



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:08 AM UTC

PDB ID : 7COW / pdb_00007cow
Title : 353 bp di-nucleosome harboring cohesive DNA termini with linker histone H1.0
Authors : Adhireksan, Z.; Sharma, D.; Lee, P.L.; Davey, C.A.
Deposited on : 2020-08-05
Resolution : 2.86 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

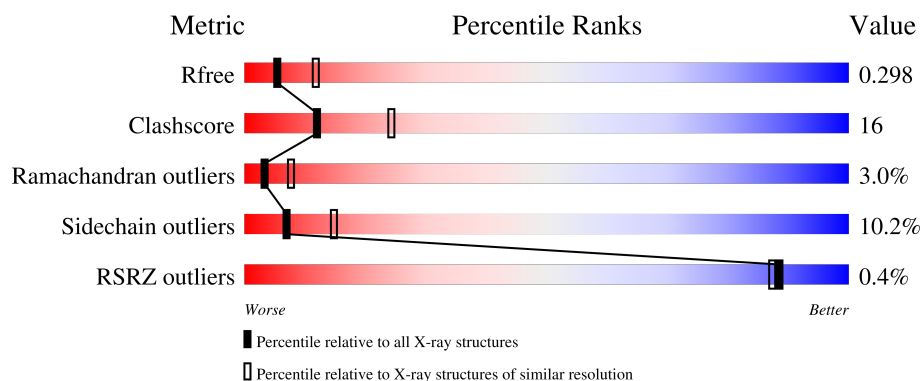
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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.



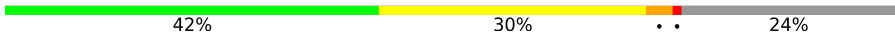
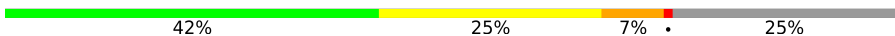
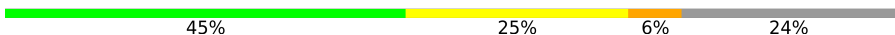
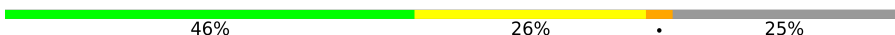
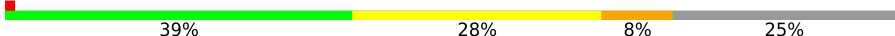
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	I	353	
2	J	353	
3	A	138	
3	E	138	
3	K	138	

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Mol	Chain	Length	Quality of chain
3	O	138	
4	B	105	
4	F	105	
4	L	105	
4	P	105	
5	C	132	
5	G	132	
5	M	132	
5	Q	132	
6	D	128	
6	H	128	
6	N	128	
6	R	128	
7	S	195	
7	T	195	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CL	C	201	-	-	X	-
10	CL	Q	201	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 27785 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 DNA (353-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	353	Total	C	N	O	P	0	0	0
			7230	3428	1369	2080	353			

- Molecule 2 is a DNA chain called DNA (353-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	353	Total	C	N	O	P	0	0	0
			7245	3446	1288	2158	353			

- Molecule 3 is a protein called Histone H3.1.

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

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	80	Total	C	N	O	S	0	0	0
			638	401	125	111	1			
4	F	82	Total	C	N	O	S	0	0	0
			653	412	127	113	1			
4	L	80	Total	C	N	O	S	0	0	0
			638	401	125	111	1			
4	P	80	Total	C	N	O	S	0	0	0
			638	401	125	111	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	expression tag	UNP P62805
B	-1	HIS	-	expression tag	UNP P62805
F	-2	SER	-	expression tag	UNP P62805
F	-1	HIS	-	expression tag	UNP P62805
L	-2	SER	-	expression tag	UNP P62805
L	-1	HIS	-	expression tag	UNP P62805
P	-2	SER	-	expression tag	UNP P62805
P	-1	HIS	-	expression tag	UNP P62805

- Molecule 5 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	107	Total	C	N	O	0	0	0
			828	523	162	143			
5	G	106	Total	C	N	O	0	0	0
			819	517	160	142			
5	M	108	Total	C	N	O	0	0	0
			833	526	163	144			
5	Q	107	Total	C	N	O	0	0	0
			824	520	161	143			

