



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:55 PM UTC

PDB ID : 2H8R / pdb_00002h8r
Title : Hepatocyte Nuclear Factor 1b bound to DNA: MODY5 Gene Product
Authors : Lu, P.; Rha, G.B.; Chi, Y.I.
Deposited on : 2006-06-07
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

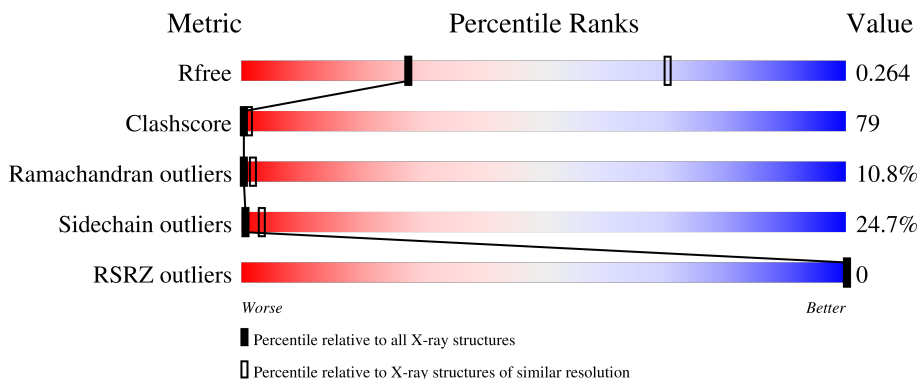
1 Overall quality at a glance

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	E	20	
2	F	20	
3	A	221	
3	B	221	

2 Entry composition

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	E	1	Total	O	0	0
			1	1		
4	F	2	Total	O	0	0
			2	2		

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

3 Residue-property plots

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

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

Chain E: 

G1 T2 T3 G4 G5 T6 T7 T8 A9 T10 T11 A12 T13 T14 T15 A16 A17 C18 C19 A20 A21

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

Chain F: 

G2 C3 T4 G5 G6 T7 T8 A9 T10 T11 A12 T13 T14 T15 A16 A17 C18 C19 A20 A21

- Molecule 3: Hepatocyte nuclear factor 1-beta

Chain A: 

S90 L150 S151 Q152 R153 L154 N155 Q156 A157 T158 P159 M160 K161 T162 Q163 A164 R165 A166 L168 Y169 T170 D171 R172 Y173 R174 K175 E176 R177 E178 I179 R180 R181 A182 F183 R184 Q185 T186 K187 G188 Y189 G190 S191 Q192 R193 L194 N195 Q196 A197 T198 P199 M200 K201 T202 Q203 A204 R205 A206 L208 Y209 T210 D211 R212 Y213 R214 K215 E216 R217 E218 I219 R220 R221 A222 F223 R224 Q225 T226 K227 E228 I229 R230 R231 A232 S233 Q234 R235 E236 R237 E238 I239 R240 R241 A242 S243 Q244 R245 T246 K247 Y248 Q249 S250 D251 G252 A253 T254 N255 P256 S257 K258 S259 E260 R261 E262 A263 L264 V265 E266 E267 C268 R269

- Molecule 3: Hepatocyte nuclear factor 1-beta

Chain B: 

S90 L150 S151 Q152 R153 L154 N155 Q156 A157 T158 P159 M160 K161 T162 Q163 A164 R165 A166 L168 Y169 T170 D171 R172 Y173 R174 K175 E176 R177 E178 I179 R180 R181 A182 F183 R184 Q185 T186 K187 G188 Y189 G190 S191 Q192 R193 L194 N195 Q196 A197 T198 P199 M200 K201 T202 Q203 A204 R205 A206 L208 Y209 T210 D211 R212 Y213 R214 K215 E216 R217 E218 I219 R220 R221 A222 F223 R224 Q225 T226 K227 E228 I229 R230 R231 A232 S233 Q234 R235 E236 R237 E238 I239 R240 R241 A242 S243 Q244 R245 T246 K247 Y248 Q249 S250 D251 G252 A253 T254 N255 P256 S257 K258 S259 E260 R261 E262 A263 L264 V265 E266 E267 C268 R269

R270	R271	R272	R273	R274	R275	R276	R277	R278	R279	R280	R281	R282	R283	R284	R285	R286	R287	R288	R289	R290	R291	R292	R293	R294	R295	R296	R297	R298	R299	R300	R301	R302	R303	R304	R305	R306	R307	R308	R309	R310																				
SER	GLN	GLN	SER	SER	GLY	GLY	GLN	SER	SER	ASP	ASP	ALA	CYS	SER	SER	GLU	PRO	THR	ASN	LYS	LYS	R231	R232	R233	R234	R235	R236	R237	R238	R239	R240	R241	R242	R243	R244	R245	R246	R247	R248	R249	R250	R251	R252	R253	R254	R255	R256	R257	R258	R259	R260	R261	R262	R263	R264	R265	R266	R267	R268	R269

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	174.69Å 174.69Å 72.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.20 20.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-3.20) 93.2 (20.00-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.223 , 0.290 0.195 , 0.264	Depositor DCC
R_{free} test set	691 reflections (4.23%)	wwPDB-VP
Wilson B-factor (Å ²)	79.5	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.98	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	E	3.28	56/453 (12.4%)	3.98	137/697 (19.7%)
2	F	3.14	48/459 (10.5%)	3.78	134/707 (19.0%)
3	A	3.95	286/1478 (19.4%)	2.98	181/1986 (9.1%)
3	B	4.20	303/1488 (20.4%)	2.88	155/1996 (7.8%)
All	All	3.89	693/3878 (17.9%)	3.20	607/5386 (11.3%)

