



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:27 AM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

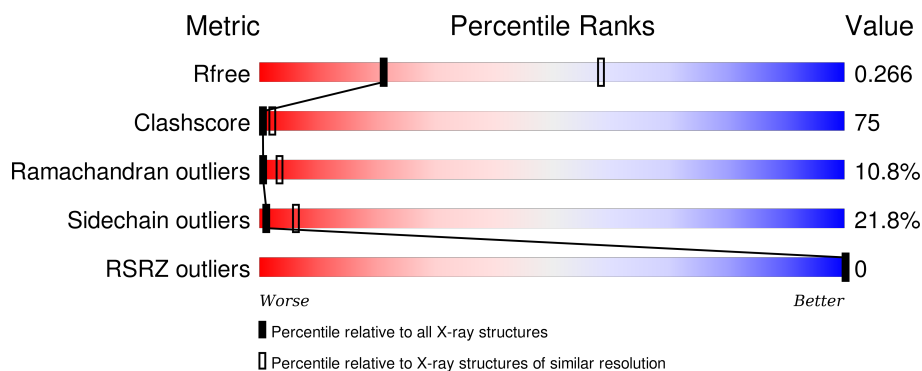
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	20	<div> <div style="width: 15%;"></div> <div style="width: 85%;"></div> </div>
2	F	20	<div> <div style="width: 10%;"></div> <div style="width: 90%;"></div> </div>
3	A	221	<div> <div style="width: 8%;"></div> <div style="width: 20%;"></div> <div style="width: 38%;"></div> <div style="width: 14%;"></div> <div style="width: 20%;"></div> </div>
3	B	221	<div> <div style="width: 6%;"></div> <div style="width: 22%;"></div> <div style="width: 39%;"></div> <div style="width: 13%;"></div> <div style="width: 20%;"></div> </div>

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*AP*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
			405	196	71	119	19			

- Molecule 2 is a DNA chain called 5'-D(*GP*CP*TP*GP*GP*TP*GP*AP*AP*TP*TP*AP*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
			409	197	76	117	19			

- 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
			1453	898	281	267	7			
3	B	176	Total	C	N	O	S	0	0	0
			1462	904	284	267	7			

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	A	1	Total	O	0	0
			1	1		
4	B	3	Total	O	0	0
			3	3		

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

3 Residue-property plots

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

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

Chain E: 

C1 T2 T3 T4 G4 G5 T6 T7 T8 A8 A9 A10 A11 A12 A13 A14 A15 A16 A17 C18 C19 A19 A20 G20

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

Chain F: 

G2 C3 G4 G5 G6 T7 G8 A9 A10 A11 A12 A13 A14 A15 A16 A17 C18 C19 A20 A21

- Molecule 3: Hepatocyte nuclear factor 1-beta

Chain A: 

S90 I91 I92 K93 E94 L95 Q96 A97 T98 L98 I99 T100 T101 E101 E102 A103 A104 E105 Q106 Q107 A108 A109 E110 D111 R112 Y112 M113 L114 S115 E116 E117 P118 P119 W119 W120 R121 A122 K123 F124 M125 I126 K126 G127 Y128 Y129 Q130 Q131 H132 H133 I134 P135 Q136 R137 E138 V139 V140 D141 Y142 T143 G144 L145 N146 Q147 S148 H149

L150 S151 Q152 H153 L154 M155 K156 A157 T158 P159 M160 T162 Q163 K164 A166 A167 L168 Y169 Y170 W171 Y172 V173 R174 K175 Q176 R177 E178 I179 L180 R181 Q182 K183 M184 Q185 T186 T187 G188 G189 SER GLN SER Y250 GLY Q251 ASN Q252 MET THR ASP LYS SER SER GLN ASP GLN LEU PHE LEU PHE PRO GLU PHE

SER GLN GLN SER HIS GLY PRO GLY GLN SER ASP ASP ALA CYS SER GLU PRO THR ASN LYS LYS M231 R232 Y232 E233 R234 R235 F236 Y237 N238 W239 F300 A301 A302 R303 R304 K305 I325 K126 G127 Y128 Q248 Y250 D251 R252 Q253 R254 M255 P256 S257 R258 E259 E260 E261 E262 A263 L264 V265 E266 E267 C268 M269

R270 A271 E272 C273 L274 Q275 R276 G277 V278 N279 S281 S282 A283 G284 L286 G287 S288 N289 L290 D111 R112 T291 E293 M113 L114 S115 E116 P118 W119 W120 R121 A122 K123 F124 M125 I126 K126 G127 Y128 Q248 Y250 D251 R252 Q253 R254 M255 P256 S257 R258 E259 E260 E261 E262 A263 L264 V265 E266 E267 C268 M269

