



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:53 PM UTC

PDB ID : 3AZI / pdb_00003azi
Title : Crystal Structure of Human Nucleosome Core Particle Containing H4K31Q mutation
Authors : Iwasaki, W.; Tachiwana, H.; Kawaguchi, K.; Shibata, T.; Kagawa, W.; Kurumizaka, H.
Deposited on : 2011-05-25
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

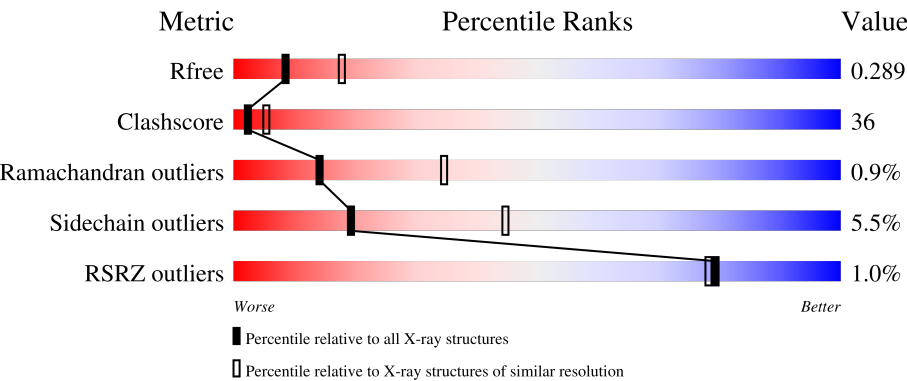
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	139	% 38% 28% . 29%
1	E	139	39% 31% . 29%
2	B	106	% 40% 31% . 26%
2	F	106	51% 27% . 21%
3	C	133	% 51% 23% 7% 19%

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Mol	Chain	Length	Quality of chain
3	G	133	2%47%29%•22%
4	D	129	2%43%26%•26%
4	H	129	%41%28%•28%
5	I	146	10%90%•
5	J	146	%95%••

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12053 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	E	99	Total	C	N	O	S	0	0	0
			816	514	158	140	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P68431
A	-2	SER	-	expression tag	UNP P68431
A	-1	HIS	-	expression tag	UNP P68431
E	-3	GLY	-	expression tag	UNP P68431
E	-2	SER	-	expression tag	UNP P68431
E	-1	HIS	-	expression tag	UNP P68431

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	78	Total	C	N	O	S	0	0	0
			619	390	120	108	1			
2	F	84	Total	C	N	O	S	0	0	0
			673	423	133	116	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P62805
B	-2	SER	-	expression tag	UNP P62805
B	-1	HIS	-	expression tag	UNP P62805
B	31	GLN	LYS	engineered mutation	UNP P62805
F	-3	GLY	-	expression tag	UNP P62805
F	-2	SER	-	expression tag	UNP P62805

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	HIS	-	expression tag	UNP P62805
F	31	GLN	LYS	engineered mutation	UNP P62805

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	108	Total	C	N	O	0	0	0
			835	526	165	144			
3	G	104	Total	C	N	O	0	0	0
			805	508	157	140			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP P04908
C	-2	SER	-	expression tag	UNP P04908
C	-1	HIS	-	expression tag	UNP P04908
G	-3	GLY	-	expression tag	UNP P04908
G	-2	SER	-	expression tag	UNP P04908
G	-1	HIS	-	expression tag	UNP P04908

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	95	Total	C	N	O	S	0	0	0
			745	468	136	139	2			
4	H	93	Total	C	N	O	S	0	0	0
			725	456	130	137	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP P06899
D	-2	SER	-	expression tag	UNP P06899
D	-1	HIS	-	expression tag	UNP P06899
H	-3	GLY	-	expression tag	UNP P06899
H	-2	SER	-	expression tag	UNP P06899
H	-1	HIS	-	expression tag	UNP P06899

- Molecule 5 is a DNA chain called 146-MER DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	145	Total	C	N	O	P	0	0	0
			2970	1421	538	867	144			
5	J	145	Total	C	N	O	P	0	0	0
			2969	1421	535	869	144			

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	C	1	Total	Cl	0	0
			1	1		
6	E	1	Total	Cl	0	0
			1	1		
6	G	1	Total	Cl	0	0
			1	1		

- Molecule 7 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	1	Total	Mn	0	0
			1	1		
7	I	5	Total	Mn	0	0
			5	5		
7	J	7	Total	Mn	0	0
			7	7		

- Molecule 8 is water.

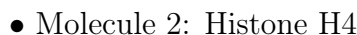
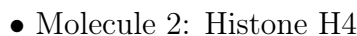
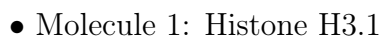
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	6	Total	O	0	0
			6	6		
8	B	6	Total	O	0	0
			6	6		
8	C	11	Total	O	0	0
			11	11		
8	D	3	Total	O	0	0
			3	3		
8	E	18	Total	O	0	0
			18	18		
8	F	12	Total	O	0	0
			12	12		

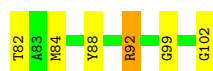
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	7	Total 7	O 7	0	0
8	H	2	Total 2	O 2	0	0
8	I	3	Total 3	O 3	0	0
8	J	4	Total 4	O 4	0	0

- Molecule 1: Histone H3.1

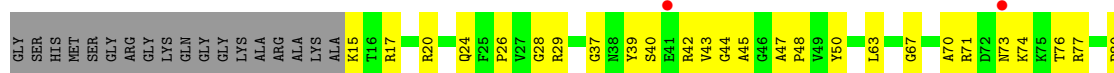




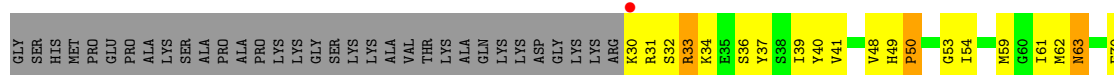
• Molecule 3: Histone H2A type 1-B/E



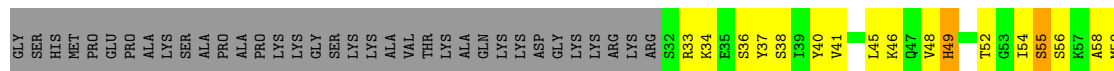
• Molecule 3: Histone H2A type 1-B/E



• Molecule 4: Histone H2B type 1-J



• Molecule 4: Histone H2B type 1-J



• Molecule 5: 146-MER DNA



- Molecule 5: 146-MER DNA



G267	A207	DA
G268	T208	T148
G269	G209	C149
G270	T210	A150
G271	T211	A151
A272	C212	T152
A273	A213	A153
T274	G214	T154
C275	C215	C155
T276	T216	C156
G277	G217	A157
G278	A218	C158
A279	A219	C159
G280	T220	T160
G281	T221	G161
G282	C222	C162
G283	A223	A163
G284	G224	G164
A285	C225	A165
T286	T226	T166
A287	G227	T167
T288	A228	C168
T289	A229	T169
G290	C230	A170
A291	A231	C171
T292	T232	C172
	G233	A173
	C234	A174
	A235	A175
	T236	A176
	T237	G177
	T238	T178
	T239	G179
	G240	T180
	A241	A181
	T242	T182
	G243	T183
	G244	T184
	A245	G185
	G246	G186
	C247	A187
	A248	A188
	G249	A189
	T250	C190
	T251	T191
	T252	G192
	C253	C193
	C254	T194
	A255	C195
	A256	C196
	A257	A197
	T258	T198
	A259	C199
	C260	A200
	A261	A201
	C262	A202
	T263	A203
	T264	G204
	T265	G205
	T266	C206

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.36Å 109.45Å 176.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.14 – 2.70 38.14 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (38.14-2.70) 99.5 (38.14-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.230 , 0.289 0.230 , 0.289	Depositor DCC
R_{free} test set	2874 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 73.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.033 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12053	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MN

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	A	0.51	0/819	0.95	1/1097 (0.1%)
1	E	0.64	0/828	1.06	4/1109 (0.4%)
2	B	0.53	0/626	0.99	1/838 (0.1%)
2	F	0.62	0/680	1.08	2/909 (0.2%)
3	C	0.60	0/845	1.00	5/1139 (0.4%)
3	G	0.52	0/815	0.93	0/1100
4	D	0.61	0/756	1.12	3/1015 (0.3%)
4	H	0.56	0/736	1.08	6/990 (0.6%)
5	I	0.30	0/3332	0.72	0/5141
5	J	0.30	0/3330	0.74	2/5138 (0.0%)
All	All	0.45	0/12767	0.87	24/18476 (0.1%)

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	C	0	1

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	92	GLU	N-CA-C	8.06	119.69	111.07
3	C	39	TYR	N-CA-C	-7.79	103.90	113.41
1	E	64	LYS	N-CA-C	6.94	118.54	110.97
1	E	114	ALA	N-CA-C	-6.60	105.97	112.97
4	H	101	LEU	N-CA-C	6.44	121.40	112.45
4	D	123	SER	N-CA-C	-6.17	106.43	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	99	GLY	N-CA-C	6.11	123.09	114.85
4	H	102	LEU	CA-C-N	6.04	126.01	120.21
4	H	102	LEU	C-N-CA	6.04	126.01	120.21
4	D	101	LEU	N-CA-C	5.73	118.74	111.69
2	F	46	ILE	N-CA-C	5.61	116.08	107.77
2	B	46	ILE	N-CA-C	5.48	115.84	108.17
1	A	111	ALA	N-CA-C	-5.47	105.23	111.14
1	E	98	ALA	N-CA-C	-5.46	105.22	111.07
3	C	43	VAL	N-CA-C	5.42	115.77	108.17
4	H	49	HIS	CA-C-N	5.34	125.41	119.32
4	H	49	HIS	C-N-CA	5.34	125.41	119.32
4	D	118	VAL	N-CA-C	5.32	116.09	110.72
4	H	54	ILE	N-CA-C	5.22	115.79	108.17
1	E	88	ALA	N-CA-C	-5.21	105.61	111.28
5	J	227	DG	N9-C1'-C2'	5.15	121.23	113.50
3	C	68	ASN	N-CA-C	-5.08	105.82	111.36
5	J	266	DT	N1-C1'-C2'	5.07	121.11	113.50
3	C	87	ILE	N-CA-C	5.04	115.26	110.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	57	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	807	0	844	59	0
1	E	816	0	856	46	0
2	B	619	0	654	37	0
2	F	673	0	717	27	0
3	C	835	0	897	55	0
3	G	805	0	861	54	0
4	D	745	0	771	51	0
4	H	725	0	745	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	2970	0	1640	249	0
5	J	2969	0	1641	268	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	1	0
6	G	1	0	0	0	0
7	E	1	0	0	0	0
7	I	5	0	0	0	0
7	J	7	0	0	0	0
8	A	6	0	0	0	0
8	B	6	0	0	1	0
8	C	11	0	0	2	0
8	D	3	0	0	0	0
8	E	18	0	0	1	0
8	F	12	0	0	0	0
8	G	7	0	0	1	0
8	H	2	0	0	0	0
8	I	3	0	0	1	0
8	J	4	0	0	0	0
All	All	12053	0	9626	766	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 36.