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 (693) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	134	ILE	CG1-CD1	22.58	2.39	1.51
3	A	249	ALA	CA-CB	-19.45	1.20	1.53
3	B	231	MET	SD-CE	17.49	2.23	1.79
3	B	108	ALA	CA-CB	-16.72	1.31	1.54
3	A	166	ALA	CA-CB	-16.72	1.22	1.53
3	B	113	MET	SD-CE	-15.86	1.40	1.79
3	B	156	LYS	CD-CE	14.74	1.96	1.52
3	B	122	ALA	CA-CB	-14.59	1.30	1.53
3	B	243	GLN	CD-OE1	14.55	1.51	1.23
1	E	2	DT	O3'-P	13.82	1.81	1.61
3	A	110	VAL	CA-CB	-13.76	1.36	1.54
3	B	265	VAL	CA-CB	-13.68	1.39	1.54
3	B	165	ARG	C-O	13.52	1.39	1.24
3	B	152	GLN	CD-NE2	13.46	1.61	1.33
3	B	283	ALA	CA-CB	-13.43	1.35	1.52
3	A	150	LEU	N-CA	-13.41	1.30	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	166	ALA	CA-CB	-13.38	1.32	1.53
3	B	282	LYS	CA-C	-13.37	1.38	1.52
3	A	134	ILE	CA-CB	-13.06	1.38	1.54
3	A	180	LEU	CG-CD2	12.90	1.95	1.52
3	B	278	VAL	C-O	12.88	1.39	1.24
3	A	123	LYS	CD-CE	12.73	1.90	1.52
3	B	150	LEU	C-O	12.52	1.37	1.24
3	B	121	ALA	CA-CB	-12.52	1.33	1.53
3	A	300	PHE	CA-C	-12.51	1.39	1.53
3	B	174	ARG	NE-CZ	12.51	1.46	1.33
3	A	129	MET	CA-C	-12.45	1.35	1.52
3	B	106	GLN	C-O	-12.41	1.09	1.24
3	A	159	PRO	C-O	12.33	1.38	1.23
3	B	141	ASP	N-CA	-12.21	1.32	1.46
3	B	274	LEU	CG-CD1	12.16	1.92	1.52
3	A	91	ILE	CA-CB	-12.15	1.39	1.54
3	A	96	GLN	CG-CD	11.85	1.81	1.52
3	A	151	SER	CA-C	-11.74	1.35	1.52
3	A	253	GLN	CG-CD	11.70	1.81	1.52
3	B	264	LEU	CA-C	-11.58	1.37	1.52
3	B	159	PRO	C-O	11.53	1.36	1.23
3	B	114	LEU	CA-C	-11.51	1.36	1.52
3	B	238	TRP	C-O	-11.49	1.09	1.23
3	A	305	LYS	C-O	-11.49	1.09	1.24
1	E	18	DC	P-OP2	11.43	1.71	1.48
3	A	121	ALA	CA-CB	-11.43	1.34	1.53
3	A	241	ALA	CA-CB	-11.34	1.34	1.53
2	F	14	DT	P-OP2	11.23	1.71	1.48
3	B	130	GLN	C-O	11.19	1.38	1.24
3	B	243	GLN	CD-NE2	11.18	1.56	1.33
3	B	138	GLU	C-O	-10.94	1.10	1.24
3	B	158	THR	CA-CB	-10.93	1.34	1.53
3	A	106	GLN	C-O	-10.91	1.11	1.24
3	B	137	ARG	CA-CB	-10.89	1.35	1.53
3	A	271	ALA	CA-CB	-10.85	1.36	1.53
2	F	15	DT	P-OP2	10.77	1.70	1.48
3	A	142	VAL	CA-CB	-10.75	1.39	1.54
3	B	133	ASN	CA-C	-10.70	1.38	1.52
3	B	110	VAL	CA-C	-10.56	1.40	1.52
3	A	304	ARG	CA-C	-10.55	1.38	1.52
3	A	103	ALA	CA-CB	-10.53	1.36	1.53
3	A	113	MET	SD-CE	-10.53	1.53	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	179	ILE	CA-C	-10.48	1.38	1.52
3	B	278	VAL	CA-CB	-10.39	1.40	1.54
3	B	163	GLN	CD-NE2	10.32	1.54	1.33
3	B	283	ALA	N-CA	-10.31	1.33	1.46
3	B	310	ARG	C-OXT	10.28	1.44	1.23
3	B	180	LEU	CG-CD1	10.20	1.86	1.52
3	B	172	TYR	N-CA	-10.18	1.34	1.46
3	A	132	HIS	C-O	10.17	1.39	1.24
3	A	93	LYS	CG-CD	10.13	1.82	1.52
3	B	276	ARG	CZ-NH1	10.11	1.47	1.32
3	B	161	LYS	CG-CD	10.08	1.82	1.52
3	B	95	LEU	C-O	-9.95	1.12	1.24
3	A	232	ARG	NE-CZ	9.93	1.44	1.33
3	B	232	ARG	NE-CZ	9.93	1.44	1.33
3	A	101	GLU	CD-OE2	9.86	1.44	1.25
3	B	231	MET	CG-SD	9.86	2.05	1.80
3	B	137	ARG	CA-C	-9.85	1.39	1.52
3	A	303	ARG	CA-C	-9.84	1.39	1.52
3	B	293	GLU	CD-OE1	9.81	1.44	1.25
1	E	1	DC	O3'-P	9.74	1.75	1.61
3	B	298	ASN	CA-C	-9.73	1.39	1.52
3	B	131	GLN	C-O	9.68	1.35	1.24
3	B	116	GLU	N-CA	-9.67	1.33	1.45
3	B	165	ARG	CZ-NH2	9.64	1.46	1.33
3	A	120	ARG	NE-CZ	9.64	1.43	1.33
3	A	238	TRP	CA-CB	-9.64	1.37	1.53
3	A	170	THR	CA-CB	-9.59	1.38	1.53
3	A	95	LEU	CA-C	-9.59	1.40	1.52
3	A	179	ILE	CG1-CD1	9.58	1.89	1.51
1	E	2	DT	P-O5'	9.47	1.79	1.60
3	A	93	LYS	CD-CE	9.47	1.80	1.52
3	A	295	ARG	N-CA	-9.46	1.35	1.46
3	A	151	SER	N-CA	9.46	1.58	1.46
3	B	270	ARG	NE-CZ	9.45	1.43	1.33
3	B	297	TYR	N-CA	-9.45	1.35	1.46
3	A	120	ARG	CA-C	-9.40	1.40	1.52
3	B	301	ALA	N-CA	-9.39	1.35	1.46
3	A	100	THR	CA-CB	9.37	1.73	1.54
3	B	301	ALA	CA-CB	-9.31	1.39	1.53
3	A	248	GLN	CD-OE1	9.30	1.41	1.23
3	B	300	PHE	CA-C	-9.30	1.41	1.52
3	B	130	GLN	CD-OE1	9.29	1.41	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	298	ASN	C-O	-9.26	1.12	1.24
3	A	242	SER	C-O	-9.24	1.12	1.24
3	A	300	PHE	C-O	-9.24	1.14	1.23
3	A	172	TYR	C-O	9.21	1.34	1.24
3	A	237	LYS	CA-C	-9.12	1.42	1.52
3	A	153	HIS	CA-CB	-9.10	1.38	1.53
3	A	293	GLU	CD-OE2	9.04	1.42	1.25
2	F	10	DA	P-OP2	9.02	1.66	1.48
3	B	91	ILE	C-O	-9.01	1.13	1.24
3	A	298	ASN	C-O	-9.00	1.12	1.24
3	A	120	ARG	C-O	-8.99	1.12	1.24
1	E	2	DT	P-OP1	8.97	1.66	1.48
3	B	109	GLU	C-O	-8.96	1.13	1.24
3	B	131	GLN	CG-CD	8.93	1.74	1.52
3	B	178	GLU	N-CA	-8.90	1.34	1.46
3	A	96	GLN	CD-OE1	8.90	1.40	1.23
3	A	297	TYR	N-CA	-8.90	1.35	1.46
3	A	250	TYR	C-O	8.89	1.34	1.24
3	A	95	LEU	C-O	-8.87	1.13	1.24
3	B	150	LEU	N-CA	-8.87	1.35	1.46
3	B	96	GLN	CG-CD	8.86	1.74	1.52
3	B	129	MET	CA-C	-8.86	1.40	1.52
3	A	243	GLN	CG-CD	8.83	1.74	1.52
3	B	167	ALA	CA-CB	-8.82	1.39	1.53
3	B	120	ARG	CZ-NH2	8.80	1.44	1.33
3	B	267	GLU	CA-C	8.79	1.64	1.52
3	A	137	ARG	CA-CB	-8.78	1.39	1.53
3	B	178	GLU	CD-OE1	8.73	1.42	1.25
3	A	130	GLN	C-O	8.73	1.34	1.24
3	A	248	GLN	CG-CD	8.72	1.73	1.52
3	B	143	THR	CA-CB	8.72	1.67	1.53
3	B	170	THR	CA-CB	-8.70	1.39	1.53
3	A	142	VAL	C-O	8.68	1.34	1.24
3	A	176	GLN	CD-NE2	8.65	1.51	1.33
3	A	274	LEU	C-O	8.61	1.33	1.24
3	B	249	ALA	CA-CB	-8.60	1.40	1.53
3	A	242	SER	CA-C	-8.59	1.40	1.52
2	F	3	DC	P-OP2	8.59	1.65	1.48
2	F	2	DG	N1-C2	8.56	1.55	1.38
3	B	232	ARG	CA-C	8.49	1.64	1.52
3	B	176	GLN	C-O	-8.48	1.13	1.24
3	A	180	LEU	C-O	-8.47	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	16	DA	P-OP1	8.46	1.65	1.48
3	A	180	LEU	N-CA	-8.44	1.36	1.46
3	A	289	ASN	N-CA	-8.45	1.34	1.46
3	B	109	GLU	CD-OE2	8.44	1.41	1.25
3	A	237	LYS	CE-NZ	8.43	1.74	1.49
2	F	21	DA	C3'-O3'	8.43	1.68	1.42
1	E	17	DC	O3'-P	8.41	1.73	1.61
3	A	138	GLU	CA-CB	-8.41	1.40	1.53
3	B	152	GLN	CD-OE1	8.40	1.39	1.23
3	B	120	ARG	NE-CZ	8.39	1.42	1.33
3	B	120	ARG	CG-CD	8.36	1.77	1.52
3	B	249	ALA	C-O	-8.36	1.12	1.24
3	B	109	GLU	CA-C	-8.35	1.42	1.52
1	E	15	DC	P-OP2	8.34	1.65	1.48
2	F	20	DA	O3'-P	8.34	1.73	1.61
3	A	132	HIS	CA-CB	-8.34	1.39	1.53
3	A	286	LEU	N-CA	-8.32	1.36	1.46
3	B	158	THR	CA-C	-8.32	1.44	1.53
2	F	20	DA	P-OP2	8.31	1.65	1.48
3	B	91	ILE	CA-C	-8.31	1.42	1.52
3	A	129	MET	SD-CE	8.29	2.00	1.79
3	B	185	GLN	CB-CG	8.28	1.77	1.52
1	E	14	DT	P-OP2	8.25	1.65	1.48
3	B	150	LEU	CA-CB	-8.24	1.41	1.53
3	A	169	TYR	CA-CB	-8.23	1.40	1.53
3	B	261	ARG	CA-C	-8.23	1.42	1.52
3	B	299	TRP	CD2-CE2	8.22	1.55	1.41
3	B	299	TRP	CA-CB	-8.20	1.39	1.53
2	F	19	DC	P-OP2	8.19	1.64	1.48
3	A	177	ARG	NE-CZ	8.17	1.42	1.33
3	A	254	LYS	CB-CG	8.16	1.76	1.52
3	A	303	ARG	CZ-NH1	8.15	1.44	1.32
3	B	282	LYS	N-CA	-8.14	1.36	1.46
3	A	299	TRP	CA-CB	-8.14	1.39	1.53
3	A	302	ASN	C-O	8.14	1.38	1.23
3	A	291	VAL	CA-C	-8.13	1.43	1.52
3	B	245	ILE	CA-C	-8.13	1.42	1.52
3	B	248	GLN	CD-OE1	8.12	1.39	1.23
3	B	279	SER	C-O	8.11	1.33	1.24
3	B	178	GLU	C-O	-8.10	1.13	1.24
3	A	94	GLU	CD-OE2	8.10	1.40	1.25
1	E	20	DG	P-OP2	8.08	1.64	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	134	ILE	C-O	8.08	1.34	1.24
3	B	135	PRO	CA-CB	-8.08	1.42	1.53
3	A	139	VAL	CA-CB	-8.07	1.44	1.54
3	B	232	ARG	N-CA	8.04	1.56	1.46
3	B	172	TYR	CA-CB	-8.02	1.41	1.53
3	A	110	VAL	CA-C	-8.02	1.41	1.52
3	B	294	VAL	CA-CB	-8.01	1.43	1.54
2	F	19	DC	P-OP1	8.01	1.64	1.48
3	B	131	GLN	CA-C	7.99	1.63	1.52
3	B	91	ILE	CA-CB	-7.99	1.43	1.54
3	B	233	ARG	NE-CZ	7.99	1.41	1.33
2	F	4	DT	P-OP1	7.98	1.64	1.48
3	B	237	LYS	CG-CD	7.98	1.76	1.52
3	B	232	ARG	CG-CD	7.97	1.76	1.52
3	A	151	SER	C-O	-7.96	1.13	1.24
3	A	123	LYS	CE-NZ	7.96	1.73	1.49
3	B	120	ARG	CZ-NH1	7.96	1.43	1.32
3	A	297	TYR	C-O	7.95	1.33	1.24
2	F	2	DG	C5-C4	7.93	1.54	1.38
3	A	257	SER	CA-C	-7.92	1.43	1.52
3	B	177	ARG	C-O	-7.92	1.14	1.24
3	B	124	MET	N-CA	-7.92	1.35	1.46
3	B	273	CYS	CA-C	-7.92	1.41	1.52
3	A	236	PHE	C-O	-7.91	1.13	1.23
3	A	105	GLU	CD-OE2	7.90	1.40	1.25
3	B	105	GLU	CA-C	7.89	1.63	1.52
3	B	138	GLU	CD-OE2	7.89	1.40	1.25
1	E	7	DT	P-OP2	7.89	1.64	1.48
3	B	293	GLU	CD-OE2	7.89	1.40	1.25
3	B	178	GLU	CD-OE2	7.88	1.40	1.25
3	B	119	TRP	CE2-CZ2	-7.88	1.23	1.39
3	B	174	ARG	CZ-NH1	7.87	1.43	1.32
3	A	300	PHE	CD1-CE1	7.86	1.62	1.38
3	A	128	TYR	N-CA	-7.86	1.36	1.46
3	A	150	LEU	CA-CB	-7.83	1.41	1.53
3	A	131	GLN	CA-C	7.83	1.63	1.52
2	F	9	DA	P-OP2	7.82	1.64	1.48
3	A	272	GLU	C-O	7.82	1.33	1.24
3	B	93	LYS	CD-CE	7.82	1.75	1.52
1	E	4	DG	O5'-C5'	7.81	1.66	1.42
3	A	137	ARG	C-O	7.81	1.33	1.24
3	A	251	ASP	CB-CG	7.80	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	293	GLU	CG-CD	7.80	1.71	1.52
1	E	3	DT	P-OP2	7.79	1.64	1.48
3	B	248	GLN	CD-NE2	7.78	1.49	1.33
3	A	245	ILE	C-O	-7.78	1.13	1.24
2	F	3	DC	P-OP1	7.77	1.64	1.48
3	A	127	GLY	CA-C	-7.76	1.41	1.51
2	F	20	DA	P-O5'	7.76	1.75	1.60
3	B	179	ILE	CA-CB	-7.75	1.45	1.54
3	B	233	ARG	CG-CD	7.75	1.75	1.52
3	B	264	LEU	C-O	-7.75	1.14	1.24
3	B	93	LYS	CE-NZ	7.74	1.72	1.49
3	B	148	SER	N-CA	-7.73	1.36	1.46
3	A	164	LYS	CA-C	-7.72	1.43	1.52
3	A	129	MET	CG-SD	7.71	2.00	1.80
3	B	237	LYS	CA-CB	-7.71	1.40	1.53
3	A	294	VAL	CA-CB	-7.69	1.43	1.54
3	A	300	PHE	CD2-CE2	7.69	1.61	1.38
3	A	135	PRO	CA-CB	-7.69	1.43	1.53
3	A	243	GLN	CD-NE2	7.68	1.49	1.33
3	A	293	GLU	CA-CB	7.68	1.66	1.53
3	B	261	ARG	CD-NE	7.62	1.56	1.46
1	E	4	DG	P-O5'	7.60	1.75	1.60
3	B	249	ALA	N-CA	-7.60	1.36	1.46
3	A	301	ALA	CA-CB	-7.58	1.41	1.53
1	E	2	DT	C2-O2	7.58	1.37	1.22
3	B	276	ARG	CA-C	-7.56	1.42	1.52
1	E	19	DA	C5-C4	7.55	1.53	1.38
3	B	112	ARG	NE-CZ	7.54	1.41	1.33
3	A	165	ARG	CA-C	-7.54	1.42	1.52
3	B	177	ARG	NE-CZ	7.53	1.41	1.33
1	E	18	DC	P-O5'	7.52	1.75	1.60
3	B	266	GLU	CD-OE1	7.51	1.39	1.25
1	E	18	DC	P-OP1	7.51	1.63	1.48
3	A	178	GLU	CD-OE1	7.50	1.39	1.25
3	B	116	GLU	C-O	7.47	1.34	1.23
3	B	242	SER	N-CA	-7.47	1.36	1.46
3	B	106	GLN	CA-C	-7.46	1.43	1.52
3	A	249	ALA	N-CA	-7.46	1.36	1.46
3	A	231	MET	CA-C	7.45	1.68	1.52
3	B	235	ARG	CZ-NH1	7.41	1.43	1.32
3	B	120	ARG	CB-CG	7.41	1.74	1.52
3	B	95	LEU	CA-C	-7.40	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	184	ASN	CA-C	-7.39	1.42	1.52
3	A	105	GLU	CD-OE1	7.35	1.39	1.25
3	B	113	MET	CG-SD	7.33	1.99	1.80
3	A	162	THR	CA-CB	-7.32	1.42	1.53
3	B	280	PRO	CA-C	-7.32	1.42	1.52
3	A	286	LEU	C-O	7.31	1.32	1.24
3	A	245	ILE	CA-CB	7.28	1.65	1.54
3	A	112	ARG	NE-CZ	7.27	1.41	1.33
3	B	296	VAL	CB-CG2	-7.27	1.28	1.52
3	B	282	LYS	CG-CD	7.26	1.74	1.52
3	B	170	THR	N-CA	-7.25	1.37	1.46
3	B	132	HIS	CA-CB	-7.24	1.40	1.53
3	B	127	GLY	CA-C	-7.23	1.41	1.51
3	B	171	TRP	CA-CB	-7.23	1.42	1.53
3	A	102	GLU	CD-OE2	7.22	1.39	1.25
3	B	235	ARG	CA-C	7.21	1.62	1.52
3	B	155	ASN	C-O	7.20	1.33	1.24
3	B	232	ARG	CD-NE	7.19	1.56	1.46
3	B	238	TRP	CA-CB	-7.19	1.41	1.53
3	B	123	LYS	CD-CE	7.19	1.74	1.52
3	A	239	GLY	C-O	7.18	1.33	1.24
1	E	19	DA	N7-C5	7.17	1.53	1.39
3	B	235	ARG	CZ-NH2	7.17	1.42	1.33
3	A	133	ASN	CB-CG	-7.16	1.34	1.52
3	B	260	GLU	C-O	7.15	1.33	1.24
3	A	303	ARG	CZ-NH2	7.14	1.42	1.33
3	B	270	ARG	CZ-NH2	7.13	1.42	1.33
3	B	291	VAL	CB-CG2	-7.13	1.29	1.52
3	A	252	ARG	C-O	-7.13	1.14	1.23
3	B	292	THR	CA-CB	7.12	1.65	1.53
3	A	290	LEU	CB-CG	7.11	1.67	1.53
3	A	237	LYS	C-O	-7.11	1.15	1.23
3	A	101	GLU	CG-CD	7.11	1.69	1.52
3	B	126	LYS	CE-NZ	7.09	1.70	1.49
3	A	125	ILE	N-CA	-7.09	1.37	1.46
3	A	140	VAL	CA-CB	-7.09	1.46	1.54
3	B	293	GLU	CB-CG	7.08	1.73	1.52
3	A	270	ARG	NE-CZ	7.08	1.40	1.33
3	A	112	ARG	N-CA	-7.06	1.37	1.46
3	A	181	ARG	NE-CZ	7.06	1.40	1.33
3	B	181	ARG	NE-CZ	7.05	1.40	1.33
3	B	96	GLN	CD-NE2	7.04	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	126	LYS	CD-CE	7.03	1.73	1.52
3	A	234	ASN	C-O	7.03	1.32	1.24
3	B	154	LEU	CG-CD2	-7.01	1.29	1.52
3	A	300	PHE	N-CA	-7.01	1.39	1.46
1	E	1	DC	O5'-C5'	7.00	1.63	1.42
3	B	282	LYS	CB-CG	7.00	1.73	1.52
3	B	152	GLN	CA-C	-6.98	1.43	1.52
3	B	293	GLU	CG-CD	6.98	1.69	1.52
3	A	93	LYS	CE-NZ	6.97	1.70	1.49
3	A	112	ARG	CA-CB	-6.96	1.42	1.53
3	B	235	ARG	NE-CZ	6.95	1.40	1.33
3	A	296	VAL	CA-C	6.95	1.61	1.52
3	B	267	GLU	C-O	6.95	1.32	1.24
3	B	272	GLU	CD-OE1	6.94	1.38	1.25
3	A	141	ASP	CA-C	-6.93	1.43	1.52
3	A	130	GLN	CD-OE1	6.93	1.36	1.23
1	E	20	DG	O5'-C5'	6.93	1.63	1.42
3	B	140	VAL	CB-CG1	-6.91	1.29	1.52
3	B	119	TRP	N-CA	-6.91	1.37	1.46
3	B	175	LYS	CA-CB	-6.91	1.41	1.53
2	F	11	DT	C2-O2	-6.90	1.08	1.22
3	B	176	GLN	CG-CD	6.88	1.69	1.52
3	B	140	VAL	CB-CG2	-6.87	1.29	1.52
3	A	307	GLU	CD-OE1	6.86	1.38	1.25
3	A	155	ASN	CG-ND2	6.86	1.47	1.33
3	A	163	GLN	CD-OE1	6.85	1.36	1.23
3	A	297	TYR	CA-CB	-6.84	1.42	1.53
2	F	11	DT	N1-C2	-6.82	1.24	1.38
3	A	98	LEU	CG-CD1	6.82	1.75	1.52
3	A	233	ARG	CD-NE	6.80	1.55	1.46
2	F	2	DG	O4'-C1'	6.79	1.55	1.41
3	A	232	ARG	CA-CB	6.79	1.65	1.53
3	B	302	ASN	C-N	-6.79	1.24	1.33
3	B	97	ALA	CA-CB	-6.79	1.42	1.53
