C4-N9-C1'	5.64	133.84	126.50
3	B	117	ASP	CB-CG-OD2	5.64	123.38	118.30
3	A	246	LEU	CB-CG-CD2	-5.63	101.43	111.00
3	B	152	GLN	CA-CB-CG	-5.63	101.02	113.40
3	A	134	ILE	CG1-CB-CG2	5.61	123.75	111.40
3	B	158	THR	CB-CA-C	-5.61	96.46	111.60
3	A	276	ARG	NH1-CZ-NH2	5.60	125.56	119.40
2	F	19	DC	N3-C4-N4	-5.60	114.08	118.00
3	A	286	LEU	N-CA-CB	-5.59	99.22	110.40
3	B	242	SER	CA-CB-OG	5.57	126.24	111.20
1	E	16	DA	N3-C4-C5	5.57	130.70	126.80
2	F	7	DT	C5-C6-N1	5.56	127.04	123.70
3	B	123	LYS	CG-CD-CE	5.56	128.59	111.90
3	B	290	LEU	CB-CA-C	-5.56	99.64	110.20
3	A	239	GLY	N-CA-C	-5.56	99.20	113.10
3	B	175	LYS	N-CA-CB	-5.55	100.62	110.60
3	A	186	THR	N-CA-C	5.54	125.97	111.00
3	A	120	ARG	CA-CB-CG	-5.54	101.21	113.40
1	E	2	DT	C5-C6-N1	5.54	127.02	123.70
2	F	10	DA	OP2-P-O3'	5.53	117.37	105.20
1	E	9	DA	C4-N9-C1'	5.53	136.25	126.30
3	A	299	TRP	CB-CA-C	-5.50	99.41	110.40
2	F	21	DA	N9-C4-C5	-5.49	103.60	105.80
1	E	13	DT	OP1-P-O3'	-5.48	93.14	105.20
3	B	174	ARG	NE-CZ-NH2	5.48	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	110	VAL	N-CA-CB	5.47	123.54	111.50
3	B	119	TRP	CH2-CZ2-CE2	-5.46	111.94	117.40
1	E	11	DA	O4'-C1'-N9	-5.46	104.18	108.00
3	B	247	TYR	OH-CZ-CE2	-5.46	105.36	120.10
2	F	2	DG	N9-C4-C5	-5.46	103.22	105.40
3	A	140	VAL	CG1-CB-CG2	-5.46	102.17	110.90
2	F	10	DA	O5'-P-OP1	-5.44	100.81	105.70
3	B	177	ARG	CB-CA-C	-5.44	99.52	110.40
3	B	243	GLN	CA-CB-CG	-5.44	101.44	113.40
3	B	176	GLN	CA-CB-CG	5.43	125.35	113.40
1	E	9	DA	N7-C8-N9	-5.43	111.08	113.80
1	E	14	DT	C6-N1-C1'	5.43	128.54	120.40
3	A	249	ALA	N-CA-CB	-5.43	102.50	110.10
3	B	283	ALA	O-C-N	-5.43	114.02	122.70
2	F	5	DG	C6-C5-N7	-5.42	127.15	130.40
1	E	17	DC	O5'-P-OP1	-5.41	100.83	105.70
3	A	184	ASN	O-C-N	5.41	131.36	122.70
2	F	9	DA	C5'-C4'-O4'	5.41	119.58	109.30
3	B	115	SER	CB-CA-C	-5.41	99.82	110.10
1	E	20	DG	C8-N9-C4	-5.40	104.24	106.40
1	E	9	DA	C5-C6-N6	5.39	128.01	123.70
3	A	291	VAL	CB-CA-C	-5.39	101.15	111.40
2	F	9	DA	C4'-C3'-C2'	-5.39	98.25	103.10
2	F	8	DG	P-O5'-C5'	-5.38	112.29	120.90
3	B	237	LYS	CB-CA-C	-5.38	99.65	110.40
1	E	7	DT	O3'-P-O5'	-5.37	93.79	104.00
3	A	241	ALA	N-CA-CB	-5.37	102.59	110.10
3	A	128	TYR	CB-CG-CD1	5.37	124.22	121.00
1	E	20	DG	OP1-P-OP2	5.36	127.64	119.60
2	F	19	DC	C5'-C4'-O4'	5.36	119.48	109.30
1	E	20	DG	C2-N3-C4	-5.35	109.22	111.90
1	E	18	DC	C6-N1-C2	5.34	122.44	120.30
2	F	4	DT	N3-C2-O2	5.33	125.50	122.30
2	F	11	DT	OP2-P-O3'	5.33	116.93	105.20
1	E	3	DT	C4-C5-C6	5.33	121.20	118.00
3	A	182	GLN	N-CA-C	-5.33	96.61	111.00
1	E	10	DT	N3-C2-O2	-5.32	119.11	122.30
2	F	16	DA	C4-C5-C6	-5.32	114.34	117.00
3	A	138	GLU	OE1-CD-OE2	-5.30	116.94	123.30
3	A	168	LEU	CB-CA-C	5.29	120.25	110.20
3	B	263	ALA	CA-C-N	-5.29	105.57	117.20
3	A	162	THR	OG1-CB-CG2	-5.27	97.88	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	9	DA	OP2-P-O3'	5.26	116.77	105.20
3	B	154	LEU	CA-CB-CG	5.25	127.39	115.30
3	A	173	VAL	CG1-CB-CG2	-5.25	102.50	110.90
3	B	247	TYR	CG-CD1-CE1	-5.24	117.11	121.30
1	E	11	DA	C2-N3-C4	-5.24	107.98	110.60
3	B	247	TYR	CG-CD2-CE2	5.23	125.48	121.30
2	F	6	DG	C5-N7-C8	5.23	106.92	104.30
1	E	14	DT	C4'-C3'-C2'	-5.23	98.39	103.10
3	B	109	GLU	OE1-CD-OE2	5.23	129.57	123.30
3	B	114	LEU	CB-CG-CD2	-5.22	102.12	111.00
2	F	20	DA	OP2-P-O3'	5.22	116.69	105.20
1	E	13	DT	C6-N1-C1'	5.22	128.23	120.40
2	F	7	DT	C5'-C4'-C3'	5.22	123.49	114.10
3	B	161	LYS	N-CA-CB	-5.22	101.21	110.60
1	E	12	DA	C5-N7-C8	5.21	106.51	103.90
3	B	174	ARG	N-CA-CB	-5.21	101.22	110.60
3	A	176	GLN	CG-CD-OE1	-5.21	111.19	121.60
1	E	20	DG	O5'-C5'-C4'	5.20	123.99	111.00
2	F	17	DA	C1'-O4'-C4'	-5.20	104.91	110.10
2	F	3	DC	O3'-P-O5'	-5.18	94.15	104.00
2	F	17	DA	P-O3'-C3'	-5.18	113.48	119.70
3	B	121	ALA	N-CA-CB	-5.17	102.86	110.10
3	A	270	ARG	N-CA-C	-5.17	97.04	111.00
1	E	16	DA	O3'-P-O5'	-5.16	94.19	104.00
3	B	128	TYR	CZ-CE2-CD2	5.15	124.44	119.80
1	E	9	DA	P-O5'-C5'	5.15	129.15	120.90
2	F	2	DG	C4'-C3'-C2'	5.15	107.73	103.10
2	F	8	DG	N3-C4-C5	-5.15	126.03	128.60
2	F	13	DA	P-O5'-C5'	-5.14	112.67	120.90
2	F	6	DG	C8-N9-C4	-5.14	104.34	106.40
3	A	252	ARG	NH1-CZ-NH2	5.14	125.05	119.40
1	E	16	DA	C5'-C4'-O4'	-5.13	99.55	109.30
2	F	13	DA	O4'-C1'-C2'	-5.12	101.80	105.90
3	A	126	LYS	CA-CB-CG	5.11	124.63	113.40
1	E	6	DT	O4'-C1'-C2'	-5.10	101.82	105.90
3	A	92	LEU	C-N-CA	-5.10	108.94	121.70
2	F	15	DT	C4-C5-C6	-5.10	114.94	118.00
3	A	151	SER	CB-CA-C	-5.10	100.41	110.10
2	F	20	DA	C4-C5-N7	-5.09	108.15	110.70
2	F	5	DG	N7-C8-N9	-5.08	110.56	113.10
1	E	18	DC	N1-C2-O2	5.08	121.95	118.90
3	B	141	ASP	CB-CG-OD1	5.06	122.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	12	DA	O3'-P-O5'	-5.05	94.41	104.00
3	B	247	TYR	CE1-CZ-OH	5.04	133.71	120.10
1	E	4	DG	C4-C5-C6	5.03	121.81	118.80
3	B	263	ALA	C-N-CA	5.01	134.24	121.70
2	F	6	DG	N3-C2-N2	5.00	123.40	119.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	183	PHE	Peptide
3	A	286	LEU	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	E	405	0	228	41	0
2	F	409	0	224	43	0
3	A	1453	0	1444	217	0
3	B	1462	0	1450	243	0
4	A	1	0	0	0	0
4	B	3	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
All	All	3736	0	3346	526	0

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 75.