All (766) 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)
1:E:134:ARG:HH11	1:E:134:ARG:HB3	1.04	1.16
5:I:55:DA:H2"	5:I:56:DA:H5'	1.27	1.14
5:J:185:DG:H2"	5:J:186:DG:H5"	1.24	1.14
5:J:188:DA:H2"	5:J:189:DA:H5'	1.23	1.13
5:I:136:DT:H2"	5:I:137:DG:H5"	1.14	1.09
5:J:152:DT:H2"	5:J:153:DA:H5"	1.30	1.09
5:I:71:DG:H2"	5:I:72:DA:H5"	1.27	1.07
5:J:285:DA:H2"	5:J:286:DT:H5'	1.37	1.07
5:J:214:DG:H2"	5:J:215:DC:H5"	1.31	1.06
5:I:9:DC:H2"	5:I:10:DC:H5"	1.36	1.05
5:I:31:DG:H2"	5:I:32:DT:H5"	1.34	1.04
5:J:190:DC:H2"	5:J:191:DT:H5'	1.40	1.03
5:I:128:DT:H2"	5:I:129:DC:H5"	1.42	1.02
5:J:181:DA:H2"	5:J:182:DT:H5"	1.42	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:91:DT:H2''	5:I:92:DT:H5'	1.43	1.01
1:E:134:ARG:HB3	1:E:134:ARG:NH1	1.76	1.00
5:J:286:DT:H4'	5:J:287:DA:OP1	1.58	1.00
5:I:52:DT:H2''	5:I:53:DC:H5'	1.42	0.99
5:J:182:DT:H2''	5:J:183:DT:H5'	1.40	0.99
5:J:264:DT:H2''	5:J:265:DT:H5'	1.44	0.98
5:I:72:DA:H2''	5:I:73:DA:H5'	1.42	0.96
5:J:168:DC:H2''	5:J:169:DT:H5''	1.46	0.96
5:I:62:DT:H2''	5:I:63:DG:H5'	1.44	0.96
5:J:179:DG:H2''	5:J:180:DT:H5''	1.47	0.95
5:J:281:DG:H2''	5:J:282:DT:H5'	1.49	0.94
5:J:170:DA:H2''	5:J:171:DC:H5''	1.51	0.93
5:J:152:DT:C2'	5:J:153:DA:H5''	1.99	0.93
5:J:185:DG:C2'	5:J:186:DG:H5''	1.99	0.93
5:J:273:DA:H2''	5:J:274:DT:H5'	1.51	0.93
3:C:84:GLN:HE22	3:C:88:ARG:HE	1.16	0.93
5:I:136:DT:C2'	5:I:137:DG:H5''	1.98	0.92
2:B:25:ASN:N	2:B:25:ASN:HD22	1.69	0.90
5:I:71:DG:C2'	5:I:72:DA:H5''	2.00	0.90
5:J:170:DA:H2''	5:J:171:DC:C5'	2.02	0.90
5:J:223:DA:H2''	5:J:224:DG:N7	1.86	0.90
5:I:98:DG:H2''	5:I:99:DA:N7	1.86	0.90
5:I:127:DA:H2''	5:I:128:DT:H5''	1.53	0.89
5:I:125:DG:N3	5:I:126:DA:N7	2.20	0.88
5:J:156:DC:H2''	5:J:157:DA:H5''	1.53	0.87
5:I:57:DA:H2''	5:I:58:DG:C8	2.08	0.87
5:J:166:DT:H2''	5:J:167:DT:H5''	1.56	0.87
4:H:36:SER:HB2	4:H:63:ASN:HD21	1.37	0.86
1:E:134:ARG:HH11	1:E:134:ARG:CB	1.87	0.86
3:G:17:ARG:HH21	3:G:28:GLY:HA2	1.41	0.85
1:E:119:ILE:HD13	2:F:43:VAL:HG11	1.55	0.85
5:I:31:DG:C2'	5:I:32:DT:H5''	2.06	0.85
5:J:179:DG:C2'	5:J:180:DT:H5''	2.06	0.84
5:J:190:DC:H2''	5:J:191:DT:C5'	2.06	0.84
5:I:9:DC:C2'	5:I:10:DC:H5''	2.05	0.84
5:I:135:DG:H1'	5:I:136:DT:H5''	1.60	0.84
3:C:39:TYR:HB3	4:D:78:SER:HB2	1.60	0.84
5:I:46:DG:H2''	5:I:47:DC:OP2	1.78	0.83
1:A:58:THR:HG21	3:G:81:ARG:HG2	1.61	0.83
5:J:246:DG:H1'	5:J:247:DC:H5''	1.60	0.83
3:G:24:GLN:HE21	3:G:24:GLN:HA	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:166:DT:H2''	5:J:167:DT:C5'	2.08	0.83
5:I:4:DA:H4'	5:I:5:DA:OP1	1.77	0.83
5:J:264:DT:H2''	5:J:265:DT:C5'	2.07	0.83
3:C:87:ILE:HD12	3:C:97:LEU:HD12	1.61	0.83
5:J:214:DG:C2'	5:J:215:DC:H5''	2.07	0.83
3:G:24:GLN:HA	3:G:24:GLN:NE2	1.93	0.82
5:J:270:DA:H2''	5:J:271:DG:O5'	1.78	0.82
5:I:139:DA:H2''	5:I:140:DT:H5'	1.61	0.82
5:I:126:DA:N1	5:I:127:DA:N6	2.28	0.82
5:J:251:DT:H2'	5:J:252:DT:H71	1.62	0.81
5:I:112:DT:C2	5:I:113:DA:N7	2.48	0.81
5:J:206:DC:H2''	5:J:207:DA:C8	2.16	0.81
1:E:37:LYS:NZ	5:J:291:DA:H4'	1.97	0.80
5:I:26:DC:H2''	5:I:27:DA:N7	1.96	0.80
1:E:37:LYS:HB2	1:E:38:PRO:C	2.07	0.80
5:I:128:DT:C2'	5:I:129:DC:H5''	2.11	0.80
5:J:181:DA:C2'	5:J:182:DT:H5''	2.12	0.80
5:I:47:DC:H2''	5:I:48:DT:H5''	1.65	0.79
5:I:127:DA:H2	5:I:128:DT:C2	1.99	0.79
2:F:92:ARG:NH1	2:F:92:ARG:HB3	1.96	0.79
5:J:189:DA:H2''	5:J:190:DC:O5'	1.82	0.79
5:J:260:DC:H2''	5:J:261:DA:H8	1.48	0.79
5:I:62:DT:H2''	5:I:63:DG:C5'	2.13	0.78
5:J:154:DT:H2''	5:J:155:DC:H5'	1.66	0.78
5:J:179:DG:H2''	5:J:180:DT:C5'	2.14	0.78
5:I:127:DA:H2''	5:I:128:DT:C5'	2.12	0.78
5:J:170:DA:C2'	5:J:171:DC:H5''	2.12	0.78
3:C:50:TYR:OH	4:D:95:GLN:HG3	1.83	0.78
5:J:198:DT:H2''	5:J:199:DC:H5'	1.63	0.78
5:I:45:DT:H2''	5:I:46:DG:C8	2.19	0.78
5:I:61:DA:H2''	5:I:62:DT:C5'	2.14	0.78
5:I:127:DA:N6	5:J:167:DT:H3	1.82	0.78
5:J:262:DC:H2''	5:J:263:DT:H5'	1.64	0.78
5:J:188:DA:H2''	5:J:189:DA:C5'	2.08	0.77
1:A:49:ARG:HD3	5:J:155:DC:OP1	1.84	0.77
5:J:230:DC:H2''	5:J:231:DA:H5'	1.67	0.77
5:J:276:DT:H2''	5:J:277:DG:N7	1.98	0.77
5:J:174:DA:N3	5:J:175:DA:N7	2.33	0.77
1:A:63:ARG:O	1:A:66:PRO:HD2	1.84	0.77
3:C:25:PHE:CZ	3:C:59:THR:HG21	2.19	0.76
5:I:83:DA:H2''	5:I:84:DC:C5'	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:83:DA:H2''	5:I:84:DC:H5'	1.65	0.76
2:B:64:ASN:HD22	2:B:67:ARG:HH12	1.30	0.76
5:I:128:DT:H2''	5:I:129:DC:C5'	2.15	0.76
5:J:273:DA:H2''	5:J:274:DT:C5'	2.15	0.76
1:E:122:LYS:HB2	6:E:1001:CL:CL	2.22	0.75
5:I:61:DA:H2''	5:I:62:DT:H5''	1.68	0.75
3:C:26:PRO:HD3	4:D:40:TYR:CD1	2.21	0.75
5:I:95:DA:H1'	5:I:96:DT:H5'	1.67	0.75
4:D:33:ARG:HD2	5:J:269:DT:H4'	1.68	0.74
5:J:286:DT:C4'	5:J:287:DA:OP1	2.35	0.74
1:A:64:LYS:HB2	1:A:64:LYS:NZ	2.03	0.74
5:I:26:DC:H2''	5:I:27:DA:C5	2.22	0.74
5:J:282:DT:H2''	5:J:283:DG:H5'	1.70	0.74
5:I:139:DA:H2''	5:I:140:DT:C5'	2.18	0.73
5:J:182:DT:H2''	5:J:183:DT:C5'	2.17	0.73
5:J:181:DA:H2''	5:J:182:DT:C5'	2.17	0.73
3:C:102:ILE:HG23	4:D:61:ILE:HD13	1.70	0.73
5:I:51:DA:H2''	5:I:52:DT:C5'	2.18	0.73
5:I:117:DT:H1'	5:I:118:DT:H5''	1.69	0.73
5:J:158:DC:H2''	5:J:159:DC:O5'	1.87	0.73
1:A:117:VAL:HG13	3:G:115:LEU:CD2	2.19	0.73
3:G:76:THR:O	4:H:52:THR:HG23	1.88	0.73
5:I:101:DC:H2''	5:I:102:DA:H5'	1.69	0.73
5:J:244:DG:H4'	5:J:245:DA:OP1	1.88	0.73
5:I:71:DG:H2''	5:I:72:DA:C5'	2.13	0.72
1:E:37:LYS:HZ2	5:J:291:DA:H4'	1.54	0.72
5:J:249:DG:H2''	5:J:250:DT:H5'	1.69	0.72
5:J:186:DG:H4'	5:J:187:DA:OP1	1.88	0.72
3:C:25:PHE:HZ	3:C:59:THR:HG21	1.52	0.72
5:J:203:DA:H2''	5:J:204:DG:OP2	1.90	0.71
5:J:290:DG:H2''	5:J:291:DA:OP2	1.89	0.71
4:H:36:SER:HB2	4:H:63:ASN:ND2	2.05	0.71
3:G:70:ALA:HA	3:G:82:HIS:CE1	2.26	0.71