3	B	243	GLN	CA-CB	-6.77	1.42	1.53
3	B	295	ARG	CA-C	-6.77	1.43	1.52
3	B	113	MET	C-O	6.75	1.32	1.24
3	B	166	ALA	N-CA	-6.75	1.38	1.46
3	B	262	GLU	C-O	6.75	1.32	1.24
3	A	169	TYR	CB-CG	-6.75	1.36	1.51
3	A	276	ARG	N-CA	-6.72	1.38	1.46
1	E	19	DA	C3'-O3'	6.72	1.62	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	247	TYR	CD1-CE1	6.72	1.58	1.38
3	A	244	GLN	CG-CD	6.71	1.68	1.52
3	A	101	GLU	CA-CB	6.71	1.64	1.53
3	B	129	MET	SD-CE	6.71	1.96	1.79
1	E	1	DC	C2-N3	6.70	1.49	1.36
2	F	2	DG	C6-N1	6.70	1.53	1.39
1	E	2	DT	C2-N3	6.70	1.51	1.37
2	F	3	DC	P-O5'	6.68	1.73	1.60
3	A	152	GLN	CA-CB	-6.68	1.45	1.53
3	B	91	ILE	CG1-CD1	-6.67	1.25	1.51
2	F	5	DG	P-O5'	6.66	1.73	1.60
3	A	248	GLN	CD-NE2	6.66	1.47	1.33
3	A	140	VAL	N-CA	-6.63	1.38	1.46
3	A	301	ALA	C-O	-6.63	1.16	1.24
3	A	95	LEU	CA-CB	-6.62	1.42	1.53
3	A	157	GLY	CA-C	6.60	1.59	1.51
3	A	178	GLU	N-CA	-6.60	1.37	1.46
3	A	92	LEU	N-CA	-6.59	1.38	1.46
3	A	184	ASN	CG-ND2	6.59	1.47	1.33
1	E	1	DC	C2-O2	6.58	1.37	1.24
3	B	267	GLU	N-CA	6.57	1.54	1.46
3	B	119	TRP	CE3-CZ3	-6.56	1.19	1.38
3	A	106	GLN	CA-CB	-6.55	1.43	1.53
3	A	135	PRO	N-CD	-6.53	1.38	1.47
3	B	248	GLN	C-O	6.53	1.32	1.24
3	A	104	ALA	CA-CB	-6.51	1.42	1.53
3	B	289	ASN	N-CA	-6.51	1.38	1.46
3	B	265	VAL	CA-C	-6.51	1.44	1.52
3	B	236	PHE	CE1-CZ	6.50	1.58	1.38
3	A	180	LEU	CG-CD1	6.49	1.74	1.52
3	A	307	GLU	CD-OE2	6.48	1.37	1.25
3	A	111	ASP	CG-OD2	6.48	1.37	1.25
3	A	164	LYS	CA-CB	-6.48	1.43	1.53
3	B	114	LEU	C-O	-6.47	1.15	1.24
3	A	123	LYS	CB-CG	6.47	1.71	1.52
3	A	155	ASN	CA-CB	-6.47	1.45	1.53
3	B	267	GLU	CD-OE1	6.47	1.37	1.25
3	B	136	GLN	C-O	6.46	1.32	1.24
1	E	11	DA	C6-N1	6.45	1.48	1.35
2	F	8	DG	O3'-P	6.45	1.70	1.61
3	A	291	VAL	N-CA	6.45	1.53	1.46
3	B	231	MET	CA-CB	6.45	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	163	GLN	CD-OE1	6.45	1.35	1.23
3	B	140	VAL	C-O	-6.44	1.16	1.24
3	A	298	ASN	CA-C	-6.43	1.43	1.52
1	E	20	DG	P-OP1	6.41	1.61	1.48
3	B	91	ILE	CB-CG1	-6.41	1.40	1.53
2	F	3	DC	O3'-P	6.41	1.70	1.61
3	B	238	TRP	NE1-CE2	-6.40	1.30	1.37
3	B	276	ARG	NE-CZ	-6.40	1.26	1.33
1	E	2	DT	N1-C2	6.39	1.51	1.38
3	B	184	ASN	CB-CG	6.38	1.68	1.52
3	A	295	ARG	CA-CB	-6.38	1.43	1.53
3	A	105	GLU	C-O	6.37	1.31	1.24
3	A	295	ARG	CZ-NH1	6.37	1.41	1.32
3	B	118	PRO	CB-CG	-6.36	1.17	1.49
3	B	153	HIS	N-CA	-6.36	1.38	1.46
3	A	116	GLU	CD-OE2	6.35	1.37	1.25
3	B	240	PRO	C-O	-6.34	1.15	1.24
3	B	112	ARG	CA-CB	-6.33	1.43	1.53
3	A	179	ILE	CA-C	-6.33	1.43	1.52
3	A	233	ARG	NE-CZ	6.32	1.40	1.33
3	A	138	GLU	CD-OE1	6.32	1.37	1.25
1	E	20	DG	C1'-N9	6.32	1.59	1.46
3	A	141	ASP	C-O	-6.31	1.16	1.24
3	A	129	MET	C-O	-6.31	1.16	1.24
3	A	175	LYS	CA-CB	-6.30	1.42	1.53
2	F	13	DA	O3'-P	6.29	1.70	1.61
1	E	18	DC	C3'-O3'	6.28	1.61	1.42
3	A	168	LEU	CA-C	-6.28	1.44	1.52
3	A	290	LEU	CG-CD1	6.28	1.73	1.52
3	A	301	ALA	N-CA	-6.28	1.38	1.46
3	B	299	TRP	CZ3-CH2	6.28	1.56	1.40
3	A	122	ALA	CA-CB	-6.26	1.42	1.53
3	A	182	GLN	CA-C	-6.26	1.43	1.52
3	A	288	SER	N-CA	-6.25	1.38	1.46
3	B	159	PRO	CA-C	6.25	1.60	1.52
3	B	303	ARG	CA-C	-6.22	1.44	1.52
1	E	10	DT	O5'-C5'	-6.21	1.24	1.42
3	A	178	GLU	CG-CD	6.20	1.67	1.52
3	B	109	GLU	CD-OE1	6.20	1.37	1.25
3	A	245	ILE	CB-CG2	6.19	1.73	1.52
2	F	3	DC	N3-C4	6.18	1.46	1.33
2	F	20	DA	C5-C4	6.18	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	271	ALA	CA-CB	-6.18	1.43	1.53
3	A	293	GLU	CD-OE1	6.18	1.37	1.25
3	A	233	ARG	CA-C	-6.17	1.45	1.52
1	E	4	DG	P-OP2	6.17	1.60	1.48
3	A	237	LYS	CA-CB	-6.16	1.42	1.53
1	E	15	DC	P-OP1	6.16	1.60	1.48
3	A	254	LYS	CG-CD	6.16	1.71	1.52
3	A	128	TYR	CG-CD2	-6.16	1.26	1.39
3	A	303	ARG	NE-CZ	6.15	1.39	1.33
2	F	15	DT	P-OP1	6.14	1.60	1.48
3	A	156	LYS	CD-CE	6.14	1.70	1.52
3	A	235	ARG	NE-CZ	6.14	1.39	1.33
3	A	160	MET	CA-C	-6.13	1.45	1.52
3	B	112	ARG	CD-NE	6.12	1.54	1.46
3	B	134	ILE	CA-CB	-6.12	1.46	1.54
3	A	175	LYS	CA-C	-6.11	1.44	1.52
3	A	178	GLU	CA-CB	-6.11	1.43	1.53
3	B	252	ARG	CA-C	6.11	1.60	1.53
1	E	19	DA	N9-C4	6.09	1.50	1.38
3	B	270	ARG	CZ-NH1	6.09	1.41	1.32
3	A	94	GLU	N-CA	-6.09	1.38	1.46
3	A	153	HIS	N-CA	-6.08	1.38	1.46
3	A	289	ASN	CA-CB	-6.08	1.43	1.53
3	B	182	GLN	N-CA	-6.08	1.38	1.46
1	E	16	DA	C5'-C4'	-6.07	1.40	1.52
2	F	2	DG	C2-N3	6.07	1.45	1.33
3	A	105	GLU	CG-CD	6.07	1.67	1.52
3	A	158	THR	CA-CB	-6.06	1.41	1.53
3	B	170	THR	C-O	6.06	1.31	1.24
3	B	185	GLN	CD-OE1	6.05	1.35	1.23
3	A	107	ARG	C-O	6.05	1.31	1.24
3	A	138	GLU	CD-OE2	6.05	1.36	1.25
3	B	237	LYS	CA-C	-6.04	1.45	1.52
3	A	174	ARG	CG-CD	6.03	1.70	1.52
3	A	100	THR	CB-CG2	6.02	1.72	1.52
3	B	272	GLU	CD-OE2	6.02	1.36	1.25
3	A	251	ASP	CG-OD1	6.01	1.36	1.25
3	B	184	ASN	CG-OD1	6.00	1.34	1.23
3	B	302	ASN	CA-C	-6.00	1.44	1.52
3	B	238	TRP	CA-C	-5.98	1.45	1.52
3	A	306	GLU	N-CA	-5.98	1.39	1.46
1	E	13	DT	P-OP2	5.97	1.60	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	143	THR	N-CA	5.97	1.53	1.46
3	A	135	PRO	C-O	5.97	1.31	1.23
3	A	179	ILE	C-O	-5.96	1.17	1.24
3	B	169	TYR	CB-CG	-5.95	1.38	1.51
1	E	9	DA	P-OP2	5.94	1.60	1.48
1	E	17	DC	P-OP2	5.93	1.60	1.48
2	F	6	DG	C6-N1	-5.93	1.27	1.39
3	B	299	TRP	CG-CD1	5.91	1.51	1.36
3	B	130	GLN	CD-NE2	5.90	1.45	1.33
3	B	148	SER	CB-OG	5.89	1.53	1.42
2	F	18	DC	O3'-P	5.89	1.70	1.61
3	A	176	GLN	N-CA	-5.89	1.39	1.46
2	F	18	DC	C3'-O3'	5.88	1.60	1.42
2	F	5	DG	P-OP1	5.86	1.60	1.48
3	A	250	TYR	CD2-CE2	5.86	1.56	1.38
1	E	19	DA	O3'-P	5.85	1.70	1.61
3	B	159	PRO	CB-CG	5.85	1.78	1.49
3	A	119	TRP	N-CA	-5.85	1.38	1.46
3	A	232	ARG	CZ-NH1	5.84	1.41	1.32
1	E	1	DC	N1-C2	5.84	1.52	1.40
2	F	5	DG	P-OP2	5.83	1.60	1.48
3	A	305	LYS	CG-CD	5.82	1.70	1.52
3	A	253	GLN	CD-NE2	5.81	1.45	1.33
3	A	245	ILE	N-CA	-5.81	1.38	1.46
3	A	170	THR	N-CA	5.80	1.52	1.46
3	A	270	ARG	CG-CD	5.80	1.69	1.52
3	A	298	ASN	N-CA	-5.80	1.38	1.46
3	B	174	ARG	CA-CB	-5.80	1.44	1.53
3	A	114	LEU	CA-C	-5.79	1.43	1.52
3	B	184	ASN	C-O	5.79	1.31	1.24
3	B	174	ARG	C-O	-5.79	1.17	1.24
3	A	126	LYS	CA-C	-5.78	1.44	1.52
3	B	267	GLU	CD-OE2	5.78	1.36	1.25
3	B	106	GLN	CA-CB	-5.76	1.44	1.53
2	F	20	DA	C5-C6	5.75	1.52	1.41
3	B	182	GLN	CA-CB	-5.74	1.43	1.53
3	A	184	ASN	CG-OD1	5.73	1.34	1.23
3	A	234	ASN	CG-OD1	-5.72	1.12	1.23
3	A	300	PHE	C-N	-5.72	1.26	1.33
3	B	178	GLU	CG-CD	5.71	1.66	1.52
3	B	125	ILE	CA-C	-5.71	1.45	1.52
2	F	5	DG	O5'-C5'	5.70	1.59	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	112	ARG	CG-CD	5.68	1.69	1.52
3	B	107	ARG	C-O	5.68	1.31	1.24
3	B	259	GLU	CD-OE1	5.68	1.36	1.25
1	E	9	DA	N3-C4	-5.68	1.23	1.34
3	B	104	ALA	N-CA	5.67	1.53	1.46
3	A	164	LYS	C-N	-5.66	1.26	1.33
3	B	119	TRP	CA-CB	-5.66	1.44	1.53
3	B	244	GLN	CD-NE2	5.66	1.45	1.33
3	B	237	LYS	N-CA	-5.66	1.39	1.46
3	B	295	ARG	CA-CB	-5.66	1.44	1.53
2	F	2	DG	O5'-C5'	5.66	1.59	1.42
3	A	155	ASN	CA-C	5.65	1.58	1.53
3	A	184	ASN	CB-CG	5.64	1.66	1.52
2	F	21	DA	C4'-C3'	5.64	1.64	1.52
3	A	248	GLN	CA-C	5.63	1.60	1.52
2	F	2	DG	C4'-O4'	5.63	1.56	1.45
1	E	4	DG	P-OP1	5.63	1.59	1.48
3	A	131	GLN	CG-CD	5.62	1.66	1.52
3	A	138	GLU	CG-CD	5.62	1.66	1.52
3	B	137	ARG	NE-CZ	-5.61	1.26	1.33
3	A	150	LEU	C-O	5.61	1.30	1.24
1	E	14	DT	C2-O2	-5.59	1.11	1.22
3	A	232	ARG	CZ-NH2	5.59	1.40	1.33
3	A	120	ARG	CZ-NH1	5.59	1.40	1.32
3	B	143	THR	CB-OG1	5.59	1.52	1.43
2	F	20	DA	P-OP1	5.59	1.59	1.48
3	B	126	LYS	C-O	5.58	1.31	1.24
3	A	305	LYS	CA-CB	5.58	1.62	1.53
2	F	12	DT	C3'-O3'	-5.57	1.25	1.42
3	A	156	LYS	C-O	5.56	1.30	1.24
1	E	20	DG	P-O5'	5.56	1.71	1.60
3	A	177	ARG	CD-NE	5.56	1.54	1.46
3	B	173	VAL	CA-CB	5.55	1.61	1.54
3	A	295	ARG	CZ-NH2	5.55	1.40	1.33
3	B	123	LYS	CE-NZ	5.54	1.66	1.49
3	B	266	GLU	CA-CB	5.54	1.62	1.53
3	B	119	TRP	CG-CD2	-5.53	1.33	1.43
2	F	3	DC	C4-C5	5.53	1.54	1.43
3	B	90	SER	CB-OG	5.51	1.53	1.42
3	B	148	SER	CA-C	5.51	1.60	1.52
1	E	12	DA	C3'-C2'	-5.51	1.42	1.52
3	A	251	ASP	CG-OD2	5.51	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	119	TRP	CA-C	-5.51	1.44	1.52
3	B	172	TYR	CG-CD1	5.51	1.50	1.39
3	A	126	LYS	CE-NZ	5.50	1.65	1.49
3	A	288	SER	C-O	5.49	1.30	1.24
3	B	236	PHE	CA-C	-5.49	1.46	1.52
3	B	105	GLU	CD-OE2	5.48	1.35	1.25
3	A	128	TYR	CZ-OH	5.48	1.49	1.38
3	A	276	ARG	CZ-NH1	5.47	1.40	1.32
3	A	175	LYS	N-CA	-5.47	1.39	1.46
3	B	246	LEU	C-O	5.47	1.30	1.24
3	A	120	ARG	C-N	-5.47	1.26	1.33
3	A	305	LYS	CA-C	-5.47	1.45	1.52
3	B	300	PHE	C-N	-5.46	1.26	1.33
3	A	253	GLN	N-CA	5.46	1.53	1.46
3	B	146	ASN	CG-ND2	5.45	1.44	1.33
1	E	20	DG	N1-C2	5.44	1.48	1.38
3	A	155	ASN	N-CA	5.43	1.54	1.47
3	B	250	TYR	CZ-OH	5.43	1.49	1.38
2	F	3	DC	C2-N3	5.43	1.47	1.36
3	B	238	TRP	CE2-CZ2	-5.42	1.28	1.39
1	E	11	DA	C6-N6	5.41	1.45	1.34
3	B	275	GLN	CD-OE1	5.41	1.33	1.23
3	A	134	ILE	C-N	-5.41	1.26	1.33
3	B	123	LYS	CG-CD	5.41	1.68	1.52
3	A	287	GLY	CA-C	-5.40	1.44	1.51
3	A	288	SER	CA-CB	-5.39	1.44	1.53
3	B	298	ASN	CG-ND2	-5.39	1.22	1.33
3	A	174	ARG	CA-CB	-5.38	1.45	1.53
3	B	166	ALA	C-O	5.38	1.30	1.24
3	A	108	ALA	CA-CB	-5.38	1.44	1.53
3	A	164	LYS	N-CA	-5.38	1.40	1.46
1	E	20	DG	C6-O6	5.37	1.35	1.24
3	A	92	LEU	C-O	5.37	1.30	1.24
3	A	270	ARG	CA-C	-5.37	1.45	1.52
3	A	174	ARG	CZ-NH1	-5.37	1.25	1.32
3	B	233	ARG	CZ-NH1	5.37	1.40	1.32
3	A	172	TYR	CA-CB	-5.35	1.45	1.53
3	B	91	ILE	N-CA	5.35	1.53	1.46
2	F	20	DA	O5'-C5'	5.35	1.58	1.42
2	F	2	DG	N9-C8	5.34	1.48	1.37
1	E	11	DA	N9-C4	-5.34	1.27	1.38
3	B	116	GLU	CA-C	5.34	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	141	ASP	N-CA	5.34	1.53	1.46
3	A	112	ARG	C-O	-5.33	1.17	1.24
3	B	181	ARG	CZ-NH2	5.33	1.40	1.33
3	B	140	VAL	C-N	-5.33	1.27	1.33
3	B	106	GLN	CD-NE2	5.33	1.44	1.33
3	B	98	LEU	CA-C	-5.32	1.45	1.52
3	B	297	TYR	CZ-OH	5.32	1.49	1.38
3	A	115	SER	C-O	-5.30	1.17	1.24
3	A	299	TRP	CG-CD1	5.29	1.50	1.36
3	A	272	GLU	CD-OE1	5.28	1.35	1.25
1	E	17	DC	C3'-O3'	5.26	1.58	1.42
3	A	128	TYR	CA-CB	-5.26	1.45	1.53
3	A	165	ARG	N-CA	-5.26	1.40	1.46
3	B	139	VAL	CA-CB	5.26	1.61	1.54
1	E	1	DC	C5'-C4'	5.26	1.62	1.52
3	B	114	LEU	CG-CD1	-5.26	1.35	1.52
1	E	16	DA	O5'-C5'	-5.26	1.26	1.42
3	A	245	ILE	C-N	-5.26	1.26	1.33
3	A	186	THR	C-O	5.25	1.29	1.23
3	A	93	LYS	CA-C	5.25	1.59	1.52
3	A	244	GLN	C-N	-5.25	1.28	1.34
3	B	169	TYR	CD2-CE2	5.24	1.54	1.38
3	A	111	ASP	CG-OD1	5.24	1.35	1.25
3	A	156	LYS	CA-CB	-5.24	1.44	1.53
3	B	288	SER	CA-C	5.24	1.59	1.52
3	B	92	LEU	N-CA	-5.23	1.40	1.46
3	B	128	TYR	CD1-CE1	5.22	1.54	1.38
3	B	246	LEU	CG-CD2	-5.22	1.35	1.52
3	B	95	LEU	CA-CB	-5.22	1.45	1.53
3	B	146	ASN	C-N	-5.21	1.26	1.34
3	B	299	TRP	CG-CD2	-5.21	1.34	1.43
1	E	5	DG	P-OP1	5.21	1.58	1.48
1	E	18	DC	N1-C2	5.20	1.50	1.40
3	B	274	LEU	N-CA	-5.19	1.40	1.46
3	B	120	ARG	CD-NE	5.18	1.53	1.46
3	B	128	TYR	CA-CB	-5.18	1.45	1.53
2	F	4	DT	P-O5'	5.17	1.70	1.60
3	A	179	ILE	C-N	-5.17	1.27	1.33
3	A	255	ASN	CG-OD1	5.16	1.33	1.23
3	A	164	LYS	CD-CE	5.16	1.68	1.52
3	B	94	GLU	CD-OE2	5.16	1.35	1.25
3	A	245	ILE	CA-C	-5.15	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	112	ARG	CZ-NH2	5.15	1.40	1.33
3	B	126	LYS	CD-CE	5.15	1.68	1.52
3	B	301	ALA	C-N	-5.15	1.26	1.33
3	B	265	VAL	C-O	-5.15	1.18	1.24
3	B	152	GLN	C-N	-5.15	1.26	1.33
3	A	165	ARG	CG-CD	-5.14	1.37	1.52
3	A	183	PHE	N-CA	-5.14	1.39	1.46
3	B	247	TYR	N-CA	-5.14	1.40	1.46
3	B	177	ARG	N-CA	5.14	1.52	1.46
3	B	110	VAL	N-CA	-5.14	1.41	1.46
3	A	130	GLN	CB-CG	5.13	1.67	1.52
3	A	181	ARG	CG-CD	5.13	1.67	1.52
3	B	270	ARG	CB-CG	5.13	1.67	1.52
3	B	161	LYS	CA-CB	-5.13	1.45	1.53
1	E	5	DG	P-OP2	5.13	1.58	1.48
3	A	299	TRP	C-O	-5.13	1.17	1.24
3	A	182	GLN	CA-CB	-5.12	1.44	1.53
3	A	299	TRP	C-N	-5.12	1.27	1.33
3	B	144	GLY	C-O	5.11	1.30	1.23
3	B	252	ARG	CD-NE	5.11	1.53	1.46
2	F	10	DA	P-OP1	5.11	1.58	1.48
3	A	113	MET	CA-CB	-5.11	1.44	1.53
3	B	275	GLN	CA-CB	5.09	1.61	1.53
3	B	247	TYR	CD2-CE2	5.09	1.53	1.38
3	B	270	ARG	CG-CD	5.08	1.67	1.52
3	B	234	ASN	CB-CG	5.07	1.64	1.52
3	B	137	ARG	N-CA	-5.07	1.40	1.46
3	B	273	CYS	C-O	-5.07	1.17	1.24
3	A	134	ILE	CG1-CD1	5.07	1.71	1.51
3	B	179	ILE	N-CA	-5.07	1.40	1.46
3	A	91	ILE	CB-CG1	-5.06	1.43	1.53
1	E	12	DA	C1'-N9	5.06	1.56	1.46
3	B	275	GLN	CD-NE2	5.06	1.43	1.33
3	B	284	HIS	CB-CG	5.06	1.57	1.50
2	F	13	DA	O5'-C5'	-5.05	1.27	1.42
3	A	244	GLN	CD-OE1	5.05	1.33	1.23
3	B	90	SER	C-O	-5.05	1.13	1.23
3	A	299	TRP	CD2-CE2	5.04	1.50	1.41
2	F	4	DT	N3-C4	5.03	1.48	1.38
3	B	111	ASP	CG-OD2	5.03	1.34	1.25
3	A	169	TYR	CG-CD1	-5.03	1.28	1.39
3	A	171	TRP	CD2-CE3	-5.03	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	111	ASP	CG-OD1	5.03	1.34	1.25
3	B	101	GLU	C-N	5.03	1.40	1.33
3	A	246	LEU	N-CA	-5.02	1.40	1.46
3	B	237	LYS	CD-CE	5.01	1.67	1.52
3	B	133	ASN	C-O	-5.00	1.17	1.24