- Molecule 3: Hepatocyte nuclear factor 1-beta

Chain B: 

S90 I91 I92 K93 E94 L95 Q96 A97 T98 L98 I99 T100 T101 E101 E102 A103 A104 E105 Q106 Q107 A108 A109 E110 D111 R112 Y112 M113 L114 S115 E116 P118 W119 W120 R121 A122 K123 F124 M125 I126 K126 G127 Y128 Y129 Q130 Q131 H132 H133 I134 P135 Q136 R137 E138 V139 V140 D141 Y142 T143 G144 L145 N146 Q147 S148 H149

L150	SER	R270
S151	GLN	A271
Q152	GLN	E272
H153	SER	C273
L154	HIS	L274
N155	GLY	Q275
K156	PRO	R276
Q157	GLY	G277
T158	GLN	V278
P159	SER	S279
M160	ASP	P280
K161	ASP	S281
T162	ALA	K282
Q163	CYS	A283
K164	SER	H284
R165	GLU	G285
A166	PRO	L286
A167	THR	G287
ASN	ASN	S288
L168	LYS	H289
Y169	LYS	L290
W171	M231	V291
Y172	R232	T292
V173	R233	E293
R174	N234	V294
K175	R235	R295
Q176	F236	V296
R177	R237	Y297
E178	W238	N298
I179	Q239	N299
L180	P240	F300
R181	A241	A301
Q182	S242	N302
F183	Q243	R303
N184	Q244	R304
K185	I245	K305
THR	L246	E306
VAL	Y247	E307
GLN	Q248	A308
SER	A249	F309
SER	Y250	R310
GLY	D251	
ASN	R252	
MET	Q253	
THR	K254	
ASP	N255	
LYS	P256	
SER	S257	
SER	K258	
GLN	E259	
ASP	E260	
GLN	R261	
LEU	E262	
PHE	A263	
PHE	L264	
LEU	V265	
PHE	E266	
PRO	E267	
GLU	C268	
PHE	N269	

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	174.69 Å 174.69 Å 72.43 Å 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
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.00 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.223 , 0.290 0.191 , 0.266	Depositor DCC
R_{free} test set	637 reflections (5.31%)	DCC
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
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 13666 reflections	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
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 ⓘ