There are 8 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-1	HIS	-	expression tag	UNP P04908
Q	-2	SER	-	expression tag	UNP P04908
Q	-1	HIS	-	expression tag	UNP P04908

- Molecule 6 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
6	H	97	Total	C	N	O	S	0	0	0
			766	480	142	142	2			
6	N	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
6	R	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 7 is a protein called Histone H1.0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	S	75	Total	C	N	O	S	0	0	0
			575	358	108	108	1			
7	T	75	Total	C	N	O	S	0	0	0
			575	358	108	108	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	0	GLY	-	expression tag	UNP P07305
S	1	PRO	-	expression tag	UNP P07305
T	0	GLY	-	expression tag	UNP P07305

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Chain	Residue	Modelled	Actual	Comment	Reference
T	1	PRO	-	expression tag	UNP P07305

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	I	2	Total Ca 2 2	0	0
8	J	1	Total Ca 1 1	0	0

- Molecule 9 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	I	2	Total K 2 2	0	0
9	J	3	Total K 3 3	0	0

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total Cl 1 1	0	0
10	G	1	Total Cl 1 1	0	0
10	M	1	Total Cl 1 1	0	0
10	Q	1	Total Cl 1 1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total O 1 1	0	0
11	E	1	Total O 1 1	0	0
11	F	1	Total O 1 1	0	0
11	K	1	Total O 1 1	0	0

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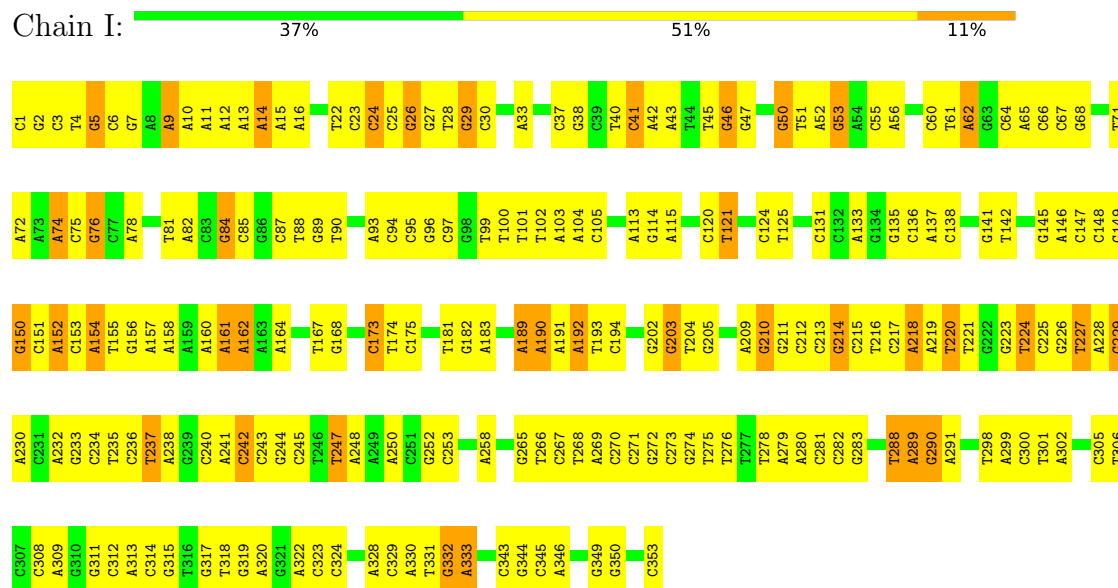
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	2	Total	O	0	0
			2	2		
11	P	3	Total	O	0	0
			3	3		