All (607) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	281	SER	CA-C-N	-17.89	94.75	121.76
3	B	281	SER	C-N-CA	-17.89	94.75	121.76
1	E	16	DA	P-O5'-C5'	-15.30	97.05	120.00
3	A	168	LEU	N-CA-C	-14.98	94.56	113.43
3	A	181	ARG	N-CA-C	-14.29	95.25	113.12
1	E	10	DT	C5'-C4'-C3'	14.01	135.91	114.90
3	A	182	GLN	N-CA-C	-13.34	96.61	113.16
3	A	308	ALA	CA-C-O	-12.91	98.86	120.80
3	B	284	HIS	N-CA-C	-12.90	93.52	113.89
3	A	289	ASN	N-CA-C	-12.67	97.82	113.02
2	F	20	DA	C5'-C4'-C3'	-12.63	95.95	114.90
1	E	17	DC	O3'-P-O5'	-12.38	85.43	104.00
3	A	251	ASP	N-CA-C	-12.13	98.76	113.19
1	E	9	DA	O4'-C1'-N9	-11.79	90.71	108.40
3	B	91	ILE	CB-CA-C	-11.73	92.06	111.29
3	B	140	VAL	N-CA-C	-11.63	99.59	110.53
3	A	136	GLN	N-CA-C	-11.57	98.54	112.89
1	E	9	DA	C5'-C4'-C3'	11.53	132.20	114.90
1	E	6	DT	O3'-P-O5'	-11.46	86.81	104.00
1	E	3	DT	C2-N1-C1'	-11.26	102.47	119.35
1	E	9	DA	C6-N1-C2	-11.18	102.04	118.80
3	A	270	ARG	N-CA-C	-11.08	97.04	112.45
3	A	101	GLU	N-CA-C	-11.03	98.95	110.97
3	B	276	ARG	NE-CZ-NH2	-10.99	109.31	119.20
1	E	14	DT	O3'-P-O5'	-10.88	87.68	104.00
2	F	4	DT	O3'-P-O5'	10.84	120.26	104.00
2	F	18	DC	N3-C4-N4	10.66	133.90	117.90
1	E	1	DC	C5'-C4'-C3'	10.64	130.87	114.90
3	B	266	GLU	N-CA-C	-10.44	99.07	112.23
2	F	10	DA	C5'-C4'-O4'	-10.40	93.80	109.40
2	F	7	DT	P-O3'-C3'	-10.39	104.61	120.20
2	F	19	DC	OP1-P-O3'	-10.39	76.83	108.00
3	A	186	THR	N-CA-C	10.37	125.97	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	125	ILE	CB-CA-C	-10.36	98.35	112.24
3	A	162	THR	N-CA-C	10.26	123.42	111.11
2	F	10	DA	C5-N7-C8	10.23	119.25	103.90
3	A	117	ASP	CA-C-O	10.19	129.12	119.24
2	F	5	DG	C5'-C4'-O4'	10.18	124.67	109.40
1	E	19	DA	C5'-C4'-C3'	-10.12	99.72	114.90
3	A	134	ILE	N-CA-CB	-10.09	100.81	111.61
1	E	10	DT	C4-C5-C6	-10.07	104.10	119.20
3	B	261	ARG	N-CA-C	-10.06	99.87	111.03
2	F	5	DG	P-O3'-C3'	-10.05	105.13	120.20
2	F	2	DG	C5'-C4'-O4'	10.04	124.45	109.40
1	E	15	DC	O4'-C1'-N1	9.95	123.32	108.40
3	A	174	ARG	NE-CZ-NH2	9.94	128.15	119.20
3	A	245	ILE	CA-C-N	-9.94	106.92	120.44
3	A	245	ILE	C-N-CA	-9.94	106.92	120.44
1	E	4	DG	N1-C2-N2	-9.93	101.40	116.30
3	B	247	TYR	N-CA-C	-9.91	100.44	111.14
1	E	13	DT	N3-C4-O4	-9.89	107.76	122.60
3	B	173	VAL	CB-CA-C	-9.87	99.11	112.04
3	A	283	ALA	N-CA-C	-9.84	99.79	113.37
3	B	263	ALA	CA-C-N	9.82	134.24	120.29
3	B	263	ALA	C-N-CA	9.82	134.24	120.29
1	E	8	DA	C2'-C3'-O3'	9.78	126.17	111.50
2	F	8	DG	C5-C6-O6	-9.77	113.64	128.30
1	E	6	DT	P-O3'-C3'	-9.72	105.61	120.20
3	B	283	ALA	N-CA-CB	-9.70	95.70	110.25
2	F	3	DC	C2'-C3'-O3'	-9.65	97.03	111.50
2	F	18	DC	N1-C2-O2	-9.64	104.73	119.20
2	F	20	DA	C5'-C4'-O4'	9.54	123.72	109.40
1	E	7	DT	C3'-C2'-C1'	9.52	115.88	101.60
2	F	11	DT	C5'-C4'-O4'	-9.48	95.18	109.40
1	E	9	DA	N3-C4-C5	-9.44	112.73	126.90
1	E	18	DC	C5'-C4'-O4'	9.44	123.56	109.40
2	F	5	DG	N1-C2-N2	-9.43	102.16	116.30
2	F	11	DT	O4'-C1'-C2'	-9.41	92.29	106.40
3	A	126	LYS	N-CA-C	-9.38	99.74	111.75
3	B	253	GLN	OE1-CD-NE2	-9.38	113.22	122.60
3	B	305	LYS	N-CA-C	-9.34	100.76	112.72
2	F	18	DC	C5'-C4'-O4'	9.32	123.38	109.40
1	E	12	DA	C6-N1-C2	-9.26	104.92	118.80
3	A	107	ARG	N-CA-C	9.20	123.52	111.75
3	A	250	TYR	N-CA-C	9.18	122.59	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	119	TRP	N-CA-C	-9.16	101.87	113.23
3	A	184	ASN	N-CA-C	-9.07	99.85	112.45
2	F	4	DT	C5'-C4'-C3'	-9.04	101.35	114.90
1	E	3	DT	C6-N1-C1'	9.03	132.89	119.35
1	E	10	DT	P-O3'-C3'	-9.02	106.67	120.20
1	E	9	DA	N1-C6-N6	-8.99	105.51	119.00
2	F	11	DT	C5'-C4'-C3'	8.89	128.24	114.90
2	F	14	DT	N3-C4-C5	8.88	128.12	114.80
3	A	92	LEU	CA-C-N	-8.87	108.94	120.65
3	A	92	LEU	C-N-CA	-8.87	108.94	120.65
3	B	265	VAL	CB-CA-C	-8.87	100.53	111.88
1	E	20	DG	P-O5'-C5'	8.82	133.23	120.00
2	F	17	DA	P-O5'-C5'	-8.81	106.78	120.00
1	E	20	DG	O5'-C5'-C4'	8.79	123.99	110.80
1	E	18	DC	P-O5'-C5'	8.73	133.10	120.00
1	E	1	DC	N1-C1'-C2'	8.73	126.59	113.50
3	A	256	PRO	CA-C-N	-8.71	110.31	122.93
3	A	256	PRO	C-N-CA	-8.71	110.31	122.93
3	B	173	VAL	N-CA-CB	8.67	121.30	110.47
1	E	19	DA	O3'-P-O5'	-8.64	91.03	104.00
3	B	280	PRO	N-CD-CG	-8.56	90.36	103.20
1	E	2	DT	P-O5'-C5'	8.51	132.77	120.00
2	F	19	DC	OP1-P-OP2	8.50	145.51	120.00
2	F	14	DT	C2'-C3'-O3'	8.50	124.25	111.50
2	F	20	DA	P-O3'-C3'	-8.47	107.49	120.20
1	E	9	DA	N9-C4-C5	8.45	118.37	105.70
1	E	2	DT	O5'-C5'-C4'	8.44	123.46	110.80
3	B	153	HIS	CA-C-N	-8.43	107.00	122.09
3	B	153	HIS	C-N-CA	-8.43	107.00	122.09
2	F	5	DG	C2'-C3'-O3'	-8.41	98.89	111.50
1	E	4	DG	C2-N3-C4	-8.39	99.22	111.80
3	A	176	GLN	CA-C-O	-8.38	112.27	120.90
3	A	175	LYS	CD-CE-NZ	8.38	138.70	111.90
1	E	6	DT	C2'-C3'-O3'	8.29	123.93	111.50
3	B	158	THR	CB-CA-C	-8.26	96.46	109.42
2	F	11	DT	C1'-O4'-C4'	8.23	122.05	109.70
3	B	175	LYS	N-CA-C	-8.22	103.15	113.01
2	F	11	DT	C4-C5-C6	-8.22	106.87	119.20
1	E	9	DA	O5'-C5'-C4'	-8.19	98.52	110.80
3	A	288	SER	N-CA-C	8.19	120.28	111.36
3	B	172	TYR	N-CA-CB	-8.15	98.19	110.01
2	F	12	DT	N1-C1'-C2'	8.11	125.66	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	135	PRO	CA-C-N	-8.08	107.00	121.14
3	A	135	PRO	C-N-CA	-8.08	107.00	121.14
2	F	7	DT	N1-C1'-C2'	8.07	125.61	113.50
3	A	257	SER	O-C-N	8.05	133.43	123.21
3	B	152	GLN	N-CA-C	8.02	121.18	111.40
2	F	8	DG	C6-N1-C2	-7.99	112.92	124.90
3	A	179	ILE	CA-C-N	-7.98	109.88	122.73
3	A	179	ILE	C-N-CA	-7.98	109.88	122.73
2	F	11	DT	O4'-C4'-C3'	-7.96	93.47	105.40
1	E	8	DA	O4'-C1'-C2'	7.95	118.32	106.40
3	A	162	THR	CB-CA-C	-7.93	98.12	110.81
2	F	3	DC	C5'-C4'-O4'	-7.92	97.53	109.40
2	F	4	DT	O4'-C1'-N1	7.92	120.27	108.40
1	E	3	DT	N1-C1'-C2'	7.90	125.35	113.50
2	F	20	DA	C2'-C3'-O3'	7.89	123.33	111.50
3	A	168	LEU	CA-C-N	-7.87	109.74	120.44
3	A	168	LEU	C-N-CA	-7.87	109.74	120.44
2	F	3	DC	C4'-C3'-C2'	7.87	114.20	102.40
2	F	16	DA	C5-N7-C8	-7.86	92.12	103.90
1	E	18	DC	O5'-P-OP2	7.85	131.54	108.00
1	E	12	DA	N1-C2-N3	7.78	140.67	129.00
2	F	17	DA	O5'-C5'-C4'	-7.72	99.22	110.80
2	F	14	DT	N3-C4-O4	-7.70	111.06	122.60
2	F	15	DT	C5'-C4'-C3'	-7.69	103.36	114.90
1	E	4	DG	N1-C2-N3	7.66	135.49	124.00
3	A	130	GLN	N-CA-CB	-7.62	98.91	110.12
1	E	18	DC	O5'-C5'-C4'	-7.61	99.39	110.80
3	A	291	VAL	CB-CA-C	-7.59	101.15	111.63
3	B	276	ARG	NH1-CZ-NH2	7.59	129.17	119.30
3	B	242	SER	N-CA-C	-7.58	103.02	111.82
3	B	242	SER	CA-CB-OG	7.57	126.24	111.10
3	A	278	VAL	CB-CA-C	-7.55	98.91	111.29
3	B	288	SER	N-CA-CB	-7.55	98.21	110.14
2	F	10	DA	C4-C5-N7	-7.55	99.38	110.70
1	E	20	DG	O4'-C1'-N9	7.54	119.71	108.40
3	B	281	SER	N-CA-CB	7.53	121.62	110.33
3	A	304	ARG	N-CA-C	-7.52	94.78	110.80
3	B	123	LYS	CG-CD-CE	7.52	128.59	111.30
3	B	116	GLU	N-CA-CB	-7.47	99.58	110.26
1	E	9	DA	C2-N3-C4	7.47	122.00	110.80
3	A	244	GLN	CA-C-O	7.42	128.79	121.00
3	B	298	ASN	N-CA-C	-7.41	103.50	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	286	LEU	N-CA-CB	-7.39	99.22	110.16
3	A	307	GLU	N-CA-C	-7.39	103.67	114.39
1	E	7	DT	C2'-C3'-O3'	-7.38	100.43	111.50
1	E	5	DG	O4'-C1'-N9	7.36	119.44	108.40
3	A	245	ILE	N-CA-C	-7.34	101.76	112.04
2	F	19	DC	C5-C6-N1	-7.34	109.99	121.00
3	B	156	LYS	CD-CE-NZ	7.31	135.29	111.90
3	A	167	ALA	CA-C-N	-7.29	107.49	122.58
3	A	167	ALA	C-N-CA	-7.29	107.49	122.58
3	B	159	PRO	CB-CG-CD	-7.25	82.91	106.10
2	F	10	DA	N7-C8-N9	-7.25	102.93	113.80
3	B	161	LYS	CA-C-O	7.24	129.18	120.92
3	B	137	ARG	CA-CB-CG	-7.24	99.62	114.10
3	A	137	ARG	NE-CZ-NH2	-7.23	112.69	119.20
3	A	159	PRO	CB-CA-C	-7.22	102.14	111.46
2	F	8	DG	C5-N7-C8	-7.21	93.39	104.20
3	B	276	ARG	N-CA-C	-7.20	104.09	113.17
3	B	233	ARG	CA-C-O	-7.17	113.09	120.84
3	A	151	SER	CA-C-O	-7.16	111.16	119.61
2	F	13	DA	C4'-C3'-C2'	-7.14	91.68	102.40
3	A	293	GLU	CA-C-N	-7.13	109.20	120.47
3	A	293	GLU	C-N-CA	-7.13	109.20	120.47
3	B	281	SER	N-CA-C	-7.11	103.58	112.90
3	A	113	MET	CG-SD-CE	7.11	116.54	100.90
3	B	237	LYS	CB-CG-CD	7.08	127.58	111.30
1	E	6	DT	OP1-P-O3'	-7.06	86.81	108.00
3	B	176	GLN	N-CA-C	-7.06	103.63	111.82
1	E	3	DT	O4'-C1'-N1	-7.06	97.81	108.40
3	A	242	SER	N-CA-C	-7.05	102.72	111.75
1	E	14	DT	N1-C2-N3	7.02	125.33	114.80
3	A	170	THR	CB-CA-C	-7.00	99.22	110.84
1	E	10	DT	N3-C4-C5	7.00	125.30	114.80
3	B	98	LEU	N-CA-C	-6.97	104.64	113.01
1	E	10	DT	C5-C6-N1	6.95	133.23	122.80
1	E	17	DC	N3-C4-C5	-6.93	111.40	121.80
1	E	19	DA	C2'-C3'-O3'	6.93	121.89	111.50
2	F	3	DC	O4'-C1'-C2'	6.93	116.79	106.40
1	E	7	DT	O4'-C1'-C2'	-6.92	96.02	106.40
2	F	9	DA	P-O3'-C3'	-6.92	109.83	120.20
2	F	5	DG	O5'-C5'-C4'	6.91	121.16	110.80
1	E	9	DA	C4-C5-N7	-6.90	100.35	110.70
2	F	6	DG	C1'-O4'-C4'	-6.88	99.39	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	11	DA	C5'-C4'-C3'	6.86	125.19	114.90
1	E	18	DC	P-O3'-C3'	6.81	130.42	120.20
3	B	270	ARG	N-CA-C	-6.81	103.93	111.36
1	E	7	DT	O3'-P-O5'	-6.81	93.79	104.00
3	B	235	ARG	O-C-N	-6.80	115.08	123.04
1	E	11	DA	C8-N9-C4	-6.80	95.70	105.90
3	B	148	SER	N-CA-C	-6.79	103.94	111.82
2	F	9	DA	C5'-C4'-O4'	6.79	119.58	109.40
2	F	16	DA	N7-C8-N9	6.79	123.98	113.80
3	A	286	LEU	O-C-N	6.78	129.88	122.15
1	E	4	DG	P-O3'-C3'	-6.78	110.04	120.20
1	E	7	DT	N3-C2-O2	-6.77	111.84	122.00
3	B	165	ARG	O-C-N	6.76	129.12	122.09
3	B	271	ALA	N-CA-C	6.75	118.64	111.28
2	F	13	DA	C6-N1-C2	-6.75	108.68	118.80
3	B	163	GLN	N-CA-CB	-6.74	99.10	110.49
3	A	170	THR	CA-CB-OG1	-6.74	99.50	109.60
2	F	19	DC	N3-C2-O2	-6.73	111.80	121.90
3	A	134	ILE	CA-C-N	6.73	126.77	119.90
3	A	134	ILE	C-N-CA	6.73	126.77	119.90
2	F	19	DC	C5'-C4'-O4'	6.72	119.48	109.40
3	A	130	GLN	CA-CB-CG	6.71	127.52	114.10
3	B	177	ARG	CB-CA-C	-6.71	99.52	110.79
2	F	18	DC	P-O5'-C5'	-6.70	109.94	120.00
2	F	7	DT	C4-C5-C6	-6.70	109.16	119.20
3	A	101	GLU	CB-CG-CD	6.69	123.98	112.60
1	E	12	DA	C8-N9-C4	-6.69	95.86	105.90
1	E	7	DT	C4'-C3'-O3'	6.68	120.03	110.00
3	B	252	ARG	N-CA-CB	-6.68	101.76	111.91
3	A	154	LEU	CA-C-O	-6.66	111.87	120.00
1	E	20	DG	C5-N7-C8	6.66	114.19	104.20
3	B	121	ALA	N-CA-C	6.65	119.09	111.11
3	B	109	GLU	N-CA-C	-6.64	104.13	111.36
2	F	21	DA	C2'-C3'-O3'	6.62	121.43	111.50
2	F	10	DA	N9-C1'-C2'	6.61	123.41	113.50
3	B	249	ALA	N-CA-C	-6.60	105.53	112.93
1	E	2	DT	C4'-C3'-O3'	6.60	119.90	110.00
1	E	15	DC	O5'-P-OP1	6.60	128.81	109.00
2	F	6	DG	N1-C2-N2	-6.60	106.41	116.30
3	A	305	LYS	N-CA-CB	6.59	121.64	110.49
3	B	302	ASN	CA-CB-CG	-6.58	106.02	112.60
3	B	276	ARG	CG-CD-NE	-6.57	97.55	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	16	DA	C5'-C4'-O4'	-6.57	99.55	109.40
2	F	3	DC	O3'-P-O5'	-6.57	94.15	104.00
3	B	274	LEU	N-CA-C	-6.56	103.23	111.11
1	E	16	DA	OP1-P-OP2	6.54	139.62	120.00
1	E	16	DA	O3'-P-O5'	-6.54	94.19	104.00
3	B	152	GLN	CA-CB-CG	-6.54	101.02	114.10
1	E	10	DT	C6-N1-C1'	6.54	129.15	119.35
2	F	21	DA	C5'-C4'-C3'	6.52	124.67	114.90
1	E	3	DT	C4'-C3'-O3'	-6.51	100.23	110.00
2	F	2	DG	OP2-P-O3'	-6.51	88.48	108.00
3	A	126	LYS	CB-CA-C	-6.49	97.86	110.46
2	F	12	DT	C2'-C3'-O3'	-6.49	101.77	111.50
2	F	6	DG	O5'-P-OP1	-6.47	89.58	109.00
3	B	235	ARG	NE-CZ-NH1	-6.47	115.03	121.50
3	B	275	GLN	CA-CB-CG	6.47	127.05	114.10
1	E	15	DC	P-O3'-C3'	6.46	129.89	120.20
2	F	6	DG	C5-C6-O6	6.46	137.99	128.30
3	A	134	ILE	CA-C-O	6.45	123.77	119.38
3	A	178	GLU	N-CA-CB	-6.45	99.59	110.49
3	A	120	ARG	CA-CB-CG	-6.44	101.21	114.10
3	A	239	GLY	N-CA-C	-6.44	99.20	112.34
1	E	1	DC	OP2-P-O3'	-6.44	88.69	108.00
3	B	177	ARG	CG-CD-NE	6.43	126.14	112.00
1	E	5	DG	C4-C5-C6	6.42	128.73	119.10
3	A	257	SER	N-CA-CB	6.42	121.02	110.69
3	B	253	GLN	CG-CD-NE2	6.42	126.03	116.40
3	B	290	LEU	CB-CA-C	-6.41	99.64	109.89
1	E	20	DG	C5-C6-N1	-6.40	102.09	111.70
2	F	7	DT	N3-C4-C5	6.40	124.40	114.80
3	B	297	TYR	CA-CB-CG	-6.40	102.38	113.90
1	E	12	DA	O3'-P-O5'	-6.40	94.41	104.00
3	A	167	ALA	N-CA-C	-6.39	105.35	113.02
2	F	18	DC	N3-C4-C5	-6.38	112.22	121.80
3	A	280	PRO	CA-N-CD	-6.38	103.06	112.00
3	A	129	MET	N-CA-C	-6.37	104.20	112.23
2	F	5	DG	N3-C2-N2	6.36	129.23	119.70
3	B	91	ILE	CG1-CB-CG2	-6.34	91.68	110.70
1	E	9	DA	C2'-C3'-O3'	-6.34	101.99	111.50
3	B	243	GLN	CA-CB-CG	-6.33	101.44	114.10
3	A	123	LYS	CD-CE-NZ	6.33	132.15	111.90
3	A	92	LEU	N-CA-C	-6.32	103.69	111.40
3	A	114	LEU	CB-CA-C	-6.32	101.51	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	98	LEU	CA-C-N	-6.31	111.00	121.92
3	B	98	LEU	C-N-CA	-6.31	111.00	121.92
3	A	168	LEU	CB-CA-C	6.31	120.25	109.65
3	B	134	ILE	N-CA-CB	-6.31	102.38	111.21
3	B	122	ALA	CA-C-O	6.30	127.65	120.90
2	F	8	DG	N1-C2-N3	6.30	133.45	124.00
1	E	3	DT	O3'-P-O5'	6.29	113.44	104.00
1	E	12	DA	C4-N9-C1'	6.29	136.48	127.05
1	E	11	DA	N7-C8-N9	6.29	123.23	113.80
3	B	159	PRO	N-CD-CG	6.27	112.61	103.20
3	A	254	LYS	CA-C-N	-6.27	114.21	122.74
3	A	254	LYS	C-N-CA	-6.27	114.21	122.74
3	B	289	ASN	N-CA-C	-6.27	104.94	112.59
3	B	161	LYS	N-CA-C	6.26	119.42	110.10
3	B	300	PHE	CA-C-N	-6.25	112.31	120.44
3	B	300	PHE	C-N-CA	-6.25	112.31	120.44
2	F	4	DT	C2'-C3'-O3'	6.24	120.86	111.50