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:CB	3:B:120:ARG:CG	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:CD	3:B:93:LYS:CE	1.75	1.59
3:B:232:ARG:CG	3:B:232:ARG:CD	1.76	1.57
3:A:93:LYS:CE	3:A:93:LYS:CD	1.80	1.56
3:A:93:LYS:CG	3:A:93:LYS:CD	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:CG	3:B:180:LEU:CD1	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:CG1	3:A:179:ILE:CD1	1.89	1.50
3:A:123:LYS:NZ	3:A:123:LYS:CE	1.73	1.50
3:B:93:LYS:NZ	3:B:93:LYS:CE	1.72	1.50
3:A:237:LYS:NZ	3:A:237:LYS:CE	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:CD	3:A:96:GLN:CG	1.81	1.46
1:E:1:DC:C5'	1:E:1:DC:O5'	1.63	1.46
3:A:180:LEU:CG	3:A:180:LEU:CD2	1.95	1.45
3:A:253:GLN:CG	3:A:253:GLN:CD	1.81	1.45
1:E:20:DG:C5'	1:E:20:DG:O5'	1.63	1.44
3:B:156:LYS:CD	3:B:156:LYS:CE	1.96	1.43
1:E:4:DG:C5'	1:E:4:DG:O5'	1.66	1.42
3:B:231:MET:SD	3:B:231:MET:CG	2.05	1.41
2:F:21:DA:C3'	2:F:21:DA:O3'	1.67	1.41
3:B:231:MET:CE	3:B:231:MET:SD	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
3:A:186:THR:HG23	3:A:187:VAL:H	1.10	1.08
2:F:18:DC:OP1	2:F:18:DC:H4'	1.40	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:O	3:B:303:ARG:HD2	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:CB	3:B:254:LYS:NZ	2.33	0.90
3:B:254:LYS:HZ2	3:B:254:LYS:HB3	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:B:179:ILE:O	3:B:179:ILE:HG23	1.73	0.87
3:A:104:ALA:HA	3:A:107:ARG:HH12	1.38	0.87
3:A:98:LEU:CD1	3:A:98:LEU:HG	2.04	0.87
3:B:91:ILE:O	3:B:91:ILE:HG22	1.73	0.87
3:B:106:GLN:O	3:B:108:ALA:N	2.08	0.86
3:A:110:VAL:HG23	3:A:173:VAL:HG21	1.56	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:B:153:HIS:HB2	3:B:158:THR:O	1.77	0.84
3:A:107:ARG:O	3:A:111:ASP:HB2	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
3:B:158:THR:HG22	3:B:159:PRO:HD2	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3:DC:OP1	2:F:4:DT:OP2	1.98	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:B:242:SER:HB3	3:B:268:CYS:SG	2.22	0.79
3:A:282:LYS:C	3:A:284:HIS:H	1.84	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:B:239:GLY:O	3:B:243:GLN:HG3	1.85	0.77
3:A:287:GLY:O	3:A:290:LEU:HB2	1.84	0.77
3:A:116:GLU:N	3:A:116:GLU:OE2	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
3:B:235:ARG:NH1	3:B:235:ARG:HG3	1.98	0.76
2:F:6:DG:C2'	2:F:7:DT:H5''	2.15	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:293:GLU:HG3	3:B:294:VAL:HG23	1.73	0.71
3:B:279:SER:O	3:B:281:SER:N	2.24	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:257:SER:O	3:A:260:GLU:N	2.25	0.70
3:A:177:ARG:O	3:A:178:GLU:C	2.28	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:186:THR:HG23	3:A:187:VAL:N	1.87	0.70
3:A:125:ILE:CG2	3:A:125:ILE:O	2.38	0.70
3:A:159:PRO:HG2	3:A:159:PRO:O	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:HG2	3:A:306:GLU:O	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:B:112:ARG:HG3	3:B:113:MET:H	1.57	0.68
3:A:250:TYR:C	3:A:252:ARG:N	2.47	0.68
1:E:18:DC:H2''	1:E:19:DA:N7	2.09	0.68
3:B:235:ARG:CG	3:B:235:ARG:HH11	2.08	0.67
3:B:305:LYS:O	3:B:306:GLU:O	2.13	0.67
3:A:107:ARG:HH11	3:A:107:ARG:HG3	1.60	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:H2'	2:F:4:DT:O5'	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
3:B:103:ALA:C	3:B:107:ARG:HH12	2.00	0.65
1:E:2:DT:H2''	1:E:3:DT:C6	2.32	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:HO5'	1:E:1:DC:C5'	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:CB	3:B:254:LYS:HZ3	2.02	0.63
3:A:141:ASP:OD2	3:A:141:ASP:N	2.29	0.63
3:B:257:SER:O	3:B:260:GLU:N	2.31	0.63