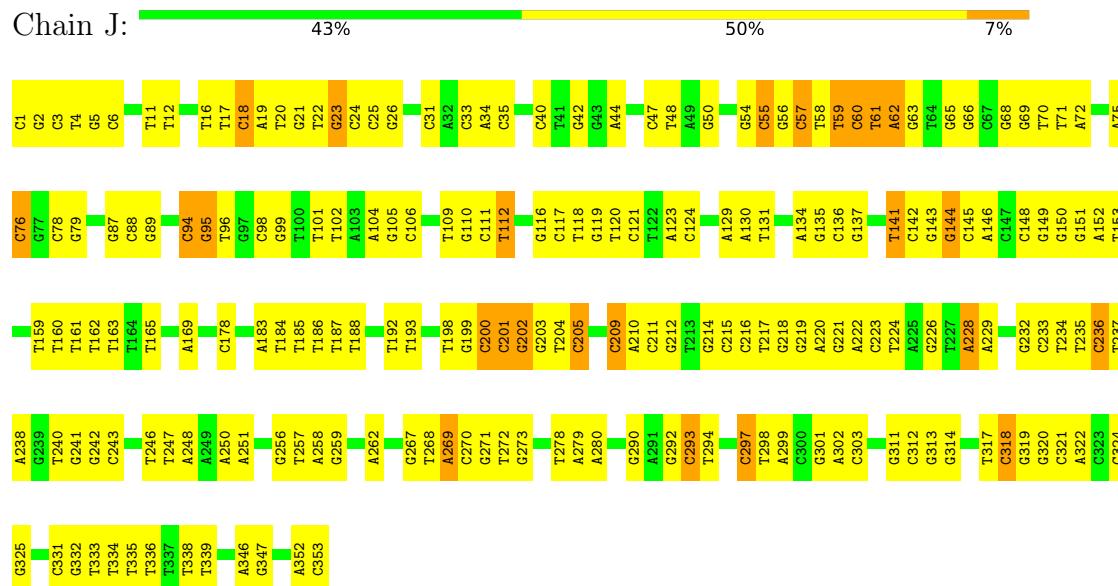
3 Residue-property plots

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: DNA (353-MER)

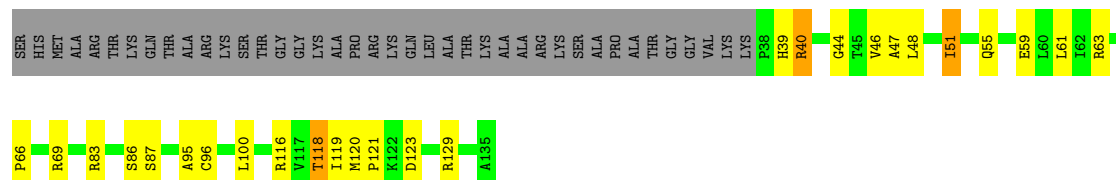


• Molecule 2: DNA (353-MER)



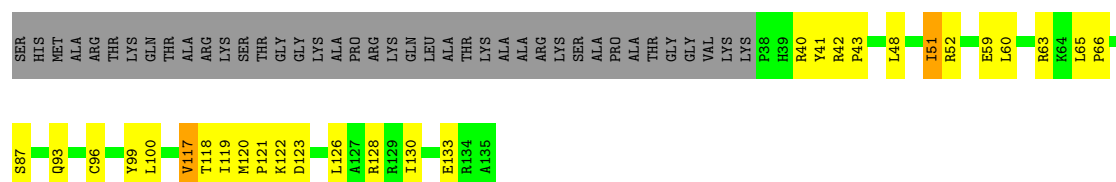
- Molecule 3: Histone H3.1

Chain A: 



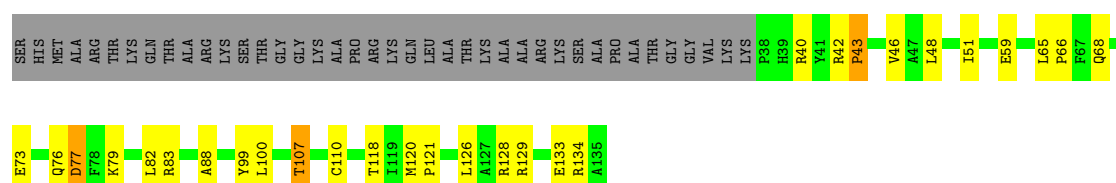
- Molecule 3: Histone H3.1

Chain E: 