2	F	14	DT	O3'-P-O5'	-6.24	94.64	104.00
3	B	298	ASN	CA-C-N	-6.24	110.23	121.14
3	B	298	ASN	C-N-CA	-6.24	110.23	121.14
2	F	2	DG	O3'-P-O5'	-6.23	94.65	104.00
1	E	3	DT	N3-C2-O2	6.22	131.33	122.00
2	F	7	DT	N3-C2-O2	-6.22	112.67	122.00
2	F	15	DT	C5'-C4'-O4'	-6.22	100.08	109.40
2	F	7	DT	C5'-C4'-O4'	-6.21	100.08	109.40
3	A	301	ALA	N-CA-C	6.21	118.85	111.33
3	A	243	GLN	CB-CG-CD	6.21	123.16	112.60
3	A	162	THR	CA-C-N	-6.21	111.88	120.38
3	A	162	THR	C-N-CA	-6.21	111.88	120.38
1	E	19	DA	O5'-C5'-C4'	-6.20	101.50	110.80
2	F	18	DC	O4'-C4'-C3'	-6.20	96.10	105.40
3	B	170	THR	CA-CB-CG2	-6.19	99.98	110.50
2	F	4	DT	N1-C2-O2	-6.19	113.92	123.20
2	F	14	DT	C4-C5-C6	-6.18	109.94	119.20
3	A	184	ASN	O-C-N	6.18	131.36	122.28
1	E	17	DC	N3-C4-N4	6.14	127.11	117.90
3	A	158	THR	CB-CA-C	-6.14	99.54	109.67
3	A	233	ARG	N-CA-C	-6.14	98.52	108.52
1	E	9	DA	C4-N9-C1'	6.13	136.25	127.05
1	E	14	DT	C6-N1-C1'	6.13	128.54	119.35
2	F	13	DA	N1-C6-N6	-6.12	109.81	119.00
2	F	7	DT	N3-C4-O4	-6.12	113.42	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	100	THR	N-CA-C	-6.12	100.04	109.52
3	A	290	LEU	N-CA-C	6.11	119.34	110.42
1	E	9	DA	P-O5'-C5'	6.10	129.15	120.00
1	E	12	DA	C3'-C2'-C1'	6.09	110.74	101.60
3	B	171	TRP	CA-CB-CG	-6.09	102.02	113.60
1	E	5	DG	C5'-C4'-C3'	-6.09	105.76	114.90
2	F	9	DA	C4'-C3'-O3'	-6.09	100.86	110.00
2	F	13	DA	N1-C2-N3	6.08	138.12	129.00
3	B	90	SER	N-CA-CB	6.07	120.83	110.50
1	E	13	DT	N3-C4-C5	6.07	123.91	114.80
1	E	5	DG	N1-C2-N2	-6.07	107.19	116.30
3	A	290	LEU	CA-C-O	-6.07	114.88	120.95
3	B	145	LEU	CD1-CG-CD2	-6.07	97.45	110.80
3	A	152	GLN	N-CA-C	6.07	120.44	111.04
3	B	309	PHE	N-CA-C	6.06	116.28	108.34
3	B	110	VAL	N-CA-C	-6.04	105.43	112.98
3	B	120	ARG	NE-CZ-NH1	-6.03	115.47	121.50
1	E	15	DC	OP2-P-O3'	-6.03	89.92	108.00
1	E	14	DT	O5'-C5'-C4'	6.02	119.83	110.80
1	E	20	DG	C4'-C3'-O3'	6.02	119.03	110.00
2	F	8	DG	C6-C5-N7	-6.01	121.08	130.10
2	F	6	DG	N1-C6-O6	-6.01	110.99	120.00
1	E	14	DT	C4-C5-C6	-6.01	110.19	119.20
3	A	287	GLY	O-C-N	6.01	130.51	122.70
3	B	267	GLU	N-CA-C	6.01	117.50	111.07
3	A	265	VAL	CB-CA-C	-6.00	103.29	112.05
3	A	151	SER	O-C-N	5.98	130.11	122.33
1	E	19	DA	C5'-C4'-O4'	5.98	118.37	109.40
1	E	5	DG	C6-C5-N7	-5.97	121.15	130.10
1	E	8	DA	N1-C6-N6	-5.97	110.05	119.00
3	A	301	ALA	CA-C-N	-5.96	113.53	122.24
3	A	301	ALA	C-N-CA	-5.96	113.53	122.24
2	F	2	DG	N1-C6-O6	5.96	128.94	120.00
3	B	159	PRO	N-CA-CB	-5.96	97.80	103.34
3	B	232	ARG	CA-C-N	-5.95	114.58	122.85
3	B	232	ARG	C-N-CA	-5.95	114.58	122.85
3	B	174	ARG	N-CA-CB	-5.95	101.22	109.91
1	E	8	DA	C1'-O4'-C4'	-5.94	100.79	109.70
3	B	157	GLY	CA-C-N	-5.93	112.08	120.49
3	B	157	GLY	C-N-CA	-5.93	112.08	120.49
1	E	4	DG	C5-C6-O6	5.92	137.18	128.30
3	A	135	PRO	CB-CA-C	-5.92	104.04	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	13	DT	C6-N1-C1'	5.92	128.23	119.35
2	F	20	DA	O5'-C5'-C4'	5.91	119.66	110.80
2	F	8	DG	N1-C6-O6	5.91	128.86	120.00
3	B	243	GLN	CA-C-N	5.90	128.99	120.79
3	B	243	GLN	C-N-CA	5.90	128.99	120.79
3	A	145	LEU	N-CA-CB	-5.90	101.77	110.85
1	E	7	DT	N1-C2-O2	5.89	132.04	123.20
3	B	300	PHE	CA-CB-CG	-5.89	107.91	113.80
1	E	8	DA	P-O5'-C5'	5.89	128.84	120.00
1	E	9	DA	C5-C6-N1	5.89	126.43	117.60
1	E	8	DA	OP1-P-O3'	-5.88	90.35	108.00
1	E	12	DA	N9-C4-C5	5.88	114.51	105.70
1	E	8	DA	C3'-C2'-C1'	-5.87	92.79	101.60
3	B	272	GLU	N-CA-C	-5.87	105.37	112.54
1	E	15	DC	C5-C4-N4	-5.87	111.49	120.30
3	A	306	GLU	CA-C-O	5.87	125.49	119.97
2	F	9	DA	C1'-O4'-C4'	-5.86	100.91	109.70
3	A	90	SER	N-CA-CB	5.85	120.45	110.50
2	F	5	DG	O5'-P-OP2	-5.84	90.47	108.00
2	F	4	DT	C1'-O4'-C4'	-5.84	100.94	109.70
3	A	150	LEU	N-CA-CB	-5.83	101.62	110.07
1	E	6	DT	C5-C6-N1	5.82	131.53	122.80
3	B	260	GLU	N-CA-C	-5.82	105.28	112.38
3	A	235	ARG	N-CA-C	5.81	118.69	109.50
2	F	13	DA	N9-C4-C5	5.81	114.42	105.70
3	B	264	LEU	N-CA-C	-5.80	105.04	111.36
3	A	128	TYR	CZ-CE2-CD2	5.78	130.00	119.60
1	E	3	DT	N1-C2-O2	-5.77	114.54	123.20
3	A	112	ARG	CG-CD-NE	5.77	124.70	112.00
3	B	179	ILE	CG1-CB-CG2	-5.77	93.38	110.70
2	F	13	DA	C5'-C4'-O4'	5.77	118.05	109.40
2	F	7	DT	C5'-C4'-C3'	5.73	123.49	114.90
2	F	10	DA	O4'-C1'-N9	-5.72	99.82	108.40
1	E	6	DT	C5'-C4'-O4'	5.72	117.98	109.40
1	E	8	DA	OP2-P-O3'	5.72	125.15	108.00
3	B	237	LYS	CB-CA-C	-5.71	99.65	109.65
3	A	162	THR	OG1-CB-CG2	-5.71	97.88	109.30
3	B	278	VAL	CA-C-O	5.71	127.91	120.78
2	F	4	DT	C5'-C4'-O4'	5.70	117.95	109.40
1	E	8	DA	C5-N7-C8	5.69	112.44	103.90
2	F	14	DT	C2-N1-C1'	-5.68	110.84	119.35
2	F	15	DT	N1-C1'-C2'	5.67	122.01	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	150	LEU	N-CA-C	-5.67	105.01	111.14
3	A	159	PRO	CB-CG-CD	-5.67	87.95	106.10
3	A	160	MET	CA-C-O	-5.67	114.14	120.66
3	B	263	ALA	O-C-N	5.67	130.13	122.59
1	E	18	DC	O4'-C4'-C3'	-5.66	96.90	105.40
3	A	147	GLN	CA-C-N	-5.66	111.70	120.31
3	A	147	GLN	C-N-CA	-5.66	111.70	120.31
3	A	164	LYS	CA-C-N	-5.66	112.90	120.54
3	A	164	LYS	C-N-CA	-5.66	112.90	120.54
3	B	301	ALA	CA-C-N	-5.66	111.55	120.60
3	B	301	ALA	C-N-CA	-5.66	111.55	120.60
3	A	96	GLN	N-CA-C	-5.65	105.49	112.38
3	A	156	LYS	CB-CG-CD	5.64	124.28	111.30
1	E	15	DC	C2-N3-C4	-5.64	111.54	120.00
3	B	276	ARG	N-CA-CB	5.64	118.84	110.49
3	B	130	GLN	N-CA-CB	-5.64	101.62	110.30
3	B	176	GLN	CA-CB-CG	5.62	125.35	114.10
3	B	178	GLU	CA-C-N	-5.62	112.46	121.35
3	B	178	GLU	C-N-CA	-5.62	112.46	121.35
2	F	19	DC	C4-C5-C6	5.62	126.03	117.60
2	F	18	DC	N3-C2-O2	5.62	130.32	121.90
3	B	291	VAL	CB-CA-C	-5.61	103.89	111.63
3	A	275	GLN	CA-C-N	-5.61	113.76	122.67
3	A	275	GLN	C-N-CA	-5.61	113.76	122.67
3	A	154	LEU	CA-CB-CG	5.60	135.90	116.30
3	B	139	VAL	CA-C-N	-5.59	113.40	120.56
3	B	139	VAL	C-N-CA	-5.59	113.40	120.56
3	A	234	ASN	CA-C-O	5.59	128.50	120.51
3	A	141	ASP	CA-CB-CG	-5.58	107.02	112.60
3	B	132	HIS	N-CA-C	5.58	120.08	113.16
3	B	175	LYS	N-CA-CB	-5.58	100.62	110.39
3	B	252	ARG	CB-CA-C	5.57	119.33	111.86
3	A	178	GLU	O-C-N	-5.57	115.19	122.59
1	E	20	DG	C4-C5-N7	-5.56	102.46	110.80
1	E	11	DA	N3-C4-N9	-5.56	119.06	127.40
3	A	306	GLU	N-CA-C	-5.56	104.75	112.03
1	E	1	DC	O5'-C5'-C4'	5.55	119.13	110.80
1	E	10	DT	N3-C4-O4	-5.54	114.28	122.60
3	B	161	LYS	N-CA-CB	-5.54	101.21	109.69
2	F	11	DT	P-O3'-C3'	-5.54	111.89	120.20
3	A	243	GLN	N-CA-CB	-5.54	101.77	110.30
1	E	13	DT	O3'-P-O5'	-5.54	95.70	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	6	DT	C4-C5-C6	-5.53	110.90	119.20
1	E	18	DC	O4'-C1'-N1	5.53	116.69	108.40
3	B	283	ALA	O-C-N	-5.52	114.02	122.08
3	B	239	GLY	N-CA-C	-5.52	101.08	112.34
3	A	150	LEU	CA-C-N	-5.51	111.75	120.63
3	A	150	LEU	C-N-CA	-5.51	111.75	120.63
3	A	185	GLN	CB-CA-C	5.51	118.88	109.24
3	B	182	GLN	N-CA-C	-5.50	106.41	113.01
2	F	8	DG	O4'-C1'-C2'	-5.50	98.15	106.40
3	A	107	ARG	CA-C-O	5.49	126.35	120.20
3	B	153	HIS	N-CA-C	-5.49	105.68	112.38
3	A	164	LYS	N-CA-C	-5.49	105.21	111.14
2	F	11	DT	C5-C6-N1	5.49	131.03	122.80
2	F	20	DA	C4'-C3'-O3'	5.48	118.22	110.00
3	A	305	LYS	CA-C-N	-5.48	112.09	121.08
3	A	305	LYS	C-N-CA	-5.48	112.09	121.08
3	B	168	LEU	CA-C-N	-5.47	112.88	120.38
3	B	168	LEU	C-N-CA	-5.47	112.88	120.38
3	A	90	SER	CA-C-N	-5.47	112.49	121.19
3	A	90	SER	C-N-CA	-5.47	112.49	121.19
2	F	14	DT	P-O3'-C3'	5.47	128.40	120.20
3	A	98	LEU	CA-C-N	-5.47	115.66	123.20
3	A	98	LEU	C-N-CA	-5.47	115.66	123.20
2	F	21	DA	O5'-P-OP2	-5.46	91.61	108.00
2	F	8	DG	N7-C8-N9	5.46	121.69	113.50
3	B	128	TYR	CB-CA-C	-5.46	102.25	110.92
3	A	153	HIS	CA-C-N	-5.45	110.03	121.64
3	A	153	HIS	C-N-CA	-5.45	110.03	121.64
3	A	295	ARG	N-CA-CB	-5.45	101.95	109.91
2	F	13	DA	P-O3'-C3'	-5.45	112.03	120.20
3	A	158	THR	CA-C-N	5.45	125.37	119.76
3	A	158	THR	C-N-CA	5.45	125.37	119.76
1	E	11	DA	N1-C2-N3	5.44	137.16	129.00
2	F	21	DA	O4'-C1'-N9	5.44	116.56	108.40
3	A	288	SER	CB-CA-C	-5.44	101.61	110.85
3	B	309	PHE	CA-C-N	5.44	131.48	121.70
3	B	309	PHE	C-N-CA	5.44	131.48	121.70
3	B	94	GLU	N-CA-C	-5.43	102.46	111.37
3	A	170	THR	CA-C-N	-5.43	112.67	120.82
3	A	170	THR	C-N-CA	-5.43	112.67	120.82
1	E	4	DG	C5'-C4'-O4'	5.42	117.53	109.40
3	A	289	ASN	N-CA-CB	-5.42	102.60	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	286	LEU	O-C-N	5.40	128.54	122.22
3	B	126	LYS	CG-CD-CE	5.40	123.71	111.30
1	E	18	DC	C2'-C3'-O3'	5.39	119.59	111.50
2	F	14	DT	C2-N3-C4	-5.39	118.92	127.00
2	F	17	DA	C2'-C3'-O3'	5.38	119.58	111.50
3	B	109	GLU	CA-C-N	-5.38	112.89	121.34
3	B	109	GLU	C-N-CA	-5.38	112.89	121.34
2	F	18	DC	O4'-C1'-N1	5.38	116.46	108.40
1	E	7	DT	C1'-O4'-C4'	5.37	117.76	109.70
2	F	4	DT	O5'-C5'-C4'	5.37	118.86	110.80
2	F	7	DT	N1-C2-O2	5.37	131.26	123.20
1	E	4	DG	O5'-P-OP1	-5.37	92.89	109.00
3	A	151	SER	N-CA-C	5.37	119.32	112.34
3	B	278	VAL	CB-CA-C	-5.36	102.49	111.29
3	A	300	PHE	CA-C-N	-5.36	113.04	120.38
3	A	300	PHE	C-N-CA	-5.36	113.04	120.38
3	A	300	PHE	CA-CB-CG	-5.35	108.45	113.80
2	F	2	DG	O5'-C5'-C4'	5.35	118.82	110.80
3	B	264	LEU	CA-C-O	-5.35	114.75	120.42
3	A	252	ARG	NE-CZ-NH1	-5.34	116.16	121.50
3	B	110	VAL	CA-C-N	-5.33	111.72	121.52
3	B	110	VAL	C-N-CA	-5.33	111.72	121.52
3	B	297	TYR	CA-C-O	5.32	126.92	121.07
3	A	151	SER	N-CA-CB	5.32	119.75	110.18
3	A	298	ASN	CA-C-N	-5.32	111.21	121.58
3	A	298	ASN	C-N-CA	-5.32	111.21	121.58
1	E	10	DT	OP2-P-O3'	5.31	123.92	108.00
3	A	299	TRP	CB-CA-C	-5.30	99.41	109.95
3	B	279	SER	O-C-N	5.29	127.64	121.39
3	A	300	PHE	N-CA-C	-5.29	102.84	111.04
3	A	175	LYS	CA-CB-CG	-5.29	103.53	114.10
2	F	11	DT	C6-N1-C1'	5.29	127.28	119.35
3	A	255	ASN	CA-C-N	5.29	125.45	119.90
3	A	255	ASN	C-N-CA	5.29	125.45	119.90
3	B	175	LYS	CA-C-O	5.28	125.92	119.05
1	E	13	DT	C2-N3-C4	-5.28	119.08	127.00
3	A	101	GLU	CB-CA-C	5.28	119.09	110.96
3	A	270	ARG	NE-CZ-NH2	5.28	123.95	119.20
3	B	264	LEU	CB-CG-CD1	5.28	126.53	110.70
2	F	7	DT	O5'-C5'-C4'	5.28	118.71	110.80
3	B	97	ALA	N-CA-C	-5.28	106.90	113.55
1	E	5	DG	O5'-P-OP1	-5.27	93.20	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	110	VAL	CA-CB-CG2	-5.27	101.45	110.40
3	A	126	LYS	CA-CB-CG	5.27	124.63	114.10
2	F	4	DT	C4'-C3'-O3'	-5.26	102.11	110.00
2	F	5	DG	N9-C1'-C2'	-5.25	105.62	113.50
2	F	16	DA	O4'-C1'-C2'	-5.25	98.52	106.40
3	B	249	ALA	CA-C-N	-5.25	111.81	121.41
3	B	249	ALA	C-N-CA	-5.25	111.81	121.41
3	A	168	LEU	CA-C-O	5.24	125.88	119.64
3	B	117	ASP	N-CA-C	5.24	121.39	109.81
3	B	176	GLN	CA-C-O	-5.24	113.94	119.97
3	A	292	THR	N-CA-C	5.24	115.96	108.74
2	F	4	DT	P-O5'-C5'	5.23	127.84	120.00
3	B	122	ALA	N-CA-C	5.22	117.38	111.11
2	F	12	DT	C5'-C4'-O4'	-5.21	101.58	109.40
3	B	165	ARG	NH1-CZ-NH2	5.21	126.08	119.30
3	A	276	ARG	NE-CZ-NH2	-5.21	114.51	119.20
1	E	11	DA	N1-C6-N6	5.21	126.81	119.00
2	F	4	DT	P-O3'-C3'	-5.20	112.40	120.20
2	F	10	DA	OP1-P-OP2	5.20	135.59	120.00
3	A	115	SER	CA-C-N	5.20	129.65	120.87
3	A	115	SER	C-N-CA	5.20	129.65	120.87
2	F	11	DT	C4'-C3'-C2'	5.18	110.17	102.40
3	B	101	GLU	CB-CG-CD	5.18	121.40	112.60
3	B	127	GLY	O-C-N	5.18	129.43	122.70
3	A	288	SER	CA-CB-OG	-5.17	100.75	111.10
1	E	13	DT	N1-C2-N3	5.17	122.56	114.80
3	B	292	THR	N-CA-C	5.17	116.15	108.86
2	F	10	DA	O5'-P-OP2	-5.17	92.50	108.00
2	F	18	DC	O5'-P-OP2	-5.17	92.50	108.00
3	B	243	GLN	O-C-N	5.16	127.59	122.12
3	A	135	PRO	N-CA-CB	-5.15	98.72	103.25
3	B	130	GLN	N-CA-C	5.15	118.71	112.23
2	F	8	DG	P-O5'-C5'	-5.14	112.29	120.00
3	A	172	TYR	N-CA-C	-5.12	105.34	111.03
3	A	276	ARG	N-CA-C	-5.12	106.34	112.59
1	E	20	DG	C5-C6-O6	5.12	135.97	128.30
3	B	137	ARG	CB-CA-C	-5.11	101.35	110.70
2	F	16	DA	P-O3'-C3'	5.11	127.86	120.20
3	B	261	ARG	CB-CG-CD	5.11	123.04	111.30
1	E	5	DG	OP1-P-OP2	5.10	135.30	120.00
2	F	6	DG	O4'-C4'-C3'	5.10	113.05	105.40
2	F	15	DT	O5'-C5'-C4'	5.09	118.44	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	142	VAL	CB-CA-C	-5.09	102.94	111.29
3	A	153	HIS	N-CA-C	-5.08	105.25	111.75
1	E	14	DT	N3-C2-O2	-5.07	114.39	122.00
1	E	12	DA	O4'-C1'-C2'	-5.07	98.80	106.40
3	B	155	ASN	CA-CB-CG	-5.07	107.53	112.60
1	E	20	DG	C4-C5-C6	5.06	126.69	119.10
3	A	163	GLN	CA-C-N	5.06	127.32	120.44
3	A	163	GLN	C-N-CA	5.06	127.32	120.44
2	F	18	DC	O5'-P-OP1	5.06	124.17	109.00
3	B	248	GLN	CB-CA-C	-5.06	101.27	110.63
2	F	13	DA	C8-N9-C1'	5.05	134.63	127.05
3	A	139	VAL	O-C-N	5.05	126.77	121.87
3	A	165	ARG	CA-C-N	-5.05	112.50	120.63
3	A	165	ARG	C-N-CA	-5.05	112.50	120.63
2	F	5	DG	C6-N1-C2	-5.05	117.33	124.90
3	A	125	ILE	CA-CB-CG2	-5.05	101.92	110.50
3	B	282	LYS	O-C-N	5.04	129.90	123.24
3	B	270	ARG	CA-C-N	5.04	127.03	120.28
3	B	270	ARG	C-N-CA	5.04	127.03	120.28
3	A	132	HIS	CA-C-N	-5.03	115.13	122.78
3	A	132	HIS	C-N-CA	-5.03	115.13	122.78
1	E	1	DC	OP1-P-O3'	5.03	123.08	108.00
3	A	254	LYS	N-CA-C	-5.03	105.80	111.28
3	A	287	GLY	N-CA-C	-5.02	101.28	113.18
1	E	7	DT	OP2-P-O3'	5.01	123.04	108.00
3	A	245	ILE	CB-CG1-CD1	-5.01	103.28	113.80
2	F	21	DA	N9-C1'-C2'	5.00	121.00	113.50
3	A	100	THR	OG1-CB-CG2	-5.00	99.30	109.30