All (526) 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)
3:B:120:ARG:CG	3:B:120:ARG:CB	1.74	1.65
3:B:185:GLN:CB	3:B:185:GLN:CG	1.77	1.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:237:LYS:CD	3:B:237:LYS:CG	1.76	1.62
3:A:254:LYS:CG	3:A:254:LYS:CB	1.76	1.62
3:A:98:LEU:CD1	3:A:98:LEU:CG	1.75	1.61
3:B:93:LYS:CE	3:B:93:LYS:CD	1.75	1.59
3:B:232:ARG:CD	3:B:232:ARG:CG	1.76	1.57
3:A:93:LYS:CD	3:A:93:LYS:CE	1.80	1.56
3:A:93:LYS:CD	3:A:93:LYS:CG	1.82	1.55
3:B:120:ARG:CG	3:B:120:ARG:CD	1.77	1.55
3:A:93:LYS:CE	3:A:93:LYS:NZ	1.70	1.55
3:B:180:LEU:CD1	3:B:180:LEU:CG	1.86	1.54
3:B:233:ARG:CG	3:B:233:ARG:CD	1.75	1.54
3:B:161:LYS:CD	3:B:161:LYS:CG	1.82	1.52
3:B:126:LYS:NZ	3:B:126:LYS:CE	1.70	1.50
3:A:179:ILE:CD1	3:A:179:ILE:CG1	1.89	1.50
3:A:123:LYS:CE	3:A:123:LYS:NZ	1.73	1.50
3:B:93:LYS:CE	3:B:93:LYS:NZ	1.72	1.50
3:A:237:LYS:CE	3:A:237:LYS:NZ	1.74	1.49
3:B:159:PRO:CG	3:B:159:PRO:CB	1.78	1.47
3:B:274:LEU:CG	3:B:274:LEU:CD1	1.92	1.47
3:A:123:LYS:CE	3:A:123:LYS:CD	1.90	1.47
3:A:96:GLN:CG	3:A:96:GLN:CD	1.81	1.46
1:E:1:DC:O5'	1:E:1:DC:C5'	1.63	1.46
3:A:180:LEU:CD2	3:A:180:LEU:CG	1.95	1.45
3:A:253:GLN:CD	3:A:253:GLN:CG	1.81	1.45
1:E:20:DG:O5'	1:E:20:DG:C5'	1.63	1.44
3:B:156:LYS:CE	3:B:156:LYS:CD	1.96	1.43
1:E:4:DG:C5'	1:E:4:DG:O5'	1.66	1.42
3:B:231:MET:CG	3:B:231:MET:SD	2.05	1.41
2:F:21:DA:C3'	2:F:21:DA:O3'	1.67	1.41
3:B:231:MET:SD	3:B:231:MET:CE	2.23	1.26
3:B:254:LYS:NZ	3:B:254:LYS:HB3	1.47	1.19
3:A:186:THR:HG22	3:A:282:LYS:NZ	1.59	1.16
3:A:177:ARG:HA	3:A:180:LEU:HD12	1.27	1.09
2:F:18:DC:H4'	2:F:18:DC:OP1	1.40	1.08
3:A:186:THR:HG23	3:A:187:VAL:H	1.10	1.08
3:A:177:ARG:HA	3:A:180:LEU:CD1	1.84	1.07
2:F:5:DG:H2”	2:F:6:DG:H5”	1.33	1.05
3:A:186:THR:CG2	3:A:187:VAL:N	2.19	1.04
3:A:186:THR:CG2	3:A:187:VAL:H	1.69	1.04
3:B:257:SER:O	3:B:259:GLU:N	1.90	1.04
3:B:134:ILE:CD1	3:B:134:ILE:CG1	2.39	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:158:THR:CG2	3:B:159:PRO:HD2	1.92	0.98
2:F:6:DG:H2"	2:F:7:DT:H5"	1.41	0.98
3:B:269:ASN:ND2	3:B:290:LEU:HD12	1.78	0.97
3:B:254:LYS:HB3	3:B:254:LYS:HZ3	1.16	0.96
3:B:303:ARG:HD2	3:B:303:ARG:O	1.65	0.96
2:F:6:DG:H2"	2:F:7:DT:C5'	1.96	0.95
3:B:175:LYS:HE3	3:B:179:ILE:HD13	1.47	0.95
3:A:165:ARG:HB3	3:A:169:TYR:CE2	2.03	0.93
3:A:183:PHE:CE2	3:A:278:VAL:HG11	2.04	0.92
2:F:20:DA:C5	2:F:21:DA:N6	2.39	0.91
3:A:104:ALA:HA	3:A:107:ARG:NH1	1.85	0.91
3:A:120:ARG:NH2	3:A:123:LYS:HB3	1.85	0.91
3:A:152:GLN:HB3	3:A:158:THR:OG1	1.70	0.91
2:F:20:DA:C6	2:F:21:DA:N6	2.39	0.90
3:B:254:LYS:NZ	3:B:254:LYS:CB	2.33	0.90
3:B:254:LYS:HB3	3:B:254:LYS:HZ2	1.29	0.90
3:B:279:SER:C	3:B:281:SER:H	1.73	0.89
1:E:15:DC:OP1	3:B:237:LYS:HD2	1.73	0.89
3:B:303:ARG:NH1	3:B:307:GLU:HB2	1.88	0.88
3:A:165:ARG:HB3	3:A:169:TYR:HE2	1.35	0.88
3:A:186:THR:HG22	3:A:282:LYS:HZ1	1.32	0.88
3:A:177:ARG:CA	3:A:180:LEU:HD12	2.03	0.88
3:A:104:ALA:HA	3:A:107:ARG:HH12	1.38	0.87
3:B:179:ILE:HG23	3:B:179:ILE:O	1.73	0.87
3:A:98:LEU:CD1	3:A:98:LEU:HG	2.04	0.87
3:B:91:ILE:HG22	3:B:91:ILE:O	1.73	0.87
3:A:110:VAL:HG23	3:A:173:VAL:HG21	1.56	0.86
3:B:106:GLN:O	3:B:108:ALA:N	2.08	0.86
3:B:93:LYS:HA	3:B:96:GLN:HB2	1.58	0.86
3:A:137:ARG:HH11	3:A:137:ARG:HG2	1.40	0.86
3:B:158:THR:HG23	3:B:159:PRO:HD2	1.59	0.85
3:A:107:ARG:O	3:A:111:ASP:HB2	1.77	0.84
3:B:153:HIS:HB2	3:B:158:THR:O	1.77	0.84
3:B:281:SER:O	3:B:282:LYS:CB	2.18	0.83
3:B:269:ASN:HD22	3:B:290:LEU:HD12	1.41	0.83
3:B:303:ARG:HH11	3:B:307:GLU:H	1.25	0.83
2:F:2:DG:H2"	2:F:3:DC:O5'	1.79	0.83
3:A:282:LYS:HG3	3:A:284:HIS:HB3	1.59	0.82
3:A:120:ARG:HH21	3:A:123:LYS:HB3	1.44	0.82