5:I:125:DG:C4	5:I:126:DA:N7	2.59	0.71
1:E:69:ARG:NH2	5:I:90:DT:OP2	2.24	0.71
5:J:259:DA:H2''	5:J:260:DC:H5''	1.71	0.71
5:I:111:DA:H2''	5:I:112:DT:OP2	1.91	0.70
5:J:156:DC:C2'	5:J:157:DA:H5''	2.22	0.70
5:I:72:DA:H2''	5:I:73:DA:C5'	2.19	0.70
5:I:32:DT:H2''	5:I:33:DG:H5'	1.73	0.70
3:C:42:ARG:HG3	4:D:88:THR:HB	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:104:DT:H2''	5:I:105:DT:O5'	1.91	0.70
2:B:78:ARG:HH11	2:B:78:ARG:HB2	1.57	0.70
5:I:5:DA:H2''	5:I:6:DT:O5'	1.92	0.69
5:I:68:DG:H2''	5:I:69:DC:H5'	1.74	0.69
5:J:236:DT:H2''	5:J:237:DT:OP2	1.92	0.69
5:J:275:DC:H2'	5:J:276:DT:H71	1.74	0.69
2:F:59:LYS:O	2:F:63:GLU:HG3	1.92	0.69
2:B:30:THR:OG1	2:B:32:PRO:HG2	1.93	0.69
5:J:234:DC:H2''	5:J:235:DC:C5	2.27	0.69
5:I:132:DC:H2''	5:I:133:DA:H5'	1.75	0.69
3:G:76:THR:HG22	5:I:131:DG:P	2.33	0.69
5:I:43:DA:H1'	5:I:44:DC:H5''	1.74	0.68
5:J:168:DC:C2'	5:J:169:DT:H5''	2.22	0.68
5:J:260:DC:H2''	5:J:261:DA:C8	2.27	0.68
4:H:56:SER:HB2	5:J:166:DT:OP2	1.93	0.68
5:I:28:DA:H2''	5:I:29:DA:C8	2.28	0.68
5:I:22:DC:H1'	5:I:23:DT:H5''	1.75	0.68
3:G:47:ALA:HB3	3:G:48:PRO:HD3	1.76	0.68
5:I:106:DT:H2''	5:I:107:DC:H6	1.59	0.68
2:B:83:ALA:O	2:B:87:VAL:HG23	1.94	0.68
5:I:2:DT:H2''	5:I:3:DC:H5'	1.76	0.68
4:D:32:SER:OG	5:I:103:DG:H5''	1.94	0.68
5:I:124:DA:H1'	5:I:125:DG:H5''	1.75	0.68
5:J:153:DA:H1'	5:J:154:DT:H5''	1.75	0.67
5:J:192:DG:H2''	5:J:193:DC:H5'	1.74	0.67
1:A:48:LEU:O	1:A:52:ARG:HG3	1.94	0.67
4:H:37:TYR:O	4:H:41:VAL:HG23	1.95	0.67
5:I:132:DC:H2''	5:I:133:DA:C5'	2.23	0.67
1:A:108:ASN:O	1:A:112:ILE:HG12	1.94	0.67
5:I:89:DC:H2''	5:I:90:DT:H71	1.76	0.67
5:J:275:DC:H2'	5:J:276:DT:C7	2.25	0.67
3:G:76:THR:CG2	5:I:130:DT:H3'	2.24	0.67
5:I:133:DA:H2''	5:I:134:DG:H5'	1.77	0.67
5:J:174:DA:C5	5:J:175:DA:N6	2.62	0.66
5:J:283:DG:H1'	5:J:284:DG:C8	2.30	0.66
2:B:31:GLN:N	2:B:32:PRO:HD2	2.11	0.66
5:I:101:DC:H2''	5:I:102:DA:C5'	2.26	0.66
4:H:88:THR:HG22	5:J:186:DG:P	2.36	0.66
5:I:141:DA:H1'	5:I:142:DT:H5''	1.78	0.66
5:I:12:DC:H2''	5:I:13:DC:O5'	1.96	0.66
5:J:188:DA:C2'	5:J:189:DA:H5'	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:223:DA:H4'	5:J:224:DG:OP1	1.95	0.66
1:A:64:LYS:HB2	1:A:64:LYS:HZ3	1.60	0.65
5:I:101:DC:H1'	5:I:102:DA:H5''	1.78	0.65
5:I:94:DG:H2''	5:I:95:DA:H8	1.62	0.65
5:J:285:DA:H2''	5:J:286:DT:C5'	2.21	0.65
3:G:17:ARG:NH2	3:G:28:GLY:HA2	2.09	0.65
3:C:26:PRO:HD3	4:D:40:TYR:CE1	2.32	0.65
2:B:68:ASP:OD2	2:B:92:ARG:HD3	1.96	0.65
5:I:55:DA:H2''	5:I:56:DA:C5'	2.18	0.65
5:I:2:DT:C6	5:I:3:DC:H5	2.15	0.65
5:I:85:DA:H1'	5:I:86:DT:H5''	1.79	0.65
1:A:117:VAL:HG13	3:G:115:LEU:HD21	1.77	0.64
5:I:126:DA:C2	5:I:127:DA:C5	2.85	0.64
5:I:127:DA:C2'	5:I:128:DT:H5''	2.24	0.64
3:C:30:VAL:HG13	4:D:70:PHE:HE1	1.61	0.64
3:G:26:PRO:HD3	4:H:40:TYR:CD1	2.32	0.64
5:I:52:DT:C2'	5:I:53:DC:H5'	2.23	0.64
5:J:209:DG:H2''	5:J:210:DT:H5'	1.79	0.64
5:I:8:DT:H1'	5:I:9:DC:H5''	1.79	0.64
5:J:247:DC:H2''	5:J:248:DA:C8	2.33	0.64
1:A:117:VAL:HG12	1:A:117:VAL:O	1.96	0.64
1:A:67:PHE:CD2	1:A:93:GLN:HG3	2.32	0.64
3:G:76:THR:HG22	5:I:130:DT:H3'	1.80	0.64
5:I:127:DA:C2	5:I:128:DT:C2	2.84	0.64
5:I:136:DT:H2''	5:I:137:DG:C5'	2.08	0.64
2:B:78:ARG:HH11	2:B:78:ARG:CB	2.10	0.64
5:I:51:DA:H2''	5:I:52:DT:H5'	1.79	0.63
1:A:134:ARG:HB2	1:A:134:ARG:NH1	2.13	0.63
4:D:33:ARG:O	4:D:33:ARG:HG3	1.98	0.63
5:I:37:DT:H2''	5:I:38:DT:C7	2.29	0.63
1:A:134:ARG:NH1	1:A:134:ARG:CB	2.61	0.63
1:E:108:ASN:O	1:E:112:ILE:HG12	1.99	0.63
5:J:274:DT:H2''	5:J:275:DC:H5''	1.80	0.63
3:C:114:VAL:HG23	8:C:2010:HOH:O	1.97	0.63
5:I:127:DA:N6	5:J:167:DT:N3	2.46	0.63
3:C:84:GLN:HE22	3:C:88:ARG:NE	1.92	0.62
5:I:37:DT:H2''	5:I:38:DT:H71	1.80	0.62
4:H:88:THR:HG22	5:J:186:DG:OP2	2.00	0.62
3:G:43:VAL:O	5:I:111:DA:H3'	2.00	0.62
5:I:103:DG:H2''	5:I:104:DT:C5'	2.29	0.62
5:J:263:DT:H2''	5:J:264:DT:O5'	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:67:DA:C2	5:J:227:DG:N2	2.68	0.62
5:J:185:DG:H2''	5:J:186:DG:C5'	2.14	0.62
5:I:94:DG:H2''	5:I:95:DA:C8	2.35	0.62
5:J:208:DT:H2''	5:J:209:DG:H5'	1.82	0.62
4:D:54:ILE:HG21	4:D:59:MET:HE2	1.80	0.61
4:D:88:THR:HG22	5:I:39:DG:OP1	1.99	0.61
5:J:151:DA:H2''	5:J:152:DT:O5'	2.00	0.61
5:J:225:DC:H2''	5:J:226:DT:H71	1.81	0.61
2:B:25:ASN:N	2:B:25:ASN:ND2	2.42	0.61
5:I:91:DT:H2''	5:I:92:DT:C5'	2.26	0.61
5:I:115:DA:H2''	5:I:116:DC:OP2	2.01	0.61
5:J:197:DA:H2''	5:J:198:DT:H5'	1.82	0.61
1:A:134:ARG:HH11	1:A:134:ARG:HB3	1.65	0.61
3:C:40:SER:HB3	4:D:89:ILE:HG13	1.82	0.61
5:J:152:DT:C3'	5:J:153:DA:H5''	2.30	0.61
5:J:153:DA:H2''	5:J:154:DT:C5'	2.31	0.61
5:J:282:DT:H1'	5:J:283:DG:H5''	1.83	0.61
3:C:62:ILE:C	3:C:62:ILE:HD12	2.26	0.60
5:I:8:DT:C2'	5:I:9:DC:H5''	2.31	0.60
5:I:130:DT:H2''	5:I:131:DG:H5''	1.82	0.60
3:G:29:ARG:NH1	4:H:36:SER:O	2.34	0.60
5:I:61:DA:H2''	5:I:62:DT:H5'	1.81	0.60
5:J:200:DA:H2''	5:J:201:DA:OP2	2.02	0.60
5:I:18:DG:H2''	5:I:19:DA:H8	1.67	0.60
5:I:42:DA:H2''	5:I:43:DA:C8	2.36	0.60
5:I:51:DA:H2''	5:I:52:DT:H5''	1.83	0.60
5:J:164:DG:H2''	5:J:165:DA:H5''	1.83	0.60
5:J:186:DG:H2''	5:J:187:DA:N7	2.16	0.60
5:J:155:DC:H2''	5:J:156:DC:OP2	2.02	0.60
5:J:280:DG:H1'	5:J:281:DG:H5''	1.84	0.60
5:I:26:DC:H2''	5:I:27:DA:C8	2.36	0.59
5:J:235:DC:H2''	5:J:236:DT:OP2	2.01	0.59
5:J:287:DA:H1'	5:J:288:DT:H5'	1.82	0.59
5:J:154:DT:C2'	5:J:155:DC:H5'	2.33	0.59
5:J:241:DA:H2''	5:J:242:DT:O5'	2.01	0.59
1:A:134:ARG:CB	1:A:134:ARG:HH11	2.16	0.59
5:I:92:DT:H2''	5:I:93:DT:H5'	1.85	0.59
5:I:38:DT:H1'	5:I:39:DG:H5'	1.85	0.59
5:J:175:DA:C2	5:J:176:DA:N6	2.71	0.59
5:I:41:DA:OP1	5:I:41:DA:C4'	2.50	0.59