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:107:ARG:NH1	3:A:107:ARG:HG3	2.14	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
3:B:173:VAL:HG23	3:B:174:ARG:N	2.13	0.62
2:F:20:DA:C6	2:F:21:DA:C6	2.87	0.62
3:B:303:ARG:NH1	3:B:307:GLU:CB	2.63	0.62
3:B:112:ARG:CG	3:B:113:MET:N	2.62	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: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:HZ2	3:B:254:LYS:CB	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:B:109:GLU:HG2	3:B:173:VAL:CG1	2.29	0.62
3:A:110:VAL:HG23	3:A:173:VAL:CG2	2.30	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:B:158:THR:CG2	3:B:159:PRO:CD	2.69	0.61
3:B:163:GLN:OE1	3:B:163:GLN:HA	2.01	0.61
3:A:256:PRO:HG2	3:A:300:PHE:CE1	2.35	0.61
3:B:120:ARG:CA	3:B:120:ARG:CG	2.73	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:179:ILE:CG2	3:A:179:ILE:O	2.48	0.61
3:A:279:SER:O	3:A:281:SER:O	2.19	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:B:303:ARG:HH12	3:B:307:GLU:HB2	1.66	0.60
3:B:258:LYS:HA	3:B:261:ARG:HG3	1.83	0.60
3:A:165:ARG:C	3:A:167:ALA:N	2.51	0.60
2:F:18:DC:OP1	2:F:18:DC:C4'	2.33	0.60
3:A:279:SER:C	3:A:281:SER:N	2.53	0.60
1:E:12:DA:OP2	3:A:151:SER:HB3	2.02	0.60
1:E:12:DA:H2''	1:E:13:DT:C5'	2.32	0.60
3:A:242:SER:O	3:A:246:LEU:HD12	2.02	0.60
3:A:240:PRO:O	3:A:243:GLN:HB3	2.02	0.60
3:B:253:GLN:O	3:B:254:LYS:C	2.39	0.60
2:F:10:DA:H2''	2:F:11:DT:O5'	2.02	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:B:303:ARG:HD2	3:B:303:ARG:C	2.15	0.59
3:A:299:TRP:O	3:A:299:TRP:CD2	2.56	0.59
3:B:104:ALA:O	3:B:105:GLU:C	2.40	0.59
3:B:274:LEU:CD1	3:B:274:LEU:HG	2.24	0.58
3:B:269:ASN:HD21	3:B:291:VAL:H	1.50	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:282:LYS:HB2	3:B:284:HIS:CE1	2.38	0.58
3:B:240:PRO:CD	3:B:241:ALA:H	2.16	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:B:161:LYS:O	3:B:162:THR:C	2.41	0.57
3:A:303:ARG:HH11	3:A:303:ARG:HG2	1.70	0.57
3:A:169:TYR:O	3:A:172:TYR:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:152:GLN:OE1	3:A:152:GLN:CA	2.53	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
3:B:106:GLN:C	3:B:108:ALA:H	2.04	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: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:CG	3:A:306:GLU:O	2.52	0.57
2:F:9:DA:H1'	2:F:10:DA:H5''	1.87	0.57
3:B:158:THR:HG22	3:B:159:PRO:N	2.16	0.57
1:E:5:DG:H1'	1:E:6:DT:H5'	1.86	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:250:TYR:HA	3:B:253:GLN:HG2	1.86	0.56
3:B:240:PRO:O	3:B:243:GLN:HB2	2.05	0.56
2:F:5:DG:H2''	2:F:6:DG:C5'	2.21	0.56
3:A:116:GLU:CD	3:A:116:GLU:N	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
3:B:175:LYS:HG3	3:B:175:LYS:O	2.02	0.55
3:B:106:GLN:CG	3:B:177:ARG:HH12	2.20	0.55
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:159:PRO:HG2	3:B:159:PRO:O	2.06	0.55
3:A:237:LYS:CD	3:A:237:LYS:NZ	2.66	0.55
3:B:91:ILE:HA	3:B:94:GLU:HB3	1.88	0.55
3:B:240:PRO:HD2	3:B:241:ALA:H	1.70	0.55
3:B:143:THR:HB	3:B:145:LEU:HG	1.89	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
2:F:5:DG:C2'	2:F:6:DG:H5''	2.24	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)
3:A:93:LYS:O	3:A:94:GLU:C	2.46	0.54
1:E:12:DA:C1'	1:E:13:DT:H5''	2.35	0.54
3:A:120:ARG:NH1	3:A:120:ARG:HB3	2.22	0.54
3:B:281:SER:O	3:B:282:LYS:HG2	2.07	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:A:131:GLN:HE21	3:A:276:ARG:HA	1.72	0.54
3:B:168:LEU:O	3:B:171:TRP:HB3	2.07	0.54
3:A:247:TYR:HE2	3:A:303:ARG:HE	1.54	0.54
3:A:170:THR:O	3:A:171:TRP:C	2.44	0.54
3:B:112:ARG:CG	3:B:113:MET:H	2.20	0.54
3:B:233:ARG:CD	3:B:233:ARG:CB	2.82	0.54
3:B:153:HIS:HA	3:B:158:THR:N	2.22	0.54
2:F:20:DA:C5	2:F:21:DA:C6	2.95	0.54