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	230	0
3	B	1462	0	1450	258	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	554	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 79.

All (554) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:120:ARG:CG	3:B:120:ARG:CB	1.74	1.65
3:B:185:GLN:CB	3:B:185:GLN:CG	1.77	1.63
3:B:237:LYS:CD	3:B:237:LYS:CG	1.76	1.62
3:A:254:LYS:CG	3:A:254:LYS:CB	1.76	1.62
3:A:98:LEU:CD1	3:A:98:LEU:CG	1.75	1.61
3:B:93:LYS:CE	3:B:93:LYS:CD	1.75	1.59
3:B:232:ARG:CD	3:B:232:ARG:CG	1.76	1.57
3:A:93:LYS:CD	3:A:93:LYS:CE	1.80	1.56
3:A:93:LYS:CD	3:A:93:LYS:CG	1.82	1.55
3:B:120:ARG:CG	3:B:120:ARG:CD	1.77	1.55
3:A:93:LYS:CE	3:A:93:LYS:NZ	1.70	1.55
3:B:180:LEU:CD1	3:B:180:LEU:CG	1.86	1.54
3:B:233:ARG:CG	3:B:233:ARG:CD	1.75	1.54
3:B:161:LYS:CD	3:B:161:LYS:CG	1.82	1.52
3:A:96:GLN:CG	3:A:96:GLN:CD	1.81	1.51
3:B:126:LYS:NZ	3:B:126:LYS:CE	1.70	1.50
3:A:179:ILE:CD1	3:A:179:ILE:CG1	1.89	1.50
3:A:123:LYS:CE	3:A:123:LYS:NZ	1.73	1.50
3:B:93:LYS:CE	3:B:93:LYS:NZ	1.72	1.50
3:A:237:LYS:CE	3:A:237:LYS:NZ	1.74	1.49
3:A:253:GLN:CD	3:A:253:GLN:CG	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:DC:O5'	1:E:1:DC:C5'	1.63	1.46
3:A:180:LEU:CD2	3:A:180:LEU:CG	1.95	1.45
1:E:20:DG:O5'	1:E:20:DG:C5'	1.63	1.44
3:B:156:LYS:CE	3:B:156:LYS:CD	1.96	1.43
1:E:4:DG:C5'	1:E:4:DG:O5'	1.66	1.42
3:B:231:MET:CG	3:B:231:MET:SD	2.05	1.41
2:F:21:DA:C3'	2:F:21:DA:O3'	1.67	1.41
3:B:231:MET:SD	3:B:231:MET:CE	2.23	1.26
3:B:254:LYS:NZ	3:B:254:LYS:HB3	1.47	1.19
3:A:186:THR:HG22	3:A:282:LYS:NZ	1.59	1.16
3:A:177:ARG:HA	3:A:180:LEU:HD12	1.27	1.09
2:F:18:DC:H4'	2:F:18:DC:OP1	1.40	1.08
3:A:186:THR:HG23	3:A:187:VAL:H	1.10	1.08
3:A:177:ARG:HA	3:A:180:LEU:CD1	1.84	1.07
2:F:5:DG:H2''	2:F:6:DG:H5''	1.33	1.05
3:A:186:THR:CG2	3:A:187:VAL:N	2.19	1.04
3:A:186:THR:CG2	3:A:187:VAL:H	1.69	1.04
3:B:257:SER:O	3:B:259:GLU:N	1.90	1.04
3:B:134:ILE:CD1	3:B:134:ILE:CG1	2.39	0.99
3:B:158:THR:CG2	3:B:159:PRO:HD2	1.92	0.98
2:F:6:DG:H2''	2:F:7:DT:H5''	1.41	0.98
3:B:269:ASN:ND2	3:B:290:LEU:HD12	1.78	0.97
3:B:254:LYS:HB3	3:B:254:LYS:HZ3	1.16	0.96
3:B:303:ARG:HD2	3:B:303:ARG:O	1.65	0.96
2:F:6:DG:H2''	2:F:7:DT:C5'	1.96	0.95
3:B:175:LYS:HE3	3:B:179:ILE:HD13	1.47	0.95
3:A:186:THR:HG22	3:A:282:LYS:HZ1	1.32	0.94
3:B:279:SER:C	3:B:281:SER:H	1.73	0.94
3:A:165:ARG:HB3	3:A:169:TYR:CE2	2.03	0.93
3:A:183:PHE:CE2	3:A:278:VAL:HG11	2.04	0.92
2:F:20:DA:C5	2:F:21:DA:N6	2.39	0.91
3:A:104:ALA:HA	3:A:107:ARG:NH1	1.85	0.91
3:A:120:ARG:NH2	3:A:123:LYS:HB3	1.85	0.91
3:A:152:GLN:HB3	3:A:158:THR:OG1	1.70	0.91
2:F:20:DA:C6	2:F:21:DA:N6	2.39	0.90
3:B:254:LYS:NZ	3:B:254:LYS:CB	2.33	0.90
3:B:254:LYS:HB3	3:B:254:LYS:HZ2	1.29	0.90
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:177:ARG:CA	3:A:180:LEU:HD12	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:104:ALA:HA	3:A:107:ARG:HH12	1.38	0.87
3:B:179:ILE:HG23	3:B:179:ILE:O	1.73	0.87
3:A:98:LEU:CD1	3:A:98:LEU:HG	2.04	0.87
3:B:91:ILE:HG22	3:B:91:ILE:O	1.73	0.87
3:A:110:VAL:HG23	3:A:173:VAL:HG21	1.56	0.86
3:B:106:GLN:O	3:B:108:ALA:N	2.08	0.86
3:B:93:LYS:HA	3:B:96:GLN:HB2	1.58	0.86
3:A:137:ARG:HH11	3:A:137:ARG:HG2	1.40	0.86
3:B:158:THR:HG23	3:B:159:PRO:HD2	1.59	0.85
3:A:107:ARG:O	3:A:111:ASP:HB2	1.77	0.84
3:B:153:HIS:HB2	3:B:158:THR:O	1.77	0.84
3:A:282:LYS:C	3:A:284:HIS:H	1.84	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:B:257:SER:C	3:B:259:GLU:H	1.85	0.83
3:A:282:LYS:HG3	3:A:284:HIS:HB3	1.59	0.82
3:A:120:ARG:HH21	3:A:123:LYS:HB3	1.44	0.82
3:A:111:ASP:HA	3:A:114:LEU:HD11	1.60	0.82
2:F:3:DC:OP1	2:F:4:DT:OP2	1.98	0.82
3:B:158:THR:HG22	3:B:159:PRO:HD2	1.59	0.82
3:A:300:PHE:O	3:A:303:ARG:HB2	1.78	0.82
3:B:112:ARG:HG3	3:B:113:MET:N	1.93	0.82
3:B:305:LYS:O	3:B:308:ALA:HB3	1.79	0.82
3:A:256:PRO:HB2	3:A:261:ARG:HG2	1.62	0.81
1:E:12:DA:H1'	1:E:13:DT:H5''	1.62	0.81
3:A:257:SER:O	3:A:260:GLU:HB3	1.81	0.81
2:F:16:DA:OP1	3:A:237:LYS:HD2	1.80	0.81
3:B:294:VAL:O	3:B:297:TYR:HB3	1.80	0.81
3:A:181:ARG:C	3:A:183:PHE:H	1.89	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:141:ASP:O	3:A:142:VAL:C	2.24	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:A:304:ARG:O	3:A:306:GLU:N	2.17	0.77
1:E:19:DA:O5'	1:E:19:DA:H2'	1.85	0.77
3:A:287:GLY:O	3:A:290:LEU:HB2	1.84	0.77
3:B:239:GLY:O	3:B:243:GLN:HG3	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:116:GLU:OE2	3:A:116:GLU:N	2.17	0.77
1:E:5:DG:O6	3:A:305:LYS:HE3	1.84	0.77
3:A:302:ASN:O	3:A:303:ARG:NH1	2.18	0.77
3:A:250:TYR:C	3:A:252:ARG:H	1.94	0.76
2:F:6:DG:C2'	2:F:7:DT:H5''	2.15	0.76
3:B:235:ARG:NH1	3:B:235:ARG:HG3	1.98	0.76
3:A:186:THR:HG22	3:A:187:VAL:N	1.99	0.76
3:A:183:PHE:HE2	3:A:278:VAL:HG11	1.50	0.76
3:A:248:GLN:O	3:A:250:TYR:N	2.20	0.75
2:F:13:DA:H1'	2:F:14:DT:H5'	1.69	0.75
3:A:177:ARG:O	3:A:178:GLU:C	2.28	0.75
3:A:299:TRP:O	3:A:299:TRP:CE3	2.40	0.75
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:A:260:GLU:O	3:A:261:ARG:C	2.30	0.73
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:N	2.47	0.72
3:B:279:SER:C	3:B:281:SER:N	2.43	0.72
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
3:A:165:ARG:O	3:A:168:LEU:N	2.24	0.71
1:E:1:DC:H5'	1:E:2:DT:H73	1.73	0.71
1:E:3:DT:OP2	3:A:304:ARG:NH1	2.24	0.71
3:B:279:SER:O	3:B:281:SER:N	2.24	0.71
3:B:293:GLU:HG3	3:B:294:VAL:HG23	1.73	0.71
3:B:140:VAL:O	3:B:141:ASP:C	2.25	0.71
3:B:269:ASN:ND2	3:B:291:VAL:H	1.89	0.70
3:B:299:TRP:CE3	3:B:299:TRP:C	2.69	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:B:103:ALA:C	3:B:107:ARG:HH12	2.00	0.70
3:A:257:SER:O	3:A:260:GLU:N	2.25	0.70
3:A:279:SER:HG	3:A:281:SER:HG	1.36	0.70
3:A:125:ILE:CG2	3:A:125:ILE:O	2.38	0.70
3:A:186:THR:HG23	3:A:187:VAL:N	1.87	0.70
3:A:159:PRO:O	3:A:159:PRO:HG2	1.92	0.69
3:B:297:TYR:HD2	3:B:298:ASN:ND2	1.90	0.69
3:A:102:GLU:O	3:A:105:GLU:HG2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:282:LYS:C	3:A:284:HIS:N	2.44	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:257:SER:O	3:A:260:GLU:CB	2.42	0.68
3:A:306:GLU:O	3:A:306:GLU:HG2	1.92	0.68
2:F:16:DA:OP1	3:A:237:LYS:CD	2.41	0.68
3:B:253:GLN:O	3:B:256:PRO:HD3	1.93	0.68
3:A:158:THR:HG22	3:A:159:PRO:HD2	1.75	0.68
3:B:112:ARG:HG3	3:B:113:MET:H	1.57	0.68
1:E:18:DC:H2''	1:E:19:DA:N7	2.09	0.68
3:A:248:GLN:C	3:A:250:TYR:N	2.50	0.67
3:A:248:GLN:O	3:A:249:ALA:C	2.36	0.67
3:B:102:GLU:O	3:B:103:ALA:C	2.37	0.67
3:A:181:ARG:C	3:A:183:PHE:N	2.48	0.67
3:A:107:ARG:HH11	3:A:107:ARG:HG3	1.60	0.67
3:B:235:ARG:HH11	3:B:235:ARG:CG	2.08	0.67
3:B:305:LYS:O	3:B:306:GLU:O	2.13	0.67
1:E:1:DC:C5'	1:E:2:DT:H73	2.25	0.66
3:A:125:ILE:C	3:A:127:GLY:N	2.47	0.66
3:B:177:ARG:O	3:B:178:GLU:C	2.32	0.66
3:B:177:ARG:O	3:B:180:LEU:N	2.24	0.66
3:B:299:TRP:O	3:B:303:ARG:HB2	1.95	0.66
3:B:303:ARG:HD2	3:B:303:ARG:C	2.15	0.66
3:B:297:TYR:HD2	3:B:298:ASN:HD22	1.42	0.66
3:A:239:GLY:O	3:A:243:GLN:HB2	1.96	0.65
2:F:4:DT:O5'	2:F:4:DT:H2'	1.97	0.65
3:A:110:VAL:O	3:A:110:VAL:CG1	2.41	0.65
3:A:151:SER:O	3:A:155:ASN:ND2	2.26	0.65
1:E:2:DT:H2''	1:E:3:DT:C6	2.32	0.65
3:A:165:ARG:C	3:A:167:ALA:N	2.51	0.64
3:B:253:GLN:O	3:B:254:LYS:C	2.39	0.64
3:A:120:ARG:HH21	3:A:123:LYS:CB	2.11	0.64
3:B:305:LYS:O	3:B:306:GLU:C	2.39	0.64
1:E:9:DA:H2''	1:E:10:DT:OP2	1.98	0.64
1:E:1:DC:C5'	1:E:1:DC:HO5'	2.07	0.64
3:A:294:VAL:O	3:A:297:TYR:HB3	1.98	0.64
3:A:177:ARG:HA	3:A:180:LEU:HD11	1.75	0.64
3:B:104:ALA:O	3:B:105:GLU:C	2.40	0.64
3:B:300:PHE:O	3:B:303:ARG:N	2.31	0.63
3:B:254:LYS:HZ3	3:B:254:LYS:CB	2.02	0.63
3:A:152:GLN:HB3	3:A:158:THR:HG1	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:257:SER:O	3:B:260:GLU:N	2.31	0.63
3:A:152:GLN:OE1	3:A:152:GLN:HA	1.97	0.63
3:B:95:LEU:C	3:B:97:ALA:H	2.04	0.63
3:B:106:GLN:C	3:B:108:ALA:H	2.04	0.63
3:A:107:ARG:NH1	3:A:107:ARG:HG3	2.14	0.62
3:B:251:ASP:O	3:B:253:GLN:NE2	2.32	0.62
3:B:258:LYS:HA	3:B:261:ARG:CZ	2.29	0.62
3:A:265:VAL:O	3:A:269:ASN:HB2	1.99	0.62
2:F:20:DA:C6	2:F:21:DA:C6	2.87	0.62
3:B:173:VAL:HG23	3:B:174:ARG:N	2.13	0.62
3:B:303:ARG:NH1	3:B:307:GLU:CB	2.63	0.62
3:A:111:ASP:HA	3:A:114:LEU:CD1	2.28	0.62
3:B:112:ARG:CG	3:B:113:MET:N	2.62	0.62
3:A:91:ILE:HG22	3:A:91:ILE:O	2.00	0.62
3:B:161:LYS:O	3:B:162:THR:C	2.41	0.62
3:B:254:LYS:CB	3:B:254:LYS:HZ2	2.04	0.62
3:A:98:LEU:CD1	3:A:98:LEU:CD2	2.75	0.62
3:A:165:ARG:CB	3:A:169:TYR:HE2	2.10	0.62
3:A:279:SER:C	3:A:281:SER:H	2.07	0.62
3:B:299:TRP:CE3	3:B:299:TRP:O	2.53	0.62
3:A:110:VAL:HG23	3:A:173:VAL:CG2	2.30	0.62
3:B:109:GLU:HG2	3:B:173:VAL:CG1	2.29	0.62
3:A:260:GLU:O	3:A:261:ARG:O	2.17	0.61
3:A:279:SER:C	3:A:281:SER:N	2.53	0.61
3:A:141:ASP:N	3:A:141:ASP:OD2	2.29	0.61
2:F:6:DG:H2''	2:F:7:DT:H5'	1.81	0.61
3:A:165:ARG:C	3:A:167:ALA:H	2.06	0.61
3:A:248:GLN:C	3:A:250:TYR:H	2.05	0.61
3:A:256:PRO:HG2	3:A:300:PHE:CE1	2.35	0.61
3:B:158:THR:CG2	3:B:159:PRO:CD	2.69	0.61
3:B:163:GLN:HA	3:B:163:GLN:OE1	2.01	0.61
3:A:179:ILE:O	3:A:179:ILE:CG2	2.48	0.61
3:A:279:SER:O	3:A:281:SER:O	2.19	0.61
3:B:120:ARG:CG	3:B:120:ARG:CA	2.73	0.61
1:E:19:DA:O5'	1:E:19:DA:C2'	2.49	0.61
3:A:116:GLU:N	3:A:116:GLU:CD	2.59	0.61
3:A:293:GLU:O	3:A:294:VAL:C	2.42	0.61
3:B:137:ARG:CZ	3:B:137:ARG:HB3	2.31	0.60
3:B:258:LYS:HA	3:B:261:ARG:HG3	1.83	0.60
3:B:303:ARG:HH12	3:B:307:GLU:HB2	1.66	0.60
2:F:18:DC:OP1	2:F:18:DC:C4'	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:DA:H2''	1:E:13:DT:C5'	2.32	0.60
1:E:12:DA:OP2	3:A:151:SER:HB3	2.02	0.60
3:A:240:PRO:O	3:A:243:GLN:HB3	2.02	0.60
3:A:242:SER:O	3:A:246:LEU:HD12	2.02	0.60
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
2:F:7:DT:OP1	3:A:161:LYS:HD2	2.03	0.59
3:B:93:LYS:O	3:B:94:GLU:C	2.45	0.59
2:F:4:DT:C4'	2:F:5:DG:OP1	2.47	0.59
3:B:300:PHE:O	3:B:301:ALA:C	2.45	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:A:93:LYS:O	3:A:94:GLU:C	2.46	0.59
3:A:299:TRP:O	3:A:299:TRP:CD2	2.56	0.59
3:B:269:ASN:HD21	3:B:291:VAL:H	1.50	0.58
3:B:274:LEU:CD1	3:B:274:LEU:HG	2.24	0.58
2:F:19:DC:H2''	2:F:20:DA:C8	2.38	0.58
2:F:17:DA:H2''	2:F:18:DC:C6	2.39	0.58
3:B:175:LYS:CE	3:B:179:ILE:HD13	2.28	0.58
3:B:240:PRO:CD	3:B:241:ALA:H	2.16	0.58
3:B:282:LYS:HB2	3:B:284:HIS:CE1	2.38	0.58
3:A:165:ARG:O	3:A:167:ALA:N	2.37	0.57
3:B:306:GLU:O	3:B:307:GLU:C	2.47	0.57
3:A:303:ARG:HG2	3:A:303:ARG:HH11	1.70	0.57
3:A:152:GLN:OE1	3:A:152:GLN:CA	2.53	0.57
3:A:169:TYR:O	3:A:172:TYR:N	2.37	0.57
3:A:170:THR:O	3:A:171:TRP:C	2.44	0.57
3:B:90:SER:O	3:B:93:LYS:N	2.36	0.57
3:B:307:GLU:O	3:B:309:PHE:N	2.37	0.57
2:F:2:DG:C2'	2:F:3:DC:O5'	2.52	0.57
3:A:137:ARG:HG2	3:A:137:ARG:NH1	2.15	0.57
3:A:279:SER:O	3:A:281:SER:N	2.37	0.57
3:B:181:ARG:C	3:B:183:PHE:N	2.60	0.57
3:A:186:THR:C	3:A:282:LYS:HZ2	2.12	0.57
3:A:261:ARG:O	3:A:263:ALA:N	2.37	0.57
3:A:306:GLU:O	3:A:306:GLU:CG	2.52	0.57
2:F:9:DA:H1'	2:F:10:DA:H5''	1.87	0.57
1:E:5:DG:H1'	1:E:6:DT:H5'	1.86	0.57
3:B:158:THR:HG22	3:B:159:PRO:N	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:240:PRO:O	3:B:243:GLN:HB2	2.05	0.56
3:B:250:TYR:HA	3:B:253:GLN:HG2	1.86	0.56
3:B:281:SER:C	3:B:282:LYS:CG	2.78	0.56
2:F:5:DG:H2''	2:F:6:DG:C5'	2.21	0.56
3:B:106:GLN:O	3:B:107:ARG:C	2.45	0.56
3:B:170:THR:HG22	3:B:171:TRP:N	2.03	0.56
3:B:162:THR:O	3:B:163:GLN:C	2.49	0.56