3:A:111:ASP:HA	3:A:114:LEU:HD11	1.60	0.82
2:F:3:DC:OP1	2:F:4:DT:OP2	1.98	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:158:THR:HG22	3:B:159:PRO:HD2	1.59	0.82
3:A:300:PHE:O	3:A:303:ARG:HB2	1.78	0.82
3:B:112:ARG:HG3	3:B:113:MET:N	1.93	0.82
3:B:305:LYS:O	3:B:308:ALA:HB3	1.79	0.82
3:A:256:PRO:HB2	3:A:261:ARG:HG2	1.62	0.81
1:E:12:DA:H1'	1:E:13:DT:H5"	1.62	0.81
3:A:257:SER:O	3:A:260:GLU:HB3	1.81	0.81
2:F:16:DA:OP1	3:A:237:LYS:HD2	1.80	0.81
3:B:294:VAL:O	3:B:297:TYR:HB3	1.80	0.81
3:B:149:HIS:NE2	3:B:160:MET:HG3	1.96	0.81
3:B:158:THR:HG22	3:B:159:PRO:CD	2.11	0.80
3:A:282:LYS:C	3:A:284:HIS:H	1.84	0.79
3:B:242:SER:HB3	3:B:268:CYS:SG	2.22	0.79
3:A:268:CYS:O	3:A:271:ALA:N	2.15	0.79
3:A:301:ALA:HA	3:A:304:ARG:HG3	1.65	0.78
3:B:257:SER:C	3:B:259:GLU:H	1.85	0.78
3:A:304:ARG:O	3:A:306:GLU:N	2.17	0.77
1:E:19:DA:O5'	1:E:19:DA:H2'	1.85	0.77
3:A:287:GLY:O	3:A:290:LEU:HB2	1.84	0.77
3:B:239:GLY:O	3:B:243:GLN:HG3	1.85	0.77
3:A:116:GLU:OE2	3:A:116:GLU:N	2.17	0.77
1:E:5:DG:O6	3:A:305:LYS:HE3	1.84	0.77
3:A:302:ASN:O	3:A:303:ARG:NH1	2.18	0.77
2:F:6:DG:C2'	2:F:7:DT:H5"	2.15	0.76
3:B:235:ARG:NH1	3:B:235:ARG:HG3	1.98	0.76
3:A:186:THR:HG22	3:A:187:VAL:N	1.99	0.76
3:A:183:PHE:HE2	3:A:278:VAL:HG11	1.50	0.76
3:A:248:GLN:O	3:A:250:TYR:N	2.20	0.75
2:F:13:DA:H1'	2:F:14:DT:H5'	1.69	0.75
3:A:299:TRP:O	3:A:299:TRP:CE3	2.40	0.75
3:A:141:ASP:O	3:A:142:VAL:C	2.24	0.74
1:E:15:DC:OP1	3:B:237:LYS:CD	2.35	0.74
3:B:281:SER:O	3:B:282:LYS:CG	2.36	0.74
3:B:106:GLN:OE1	3:B:177:ARG:NH1	2.22	0.73
1:E:5:DG:OP2	3:B:159:PRO:HG3	1.89	0.72
3:B:282:LYS:HB2	3:B:284:HIS:ND1	2.04	0.72
3:A:102:GLU:OE2	3:A:177:ARG:HD2	1.89	0.72
3:A:250:TYR:C	3:A:252:ARG:H	1.94	0.72
3:B:279:SER:C	3:B:281:SER:N	2.43	0.71
3:A:127:GLY:O	3:A:130:GLN:HB2	1.90	0.71
3:B:303:ARG:NH1	3:B:307:GLU:H	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:165:ARG:O	3:A:168:LEU:N	2.24	0.71
3:A:181:ARG:C	3:A:183:PHE:H	1.89	0.71
1:E:1:DC:H5'	1:E:2:DT:H73	1.73	0.71
1:E:3:DT:OP2	3:A:304:ARG:NH1	2.24	0.71
3:B:279:SER:O	3:B:281:SER:N	2.24	0.71
3:B:293:GLU:HG3	3:B:294:VAL:HG23	1.73	0.71
3:B:269:ASN:ND2	3:B:291:VAL:H	1.89	0.70
3:A:111:ASP:O	3:A:114:LEU:HD12	1.91	0.70
3:B:235:ARG:HG3	3:B:235:ARG:HH11	1.55	0.70
3:A:177:ARG:O	3:A:178:GLU:C	2.28	0.70
3:A:257:SER:O	3:A:260:GLU:N	2.25	0.70
3:B:170:THR:HG22	3:B:171:TRP:N	2.03	0.70
3:A:279:SER:HG	3:A:281:SER:HG	1.36	0.70
3:A:125:ILE:CG2	3:A:125:ILE:O	2.38	0.70
3:A:186:THR:HG23	3:A:187:VAL:N	1.87	0.70
3:A:159:PRO:O	3:A:159:PRO:HG2	1.92	0.69
3:B:297:TYR:HD2	3:B:298:ASN:ND2	1.90	0.69
3:A:102:GLU:O	3:A:105:GLU:HG2	1.91	0.69
1:E:12:DA:H2"	1:E:13:DT:H5'	1.75	0.69
3:A:125:ILE:O	3:A:125:ILE:HG22	1.85	0.69
3:A:260:GLU:O	3:A:261:ARG:C	2.30	0.69
3:A:257:SER:O	3:A:260:GLU:CB	2.42	0.68
3:A:306:GLU:O	3:A:306:GLU:HG2	1.92	0.68
2:F:16:DA:OP1	3:A:237:LYS:CD	2.41	0.68
3:B:253:GLN:O	3:B:256:PRO:HD3	1.93	0.68
3:A:158:THR:HG22	3:A:159:PRO:HD2	1.75	0.68
3:A:282:LYS:C	3:A:284:HIS:N	2.44	0.68
3:A:250:TYR:C	3:A:252:ARG:N	2.47	0.68
3:B:112:ARG:HG3	3:B:113:MET:H	1.57	0.68
1:E:18:DC:H2"	1:E:19:DA:N7	2.09	0.68
3:A:107:ARG:HH11	3:A:107:ARG:HG3	1.60	0.67
3:B:235:ARG:HH11	3:B:235:ARG:CG	2.08	0.67
3:B:305:LYS:O	3:B:306:GLU:O	2.13	0.67
1:E:1:DC:C5'	1:E:2:DT:H73	2.25	0.66
3:B:177:ARG:O	3:B:180:LEU:N	2.24	0.66
3:B:140:VAL:O	3:B:141:ASP:C	2.25	0.66
3:B:299:TRP:CE3	3:B:299:TRP:C	2.69	0.66
3:B:299:TRP:O	3:B:303:ARG:HB2	1.95	0.66
3:B:297:TYR:HD2	3:B:298:ASN:HD22	1.42	0.66
3:A:125:ILE:C	3:A:127:GLY:N	2.47	0.65
3:A:239:GLY:O	3:A:243:GLN:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4:DT:O5'	2:F:4:DT:H2'	1.97	0.65