3:B:91:ILE:CG2	3:B:91:ILE:O	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:B:174:ARG:C	3:B:176:GLN:N	2.61	0.52
3:A:137:ARG:HH11	3:A:137:ARG:CG	2.15	0.52
3:B:95:LEU:O	3:B:97:ALA:N	2.42	0.52
3:B:231:MET:O	3:B:232:ARG:O	2.28	0.52
3:B:161:LYS:CD	3:B:161:LYS:CB	2.79	0.52
3:A:186:THR:CG2	3:A:282:LYS:NZ	2.52	0.52
3:A:175:LYS:O	3:A:175:LYS:HG3	2.09	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:B:173:VAL:CG2	3:B:174:ARG:N	2.73	0.52
3:A:104:ALA:HA	3:A:107:ARG:CZ	2.39	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:281:SER:C	3:B:282:LYS:CG	2.78	0.51
3:B:135:PRO:C	3:B:137:ARG:N	2.63	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:B:162:THR:O	3:B:163:GLN:C	2.49	0.51
3:A:256:PRO:HB2	3:A:261:ARG:CG	2.38	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:B:165:ARG:O	3:B:169:TYR:N	2.32	0.50
3:A:120:ARG:HA	3:A:120:ARG:NE	2.27	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
2:F:3:DC:P	2:F:4:DT:OP2	2.69	0.50
1:E:12:DA:C8	1:E:13:DT:C7	2.95	0.50
3:B:296:VAL:CG2	3:B:297:TYR:N	2.73	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:260:GLU:O	3:B:263:ALA:HB3	2.11	0.50
3:A:181:ARG:C	3:A:183:PHE:N	2.48	0.50
3:A:300:PHE:O	3:A:301:ALA:C	2.47	0.50
3:A:293:GLU:O	3:A:297:TYR:N	2.35	0.50
3:B:95:LEU:C	3:B:97:ALA:N	2.65	0.50
3:A:237:LYS:CG	3:A:237:LYS:NZ	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:N	3:B:231:MET:SD	2.85	0.49
3:B:302:ASN:O	3:B:306:GLU:HG3	2.12	0.49
3:B:180:LEU:CD1	3:B:180:LEU:CD2	2.86	0.49
3:A:125:ILE:C	3:A:127:GLY:H	2.14	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:B:171:TRP:CE3	3:B:172:TYR:CA	2.95	0.49
3:A:291:VAL:HG12	3:A:292:THR:N	2.26	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
3:B:120:ARG:CG	3:B:120:ARG:C	2.80	0.49
3:A:256:PRO:CG	3:A:300:PHE:CE1	2.95	0.49
2:F:21:DA:O3'	2:F:21:DA:H3'	1.96	0.49
3:B:103:ALA:HB1	3:B:107:ARG:HH12	1.78	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: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:B:128:TYR:CE2	3:B:132:HIS:CD2	3.01	0.48
3:A:186:THR:HG22	3:A:282:LYS:HZ3	1.69	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: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:N	3:A:293:GLU:OE1	2.32	0.48
3:B:167:ALA:O	3:B:168:LEU:C	2.50	0.48
3:B:297:TYR:CD2	3:B:297:TYR:C	2.86	0.48
3:B:163:GLN:O	3:B:166:ALA:HB3	2.14	0.48
3:A:158:THR:CG2	3:A:159:PRO:HD2	2.43	0.48
3:A:301:ALA:C	3:A:303:ARG:H	2.17	0.48
3:A:110:VAL:O	3:A:110:VAL:HG12	2.06	0.48
3:A:106:GLN:HB3	3:A:173:VAL:HG11	1.96	0.48
3:B:106:GLN:C	3:B:108:ALA:N	2.59	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:A:109:GLU:OE2	3:A:112:ARG:NH2	2.39	0.47
2:F:3:DC:H5'	3:B:297:TYR:OH	2.14	0.47
1:E:12:DA:H1'	1:E:13:DT:C5'	2.38	0.47
3:B:169:TYR:O	3:B:170:THR:C	2.50	0.47
3:A:257:SER:N	3:A:260:GLU:HB3	2.29	0.47
3:B:177:ARG:O	3:B:179:ILE:N	2.47	0.47
3:A:256:PRO:HB3	3:A:260:GLU:HG3	1.96	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
3:B:128:TYR:CE2	3:B:132:HIS:HD2	2.33	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:B:257:SER:O	3:B:258:LYS:C	2.49	0.47
3:A:271:ALA:O	3:A:274:LEU:HB2	2.14	0.47
2:F:13:DA:C8	2:F:14:DT:H71	2.50	0.47
2:F:3:DC:O2	2:F:3:DC:C2'	2.61	0.47
2:F:4:DT:O5'	2:F:4:DT:C2'	2.63	0.47
3:B:174:ARG:C	3:B:176:GLN:H	2.19	0.47
3:A:297:TYR:CD1	3:A:297:TYR:C	2.86	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:B:303:ARG:HD3	3:B:306:GLU:CD	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:268:CYS:O	3:A:270:ARG:N	2.49	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:242:SER:HB3	3:A:268:CYS:SG	2.55	0.46
3:A:241:ALA:C	3:A:243:GLN:N	2.64	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