5:J:217:DG:H1'	5:J:218:DA:H5'	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:244:DG:H1'	5:J:245:DA:C8	2.38	0.59
5:J:215:DC:H2''	5:J:216:DT:C6	2.38	0.58
5:I:10:DC:H2''	5:I:11:DA:C8	2.38	0.58
5:J:166:DT:C2'	5:J:167:DT:H5''	2.31	0.58
5:J:246:DG:H2''	5:J:247:DC:C5'	2.33	0.58
5:J:261:DA:H2''	5:J:262:DC:H5''	1.84	0.58
4:D:30:LYS:N	5:I:104:DT:OP1	2.36	0.58
5:J:183:DT:H1'	5:J:184:DT:H5'	1.84	0.58
1:A:42:ARG:HH21	5:I:68:DG:P	2.26	0.58
5:J:234:DC:H4'	5:J:235:DC:OP1	2.03	0.58
5:J:246:DG:H2''	5:J:247:DC:H5'	1.85	0.58
1:A:76:GLN:HA	1:A:76:GLN:HE21	1.68	0.58
4:D:92:ARG:HG2	4:D:92:ARG:HH11	1.69	0.57
5:I:4:DA:H2''	5:I:5:DA:C8	2.39	0.57
2:F:30:THR:OG1	2:F:32:PRO:HG2	2.04	0.57
3:G:67:GLY:HA3	4:H:49:HIS:CD2	2.39	0.57
5:I:124:DA:H2''	5:I:125:DG:H5''	1.85	0.57
2:F:64:ASN:N	2:F:64:ASN:HD22	2.02	0.57
3:C:51:LEU:HD13	4:D:73:ILE:HG21	1.87	0.57
5:I:53:DC:H1'	5:I:54:DA:C8	2.39	0.57
5:J:232:DT:H2''	5:J:233:DG:OP2	2.03	0.57
3:G:44:GLY:O	3:G:48:PRO:HD3	2.05	0.57
2:B:72:TYR:HE1	4:D:80:LEU:HD13	1.70	0.57
1:E:41:TYR:HA	5:J:290:DG:H5''	1.87	0.57
3:C:84:GLN:HG3	3:C:105:GLY:C	2.29	0.57
5:I:71:DG:C3'	5:I:72:DA:H5''	2.33	0.57
5:J:170:DA:H2''	5:J:171:DC:H5'	1.82	0.57
5:J:175:DA:H2''	5:J:176:DA:C8	2.40	0.56
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.39	0.56
1:A:96:CYS:SG	2:B:62:LEU:HD21	2.44	0.56
5:I:96:DT:H2''	5:I:97:DG:OP2	2.05	0.56
5:J:163:DA:H1'	5:J:164:DG:C5	2.41	0.56
5:J:177:DG:C2'	5:J:178:DT:H71	2.36	0.56
4:D:37:TYR:H	4:D:63:ASN:HD21	1.54	0.56
3:G:73:ASN:O	3:G:74:LYS:HB2	2.05	0.56
3:G:99:ARG:HD3	8:G:2003:HOH:O	2.04	0.56
5:I:18:DG:H2''	5:I:19:DA:O5'	2.06	0.56
5:I:113:DA:H2	5:I:114:DC:C2	2.23	0.56
5:I:90:DT:H1'	5:I:91:DT:H5''	1.87	0.56
5:I:103:DG:H2''	5:I:104:DT:H5'	1.86	0.56
5:J:186:DG:H2''	5:J:187:DA:C8	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:281:DG:H2''	5:J:282:DT:C5'	2.32	0.56
5:I:88:DC:H2''	5:I:89:DC:C6	2.41	0.56
3:C:11:ARG:HH12	5:J:264:DT:H1'	1.71	0.56
3:G:83:LEU:O	3:G:87:ILE:HG12	2.05	0.56
5:J:214:DG:H2''	5:J:215:DC:C5'	2.20	0.56
5:J:220:DT:H2'	5:J:221:DT:H71	1.87	0.56
1:E:116:ARG:HH22	1:E:123:ASP:CG	2.14	0.56
5:I:124:DA:C2'	5:I:125:DG:H5''	2.35	0.56
5:J:166:DT:H2''	5:J:167:DT:O5'	2.06	0.56
5:J:174:DA:C6	5:J:175:DA:N6	2.74	0.56
3:G:42:ARG:CD	4:H:88:THR:HB	2.36	0.55
5:I:31:DG:C3'	5:I:32:DT:H5''	2.36	0.55
5:J:259:DA:C2'	5:J:260:DC:H5''	2.37	0.55
3:C:26:PRO:O	3:C:30:VAL:HG23	2.05	0.55
2:F:84:MET:HE1	2:F:102:GLY:CA	2.36	0.55
5:I:9:DC:C3'	5:I:10:DC:H5''	2.37	0.55
5:J:291:DA:H2''	5:J:292:DT:H5'	1.88	0.55
1:A:76:GLN:HA	1:A:76:GLN:NE2	2.22	0.55
1:A:123:ASP:OD1	1:E:113:HIS:CE1	2.59	0.55
3:C:81:ARG:NH2	3:C:107:VAL:O	2.40	0.55
4:D:31:ARG:HD3	5:J:270:DA:O3'	2.05	0.55
1:A:70:LEU:O	1:A:74:ILE:HG12	2.07	0.55
5:I:2:DT:H2''	5:I:3:DC:C5'	2.37	0.55
5:I:11:DA:H1'	5:I:12:DC:H5''	1.88	0.55
4:H:41:VAL:HB	4:H:59:MET:HE1	1.88	0.55
5:I:51:DA:C2'	5:I:52:DT:H5''	2.37	0.55
5:I:127:DA:H2	5:I:128:DT:N1	2.05	0.55
1:A:48:LEU:CD1	3:G:117:PRO:HD3	2.36	0.55
1:A:58:THR:CG2	3:G:81:ARG:HG2	2.36	0.55
2:B:72:TYR:CE1	4:D:80:LEU:HD13	2.42	0.55
5:I:18:DG:H2''	5:I:19:DA:C8	2.42	0.55
5:I:127:DA:H62	5:J:167:DT:H3	1.53	0.55
5:J:246:DG:C1'	5:J:247:DC:H5''	2.36	0.55
2:F:92:ARG:HB3	2:F:92:ARG:HH11	1.68	0.55
5:I:129:DC:H2''	5:I:130:DT:C5	2.42	0.55
5:J:195:DC:H1'	5:J:196:DC:C6	2.42	0.55
5:J:201:DA:H2''	5:J:202:DA:OP2	2.06	0.55
5:J:225:DC:H2''	5:J:226:DT:C7	2.35	0.55
5:I:6:DT:H2''	5:I:7:DA:C8	2.41	0.55
5:J:157:DA:H2''	5:J:158:DC:H5'	1.88	0.55
5:J:167:DT:H2''	5:J:168:DC:C6	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:ARG:HH22	5:I:90:DT:P	2.30	0.54
3:C:55:LEU:O	3:C:59:THR:HG22	2.07	0.54
3:C:84:GLN:HA	3:C:84:GLN:HE21	1.72	0.54
5:I:8:DT:H2''	5:I:9:DC:H5''	1.87	0.54
5:I:143:DT:H2''	5:I:144:DG:OP2	2.07	0.54
5:J:153:DA:C2'	5:J:154:DT:H5''	2.37	0.54
5:J:185:DG:C3'	5:J:186:DG:H5''	2.37	0.54
5:J:191:DT:H2''	5:J:192:DG:C8	2.42	0.54
3:C:55:LEU:O	3:C:59:THR:CG2	2.56	0.54
5:I:35:DA:C8	5:I:36:DT:H72	2.43	0.54
5:J:182:DT:H2'	5:J:183:DT:H72	1.89	0.54
5:J:237:DT:H1'	5:J:238:DT:H5''	1.90	0.54
5:J:288:DT:H1'	5:J:289:DT:H5'	1.88	0.54
1:A:134:ARG:HB2	1:A:134:ARG:CZ	2.37	0.54
5:I:126:DA:C2	5:I:127:DA:C6	2.96	0.54
5:J:262:DC:C2'	5:J:263:DT:H5'	2.35	0.54
2:F:79:LYS:HD3	5:I:100:DG:OP1	2.08	0.54
5:J:163:DA:H2''	5:J:164:DG:N7	2.23	0.54
5:I:82:DA:H1'	5:I:83:DA:H5''	1.89	0.54
2:F:84:MET:HE1	2:F:102:GLY:HA2	1.90	0.53
3:G:77:ARG:HG2	5:I:131:DG:OP1	2.08	0.53
3:C:102:ILE:CG2	4:D:61:ILE:HD13	2.37	0.53
5:J:177:DG:H2''	5:J:178:DT:H71	1.90	0.53
1:A:117:VAL:O	1:A:117:VAL:CG1	2.56	0.53
5:I:67:DA:H2''	5:I:68:DG:O5'	2.09	0.53
5:I:8:DT:H2''	5:I:9:DC:C5'	2.38	0.53
5:J:230:DC:H2''	5:J:231:DA:C5'	2.37	0.53
2:F:31:GLN:N	2:F:32:PRO:HD2	2.24	0.53
1:A:48:LEU:HB3	1:A:52:ARG:HH12	1.72	0.53
4:H:38:SER:O	4:H:59:MET:HE3	2.09	0.53
5:I:113:DA:H2''	5:I:114:DC:O5'	2.08	0.53
5:J:193:DC:H2''	5:J:194:DT:H71	1.90	0.53
5:J:282:DT:H1'	5:J:283:DG:C5'	2.39	0.53
1:E:128:ARG:NH2	1:E:134:ARG:HD3	2.23	0.53
5:J:215:DC:H2''	5:J:216:DT:C5	2.44	0.53
5:J:219:DA:H2''	5:J:220:DT:H5'	1.91	0.53
5:I:113:DA:H2	5:I:114:DC:N3	2.06	0.52
3:G:76:THR:HG22	5:I:131:DG:OP2	2.08	0.52
5:I:55:DA:C2'	5:I:56:DA:H5'	2.18	0.52
5:J:193:DC:H4'	5:J:194:DT:OP1	2.09	0.52
1:A:65:LEU:HB3	1:A:66:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:92:ARG:HG2	4:D:92:ARG:NH1	2.24	0.52
5:I:94:DG:OP1	5:I:94:DG:H4'	2.09	0.52
5:J:153:DA:H2''	5:J:154:DT:H5''	1.91	0.52
5:J:198:DT:C2'	5:J:199:DC:H5'	2.34	0.52
5:J:271:DG:H2''	5:J:272:DA:C8	2.44	0.52
4:D:80:LEU:HD21	4:D:96:THR:HG21	1.90	0.52
1:E:65:LEU:HB3	1:E:66:PRO:HD3	1.92	0.52
1:E:116:ARG:NH1	1:E:118:THR:O	2.43	0.52