3:A:110:VAL:O	3:A:110:VAL:CG1	2.41	0.65
3:A:151:SER:O	3:A:155:ASN:ND2	2.26	0.65
1:E:2:DT:H2"	1:E:3:DT:C6	2.32	0.65
3:B:103:ALA:C	3:B:107:ARG:HH12	2.00	0.65
3:A:120:ARG:HH21	3:A:123:LYS:CB	2.11	0.64
1:E:9:DA:H2"	1:E:10:DT:OP2	1.98	0.64
1:E:1:DC:C5'	1:E:1:DC:HO5'	2.07	0.64
3:A:294:VAL:O	3:A:297:TYR:HB3	1.98	0.64
3:A:177:ARG:HA	3:A:180:LEU:HD11	1.75	0.64
3:A:152:GLN:OE1	3:A:152:GLN:HA	1.97	0.64
3:B:300:PHE:O	3:B:303:ARG:N	2.31	0.63
3:B:254:LYS:HZ3	3:B:254:LYS:CB	2.02	0.63
3:A:141:ASP:N	3:A:141:ASP:OD2	2.29	0.63
3:B:257:SER:O	3:B:260:GLU:N	2.31	0.63
3:A:107:ARG:NH1	3:A:107:ARG:HG3	2.14	0.62
3:B:251:ASP:O	3:B:253:GLN:NE2	2.32	0.62
3:B:258:LYS:HA	3:B:261:ARG:CZ	2.29	0.62
3:A:248:GLN:C	3:A:250:TYR:N	2.50	0.62
3:A:265:VAL:O	3:A:269:ASN:HB2	1.99	0.62
2:F:20:DA:C6	2:F:21:DA:C6	2.87	0.62
3:B:173:VAL:HG23	3:B:174:ARG:N	2.13	0.62
3:B:303:ARG:NH1	3:B:307:GLU:CB	2.63	0.62
3:A:111:ASP:HA	3:A:114:LEU:CD1	2.28	0.62
3:A:248:GLN:O	3:A:249:ALA:C	2.36	0.62
3:B:112:ARG:CG	3:B:113:MET:N	2.62	0.62
3:A:91:ILE:HG22	3:A:91:ILE:O	2.00	0.62
3:B:102:GLU:O	3:B:103:ALA:C	2.37	0.62
3:B:254:LYS:CB	3:B:254:LYS:HZ2	2.04	0.62
3:A:98:LEU:CD1	3:A:98:LEU:CD2	2.75	0.62
3:A:165:ARG:CB	3:A:169:TYR:HE2	2.10	0.62
3:B:299:TRP:CE3	3:B:299:TRP:O	2.53	0.62
3:A:110:VAL:HG23	3:A:173:VAL:CG2	2.30	0.62
3:B:109:GLU:HG2	3:B:173:VAL:CG1	2.29	0.62
3:B:177:ARG:O	3:B:178:GLU:C	2.32	0.61
3:A:260:GLU:O	3:A:261:ARG:O	2.17	0.61
2:F:6:DG:H2"	2:F:7:DT:H5'	1.81	0.61
3:A:256:PRO:HG2	3:A:300:PHE:CE1	2.35	0.61
3:B:158:THR:CG2	3:B:159:PRO:CD	2.69	0.61
3:B:163:GLN:HA	3:B:163:GLN:OE1	2.01	0.61
3:A:179:ILE:O	3:A:179:ILE:CG2	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:279:SER:O	3:A:281:SER:O	2.19	0.61
3:B:120:ARG:CG	3:B:120:ARG:CA	2.73	0.61
1:E:19:DA:O5'	1:E:19:DA:C2'	2.49	0.61
3:B:137:ARG:CZ	3:B:137:ARG:HB3	2.31	0.60
3:A:186:THR:HG22	3:A:282:LYS:HZ2	1.61	0.60
3:A:165:ARG:C	3:A:167:ALA:N	2.51	0.60
3:B:258:LYS:HA	3:B:261:ARG:HG3	1.83	0.60
3:B:303:ARG:HH12	3:B:307:GLU:HB2	1.66	0.60
2:F:18:DC:OP1	2:F:18:DC:C4'	2.33	0.60
1:E:12:DA:H2"	1:E:13:DT:C5'	2.32	0.60
1:E:12:DA:OP2	3:A:151:SER:HB3	2.02	0.60
3:A:240:PRO:O	3:A:243:GLN:HB3	2.02	0.60
3:A:242:SER:O	3:A:246:LEU:HD12	2.02	0.60
3:A:279:SER:C	3:A:281:SER:N	2.53	0.60
2:F:10:DA:H2"	2:F:11:DT:O5'	2.02	0.60
3:B:253:GLN:O	3:B:254:LYS:C	2.39	0.60
3:B:147:GLN:O	3:B:147:GLN:NE2	2.35	0.60
1:E:7:DT:H2"	1:E:8:DA:C8	2.37	0.59
3:B:305:LYS:O	3:B:306:GLU:C	2.39	0.59
2:F:7:DT:OP1	3:A:161:LYS:HD2	2.03	0.59
2:F:4:DT:C4'	2:F:5:DG:OP1	2.47	0.59
3:B:109:GLU:O	3:B:112:ARG:HG2	2.03	0.59
1:E:8:DA:H1'	1:E:9:DA:H5'	1.84	0.59
3:A:103:ALA:O	3:A:107:ARG:NH1	2.35	0.59
3:B:95:LEU:C	3:B:97:ALA:H	2.04	0.59
3:A:299:TRP:O	3:A:299:TRP:CD2	2.56	0.59
3:B:303:ARG:HD2	3:B:303:ARG:C	2.15	0.59
3:B:104:ALA:O	3:B:105:GLU:C	2.40	0.59
3:B:269:ASN:HD21	3:B:291:VAL:H	1.50	0.58
3:B:274:LEU:CD1	3:B:274:LEU:HG	2.24	0.58
2:F:19:DC:H2"	2:F:20:DA:C8	2.38	0.58
2:F:17:DA:H2"	2:F:18:DC:C6	2.39	0.58
3:A:248:GLN:C	3:A:250:TYR:H	2.05	0.58
3:B:175:LYS:CE	3:B:179:ILE:HD13	2.28	0.58
3:B:240:PRO:CD	3:B:241:ALA:H	2.16	0.58
3:B:282:LYS:HB2	3:B:284:HIS:CE1	2.38	0.58
3:A:165:ARG:C	3:A:167:ALA:H	2.06	0.57
3:A:165:ARG:O	3:A:167:ALA:N	2.37	0.57
3:A:303:ARG:HG2	3:A:303:ARG:HH11	1.70	0.57
3:B:161:LYS:O	3:B:162:THR:C	2.41	0.57
3:A:152:GLN:OE1	3:A:152:GLN:CA	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:169:TYR:O	3:A:172:TYR:N	2.37	0.57
3:B:90:SER:O	3:B:93:LYS:N	2.36	0.57
3:B:307:GLU:O	3:B:309:PHE:N	2.37	0.57
2:F:2:DG:C2'	2:F:3:DC:O5'	2.52	0.57