3:B:177:ARG:C	3:B:179:ILE:N	2.58	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:A:186:THR:HG22	3:A:282:LYS:HZ2	1.65	0.56
3:B:257:SER:C	3:B:259:GLU:N	2.42	0.56
2:F:21:DA:C3'	2:F:21:DA:HO3'	2.11	0.55
3:A:105:GLU:O	3:A:108:ALA:HB3	2.06	0.55
3:B:106:GLN:CG	3:B:177:ARG:HH12	2.20	0.55
3:B:175:LYS:O	3:B:175:LYS:HG3	2.02	0.55
3:B:250:TYR:C	3:B:250:TYR:CD1	2.85	0.55
3:A:237:LYS:NZ	3:A:237:LYS:CD	2.66	0.55
3:B:159:PRO:O	3:B:159:PRO:HG2	2.06	0.55
3:B:91:ILE:HA	3:B:94:GLU:HB3	1.88	0.55
3:B:109:GLU:C	3:B:111:ASP:N	2.59	0.55
3:B:143:THR:HB	3:B:145:LEU:HG	1.89	0.55
3:B:240:PRO:HD2	3:B:241:ALA:H	1.70	0.55
2:F:5:DG:C2'	2:F:6:DG:H5''	2.24	0.55
3:B:125:ILE:O	3:B:128:TYR:HB3	2.05	0.55
3:B:303:ARG:NH1	3:B:307:GLU:N	2.55	0.55
3:A:165:ARG:O	3:A:166:ALA:C	2.49	0.55
3:B:128:TYR:CD1	3:B:172:TYR:HE1	2.25	0.55
3:B:174:ARG:O	3:B:177:ARG:N	2.38	0.55
1:E:16:DA:C2	2:F:8:DG:C2	2.95	0.55
3:B:95:LEU:C	3:B:97:ALA:N	2.65	0.55
3:B:109:GLU:HG2	3:B:173:VAL:HG11	1.87	0.54
1:E:12:DA:C1'	1:E:13:DT:H5''	2.35	0.54
3:A:120:ARG:HB3	3:A:120:ARG:NH1	2.22	0.54
3:B:119:TRP:CH2	3:B:123:LYS:HD3	2.42	0.54
3:B:270:ARG:HG3	3:B:270:ARG:HH11	1.72	0.54
3:B:281:SER:O	3:B:282:LYS:HG2	2.07	0.54
3:A:125:ILE:C	3:A:127:GLY:H	2.14	0.54
3:B:174:ARG:C	3:B:176:GLN:N	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:131:GLN:HE21	3:A:276:ARG:HA	1.72	0.54
3:A:247:TYR:HE2	3:A:303:ARG:HE	1.54	0.54
3:B:168:LEU:O	3:B:171:TRP:HB3	2.07	0.54
2:F:20:DA:C5	2:F:21:DA:C6	2.95	0.54
3:B:112:ARG:CG	3:B:113:MET:H	2.20	0.54
3:B:135:PRO:C	3:B:137:ARG:N	2.63	0.54
3:B:153:HIS:HA	3:B:158:THR:N	2.22	0.54
3:B:233:ARG:CD	3:B:233:ARG:CB	2.82	0.54
3:B:120:ARG:CG	3:B:120:ARG:C	2.80	0.53
3:B:123:LYS:O	3:B:124:MET:C	2.52	0.53
3:A:116:GLU:CD	3:A:116:GLU:H	2.17	0.53
3:A:162:THR:O	3:A:163:GLN:C	2.51	0.53
3:B:91:ILE:O	3:B:91:ILE:CG2	2.46	0.53
3:B:268:CYS:O	3:B:271:ALA:HB3	2.08	0.53
1:E:9:DA:C2'	1:E:10:DT:OP2	2.51	0.53
3:B:259:GLU:C	3:B:261:ARG:N	2.65	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:297:TYR:C	3:B:297:TYR:CD2	2.86	0.53
3:B:109:GLU:C	3:B:111:ASP:H	2.16	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:A:301:ALA:C	3:A:303:ARG:H	2.17	0.52
3:B:175:LYS:O	3:B:179:ILE:HB	2.09	0.52
3:B:181:ARG:O	3:B:183:PHE:N	2.43	0.52
3:A:137:ARG:HH11	3:A:137:ARG:CG	2.15	0.52
3:B:95:LEU:O	3:B:97:ALA:N	2.42	0.52
3:B:169:TYR:O	3:B:170:THR:C	2.50	0.52
3:B:161:LYS:CD	3:B:161:LYS:CB	2.79	0.52
3:B:231:MET:O	3:B:232:ARG:O	2.28	0.52
3:A:175:LYS:HG3	3:A:175:LYS:O	2.09	0.52
3:A:186:THR:CG2	3:A:282:LYS:NZ	2.52	0.52
2:F:8:DG:OP2	3:A:146:ASN:HB2	2.10	0.52
3:A:104:ALA:HA	3:A:107:ARG:CZ	2.39	0.52
3:A:300:PHE:O	3:A:301:ALA:C	2.47	0.52
3:B:173:VAL:CG2	3:B:174:ARG:N	2.73	0.52
1:E:19:DA:C2	2:F:4:DT:N3	2.68	0.52
3:A:137:ARG:O	3:A:138:GLU:C	2.53	0.52
3:A:258:LYS:O	3:A:262:GLU:HB2	2.10	0.52
3:B:257:SER:O	3:B:258:LYS:C	2.49	0.51
3:A:256:PRO:HB2	3:A:261:ARG:CG	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:186:THR:HG22	3:A:282:LYS:HZ3	1.65	0.51
3:A:297:TYR:CD1	3:A:297:TYR:C	2.86	0.51
3:B:303:ARG:HD3	3:B:306:GLU:CD	2.36	0.51
3:B:167:ALA:O	3:B:168:LEU:C	2.50	0.51
3:B:272:GLU:OE1	3:B:276:ARG:NH2	2.44	0.51
3:A:152:GLN:C	3:A:154:LEU:N	2.66	0.51
3:A:120:ARG:HA	3:A:120:ARG:NE	2.27	0.50
3:B:165:ARG:O	3:B:169:TYR:N	2.32	0.50
1:E:2:DT:H2'	1:E:3:DT:H72	1.93	0.50
3:B:269:ASN:HD21	3:B:291:VAL:N	2.09	0.50
1:E:12:DA:C8	1:E:13:DT:C7	2.95	0.50
2:F:3:DC:P	2:F:4:DT:OP2	2.69	0.50
3:B:170:THR:O	3:B:171:TRP:C	2.53	0.50
3:A:241:ALA:C	3:A:243:GLN:N	2.64	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:164:LYS:O	3:A:165:ARG:C	2.45	0.50
3:A:293:GLU:O	3:A:297:TYR:N	2.35	0.50
3:B:299:TRP:C	3:B:299:TRP:HE3	2.19	0.50
3:A:168:LEU:O	3:A:169:TYR:C	2.54	0.50
3:A:237:LYS:NZ	3:A:237:LYS:CG	2.74	0.50
3:A:269:ASN:HD21	3:A:291:VAL:H	1.59	0.50
3:B:136:GLN:OE1	3:B:147:GLN:HG2	2.12	0.50
3:B:177:ARG:C	3:B:180:LEU:H	2.16	0.50
3:B:231:MET:SD	3:B:231:MET:N	2.85	0.49
3:B:302:ASN:O	3:B:306:GLU:HG3	2.12	0.49
3:B:180:LEU:CD1	3:B:180:LEU:CD2	2.86	0.49
3:A:150:LEU:O	3:A:151:SER:C	2.55	0.49
3:B:264:LEU:HA	3:B:267:GLU:HB3	1.93	0.49
3:B:135:PRO:C	3:B:137:ARG:H	2.20	0.49
3:A:291:VAL:HG12	3:A:292:THR:N	2.26	0.49
3:B:171:TRP:CE3	3:B:172:TYR:CA	2.95	0.49
3:B:174:ARG:C	3:B:176:GLN:H	2.19	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:135:PRO:O	3:B:136:GLN:C	2.52	0.49
3:B:137:ARG:C	3:B:139:VAL:H	2.21	0.49
2:F:21:DA:O3'	2:F:21:DA:H3'	1.96	0.49
3:A:256:PRO:CG	3:A:300:PHE:CE1	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:299:TRP:O	3:A:299:TRP:CG	2.66	0.49
3:B:103:ALA:HB1	3:B:107:ARG:HH12	1.78	0.49
3:B:181:ARG:C	3:B:183:PHE:H	2.19	0.49
3:A:172:TYR:O	3:A:173:VAL:C	2.56	0.48
3:A:141:ASP:O	3:A:143:THR:N	2.46	0.48
3:B:128:TYR:CE2	3:B:132:HIS:CD2	3.01	0.48
3:A:93:LYS:CD	3:A:93:LYS:CB	2.83	0.48
3:B:269:ASN:OD1	3:B:291:VAL:HB	2.13	0.48
3:B:291:VAL:HG12	3:B:292:THR:N	2.27	0.48
3:A:293:GLU:OE1	3:A:293:GLU:N	2.32	0.48
3:B:112:ARG:O	3:B:113:MET:C	2.54	0.48
3:B:299:TRP:C	3:B:299:TRP:CD2	2.92	0.48
3:A:158:THR:CG2	3:A:159:PRO:HD2	2.43	0.48
3:B:137:ARG:C	3:B:139:VAL:N	2.72	0.48
3:B:163:GLN:O	3:B:166:ALA:HB3	2.14	0.48
3:B:174:ARG:O	3:B:175:LYS:C	2.56	0.48
3:A:106:GLN:HB3	3:A:173:VAL:HG11	1.96	0.48
3:A:110:VAL:O	3:A:110:VAL:HG12	2.06	0.48
3:A:109:GLU:OE2	3:A:112:ARG:NH2	2.39	0.47
3:B:99:ASN:O	3:B:100:THR:O	2.31	0.47
1:E:12:DA:H1'	1:E:13:DT:C5'	2.38	0.47
2:F:3:DC:H5'	3:B:297:TYR:OH	2.14	0.47
3:B:103:ALA:C	3:B:107:ARG:NH1	2.69	0.47
3:B:236:PHE:CD2	3:B:236:PHE:C	2.90	0.47
3:A:257:SER:N	3:A:260:GLU:HB3	2.29	0.47
3:A:256:PRO:HB3	3:A:260:GLU:HG3	1.96	0.47
3:B:117:ASP:O	3:B:118:PRO:C	2.57	0.47
3:B:164:LYS:O	3:B:165:ARG:C	2.56	0.47
3:B:177:ARG:O	3:B:179:ILE:N	2.47	0.47
3:A:110:VAL:HG22	3:A:169:TYR:HB3	1.96	0.47
3:B:259:GLU:C	3:B:261:ARG:H	2.23	0.47
1:E:2:DT:H2''	1:E:3:DT:H6	1.80	0.47
2:F:4:DT:H4'	2:F:5:DG:OP1	2.15	0.47
3:A:271:ALA:O	3:A:274:LEU:HB2	2.14	0.47
3:B:128:TYR:CE2	3:B:132:HIS:HD2	2.33	0.47
2:F:3:DC:C2'	2:F:3:DC:O2	2.61	0.47
2:F:4:DT:O5'	2:F:4:DT:C2'	2.63	0.47
2:F:13:DA:C8	2:F:14:DT:H71	2.50	0.47
3:A:135:PRO:O	3:A:136:GLN:C	2.53	0.46
3:B:149:HIS:CE1	3:B:160:MET:HG3	2.48	0.46
3:A:268:CYS:O	3:A:270:ARG:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:91:ILE:O	3:A:91:ILE:CG2	2.64	0.46
3:A:291:VAL:C	3:A:292:THR:CG2	2.88	0.46
3:B:171:TRP:CE3	3:B:172:TYR:HA	2.50	0.46
3:B:90:SER:O	3:B:91:ILE:C	2.55	0.46
3:B:101:GLU:O	3:B:105:GLU:HB2	2.16	0.46
3:B:112:ARG:C	3:B:114:LEU:N	2.70	0.46
3:A:242:SER:HB3	3:A:268:CYS:SG	2.55	0.46
3:A:165:ARG:HG3	3:A:165:ARG:HH11	1.80	0.46
3:B:163:GLN:OE1	3:B:163:GLN:CA	2.64	0.46
3:B:271:ALA:O	3:B:274:LEU:HB2	2.16	0.46
1:E:19:DA:N1	2:F:4:DT:C4	2.83	0.46
3:A:258:LYS:O	3:A:259:GLU:C	2.58	0.46
3:A:273:CYS:HB3	3:A:278:VAL:HG23	1.98	0.46
3:B:233:ARG:CG	3:B:233:ARG:NE	2.67	0.46
2:F:5:DG:N7	3:B:305:LYS:NZ	2.63	0.46
3:A:283:ALA:O	3:A:286:LEU:HB2	2.15	0.46
3:A:300:PHE:O	3:A:303:ARG:N	2.49	0.46
3:B:90:SER:O	3:B:92:LEU:N	2.48	0.46
3:B:251:ASP:C	3:B:252:ARG:HG3	2.37	0.46
3:B:132:HIS:ND1	3:B:276:ARG:HD3	2.31	0.45
3:B:132:HIS:O	3:B:276:ARG:NH1	2.48	0.45
3:A:125:ILE:O	3:A:126:LYS:C	2.59	0.45
3:A:145:LEU:HD23	3:A:164:LYS:HD2	1.99	0.45
3:A:177:ARG:O	3:A:180:LEU:HD12	2.17	0.45
3:A:281:SER:O	3:A:282:LYS:C	2.58	0.45
1:E:4:DG:C5'	1:E:4:DG:P	3.02	0.45
3:B:131:GLN:O	3:B:275:GLN:NE2	2.46	0.45
3:B:302:ASN:HD22	3:B:302:ASN:HA	1.42	0.45
3:A:91:ILE:HA	3:A:94:GLU:HB3	1.98	0.45
1:E:5:DG:H2'	1:E:5:DG:H5'	1.68	0.45
3:A:96:GLN:CD	3:A:96:GLN:C	2.84	0.45
1:E:3:DT:O4	2:F:20:DA:N1	2.50	0.45
3:A:116:GLU:O	3:A:118:PRO:HD3	2.17	0.45
3:A:163:GLN:HA	3:A:163:GLN:NE2	2.32	0.45
3:A:261:ARG:H	3:A:261:ARG:HG3	1.50	0.45
3:A:304:ARG:C	3:A:306:GLU:N	2.75	0.45
1:E:8:DA:H1'	1:E:9:DA:C5'	2.46	0.45
3:B:264:LEU:O	3:B:265:VAL:C	2.58	0.45
3:B:296:VAL:O	3:B:300:PHE:HD1	2.00	0.45
1:E:12:DA:C2'	1:E:13:DT:C5'	2.95	0.45
3: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:A:174:ARG:C	3:A:176:GLN:N	2.73	0.44
3:B:120:ARG:C	3:B:120:ARG:HG2	2.43	0.44
3:A:92:LEU:O	3:A:93:LYS:C	2.58	0.44
3:A:174:ARG:O	3:A:175:LYS:C	2.57	0.44
3:B:128:TYR:C	3:B:128:TYR:CD2	2.93	0.44
3:B:155:ASN:HD22	3:B:155:ASN:HA	1.26	0.44
3:B:172:TYR:CE1	3:B:176:GLN:OE1	2.71	0.44
3:B:296:VAL:O	3:B:297:TYR:C	2.59	0.44
3:A:137:ARG:NH1	3:A:137:ARG:CG	2.73	0.44
3:B:175:LYS:HA	3:B:178:GLU:HB3	2.00	0.44
3:A:274:LEU:HD23	3:A:274:LEU:HA	1.65	0.43
3:B:258:LYS:CA	3:B:261:ARG:HG3	2.48	0.43
3:A:178:GLU:O	3:A:179:ILE:C	2.59	0.43
3:A:265:VAL:HG21	3:A:293:GLU:CD	2.44	0.43
3:A:98:LEU:HA	3:A:98:LEU:HD23	1.65	0.43
3:A:241:ALA:HB3	3:A:242:SER:H	1.53	0.43
3:B:183:PHE:O	3:B:184:ASN:C	2.61	0.43
3:B:269:ASN:HD21	3:B:290:LEU:HD12	1.74	0.43
3:B:294:VAL:HG23	3:B:294:VAL:H	1.28	0.43
3:B:181:ARG:O	3:B:182:GLN:C	2.61	0.43
3:B:296:VAL:C	3:B:299:TRP:H	2.27	0.43
3:B:165:ARG:HB3	3:B:169:TYR:CE2	2.53	0.43
3:A:95:LEU:HD12	3:A:95:LEU:HA	1.62	0.43
3:A:160:MET:HG2	3:A:164:LYS:HB2	2.00	0.43
3:A:95:LEU:C	3:A:97:ALA:N	2.76	0.43
3:B:160:MET:CE	3:B:165:ARG:HA	2.49	0.43
3:B:259:GLU:O	3:B:260:GLU:C	2.59	0.43
3:A:240:PRO:O	3:A:243:GLN:CB	2.67	0.42
3:A:301:ALA:C	3:A:303:ARG:N	2.76	0.42
3:B:91:ILE:HD13	3:B:91:ILE:HG21	1.70	0.42
3:B:150:LEU:HA	3:B:150:LEU:HD12	1.71	0.42
3:B:168:LEU:O	3:B:169:TYR:C	2.62	0.42
3:B:172:TYR:O	3:B:173:VAL:C	2.62	0.42
3:A:179:ILE:HD13	3:A:182:GLN:NE2	2.34	0.42
3:B:246:LEU:HD23	3:B:246:LEU:HA	1.59	0.42
1:E:1:DC:C5'	1:E:2:DT:C7	2.96	0.42
3:A:106:GLN:O	3:A:107:ARG:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:159:PRO:O	3:A:159:PRO:CG	2.66	0.42
3:A:177:ARG:O	3:A:178:GLU:O	2.36	0.42
3:A:172:TYR:O	3:A:175:LYS:HB3	2.20	0.42
1:E:5:DG:H4'	3:B:161:LYS:HE3	2.02	0.42
3:A:171:TRP:CE3	3:A:172:TYR:HA	2.54	0.42
3:B:297:TYR:CD2	3:B:298:ASN:ND2	2.79	0.42
3:B:296:VAL:CG2	3:B:297:TYR:N	2.73	0.42
2:F:3:DC:H3'	2:F:4:DT:C6	2.54	0.41
3:A:165:ARG:O	3:A:169:TYR:CD2	2.73	0.41
3:A:165:ARG:HG3	3:A:165:ARG:NH1	2.35	0.41
3:A:288:SER:C	3:A:290:LEU:N	2.75	0.41
3:A:300:PHE:O	3:A:303:ARG:CB	2.60	0.41
3:B:106:GLN:CG	3:B:177:ARG:NH1	2.84	0.41
3:A:147:GLN:C	3:A:147:GLN:CD	2.88	0.41
3:A:236:PHE:HE2	3:A:238:TRP:CD1	2.38	0.41
3:B:258:LYS:O	3:B:258:LYS:CG	2.68	0.41
3:B:273:CYS:O	3:B:274:LEU:C	2.62	0.41
3:B:128:TYR:O	3:B:129:MET:C	2.62	0.41
3:B:153:HIS:CB	3:B:158:THR:O	2.60	0.41
3:A:187:VAL:N	3:A:282:LYS:HZ2	2.17	0.41
3:A:105:GLU:O	3:A:106:GLN:C	2.62	0.41
3:A:113:MET:HA	3:A:116:GLU:HG2	2.02	0.41
3:A:235:ARG:HG2	3:A:236:PHE:N	2.36	0.41
3:B:111:ASP:HA	3:B:114:LEU:HD12	2.01	0.41
3:B:110:VAL:HG11	3:B:170:THR:HA	2.02	0.41
3:B:285:GLY:C	3:B:287:GLY:N	2.75	0.41
3:A:127:GLY:O	3:A:128:TYR:C	2.63	0.41
3:A:235:ARG:HG2	3:A:236:PHE:H	1.86	0.41
3:B:169:TYR:O	3:B:172:TYR:HB3	2.21	0.41
3:A:240:PRO:O	3:A:243:GLN:N	2.54	0.40
3:A:281:SER:HG	3:A:281:SER:H	1.67	0.40
3:B:261:ARG:HB2	3:B:262:GLU:H	1.67	0.40
3:A:264:LEU:O	3:A:265:VAL:C	2.60	0.40
3:B:293:GLU:O	3:B:296:VAL:HG22	2.19	0.40
3:A:303:ARG:NH1	3:A:303:ARG:HG2	2.34	0.40
3:B:166:ALA:O	3:B:167:ALA:C	2.62	0.40
3:B:126:LYS:O	3:B:130:GLN:HB3	2.21	0.40
3:B:281:SER:C	3:B:282:LYS:HG3	2.45	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%)	0	3
3	B	172/221 (78%)	125 (73%)	25 (14%)	22 (13%)	0	1
All	All	344/442 (78%)	249 (72%)	58 (17%)	37 (11%)	0	2