1:E:128:ARG:HD2	1:E:133:GLU:OE1	2.08	0.52
5:I:64:DT:H1'	5:I:65:DT:H5''	1.92	0.52
1:E:37:LYS:NZ	5:J:291:DA:C4'	2.72	0.52
1:E:60:LEU:HD13	1:E:93:GLN:CD	2.34	0.52
8:E:2018:HOH:O	2:F:59:LYS:HE3	2.09	0.52
5:I:95:DA:H2''	5:I:96:DT:OP2	2.09	0.52
4:D:80:LEU:HD21	4:D:96:THR:CG2	2.40	0.52
5:I:130:DT:C2'	5:I:131:DG:H5''	2.40	0.52
5:J:170:DA:H1'	5:J:171:DC:H5''	1.91	0.52
4:H:33:ARG:HD3	5:J:174:DA:H4'	1.92	0.52
5:J:150:DA:H2''	5:J:151:DA:OP2	2.10	0.52
3:C:62:ILE:HD11	4:D:62:MET:SD	2.49	0.52
1:E:37:LYS:HZ1	5:J:291:DA:C4'	2.23	0.52
5:J:241:DA:H4'	5:J:241:DA:OP1	2.10	0.52
1:E:68:GLN:HG3	1:E:89:VAL:HG11	1.92	0.51
3:G:20:ARG:O	4:H:120:LYS:HG2	2.10	0.51
5:I:135:DG:H1'	5:I:136:DT:C5'	2.37	0.51
5:J:197:DA:H2''	5:J:198:DT:C5'	2.40	0.51
1:A:76:GLN:HE21	1:A:76:GLN:CA	2.22	0.51
3:G:40:SER:HB3	4:H:89:ILE:HG13	1.93	0.51
5:I:20:DT:H2''	5:I:21:DT:OP2	2.10	0.51
5:I:98:DG:H2''	5:I:99:DA:C8	2.44	0.51
5:J:156:DC:H2''	5:J:157:DA:C5'	2.33	0.51
5:J:220:DT:C2'	5:J:221:DT:H71	2.40	0.51
3:C:62:ILE:HG12	4:D:62:MET:HE1	1.92	0.51
5:I:5:DA:C2'	5:I:6:DT:O5'	2.57	0.51
5:I:24:DA:H2''	5:I:25:DC:C6	2.45	0.51
5:J:174:DA:C2	5:J:175:DA:N7	2.79	0.51
3:G:42:ARG:HG3	4:H:88:THR:HB	1.91	0.51
5:I:2:DT:N1	5:I:3:DC:H5	2.08	0.51
2:B:89:ALA:O	2:B:92:ARG:HB2	2.09	0.51
3:C:40:SER:CB	4:D:89:ILE:HG13	2.39	0.51
1:E:61:LEU:HD12	2:F:37:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:THR:HA	2:F:45:ARG:HB3	1.92	0.51
5:J:169:DT:C4	5:J:170:DA:N6	2.78	0.51
5:J:218:DA:H1'	5:J:219:DA:C8	2.46	0.51
5:J:233:DG:H2''	5:J:234:DC:O5'	2.11	0.51
2:B:35:ARG:HG3	2:B:46:ILE:HD12	1.91	0.51
3:G:118:LYS:HD2	3:G:118:LYS:O	2.11	0.51
5:I:135:DG:C1'	5:I:136:DT:H5''	2.38	0.51
5:J:205:DG:H1'	5:J:206:DC:H5''	1.91	0.51
5:I:83:DA:H2''	5:I:84:DC:H5''	1.91	0.51
5:J:161:DG:H2''	5:J:162:DC:OP2	2.10	0.51
5:J:215:DC:H2''	5:J:216:DT:H71	1.91	0.51
5:J:195:DC:H1'	5:J:196:DC:C5	2.46	0.51
5:J:284:DG:H2''	5:J:285:DA:O5'	2.11	0.51
5:J:215:DC:C2'	5:J:216:DT:H71	2.41	0.50
3:G:50:TYR:OH	4:H:111:VAL:HA	2.11	0.50
5:I:19:DA:H4'	5:I:19:DA:OP1	2.11	0.50
5:I:74:DT:H2'	5:I:75:DT:H71	1.92	0.50
1:A:120:MET:C	2:B:50:ILE:HD11	2.35	0.50
1:E:65:LEU:HD23	5:I:90:DT:OP2	2.12	0.50
5:I:41:DA:H2''	5:I:42:DA:H8	1.76	0.50
5:I:126:DA:C2	5:I:127:DA:N7	2.80	0.50
3:C:90:ASP:O	3:C:91:GLU:C	2.52	0.50
5:I:11:DA:C6	5:J:283:DG:N2	2.79	0.50
5:I:33:DG:H2''	5:I:34:DT:O5'	2.11	0.50
5:I:113:DA:C2	5:I:114:DC:C4	2.99	0.50
3:C:31:HIS:NE2	3:C:35:ARG:NH1	2.58	0.50
3:G:81:ARG:O	3:G:85:LEU:HG	2.12	0.50
5:J:253:DC:H2''	5:J:254:DC:O5'	2.12	0.50
5:J:211:DT:H6	5:J:211:DT:H5'	1.76	0.50
1:A:63:ARG:C	1:A:66:PRO:HD2	2.37	0.50
3:G:71:ARG:O	3:G:74:LYS:N	2.40	0.50
5:I:61:DA:C2'	5:I:62:DT:H5''	2.40	0.50
5:J:205:DG:H2''	5:J:206:DC:H5''	1.93	0.50
1:A:63:ARG:HE	1:A:66:PRO:HG2	1.76	0.50
5:J:205:DG:C2'	5:J:206:DC:H5''	2.42	0.50
3:C:84:GLN:HA	3:C:84:GLN:NE2	2.27	0.50
5:I:111:DA:C2	5:I:112:DT:C2	3.00	0.50
4:H:36:SER:CB	4:H:63:ASN:HD21	2.15	0.49
4:H:38:SER:HA	4:H:59:MET:HE3	1.93	0.49
5:J:205:DG:H2''	5:J:206:DC:C5'	2.41	0.49
1:A:40:ARG:HH11	1:A:40:ARG:HG3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:HG21	5:J:229:DA:H3'	1.93	0.49
2:B:49:LEU:HB3	8:B:2004:HOH:O	2.11	0.49
1:E:41:TYR:OH	5:I:7:DA:H5'	2.11	0.49
4:H:76:GLU:HA	4:H:79:ARG:NH1	2.26	0.49
3:C:42:ARG:O	4:D:88:THR:HA	2.12	0.49
3:G:24:GLN:HE21	3:G:24:GLN:CA	2.13	0.49
5:J:223:DA:H2''	5:J:224:DG:C8	2.47	0.49
5:J:236:DT:H2''	5:J:237:DT:H72	1.94	0.49
5:I:8:DT:C1'	5:I:9:DC:H5''	2.42	0.49
5:J:153:DA:C1'	5:J:154:DT:H5''	2.41	0.49
3:C:29:ARG:NH2	4:D:36:SER:O	2.46	0.49
1:A:96:CYS:SG	2:B:62:LEU:CD2	3.01	0.49
3:G:45:ALA:O	3:G:48:PRO:HD2	2.12	0.49
5:I:110:DA:H2''	5:I:111:DA:OP2	2.13	0.49
5:J:175:DA:C2	5:J:176:DA:C6	3.01	0.49
3:G:50:TYR:OH	4:H:95:GLN:HG3	2.12	0.49
5:I:48:DT:H2''	5:I:49:DC:C6	2.48	0.49
3:C:62:ILE:HD13	3:C:83:LEU:CD2	2.43	0.48
5:I:105:DT:O4	5:J:187:DA:N6	2.46	0.48
5:I:57:DA:N6	5:J:235:DC:N4	2.61	0.48
5:J:170:DA:C1'	5:J:171:DC:H5''	2.42	0.48
1:A:84:PHE:CD1	2:B:81:VAL:HB	2.48	0.48
5:I:42:DA:H2''	5:I:43:DA:H8	1.77	0.48
5:I:43:DA:C1'	5:I:44:DC:H5''	2.43	0.48
5:I:108:DC:H2''	5:I:109:DA:C8	2.47	0.48
5:I:124:DA:C1'	5:I:125:DG:H5''	2.42	0.48
2:B:46:ILE:O	5:J:227:DG:H3'	2.14	0.48
2:B:84:MET:HE3	2:B:88:TYR:CZ	2.48	0.48
2:F:92:ARG:HB3	2:F:92:ARG:CZ	2.43	0.48
5:J:249:DG:H2'	5:J:250:DT:H71	1.95	0.48
5:I:1:DA:C2	5:I:2:DT:N3	2.82	0.48
5:I:28:DA:C2'	5:I:29:DA:C8	2.96	0.48
5:J:259:DA:H2''	5:J:260:DC:C5'	2.41	0.48
5:J:265:DT:H1'	5:J:266:DT:H5'	1.94	0.48
1:E:116:ARG:NH2	1:E:123:ASP:OD1	2.42	0.48
5:I:102:DA:H2''	5:I:103:DG:OP2	2.13	0.48
2:B:75:HIS:HD2	4:D:96:THR:OG1	1.97	0.48
5:I:103:DG:H1'	5:I:104:DT:H5''	1.96	0.48
1:A:99:TYR:OH	1:A:133:GLU:OE1	2.32	0.47
1:A:123:ASP:OD1	1:E:113:HIS:HE1	1.97	0.47
5:I:25:DC:H4'	5:I:25:DC:OP1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:73:DA:H2''	5:I:74:DT:H5'	1.94	0.47
1:A:48:LEU:HB3	1:A:52:ARG:NH1	2.29	0.47
3:C:32:ARG:NH1	5:I:29:DA:OP1	2.43	0.47
2:F:84:MET:HE3	2:F:88:TYR:CZ	2.50	0.47
5:I:137:DG:H2''	5:I:138:DG:C8	2.50	0.47
1:A:48:LEU:HD21	2:B:44:LYS:HD2	1.95	0.47
2:B:51:TYR:O	2:B:55:ARG:HG3	2.15	0.47
5:I:91:DT:C2'	5:I:92:DT:H5'	2.28	0.47
5:J:206:DC:H2''	5:J:207:DA:H8	1.73	0.47
1:A:63:ARG:HB2	1:A:66:PRO:HG2	1.96	0.47
3:C:81:ARG:O	3:C:81:ARG:HG3	2.11	0.47
5:I:75:DT:H2''	5:I:76:DC:OP2	2.13	0.47
5:J:209:DG:C8	5:J:210:DT:H72	2.49	0.47
4:D:48:VAL:HG23	4:D:49:HIS:ND1	2.30	0.47
1:E:37:LYS:HZ1	5:J:291:DA:H4'	1.74	0.47
5:J:159:DC:H2''	5:J:160:DT:O5'	2.15	0.47
5:J:221:DT:H1'	5:J:222:DC:H5'	1.96	0.47
1:E:37:LYS:HE2	1:E:39:HIS:HA	1.97	0.47