3:A:137:ARG:HG2	3:A:137:ARG:NH1	2.15	0.57
3:B:106:GLN:C	3:B:108:ALA:H	2.04	0.57
3:A:279:SER:O	3:A:281:SER:N	2.37	0.57
3:A:261:ARG:O	3:A:263:ALA:N	2.37	0.57
3:A:306:GLU:O	3:A:306:GLU:CG	2.52	0.57
2:F:9:DA:H1'	2:F:10:DA:H5"	1.87	0.57
1:E:5:DG:H1'	1:E:6:DT:H5'	1.86	0.57
3:B:158:THR:HG22	3:B:159:PRO:N	2.16	0.57
3:B:174:ARG:O	3:B:176:GLN:N	2.38	0.56
1:E:15:DC:H4'	3:B:235:ARG:HD3	1.88	0.56
3:A:279:SER:C	3:A:281:SER:H	2.07	0.56
3:B:240:PRO:O	3:B:243:GLN:HB2	2.05	0.56
3:B:250:TYR:HA	3:B:253:GLN:HG2	1.86	0.56
2:F:5:DG:H2"	2:F:6:DG:C5'	2.21	0.56
3:A:116:GLU:N	3:A:116:GLU:CD	2.59	0.56
3:A:293:GLU:O	3:A:294:VAL:C	2.42	0.56
3:B:106:GLN:HG3	3:B:177:ARG:HH12	1.71	0.56
1:E:1:DC:O4'	1:E:2:DT:H72	2.06	0.56
2:F:21:DA:C3'	2:F:21:DA:HO3'	2.11	0.55
3:A:105:GLU:O	3:A:108:ALA:HB3	2.06	0.55
3:B:106:GLN:CG	3:B:177:ARG:HH12	2.20	0.55
3:B:175:LYS:O	3:B:175:LYS:HG3	2.02	0.55
3:A:237:LYS:NZ	3:A:237:LYS:CD	2.66	0.55
3:B:159:PRO:O	3:B:159:PRO:HG2	2.06	0.55
3:B:91:ILE:HA	3:B:94:GLU:HB3	1.88	0.55
3:B:143:THR:HB	3:B:145:LEU:HG	1.89	0.55
3:B:240:PRO:HD2	3:B:241:ALA:H	1.70	0.55
2:F:5:DG:C2'	2:F:6:DG:H5"	2.24	0.55
3:B:125:ILE:O	3:B:128:TYR:HB3	2.05	0.55
3:B:303:ARG:NH1	3:B:307:GLU:N	2.55	0.55
3:B:128:TYR:CD1	3:B:172:TYR:HE1	2.25	0.55
3:B:93:LYS:O	3:B:94:GLU:C	2.45	0.55
3:B:174:ARG:O	3:B:177:ARG:N	2.38	0.55
3:B:300:PHE:O	3:B:301:ALA:C	2.45	0.55
1:E:16:DA:C2	2:F:8:DG:C2	2.95	0.55
3:B:109:GLU:HG2	3:B:173:VAL:HG11	1.87	0.54
3:B:177:ARG:C	3:B:179:ILE:N	2.58	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:DA:C1'	1:E:13:DT:H5"	2.35	0.54
3:A:93:LYS:O	3:A:94:GLU:C	2.46	0.54
3:A:120:ARG:HB3	3:A:120:ARG:NH1	2.22	0.54
3:B:119:TRP:CH2	3:B:123:LYS:HD3	2.42	0.54
3:B:270:ARG:HG3	3:B:270:ARG:HH11	1.72	0.54
3:B:281:SER:O	3:B:282:LYS:HG2	2.07	0.54
3:A:131:GLN:HE21	3:A:276:ARG:HA	1.72	0.54
3:A:170:THR:O	3:A:171:TRP:C	2.44	0.54
3:A:247:TYR:HE2	3:A:303:ARG:HE	1.54	0.54
3:B:168:LEU:O	3:B:171:TRP:HB3	2.07	0.54
2:F:20:DA:C5	2:F:21:DA:C6	2.95	0.54
3:B:112:ARG:CG	3:B:113:MET:H	2.20	0.54
3:B:153:HIS:HA	3:B:158:THR:N	2.22	0.54
3:B:233:ARG:CD	3:B:233:ARG:CB	2.82	0.54
3:B:91:ILE:O	3:B:91:ILE:CG2	2.46	0.53
3:B:268:CYS:O	3:B:271:ALA:HB3	2.08	0.53
1:E:9:DA:C2'	1:E:10:DT:OP2	2.51	0.53
3:B:167:ALA:O	3:B:170:THR:HB	2.08	0.53
3:B:249:ALA:O	3:B:253:GLN:HG2	2.09	0.53
3:B:306:GLU:O	3:B:307:GLU:C	2.47	0.53
3:B:137:ARG:O	3:B:139:VAL:N	2.42	0.53
2:F:13:DA:C8	2:F:14:DT:C7	2.91	0.52
3:B:257:SER:C	3:B:259:GLU:N	2.42	0.52
3:B:175:LYS:O	3:B:179:ILE:HB	2.09	0.52
3:B:181:ARG:O	3:B:183:PHE:N	2.43	0.52
3:A:137:ARG:HH11	3:A:137:ARG:CG	2.15	0.52
3:B:174:ARG:C	3:B:176:GLN:N	2.61	0.52
3:B:95:LEU:O	3:B:97:ALA:N	2.42	0.52
3:B:161:LYS:CD	3:B:161:LYS:CB	2.79	0.52
3:B:231:MET:O	3:B:232:ARG:O	2.28	0.52
3:A:175:LYS:HG3	3:A:175:LYS:O	2.09	0.52
3:A:186:THR:CG2	3:A:282:LYS:NZ	2.52	0.52
3:B:181:ARG:C	3:B:183:PHE:N	2.60	0.52
2:F:8:DG:OP2	3:A:146:ASN:HB2	2.10	0.52
3:A:104:ALA:HA	3:A:107:ARG:CZ	2.39	0.52
3:B:173:VAL:CG2	3:B:174:ARG:N	2.73	0.52
1:E:19:DA:C2	2:F:4:DT:N3	2.68	0.52
3:A:258:LYS:O	3:A:262:GLU:HB2	2.10	0.52
3:B:135:PRO:C	3:B:137:ARG:N	2.63	0.51
3:B:281:SER:C	3:B:282:LYS:CG	2.78	0.51
3:B:106:GLN:O	3:B:107:ARG:C	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:256:PRO:HB2	3:A:261:ARG:CG	2.38	0.51
3:B:162:THR:O	3:B:163:GLN:C	2.49	0.51
3:A:104:ALA:CA	3:A:107:ARG:HH12	2.17	0.51
3:A:272:GLU:O	3:A:276:ARG:HG2	2.10	0.51
3:B:109:GLU:C	3:B:111:ASP:N	2.59	0.51
3:B:272:GLU:OE1	3:B:276:ARG:NH2	2.44	0.51
3:B:250:TYR:C	3:B:250:TYR:CD1	2.85	0.51
3:A:120:ARG:HA	3:A:120:ARG:NE	2.27	0.50