3:A:165:ARG:HG3	3:A:165:ARG:HH11	1.80	0.46
3:B:233:ARG:CG	3:B:233:ARG:NE	2.67	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:90:SER:O	3:B:92:LEU:N	2.48	0.46
3:A:300:PHE:O	3:A:303:ARG:N	2.49	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:B:170:THR:O	3:B:171:TRP:C	2.53	0.45
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:A:177:ARG:O	3:A:180:LEU:HD12	2.17	0.45
3:A:145:LEU:HD23	3:A:164:LYS:HD2	1.99	0.45
3:B:181:ARG:C	3:B:183:PHE:H	2.19	0.45
3:B:302:ASN:HA	3:B:302:ASN:HD22	1.42	0.45
1:E:4:DG:P	1:E:4:DG:C5'	3.02	0.45
3:B:131:GLN:O	3:B:275:GLN:NE2	2.46	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
3:B:177:ARG:C	3:B:180:LEU:H	2.16	0.45
3:A:261:ARG:H	3:A:261:ARG:HG3	1.50	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:NE2	3:A:163:GLN:HA	2.32	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
3:A:150:LEU:O	3:A:151:SER:C	2.55	0.45
1:E:12:DA:C2'	1:E:13:DT:C5'	2.95	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:172:TYR:CE1	3:B:176:GLN:OE1	2.71	0.44
3:B:155:ASN:HD22	3:B:155:ASN:HA	1.26	0.44
3:B:175:LYS:HA	3:B:178:GLU:HB3	2.00	0.44
3:A:137:ARG:CG	3:A:137:ARG:NH1	2.73	0.44
3:A:274:LEU:HD23	3:A:274:LEU:HA	1.65	0.43
3:B:299:TRP:CD2	3:B:299:TRP:C	2.92	0.43
3:B:258:LYS:CA	3:B:261:ARG:HG3	2.48	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:B:294:VAL:HG23	3:B:294:VAL:H	1.28	0.43
3:B:269:ASN:HD21	3:B:290:LEU:HD12	1.74	0.43
3:A:241:ALA:HB3	3:A:242:SER:H	1.53	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:160:MET:HG2	3:A:164:LYS:HB2	2.00	0.43
3:A:95:LEU:HD12	3:A:95:LEU:HA	1.62	0.43
3:B:160:MET:CE	3:B:165:ARG:HA	2.49	0.43
3:B:236:PHE:C	3:B:236:PHE:CD2	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:HA	3:B:246:LEU:HD23	1.59	0.42
1:E:1:DC:C5'	1:E:2:DT:C7	2.96	0.42
3:A:159:PRO:CG	3:A:159:PRO:O	2.66	0.42
3:A:135:PRO:O	3:A:136:GLN:C	2.53	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:B:297:TYR:CD2	3:B:298:ASN:ND2	2.79	0.42
3:B:299:TRP:HE3	3:B:299:TRP:C	2.19	0.42
3:A:171:TRP:CE3	3:A:172:TYR:HA	2.54	0.42
3:B:90:SER:O	3:B:91:ILE:C	2.55	0.41
3:A:300:PHE:O	3:A:303:ARG:CB	2.60	0.41
2:F:3:DC:H3'	2:F:4:DT:C6	2.54	0.41
3:A:165:ARG:HG3	3:A:165:ARG:NH1	2.35	0.41
3:A:165:ARG:O	3:A:169:TYR:CD2	2.73	0.41
3:B:106:GLN:CG	3:B:177:ARG:NH1	2.84	0.41
3:B:258:LYS:O	3:B:258:LYS:CG	2.68	0.41
3:A:236:PHE:HE2	3:A:238:TRP:CD1	2.38	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:B:111:ASP:HA	3:B:114:LEU:HD12	2.01	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: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:B:169:TYR:O	3:B:172:TYR:HB3	2.21	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: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:HG2	3:A:303:ARG:NH1	2.34	0.40
3:A:304:ARG:C	3:A:306:GLU:N	2.75	0.40
3:B:126:LYS:O	3:B:130:GLN:HB3	2.21	0.40
3:A:152:GLN:HB3	3:A:158:THR:HG1	1.81	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	5
3	B	172/221 (78%)	125 (73%)	25 (14%)	22 (13%)	0	2
All	All	344/442 (78%)	249 (72%)	58 (17%)	37 (11%)	0	3

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 ⓘ

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%)	1	3
3	B	154/195 (79%)	125 (81%)	29 (19%)	2	10
All	All	308/390 (79%)	241 (78%)	67 (22%)	1	6

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

Some 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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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%)	-0.66	0 100 100	29, 65, 100, 108	0
3	B	176/221 (79%)	-0.72	0 100 100	36, 65, 99, 108	0
All	All	392/482 (81%)	-0.72	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.