5:I:43:DA:C2'	5:I:44:DC:H5''	2.44	0.47
1:E:85:GLN:O	1:E:86:SER:C	2.56	0.47
5:I:83:DA:C2'	5:I:84:DC:H5''	2.45	0.47
5:I:127:DA:C1'	5:I:128:DT:H5''	2.45	0.47
2:F:78:ARG:NH1	2:F:82:THR:HG23	2.30	0.46
5:I:53:DC:H4'	5:I:54:DA:OP1	2.15	0.46
5:I:129:DC:H2''	5:I:130:DT:H72	1.97	0.46
5:J:203:DA:H1'	5:J:204:DG:H5'	1.97	0.46
5:J:264:DT:H2'	5:J:265:DT:H72	1.96	0.46
3:C:26:PRO:HD3	4:D:40:TYR:CG	2.48	0.46
5:I:88:DC:N4	5:J:204:DG:O6	2.49	0.46
3:C:42:ARG:CG	4:D:88:THR:HB	2.44	0.46
3:G:76:THR:HG21	5:I:130:DT:H3'	1.95	0.46
4:H:89:ILE:O	4:H:89:ILE:HG22	2.15	0.46
5:J:193:DC:H2''	5:J:194:DT:C7	2.45	0.46
5:I:49:DC:H2''	5:I:50:DC:OP2	2.15	0.46
5:J:235:DC:H2''	5:J:236:DT:H72	1.96	0.46
5:J:268:DG:H2''	5:J:269:DT:C6	2.49	0.46
5:I:125:DG:N2	5:J:169:DT:O2	2.49	0.46
5:J:209:DG:C2'	5:J:210:DT:H5'	2.44	0.46
5:J:209:DG:H2'	5:J:210:DT:H72	1.98	0.46
3:C:62:ILE:CG1	4:D:62:MET:HE1	2.46	0.46
4:H:55:SER:OG	4:H:56:SER:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:251:DT:H2''	5:J:252:DT:O5'	2.15	0.46
1:E:120:MET:HG2	2:F:47:SER:HB2	1.98	0.46
5:I:41:DA:OP1	5:I:41:DA:O4'	2.33	0.46
1:E:37:LYS:CE	1:E:39:HIS:HA	2.45	0.46
2:F:31:GLN:O	2:F:32:PRO:C	2.59	0.46
4:H:68:ASP:O	4:H:72:ARG:HG3	2.16	0.46
5:I:73:DA:H1'	5:I:74:DT:H5''	1.97	0.46
5:I:93:DT:H2''	5:I:94:DG:O5'	2.16	0.46
5:I:106:DT:H2''	5:I:107:DC:O5'	2.15	0.46
5:J:179:DG:C1'	5:J:180:DT:H5''	2.46	0.46
5:I:19:DA:H2'	5:I:20:DT:C6	2.51	0.45
5:J:173:DA:C2	5:J:174:DA:C2	3.04	0.45
5:J:175:DA:H2''	5:J:176:DA:O5'	2.16	0.45
5:J:251:DT:H2'	5:J:252:DT:C7	2.40	0.45
5:I:84:DC:C5	5:I:85:DA:N6	2.85	0.45
5:I:121:DG:H2''	5:I:122:DG:OP2	2.16	0.45
5:J:244:DG:C2	5:J:245:DA:C2	3.05	0.45
5:J:172:DC:H2''	5:J:173:DA:N7	2.31	0.45
5:I:10:DC:H1'	5:I:11:DA:N7	2.32	0.45
5:I:58:DG:H2''	5:I:59:DG:C8	2.50	0.45
5:J:148:DT:H2''	5:J:149:DC:H5'	1.98	0.45
1:E:73:GLU:OE1	2:F:25:ASN:HB2	2.16	0.45
4:H:106:LEU:HD12	4:H:106:LEU:HA	1.85	0.45
5:I:62:DT:C2'	5:I:63:DG:C5'	2.88	0.45
3:G:15:LYS:HE2	5:J:178:DT:H5''	1.99	0.45
5:I:57:DA:H2''	5:I:58:DG:N7	2.29	0.45
5:J:209:DG:H5'	5:J:209:DG:H8	1.81	0.45
5:J:284:DG:H2''	5:J:285:DA:H8	1.81	0.45
1:A:85:GLN:HG3	2:B:82:THR:HA	1.99	0.45
4:D:31:ARG:O	4:D:32:SER:HB2	2.17	0.45
5:I:131:DG:H2''	5:I:132:DC:C6	2.52	0.45
5:J:197:DA:H1'	5:J:198:DT:H5''	1.99	0.45
2:B:31:GLN:N	2:B:32:PRO:CD	2.78	0.45
3:G:67:GLY:O	3:G:70:ALA:N	2.49	0.45
4:H:102:LEU:HA	4:H:103:PRO:HD3	1.83	0.45
5:I:130:DT:H2''	5:I:131:DG:C5'	2.46	0.45
3:C:57:TYR:HB2	4:D:113:GLU:OE2	2.17	0.45
4:H:78:SER:HA	4:H:89:ILE:HD11	1.99	0.45
5:I:34:DT:H2''	5:I:35:DA:H5'	1.99	0.45
5:J:152:DT:H2'	5:J:153:DA:C8	2.52	0.45
4:D:31:ARG:CG	5:J:270:DA:H4'	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:116:DC:H2'	5:I:117:DT:C7	2.46	0.44
3:C:102:ILE:HB	8:C:2008:HOH:O	2.16	0.44
2:F:51:TYR:O	2:F:55:ARG:HG3	2.17	0.44
3:G:26:PRO:HD3	4:H:40:TYR:CE1	2.52	0.44
5:I:34:DT:H2''	5:I:35:DA:H8	1.82	0.44
5:J:165:DA:C8	5:J:166:DT:H72	2.51	0.44
5:I:37:DT:H4'	5:I:38:DT:OP1	2.18	0.44
5:I:127:DA:H1'	5:I:128:DT:H5''	1.99	0.44
5:I:132:DC:H2''	5:I:133:DA:H5''	1.95	0.44
5:J:215:DC:C2'	5:J:216:DT:C7	2.96	0.44
5:J:243:DG:H2''	5:J:244:DG:OP2	2.17	0.44
1:A:50:GLU:OE2	2:B:35:ARG:NH2	2.50	0.44
2:B:56:GLY:O	2:B:60:VAL:HG23	2.18	0.44
3:G:73:ASN:O	3:G:73:ASN:ND2	2.50	0.44
5:J:260:DC:C2'	5:J:261:DA:C8	3.00	0.44
5:J:282:DT:C2'	5:J:283:DG:H5'	2.42	0.44
3:C:114:VAL:O	3:C:114:VAL:HG12	2.18	0.44
2:B:78:ARG:HB2	2:B:78:ARG:NH1	2.29	0.44
1:E:116:ARG:HD2	1:E:120:MET:HE3	1.98	0.44
5:J:163:DA:H1'	5:J:164:DG:C4	2.52	0.44
2:B:75:HIS:CD2	4:D:96:THR:OG1	2.71	0.44
3:C:62:ILE:HD13	3:C:83:LEU:HD22	1.99	0.44
5:I:64:DT:H2''	5:I:65:DT:H5'	2.00	0.44
3:G:63:LEU:HD22	4:H:45:LEU:HD13	2.00	0.44
5:J:286:DT:H1'	5:J:287:DA:C8	2.53	0.44
1:A:46:VAL:O	1:A:49:ARG:HB3	2.18	0.43
4:D:90:THR:OG1	4:D:92:ARG:HB3	2.18	0.43
1:E:48:LEU:HD21	2:F:44:LYS:HD2	2.00	0.43
5:I:125:DG:N2	5:J:169:DT:C2	2.86	0.43
5:J:236:DT:C2'	5:J:237:DT:H72	2.48	0.43
5:J:270:DA:C2'	5:J:271:DG:O5'	2.60	0.43
3:C:84:GLN:HG3	3:C:105:GLY:HA3	2.00	0.43
5:I:25:DC:H2''	5:I:26:DC:O5'	2.17	0.43
5:I:116:DC:H2'	5:I:117:DT:H72	2.00	0.43
5:J:229:DA:H1'	5:J:230:DC:H5''	1.99	0.43
5:J:236:DT:H2''	5:J:237:DT:C7	2.48	0.43
5:J:246:DG:C2'	5:J:247:DC:H5''	2.48	0.43
5:J:262:DC:H1'	5:J:263:DT:C5'	2.48	0.43
5:I:94:DG:C6	5:I:95:DA:N6	2.86	0.43
5:J:235:DC:C2'	5:J:236:DT:H72	2.48	0.43
5:J:287:DA:C2	5:J:288:DT:C2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:86:ARG:N	4:D:86:ARG:HD2	2.32	0.43
3:G:93:LEU:HD23	4:H:106:LEU:HD21	2.00	0.43
5:J:153:DA:H2''	5:J:154:DT:H5'	1.99	0.43
5:J:188:DA:C2'	5:J:189:DA:C5'	2.88	0.43
5:J:264:DT:H2''	5:J:265:DT:H5''	1.97	0.43
5:J:277:DG:H2''	5:J:278:DC:C5'	2.48	0.43
3:C:62:ILE:HD11	4:D:62:MET:CE	2.49	0.43
5:I:142:DT:H2''	5:I:143:DT:O5'	2.17	0.43
5:J:231:DA:H1'	5:J:232:DT:H5'	2.00	0.43
5:J:234:DC:H2''	5:J:235:DC:H5	1.82	0.43
3:C:77:ARG:HA	4:D:53:GLY:O	2.18	0.43
3:C:84:GLN:CG	3:C:105:GLY:HA3	2.49	0.43
5:I:28:DA:H2''	5:I:29:DA:H8	1.78	0.43
5:J:264:DT:C2'	5:J:265:DT:C5'	2.91	0.43
1:A:43:PRO:HA	5:J:229:DA:H5'	2.00	0.43
2:B:26:ILE:HG23	2:B:27:GLN:N	2.34	0.43
3:G:80:PRO:HB2	3:G:104:GLN:O	2.18	0.43
5:J:215:DC:H2''	5:J:216:DT:C7	2.47	0.43
3:C:31:HIS:CE1	3:C:35:ARG:NH1	2.87	0.43
1:E:39:HIS:ND1	1:E:40:ARG:N	2.66	0.43
1:A:111:ALA:O	1:A:112:ILE:C	2.62	0.43
1:A:134:ARG:O	1:A:135:ALA:C	2.62	0.43
1:E:97:GLU:HG2	2:F:37:LEU:HD21	1.99	0.43
5:J:211:DT:H2''	5:J:212:DC:O5'	2.19	0.43
5:J:255:DA:H2''	5:J:256:DA:OP2	2.19	0.43
1:A:119:ILE:HD13	2:B:43:VAL:HG21	2.00	0.42
3:C:58:LEU:HD11	4:D:102:LEU:HD11	2.00	0.42
3:G:40:SER:CB	4:H:89:ILE:HG13	2.49	0.42