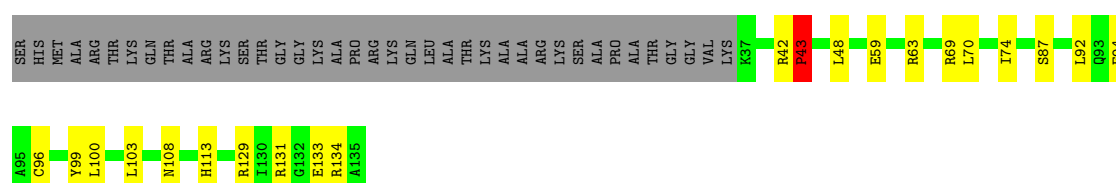
- Molecule 3: Histone H3.1

Chain K: 



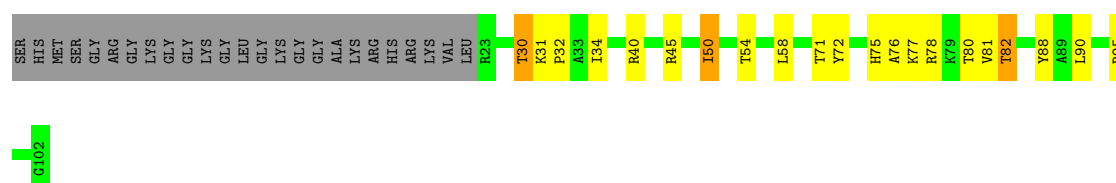
- Molecule 3: Histone H3.1

Chain O: 

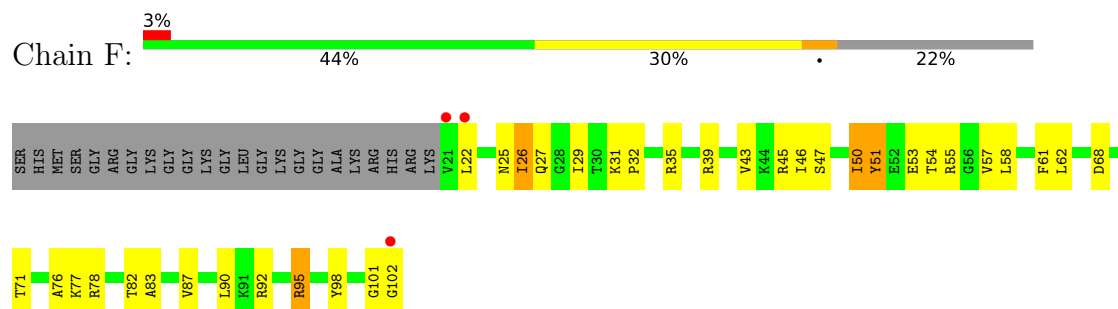


- Molecule 4: Histone H4

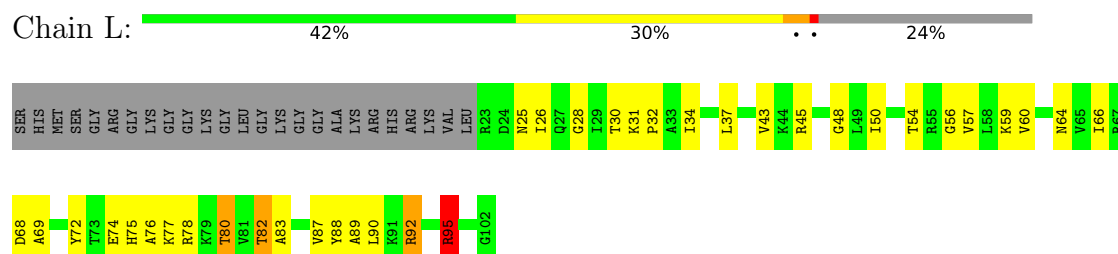
Chain B: 