3:B:165:ARG:O	3:B:169:TYR:N	2.32	0.50
1:E:2:DT:H2'	1:E:3:DT:H72	1.93	0.50
3:B:269:ASN:HD21	3:B:291:VAL:N	2.09	0.50
1:E:12:DA:C8	1:E:13:DT:C7	2.95	0.50
2:F:3:DC:P	2:F:4:DT:OP2	2.69	0.50
3:A:165:ARG:O	3:A:166:ALA:C	2.49	0.50
3:A:292:THR:O	3:A:296:VAL:HG23	2.10	0.50
3:B:296:VAL:CG2	3:B:297:TYR:N	2.73	0.50
3:A:181:ARG:C	3:A:183:PHE:N	2.48	0.50
3:B:260:GLU:O	3:B:263:ALA:HB3	2.11	0.50
3:A:293:GLU:O	3:A:297:TYR:N	2.35	0.50
3:A:300:PHE:O	3:A:301:ALA:C	2.47	0.50
3:B:95:LEU:C	3:B:97:ALA:N	2.65	0.50
3:A:237:LYS:NZ	3:A:237:LYS:CG	2.74	0.50
3:A:269:ASN:HD21	3:A:291:VAL:H	1.59	0.50
3:B:136:GLN:OE1	3:B:147:GLN:HG2	2.12	0.50
3:B:231:MET:SD	3:B:231:MET:N	2.85	0.49
3:B:302:ASN:O	3:B:306:GLU:HG3	2.12	0.49
3:A:125:ILE:C	3:A:127:GLY:H	2.14	0.49
3:B:180:LEU:CD1	3:B:180:LEU:CD2	2.86	0.49
3:B:109:GLU:C	3:B:111:ASP:H	2.16	0.49
3:B:264:LEU:HA	3:B:267:GLU:HB3	1.93	0.49
3:A:291:VAL:HG12	3:A:292:THR:N	2.26	0.49
3:B:171:TRP:CE3	3:B:172:TYR:CA	2.95	0.49
3:B:107:ARG:HG3	3:B:107:ARG:HH11	1.75	0.49
3:B:109:GLU:HG2	3:B:173:VAL:HG12	1.94	0.49
2:F:21:DA:O3'	2:F:21:DA:H3'	1.96	0.49
3:A:256:PRO:CG	3:A:300:PHE:CE1	2.95	0.49
3:B:120:ARG:CG	3:B:120:ARG:C	2.80	0.49
3:A:116:GLU:CD	3:A:116:GLU:H	2.17	0.49
3:A:299:TRP:O	3:A:299:TRP:CG	2.66	0.49
3:B:103:ALA:HB1	3:B:107:ARG:HH12	1.78	0.49
3:B:123:LYS:O	3:B:124:MET:C	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:259:GLU:C	3:B:261:ARG:N	2.65	0.48
3:A:141:ASP:O	3:A:143:THR:N	2.46	0.48
3:A:162:THR:O	3:A:163:GLN:C	2.51	0.48
3:A:186:THR:HG22	3:A:282:LYS:HZ3	1.69	0.48
3:B:128:TYR:CE2	3:B:132:HIS:CD2	3.01	0.48
3:A:93:LYS:CD	3:A:93:LYS:CB	2.83	0.48
3:B:269:ASN:OD1	3:B:291:VAL:HB	2.13	0.48
3:B:291:VAL:HG12	3:B:292:THR:N	2.27	0.48
3:A:293:GLU:OE1	3:A:293:GLU:N	2.32	0.48
3:B:167:ALA:O	3:B:168:LEU:C	2.50	0.48
3:B:297:TYR:C	3:B:297:TYR:CD2	2.86	0.48
3:A:158:THR:CG2	3:A:159:PRO:HD2	2.43	0.48
3:B:163:GLN:O	3:B:166:ALA:HB3	2.14	0.48
3:A:301:ALA:C	3:A:303:ARG:H	2.17	0.48
3:A:106:GLN:HB3	3:A:173:VAL:HG11	1.96	0.48
3:A:110:VAL:O	3:A:110:VAL:HG12	2.06	0.48
3:A:109:GLU:OE2	3:A:112:ARG:NH2	2.39	0.47
3:A:187:VAL:N	3:A:282:LYS:HZ2	2.12	0.47
3:B:99:ASN:O	3:B:100:THR:O	2.31	0.47
3:B:106:GLN:C	3:B:108:ALA:N	2.59	0.47
1:E:12:DA:H1'	1:E:13:DT:C5'	2.38	0.47
2:F:3:DC:H5'	3:B:297:TYR:OH	2.14	0.47
3:A:257:SER:N	3:A:260:GLU:HB3	2.29	0.47
3:B:169:TYR:O	3:B:170:THR:C	2.50	0.47
3:A:256:PRO:HB3	3:A:260:GLU:HG3	1.96	0.47
3:B:177:ARG:O	3:B:179:ILE:N	2.47	0.47
3:A:110:VAL:HG22	3:A:169:TYR:HB3	1.96	0.47
3:A:137:ARG:O	3:A:138:GLU:C	2.53	0.47
1:E:2:DT:H2"	1:E:3:DT:H6	1.80	0.47
2:F:4:DT:H4'	2:F:5:DG:OP1	2.15	0.47
3:A:271:ALA:O	3:A:274:LEU:HB2	2.14	0.47
3:B:128:TYR:CE2	3:B:132:HIS:HD2	2.33	0.47
3:B:257:SER:O	3:B:258:LYS:C	2.49	0.47
2:F:3:DC:C2'	2:F:3:DC:O2	2.61	0.47
2:F:4:DT:O5'	2:F:4:DT:C2'	2.63	0.47
2:F:13:DA:C8	2:F:14:DT:H71	2.50	0.47
3:A:297:TYR:CD1	3:A:297:TYR:C	2.86	0.47
3:B:174:ARG:C	3:B:176:GLN:H	2.19	0.47
3:A:186:THR:C	3:A:282:LYS:HZ2	2.18	0.46
3:B:149:HIS:CE1	3:B:160:MET:HG3	2.48	0.46
3:A:268:CYS:O	3:A:270:ARG:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:303:ARG:HD3	3:B:306:GLU:CD	2.36	0.46
3:A:91:ILE:O	3:A:91:ILE:CG2	2.64	0.46
3:B:171:TRP:CE3	3:B:172:TYR:HA	2.50	0.46
3:A:152:GLN:C	3:A:154:LEU:N	2.66	0.46
3:B:101:GLU:O	3:B:105:GLU:HB2	2.16	0.46
3:A:241:ALA:C	3:A:243:GLN:N	2.64	0.46
3:A:242:SER:HB3	3:A:268:CYS:SG	2.55	0.46
3:A:165:ARG:HG3	3:A:165:ARG:HH11	1.80	0.46
3:B:163:GLN:OE1	3:B:163:GLN:CA	2.64	0.46
3:B:271:ALA:O	3:B:274:LEU:HB2	2.16	0.46
1:E:19:DA:N1	2:F:4:DT:C4	2.83	0.46
3:A:273:CYS:HB3	3:A:278:VAL:HG23	1.98	0.46