5:I:41:DA:C2'	5:I:42:DA:H8	2.32	0.42
5:J:208:DT:H2''	5:J:209:DG:H8	1.84	0.42
2:B:64:ASN:HA	2:B:67:ARG:NH1	2.34	0.42
3:G:37:GLY:HA3	3:G:39:TYR:CE2	2.54	0.42
5:J:211:DT:H5'	5:J:211:DT:C6	2.54	0.42
5:J:242:DT:H2''	5:J:243:DG:OP2	2.20	0.42
5:J:264:DT:H2'	5:J:265:DT:C7	2.48	0.42
3:C:84:GLN:HG3	3:C:105:GLY:CA	2.48	0.42
3:G:77:ARG:O	3:G:77:ARG:HG3	2.18	0.42
4:H:48:VAL:C	4:H:49:HIS:ND1	2.78	0.42
5:I:100:DG:H2'	5:I:100:DG:O5'	2.19	0.42
5:J:256:DA:H2''	5:J:257:DA:OP2	2.19	0.42
5:J:274:DT:H1'	5:J:275:DC:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:26:PRO:HD3	4:H:40:TYR:CG	2.55	0.42
5:J:179:DG:H1'	5:J:180:DT:H5''	2.02	0.42
1:A:118:THR:HA	2:B:45:ARG:O	2.20	0.42
2:B:62:LEU:O	2:B:63:GLU:C	2.61	0.42
1:E:106:ASP:O	1:E:107:THR:C	2.61	0.42
4:H:40:TYR:O	4:H:41:VAL:C	2.62	0.42
5:I:113:DA:C2	5:I:114:DC:N3	2.86	0.42
5:J:209:DG:H1'	5:J:210:DT:H5'	2.00	0.42
5:J:212:DC:H2''	5:J:213:DA:OP2	2.20	0.42
5:J:235:DC:H2''	5:J:236:DT:C7	2.50	0.42
4:D:106:LEU:HD12	4:D:106:LEU:HA	1.84	0.42
4:H:111:VAL:O	4:H:112:SER:C	2.62	0.42
5:I:43:DA:H2''	5:I:44:DC:C5'	2.50	0.42
1:A:43:PRO:HA	5:J:229:DA:C5'	2.50	0.42
1:A:61:LEU:H	1:A:97:GLU:CD	2.28	0.42
1:A:89:VAL:C	1:A:90:MET:HE2	2.45	0.42
2:F:64:ASN:N	2:F:64:ASN:ND2	2.67	0.42
5:I:62:DT:H1'	5:I:63:DG:H5''	2.02	0.42
5:J:231:DA:H2''	5:J:232:DT:O5'	2.20	0.42
3:C:30:VAL:HG13	4:D:70:PHE:CE1	2.48	0.42
3:C:78:ILE:N	4:D:53:GLY:O	2.43	0.42
4:H:46:LYS:HD3	4:H:46:LYS:HA	1.51	0.42
5:I:54:DA:H2''	5:I:55:DA:O5'	2.19	0.42
3:C:11:ARG:HH12	5:J:264:DT:C1'	2.32	0.42
4:D:54:ILE:CG2	4:D:59:MET:HE2	2.49	0.42
2:F:35:ARG:O	2:F:39:ARG:HG2	2.20	0.42
4:H:55:SER:HB3	4:H:58:ALA:HB3	2.02	0.42
5:I:114:DC:H4'	5:I:114:DC:OP1	2.20	0.42
5:I:123:DT:H2'	8:I:2002:HOH:O	2.19	0.42
5:J:217:DG:H2''	5:J:218:DA:H5'	2.01	0.42
4:D:84:ASN:O	4:D:86:ARG:HD2	2.19	0.41
5:I:74:DT:H2''	5:I:75:DT:O5'	2.19	0.41
5:J:238:DT:H6	5:J:238:DT:H5'	1.84	0.41
1:E:113:HIS:C	1:E:115:LYS:H	2.27	0.41
1:A:48:LEU:HD11	3:G:117:PRO:HD3	2.02	0.41
1:A:85:GLN:HA	5:I:49:DC:OP1	2.20	0.41
5:I:21:DT:H1'	5:I:22:DC:H5'	2.03	0.41
3:G:77:ARG:NH1	5:I:130:DT:H4'	2.36	0.41
4:H:34:LYS:HB2	5:I:123:DT:OP1	2.21	0.41
1:E:51:ILE:O	1:E:55:GLN:HG3	2.20	0.41
3:G:67:GLY:O	3:G:70:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:86:DT:C4	5:I:87:DG:C6	3.09	0.41
5:I:116:DC:C6	5:I:117:DT:H72	2.56	0.41
1:A:46:VAL:HG13	1:A:49:ARG:HE	1.86	0.41
4:D:54:ILE:HG23	4:D:54:ILE:O	2.20	0.41
1:E:60:LEU:HD13	1:E:93:GLN:CG	2.50	0.41
1:E:96:CYS:O	1:E:99:TYR:HB3	2.21	0.41
5:I:89:DC:H2''	5:I:90:DT:C7	2.47	0.41
5:J:167:DT:H2''	5:J:168:DC:C5	2.55	0.41
5:J:199:DC:H2''	5:J:200:DA:C8	2.55	0.41
1:E:78:PHE:CE2	2:F:67:ARG:HB2	2.56	0.41
5:I:19:DA:H2''	5:I:20:DT:C5'	2.50	0.41
5:I:32:DT:C2'	5:I:33:DG:H5'	2.45	0.41
5:J:193:DC:H1'	5:J:194:DT:C5	2.56	0.41
5:J:196:DC:H2''	5:J:197:DA:OP2	2.20	0.41
1:A:59:GLU:O	1:A:59:GLU:OE2	2.39	0.41
1:A:134:ARG:O	1:A:135:ALA:OXT	2.38	0.41
2:F:19:ARG:HG2	2:F:20:LYS:N	2.36	0.41
5:I:106:DT:H2''	5:I:107:DC:C6	2.46	0.41
5:J:283:DG:H1'	5:J:284:DG:N7	2.36	0.41
1:A:82:LEU:C	1:A:83:ARG:HG3	2.46	0.41
3:C:17:ARG:HA	3:C:20:ARG:HH11	1.86	0.41
4:D:40:TYR:O	4:D:41:VAL:C	2.63	0.41
1:E:42:ARG:HB3	5:J:215:DC:OP1	2.21	0.41
1:E:108:ASN:HB2	2:F:43:VAL:HG22	2.03	0.41
3:G:42:ARG:CG	4:H:88:THR:HB	2.50	0.41
4:H:36:SER:OG	4:H:37:TYR:N	2.54	0.41
5:I:47:DC:N4	5:J:245:DA:C6	2.89	0.41
5:I:113:DA:C2	5:I:114:DC:C2	3.07	0.41
5:J:239:DT:H2''	5:J:240:DG:OP2	2.21	0.41
5:J:275:DC:H2'	5:J:276:DT:C5	2.55	0.41
2:B:33:ALA:HA	2:B:36:ARG:CZ	2.51	0.41
2:B:84:MET:SD	2:B:101:GLY:HA3	2.61	0.41
4:D:31:ARG:NE	4:D:31:ARG:HA	2.36	0.41
5:I:91:DT:H5'	5:I:91:DT:H6	1.86	0.41
5:I:116:DC:C2'	5:I:117:DT:C7	2.99	0.41
1:A:73:GLU:OE2	2:B:25:ASN:HB2	2.21	0.40
1:A:114:ALA:O	1:A:115:LYS:HB2	2.22	0.40
5:I:80:DT:H2''	5:I:81:DG:OP2	2.21	0.40
5:I:41:DA:H2''	5:I:42:DA:O5'	2.21	0.40
5:I:107:DC:H4'	5:I:107:DC:OP1	2.22	0.40
3:C:54:VAL:O	3:C:55:LEU:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:85:LEU:HD23	3:G:108:LEU:CD2	2.51	0.40
4:H:60:GLY:O	4:H:61:ILE:C	2.65	0.40
5:I:27:DA:H2''	5:I:28:DA:O5'	2.22	0.40
5:I:60:DC:H2''	5:I:61:DA:C8	2.56	0.40
5:J:195:DC:H2'	5:J:195:DC:O5'	2.22	0.40
3:G:108:LEU:HD23	3:G:108:LEU:HA	1.86	0.40
4:H:37:TYR:HA	4:H:40:TYR:HD2	1.86	0.40
4:H:80:LEU:HD11	4:H:96:THR:CG2	2.52	0.40
5:I:41:DA:OP1	5:I:41:DA:H4'	2.19	0.40
5:I:126:DA:C2	5:I:127:DA:N6	2.90	0.40
5:I:2:DT:C2	5:I:3:DC:C5	3.09	0.40
5:I:127:DA:C2	5:I:128:DT:N1	2.89	0.40
5:I:132:DC:C2'	5:I:133:DA:H5''	2.51	0.40
5:J:285:DA:C2'	5:J:286:DT:H5'	2.27	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	96/139 (69%)	87 (91%)	8 (8%)	1 (1%)	12	32
1	E	97/139 (70%)	89 (92%)	8 (8%)	0	100	100
2	B	76/106 (72%)	71 (93%)	5 (7%)	0	100	100
2	F	82/106 (77%)	79 (96%)	3 (4%)	0	100	100
3	C	106/133 (80%)	103 (97%)	3 (3%)	0	100	100
3	G	102/133 (77%)	89 (87%)	12 (12%)	1 (1%)	12	32
4	D	93/129 (72%)	85 (91%)	6 (6%)	2 (2%)	5	14
4	H	91/129 (70%)	81 (89%)	7 (8%)	3 (3%)	3	7
All	All	743/1014 (73%)	684 (92%)	52 (7%)	7 (1%)	14	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	104	GLY
3	G	113	ALA
4	H	104	GLY
4	H	55	SER
4	D	50	PRO
4	H	123	SER
1	A	117	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/113 (75%)	79 (93%)	6 (7%)	13	33
1	E	86/113 (76%)	82 (95%)	4 (5%)	23	51
2	B	63/81 (78%)	61 (97%)	2 (3%)	34	64
2	F	69/81 (85%)	66 (96%)	3 (4%)	26	54
3	C	85/102 (83%)	79 (93%)	6 (7%)	13	33
3	G	83/102 (81%)	79 (95%)	4 (5%)	23	50
4	D	81/107 (76%)	73 (90%)	8 (10%)	7	19
4	H	79/107 (74%)	77 (98%)	2 (2%)	42	71
All	All	631/806 (78%)	596 (94%)	35 (6%)	19	45