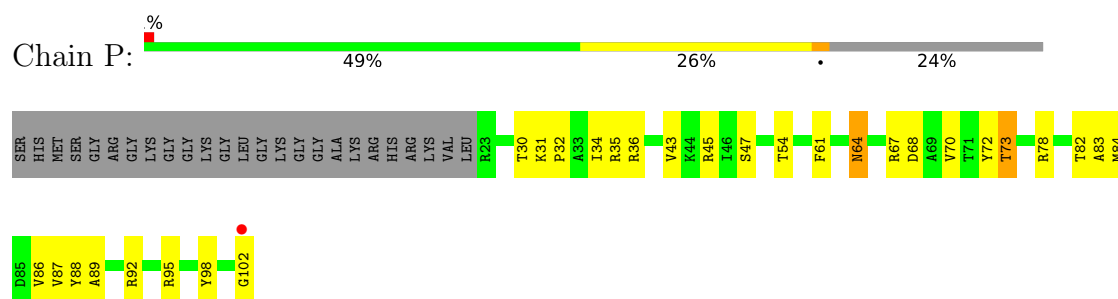
- Molecule 4: Histone H4



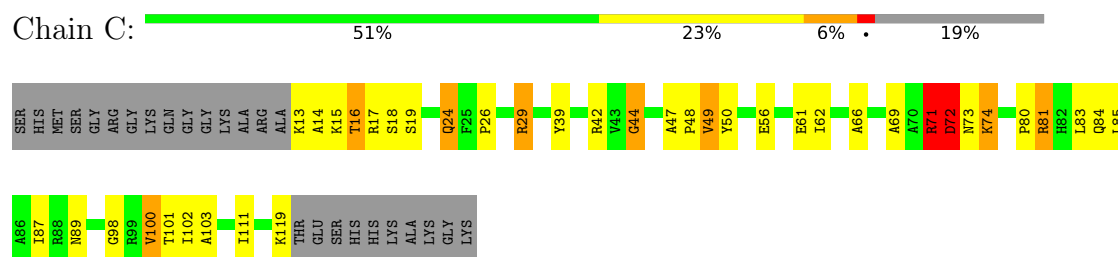
- Molecule 4: Histone H4



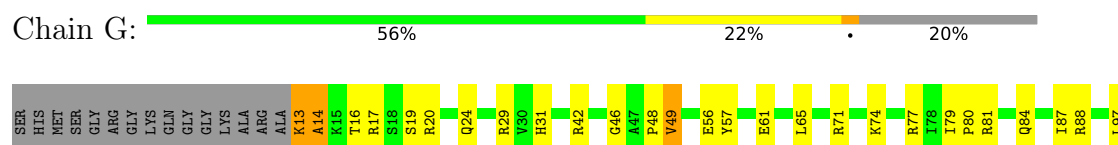
- Molecule 4: Histone H4

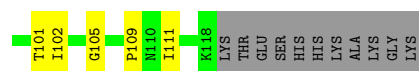


- Molecule 5: Histone H2A type 1-B/E



- Molecule 5: Histone H2A type 1-B/E

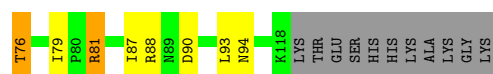




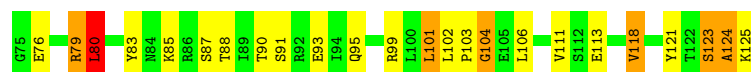
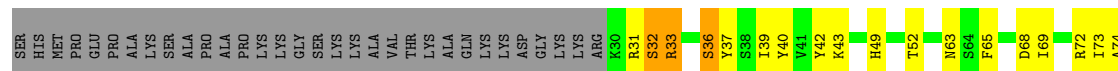
• Molecule 5: Histone H2A type 1-B/E



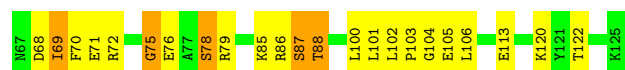
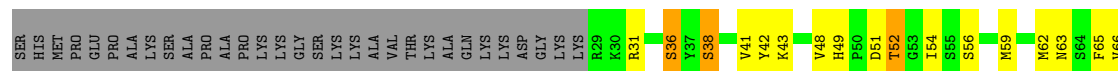
• Molecule 5: Histone H2A type 1-B/E