3:B:233:ARG:CG	3:B:233:ARG:NE	2.67	0.46
2:F:5:DG:N7	3:B:305:LYS:NZ	2.63	0.46
3:A:283:ALA:O	3:A:286:LEU:HB2	2.15	0.46
3:A:300:PHE:O	3:A:303:ARG:N	2.49	0.46
3:B:90:SER:O	3:B:92:LEU:N	2.48	0.46
3:B:132:HIS:ND1	3:B:276:ARG:HD3	2.31	0.45
3:B:132:HIS:O	3:B:276:ARG:NH1	2.48	0.45
3:B:170:THR:O	3:B:171:TRP:C	2.53	0.45
3:A:145:LEU:HD23	3:A:164:LYS:HD2	1.99	0.45
3:A:177:ARG:O	3:A:180:LEU:HD12	2.17	0.45
3:B:181:ARG:C	3:B:183:PHE:H	2.19	0.45
1:E:4:DG:C5'	1:E:4:DG:P	3.02	0.45
3:B:131:GLN:O	3:B:275:GLN:NE2	2.46	0.45
3:B:302:ASN:HD22	3:B:302:ASN:HA	1.42	0.45
3:A:91:ILE:HA	3:A:94:GLU:HB3	1.98	0.45
3:A:164:LYS:O	3:A:165:ARG:C	2.45	0.45
1:E:5:DG:H2'	1:E:5:DG:H5'	1.68	0.45
3:A:168:LEU:O	3:A:169:TYR:C	2.54	0.45
1:E:3:DT:O4	2:F:20:DA:N1	2.50	0.45
3:A:116:GLU:O	3:A:118:PRO:HD3	2.17	0.45
3:A:163:GLN:HA	3:A:163:GLN:NE2	2.32	0.45
3:A:261:ARG:H	3:A:261:ARG:HG3	1.50	0.45
3:B:177:ARG:C	3:B:180:LEU:H	2.16	0.45
3:B:135:PRO:C	3:B:137:ARG:H	2.20	0.45
1:E:8:DA:H1'	1:E:9:DA:C5'	2.46	0.45
3:B:296:VAL:O	3:B:300:PHE:HD1	2.00	0.45
1:E:12:DA:C2'	1:E:13:DT:C5'	2.95	0.45
3:A:150:LEU:O	3:A:151:SER:C	2.55	0.45
3:B:140:VAL:HG23	3:B:141:ASP:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:174:ARG:O	3:A:176:GLN:N	2.50	0.44
3:A:269:ASN:HD22	3:A:269:ASN:HA	1.43	0.44
3:B:270:ARG:HG3	3:B:270:ARG:NH1	2.32	0.44
3:A:126:LYS:O	3:A:130:GLN:HG2	2.17	0.44
3:B:135:PRO:O	3:B:136:GLN:C	2.52	0.44
3:B:112:ARG:O	3:B:113:MET:C	2.54	0.44
3:A:172:TYR:O	3:A:173:VAL:C	2.56	0.44
3:B:155:ASN:HD22	3:B:155:ASN:HA	1.26	0.44
3:B:172:TYR:CE1	3:B:176:GLN:OE1	2.71	0.44
3:A:137:ARG:NH1	3:A:137:ARG:CG	2.73	0.44
3:B:175:LYS:HA	3:B:178:GLU:HB3	2.00	0.44
3:A:274:LEU:HD23	3:A:274:LEU:HA	1.65	0.43
3:B:258:LYS:CA	3:B:261:ARG:HG3	2.48	0.43
3:B:299:TRP:C	3:B:299:TRP:CD2	2.92	0.43
3:B:174:ARG:O	3:B:175:LYS:C	2.56	0.43
3:A:177:ARG:O	3:A:178:GLU:O	2.36	0.43
3:B:137:ARG:C	3:B:139:VAL:H	2.21	0.43
3:B:137:ARG:C	3:B:139:VAL:N	2.72	0.43
3:A:98:LEU:HA	3:A:98:LEU:HD23	1.65	0.43
3:A:241:ALA:HB3	3:A:242:SER:H	1.53	0.43
3:B:269:ASN:HD21	3:B:290:LEU:HD12	1.74	0.43
3:B:294:VAL:HG23	3:B:294:VAL:H	1.28	0.43
3:B:103:ALA:C	3:B:107:ARG:NH1	2.69	0.43
3:B:165:ARG:HB3	3:B:169:TYR:CE2	2.53	0.43
3:A:95:LEU:HD12	3:A:95:LEU:HA	1.62	0.43
3:A:160:MET:HG2	3:A:164:LYS:HB2	2.00	0.43
3:B:160:MET:CE	3:B:165:ARG:HA	2.49	0.43
3:B:236:PHE:CD2	3:B:236:PHE:C	2.90	0.43
3:A:240:PRO:O	3:A:243:GLN:CB	2.67	0.42
3:B:164:LYS:O	3:B:165:ARG:C	2.56	0.42
3:B:91:ILE:HD13	3:B:91:ILE:HG21	1.70	0.42
3:B:117:ASP:O	3:B:118:PRO:C	2.57	0.42
3:B:150:LEU:HA	3:B:150:LEU:HD12	1.71	0.42
3:A:179:ILE:HD13	3:A:182:GLN:NE2	2.34	0.42
3:B:246:LEU:HD23	3:B:246:LEU:HA	1.59	0.42
1:E:1:DC:C5'	1:E:2:DT:C7	2.96	0.42
3:A:135:PRO:O	3:A:136:GLN:C	2.53	0.42
3:A:159:PRO:O	3:A:159:PRO:CG	2.66	0.42
3:A:173:VAL:HG12	3:A:174:ARG:N	2.34	0.42
3:A:291:VAL:C	3:A:292:THR:CG2	2.88	0.42
3:A:172:TYR:O	3:A:175:LYS:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:DG:H4'	3:B:161:LYS:HE3	2.02	0.42
3:A:171:TRP:CE3	3:A:172:TYR:HA	2.54	0.42
3:B:297:TYR:CD2	3:B:298:ASN:ND2	2.79	0.42
3:B:299:TRP:C	3:B:299:TRP:HE3	2.19	0.42
2:F:3:DC:H3'	2:F:4:DT:C6	2.54	0.41
3:A:165:ARG:O	3:A:169:TYR:CD2	2.73	0.41
3:A:165:ARG:HG3	3:A:165:ARG:NH1	2.35	0.41
3:A:300:PHE:O	3:A:303:ARG:CB	2.60	0.41
3:B:90:SER:O	3:B:91:ILE:C	2.55	0.41
3:B:106:GLN:CG	3:B:177:ARG:NH1	2.84	0.41
3:A:236:PHE:HE2	3:A:238:TRP:CD1	2.38	0.41
3:B:258:LYS:O	3:B:258:LYS:CG	2.68	0.41
3:B:112:ARG:C	3:B:114:LEU:N	2.70	0.41
3:B:153:HIS:CB	3:B:158:THR:O	2.60	0.41
3:B:301:ALA:O	3:B:302:ASN:C	2.56	0.41
3:A:281:SER:O	3:A:282:LYS:C	2.58	0.41