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	A	64	LYS
1	A	76	GLN
1	A	120	MET
1	A	121	PRO
1	A	129	ARG
2	B	25	ASN

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Mol	Chain	Res	Type
2	B	78	ARG
3	C	29	ARG
3	C	59	THR
3	C	62	ILE
3	C	81	ARG
3	C	84	GLN
3	C	91	GLU
4	D	33	ARG
4	D	34	LYS
4	D	39	ILE
4	D	50	PRO
4	D	63	ASN
4	D	71	GLU
4	D	86	ARG
4	D	118	VAL
1	E	79	LYS
1	E	122	LYS
1	E	129	ARG
1	E	134	ARG
2	F	21	VAL
2	F	57	VAL
2	F	92	ARG
3	G	81	ARG
3	G	95	LYS
3	G	99	ARG
3	G	114	VAL
4	H	63	ASN
4	H	105	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	113	HIS
2	B	27	GLN
2	B	31	GLN
2	B	64	ASN
2	B	75	HIS
2	B	93	GLN
3	C	24	GLN
3	C	84	GLN
3	C	94	ASN

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Mol	Chain	Res	Type
4	D	63	ASN
4	D	82	HIS
4	D	84	ASN
1	E	113	HIS
2	F	31	GLN
2	F	64	ASN
2	F	75	HIS
2	F	93	GLN
3	G	24	GLN
3	G	73	ASN
3	G	94	ASN
4	H	47	GLN
4	H	63	ASN
4	H	82	HIS
4	H	95	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 17 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	98/139 (70%)	-0.18	2 (2%) 65 62	36, 72, 99, 126	0
1	E	99/139 (71%)	-0.44	0 100 100	35, 53, 82, 118	0
2	B	78/106 (73%)	-0.18	1 (1%) 75 73	48, 67, 95, 110	0
2	F	84/106 (79%)	-0.40	0 100 100	30, 48, 65, 95	0
3	C	108/133 (81%)	-0.16	1 (0%) 81 80	33, 58, 93, 147	0
3	G	104/133 (78%)	-0.09	2 (1%) 66 63	47, 66, 102, 119	0
4	D	95/129 (73%)	-0.23	2 (2%) 63 61	29, 62, 94, 151	0
4	H	93/129 (72%)	-0.17	1 (1%) 78 76	43, 64, 108, 123	0
5	I	145/146 (99%)	0.51	0 100 100	55, 129, 159, 173	0
5	J	145/146 (99%)	0.45	1 (0%) 84 83	62, 126, 162, 171	0
All	All	1049/1306 (80%)	-0.03	10 (0%) 79 78	29, 69, 149, 173	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	124	ALA	3.6
3	C	11	ARG	2.8
1	A	135	ALA	2.6
4	H	124	ALA	2.6
3	G	73	ASN	2.5
2	B	102	GLY	2.4
5	J	187	DA	2.3
1	A	38	PRO	2.3
4	D	30	LYS	2.1
3	G	41	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MN	I	1001	1/1	0.70	0.12	161,161,161,161	0
7	MN	I	1005	1/1	0.78	0.10	138,138,138,138	0
7	MN	J	1007	1/1	0.80	0.07	197,197,197,197	0
7	MN	J	1003	1/1	0.83	0.10	201,201,201,201	0
7	MN	J	1005	1/1	0.86	0.13	138,138,138,138	0
7	MN	J	1004	1/1	0.89	0.07	140,140,140,140	0
7	MN	J	1001	1/1	0.89	0.07	142,142,142,142	0
7	MN	I	1004	1/1	0.89	0.09	120,120,120,120	0
7	MN	I	1002	1/1	0.92	0.14	112,112,112,112	0
7	MN	I	1003	1/1	0.93	0.07	134,134,134,134	0
6	CL	A	1001	1/1	0.94	0.07	80,80,80,80	0
6	CL	G	1001	1/1	0.96	0.06	81,81,81,81	0
7	MN	J	1002	1/1	0.96	0.12	100,100,100,100	0
7	MN	J	1006	1/1	0.96	0.04	127,127,127,127	0
6	CL	C	1001	1/1	0.96	0.07	65,65,65,65	0
6	CL	E	1001	1/1	0.97	0.09	63,63,63,63	0
7	MN	E	1002	1/1	0.97	0.16	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.