• Molecule 6: Histone H2B type 1-J



• Molecule 6: Histone H2B type 1-J



• Molecule 6: Histone H2B type 1-J



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.22Å 105.05Å 171.13Å 86.59° 88.95° 88.25°	Depositor
Resolution (Å)	49.35 – 2.86 49.35 – 2.86	Depositor EDS
% Data completeness (in resolution range)	97.4 (49.35-2.86) 97.4 (49.35-2.86)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.225 , 0.297 0.230 , 0.298	Depositor DCC
R_{free} test set	2099 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	81.7	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 77.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	27785	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: CA, CL, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	I	0.42	0/8122	0.96	60/12523 (0.5%)
2	J	0.41	1/8116 (0.0%)	0.98	53/12532 (0.4%)
3	A	1.01	0/819	1.55	2/1097 (0.2%)
3	E	1.02	0/819	1.51	0/1097
3	K	1.02	0/819	1.56	2/1097 (0.2%)
3	O	0.98	0/828	1.51	0/1109
4	B	1.00	0/645	1.57	0/862
4	F	1.02	0/660	1.53	0/883
4	L	1.06	0/645	1.62	2/862 (0.2%)
4	P	1.06	0/645	1.55	1/862 (0.1%)
5	C	1.03	0/838	1.52	2/1129 (0.2%)
5	G	1.02	0/829	1.54	2/1118 (0.2%)
5	M	1.02	0/843	1.53	2/1136 (0.2%)
5	Q	1.00	0/834	1.55	0/1125
6	D	1.05	0/766	1.64	4/1026 (0.4%)
6	H	1.01	0/777	1.60	4/1040 (0.4%)
6	N	1.08	0/766	1.61	4/1026 (0.4%)
6	R	1.08	1/766 (0.1%)	1.64	4/1026 (0.4%)
7	S	1.14	0/581	1.71	4/775 (0.5%)
7	T	1.12	0/581	1.55	0/775
All	All	0.76	2/29699 (0.0%)	1.26	146/43100 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	112	DT	O3'-P	-5.47	1.52	1.61
6	R	71	GLU	CD-OE2	5.26	1.35	1.25