All (37) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
3	A	241	ALA
3	A	249	ALA
3	B	133	ASN
3	B	262	GLU
3	A	280	PRO
3	B	162	THR
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%)	112 (73%)	42 (27%)	0	2
3	B	154/195 (79%)	120 (78%)	34 (22%)	1	5
All	All	308/390 (79%)	232 (75%)	76 (25%)	1	3

All (76) 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	110	VAL
3	A	114	LEU
3	A	115	SER
3	A	116	GLU
3	A	120	ARG
3	A	123	LYS
3	A	126	LYS

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Mol	Chain	Res	Type
3	A	130	GLN
3	A	141	ASP
3	A	148	SER
3	A	151	SER
3	A	152	GLN
3	A	158	THR
3	A	168	LEU
3	A	170	THR
3	A	178	GLU
3	A	180	LEU
3	A	184	ASN
3	A	187	VAL
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	290	LEU
3	A	292	THR
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	133	ASN
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

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Mol	Chain	Res	Type
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	252	ARG
3	B	253	GLN
3	B	254	LYS
3	B	261	ARG
3	B	274	LEU
3	B	276	ARG
3	B	281	SER
3	B	282	LYS
3	B	286	LEU
3	B	292	THR
3	B	293	GLU
3	B	294	VAL
3	B	295	ARG
3	B	296	VAL
3	B	303	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	96	GLN
3	A	106	GLN
3	A	130	GLN
3	A	131	GLN
3	A	133	ASN
3	A	136	GLN
3	A	146	ASN
3	A	176	GLN
3	A	182	GLN
3	A	185	GLN
3	A	243	GLN
3	A	269	ASN
3	A	298	ASN
3	B	132	HIS
3	B	152	GLN

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Mol	Chain	Res	Type
3	B	155	ASN
3	B	176	GLN
3	B	243	GLN
3	B	244	GLN
3	B	269	ASN
3	B	298	ASN
3	B	302	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	2

All chain breaks are listed below:

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

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	20/20 (100%)	-1.78	0 100 100	43, 65, 108, 112	0
2	F	20/20 (100%)	-1.78	0 100 100	48, 66, 109, 116	0
3	A	176/221 (79%)	-1.53	0 100 100	29, 65, 100, 108	0
3	B	176/221 (79%)	-1.51	0 100 100	36, 65, 99, 108	0
All	All	392/482 (81%)	-1.55	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.