3:A:113:MET:HA	3:A:116:GLU:HG2	2.02	0.41
3:A:235:ARG:HG2	3:A:236:PHE:N	2.36	0.41
3:B:111:ASP:HA	3:B:114:LEU:HD12	2.01	0.41
3:A:258:LYS:O	3:A:259:GLU:C	2.58	0.41
3:B:110:VAL:HG11	3:B:170:THR:HA	2.02	0.41
3:A:125:ILE:O	3:A:126:LYS:C	2.59	0.41
3:A:235:ARG:HG2	3:A:236:PHE:H	1.86	0.41
3:B:169:TYR:O	3:B:172:TYR:HB3	2.21	0.41
3:A:240:PRO:O	3:A:243:GLN:N	2.54	0.40
3:A:281:SER:HG	3:A:281:SER:H	1.67	0.40
3:B:261:ARG:HB2	3:B:262:GLU:H	1.67	0.40
3:B:293:GLU:O	3:B:296:VAL:HG22	2.19	0.40
3:A:303:ARG:NH1	3:A:303:ARG:HG2	2.34	0.40
3:A:304:ARG:C	3:A:306:GLU:N	2.75	0.40
3:A:152:GLN:HB3	3:A:158:THR:HG1	1.81	0.40
3:B:126:LYS:O	3:B:130:GLN:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	172/221 (78%)	124 (72%)	33 (19%)	15 (9%)	1 4
3	B	172/221 (78%)	125 (73%)	25 (14%)	22 (13%)	0 1
All	All	344/442 (78%)	249 (72%)	58 (17%)	37 (11%)	0 2

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	141	ASP
3	A	142	VAL
3	A	173	VAL
3	A	234	ASN
3	A	262	GLU
3	A	305	LYS
3	B	100	THR
3	B	232	ARG
3	B	258	LYS
3	B	306	GLU
3	B	308	ALA
3	A	113	MET
3	A	258	LYS
3	A	269	ASN
3	B	107	ARG
3	B	138	GLU
3	A	178	GLU
3	A	261	ARG
3	A	272	GLU
3	B	96	GLN
3	B	105	GLU
3	B	124	MET
3	B	151	SER
3	B	234	ASN
3	B	293	GLU
3	A	241	ALA
3	A	249	ALA
3	B	133	ASN
3	B	262	GLU
3	A	280	PRO
3	B	162	THR

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Mol	Chain	Res	Type
3	B	280	PRO
3	B	307	GLU
3	B	178	GLU
3	B	91	ILE
3	B	287	GLY
3	B	255	ASN

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
3	A	154/195 (79%)	116 (75%)	38 (25%)	0 2
3	B	154/195 (79%)	125 (81%)	29 (19%)	1 8
All	All	308/390 (79%)	241 (78%)	67 (22%)	1 5

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	90	SER
3	A	93	LYS
3	A	95	LEU
3	A	101	GLU
3	A	114	LEU
3	A	115	SER
3	A	116	GLU
3	A	120	ARG
3	A	123	LYS
3	A	133	ASN
3	A	141	ASP
3	A	148	SER
3	A	151	SER
3	A	152	GLN
3	A	158	THR
3	A	170	THR
3	A	178	GLU

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Mol	Chain	Res	Type
3	A	180	LEU
3	A	184	ASN
3	A	187	VAL
3	A	232	ARG
3	A	235	ARG
3	A	237	LYS
3	A	245	ILE
3	A	246	LEU
3	A	254	LYS
3	A	262	GLU
3	A	266	GLU
3	A	269	ASN
3	A	276	ARG
3	A	279	SER
3	A	281	SER
3	A	294	VAL
3	A	295	ARG
3	A	302	ASN
3	A	303	ARG
3	A	304	ARG
3	A	305	LYS
3	B	109	GLU
3	B	111	ASP
3	B	138	GLU
3	B	156	LYS
3	B	159	PRO
3	B	163	GLN
3	B	170	THR
3	B	174	ARG
3	B	184	ASN
3	B	185	GLN
3	B	231	MET
3	B	232	ARG
3	B	235	ARG
3	B	237	LYS
3	B	242	SER
3	B	244	GLN
3	B	247	TYR
3	B	250	TYR
3	B	253	GLN
3	B	254	LYS
3	B	261	ARG

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Mol	Chain	Res	Type
3	B	276	ARG
3	B	281	SER
3	B	282	LYS
3	B	286	LEU
3	B	292	THR
3	B	295	ARG
3	B	296	VAL
3	B	303	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	96	GLN
3	A	106	GLN
3	A	131	GLN
3	A	136	GLN
3	A	163	GLN
3	A	176	GLN
3	A	182	GLN
3	A	185	GLN
3	A	243	GLN
3	A	253	GLN
3	A	269	ASN
3	A	298	ASN
3	B	132	HIS
3	B	155	ASN
3	B	176	GLN
3	B	269	ASN
3	B	298	ASN
3	B	302	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	2:DT	O3'	3:DT	P	1.81
1	E	1:DC	O3'	2:DT	P	1.75

6 Fit of model and data [\(i\)](#)

6.1 Protein, DNA and RNA chains [\(i\)](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	20/20 (100%)	-0.91	0 [100] [100]	43, 65, 108, 112	0
2	F	20/20 (100%)	-1.00	0 [100] [100]	48, 66, 109, 116	0
3	A	176/221 (79%)	-0.67	0 [100] [100]	29, 65, 100, 108	0
3	B	176/221 (79%)	-0.73	0 [100] [100]	36, 65, 99, 108	0
All	All	392/482 (81%)	-0.73	0 [100] [100]	29, 65, 103, 116	0

There are no RSRZ outliers to report.

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.