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	16	DT	C2'-C3'-O3'	-10.03	96.45	111.50
1	I	76	DG	C2'-C3'-O3'	-8.95	98.07	111.50
1	I	192	DA	C2'-C3'-O3'	-8.86	98.22	111.50
1	I	289	DA	C2'-C3'-O3'	-8.74	98.39	111.50
2	J	70	DT	C2'-C3'-O3'	-8.60	98.60	111.50
2	J	42	DG	C2'-C3'-O3'	-8.59	98.62	111.50
1	I	210	DG	C2'-C3'-O3'	8.57	124.35	111.50
1	I	9	DA	C2'-C3'-O3'	8.49	124.24	111.50
2	J	72	DA	C4'-C3'-O3'	8.36	122.53	110.00
2	J	66	DG	C2'-C3'-O3'	-8.30	99.05	111.50
1	I	60	DC	C2'-C3'-O3'	-8.29	99.06	111.50
1	I	317	DG	C4'-C3'-O3'	8.02	122.03	110.00
2	J	57	DC	C4'-C3'-O3'	7.95	121.93	110.00
1	I	332	DG	C4'-C3'-O3'	7.95	121.93	110.00
2	J	228	DA	C2'-C3'-O3'	7.94	123.41	111.50
2	J	61	DT	C2'-C3'-O3'	-7.92	99.61	111.50
2	J	26	DG	C2'-C3'-O3'	-7.87	99.69	111.50
1	I	47	DG	C2'-C3'-O3'	-7.71	99.94	111.50
2	J	198	DT	C2'-C3'-O3'	7.65	122.97	111.50
1	I	220	DT	C4'-C3'-O3'	7.46	121.19	110.00
2	J	60	DC	C2'-C3'-O3'	-7.43	100.35	111.50
1	I	84	DG	C4'-C3'-O3'	7.36	121.04	110.00
1	I	30	DC	C2'-C3'-O3'	-7.34	100.48	111.50
1	I	224	DT	C4'-C3'-O3'	7.33	120.99	110.00
2	J	59	DT	C2'-C3'-O3'	7.26	122.40	111.50
2	J	256	DG	C2'-C3'-O3'	-7.24	100.64	111.50
2	J	297	DC	C2'-C3'-O3'	-7.11	100.84	111.50
1	I	62	DA	C2'-C3'-O3'	-7.00	101.00	111.50
1	I	60	DC	C4'-C3'-O3'	6.91	120.37	110.00
2	J	200	DC	C2'-C3'-O3'	6.91	121.86	111.50
1	I	269	DA	C2'-C3'-O3'	-6.84	101.24	111.50
1	I	164	DA	C2'-C3'-O3'	6.81	121.71	111.50
1	I	214	DG	C4'-C3'-O3'	6.63	119.94	110.00
1	I	237	DT	C2'-C3'-O3'	6.55	121.32	111.50
2	J	31	DC	C2'-C3'-O3'	-6.45	101.83	111.50
2	J	31	DC	C4'-C3'-O3'	6.44	119.66	110.00
1	I	288	DT	C2'-C3'-O3'	6.44	121.15	111.50
1	I	298	DT	C2'-C3'-O3'	-6.41	101.89	111.50
7	S	86	GLY	CA-C-O	-6.36	118.08	122.22
1	I	333	DA	C2'-C3'-O3'	6.33	120.99	111.50
2	J	226	DG	C2'-C3'-O3'	-6.30	102.05	111.50
1	I	26	DG	C2'-C3'-O3'	-6.29	102.07	111.50
2	J	76	DC	C2'-C3'-O3'	-6.27	102.09	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	18	DC	C2'-C3'-O3'	-6.26	102.11	111.50
3	K	107	THR	CA-C-N	6.23	129.48	120.38
3	K	107	THR	C-N-CA	6.23	129.48	120.38
1	I	46	DG	C2'-C3'-O3'	-6.23	102.15	111.50
2	J	23	DG	C4'-C3'-O3'	6.22	119.33	110.00
1	I	162	DA	C2'-C3'-O3'	-6.16	102.26	111.50
2	J	212	DG	C2'-C3'-O3'	-6.15	102.27	111.50
5	G	97	LEU	CA-C-N	6.15	126.94	119.99
5	G	97	LEU	C-N-CA	6.15	126.94	119.99
1	I	229	DG	C2'-C3'-O3'	-6.09	102.36	111.50
2	J	50	DG	C2'-C3'-O3'	-6.09	102.36	111.50
1	I	190	DA	C2'-C3'-O3'	-6.08	102.39	111.50
1	I	173	DC	C2'-C3'-O3'	-6.07	102.40	111.50
1	I	258	DA	C2'-C3'-O3'	-6.03	102.46	111.50
1	I	133	DA	C2'-C3'-O3'	-6.01	102.48	111.50
2	J	123	DA	C2'-C3'-O3'	6.01	120.52	111.50
4	L	95	ARG	CA-C-N	5.99	129.62	121.05
4	L	95	ARG	C-N-CA	5.99	129.62	121.05
2	J	246	DT	C2'-C3'-O3'	5.99	120.48	111.50
2	J	95	DG	C2'-C3'-O3'	5.96	120.44	111.50
1	I	29	DG	C2'-C3'-O3'	-5.95	102.57	111.50
1	I	173	DC	C4'-C3'-O3'	5.93	118.90	110.00
2	J	293	DC	C4'-C3'-O3'	5.89	118.84	110.00
1	I	14	DA	C2'-C3'-O3'	5.81	120.21	111.50
1	I	191	DA	C2'-C3'-O3'	-5.80	102.79	111.50
1	I	205	DG	C2'-C3'-O3'	-5.79	102.81	111.50
2	J	23	DG	C2'-C3'-O3'	-5.79	102.82	111.50
1	I	183	DA	C4'-C3'-O3'	5.76	118.64	110.00
3	A	86	SER	CA-C-N	5.75	128.30	120.54
3	A	86	SER	C-N-CA	5.75	128.30	120.54
1	I	53	DG	C2'-C3'-O3'	-5.70	102.95	111.50
2	J	62	DA	C2'-C3'-O3'	-5.70	102.95	111.50
2	J	61	DT	C4'-C3'-O3'	5.69	118.54	110.00
1	I	74	DA	C4'-C3'-O3'	5.69	118.53	110.00
1	I	150	DG	C2'-C3'-O3'	5.69	120.03	111.50
1	I	203	DG	C2'-C3'-O3'	5.67	120.00	111.50
1	I	121	DT	C2'-C3'-O3'	5.61	119.92	111.50
2	J	236	DC	C2'-C3'-O3'	5.60	119.90	111.50
1	I	211	DG	C2'-C3'-O3'	-5.56	103.16	111.50
2	J	62	DA	C4'-C3'-O3'	5.55	118.33	110.00
2	J	320	DG	C2'-C3'-O3'	5.55	119.83	111.50
1	I	152	DA	C2'-C3'-O3'	5.54	119.81	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	247	DT	C2'-C3'-O3'	5.51	119.76	111.50
1	I	5	DG	C2'-C3'-O3'	5.50	119.75	111.50
1	I	26	DG	C4'-C3'-O3'	5.48	118.21	110.00
1	I	161	DA	C4'-C3'-O3'	5.46	118.19	110.00
2	J	318	DC	C2'-C3'-O3'	-5.46	103.31	111.50
1	I	227	DT	C2'-C3'-O3'	5.45	119.68	111.50
1	I	320	DA	C2'-C3'-O3'	5.44	119.67	111.50
2	J	40	DC	C2'-C3'-O3'	-5.44	103.34	111.50
1	I	242	DC	C2'-C3'-O3'	5.44	119.66	111.50
6	H	78	SER	CA-C-N	5.42	127.49	120.44
6	H	78	SER	C-N-CA	5.42	127.49	120.44
6	N	48	VAL	CA-C-N	5.41	128.48	122.74
6	N	48	VAL	C-N-CA	5.41	128.48	122.74
2	J	209	DC	C4'-C3'-O3'	5.40	118.11	110.00
1	I	218	DA	C2'-C3'-O3'	-5.40	103.39	111.50
7	S	50	ILE	CA-C-N	5.40	127.52	120.28
7	S	50	ILE	C-N-CA	5.40	127.52	120.28
2	J	201	DC	C4'-C3'-O3'	5.40	118.10	110.00
2	J	292	DG	C2'-C3'-O3'	-5.40	103.40	111.50
1	I	78	DA	C4'-C3'-O3'	-5.37	101.94	110.00
2	J	290	DG	C2'-C3'-O3'	-5.36	103.46	111.50
1	I	154	DA	C2'-C3'-O3'	-5.35	103.47	111.50
2	J	169	DA	C2'-C3'-O3'	-5.35	103.47	111.50
2	J	209	DC	C2'-C3'-O3'	-5.30	103.54	111.50
6	R	71	GLU	CB-CG-CD	5.29	121.60	112.60
6	N	48	VAL	O-C-N	5.29	127.57	122.07
6	D	111	VAL	CA-C-N	5.29	128.14	120.79
6	D	111	VAL	C-N-CA	5.29	128.14	120.79
2	J	202	DG	C2'-C3'-O3'	5.28	119.42	111.50
2	J	141	DT	C4'-C3'-O3'	5.25	117.88	110.00
6	N	41	VAL	CA-C-O	-5.25	115.22	121.05
2	J	352	DA	C2'-C3'-O3'	5.23	119.34	111.50
6	R	41	VAL	N-CA-C	-5.21	105.41	110.42
6	D	63	ASN	CA-C-N	5.21	127.57	120.54
6	D	63	ASN	C-N-CA	5.21	127.57	120.54
1	I	50	DG	C2'-C3'-O3'	-5.20	103.69	111.50
6	H	113	GLU	CA-C-N	5.12	125.64	120.00
6	H	113	GLU	C-N-CA	5.12	125.64	120.00
1	I	41	DC	C2'-C3'-O3'	-5.11	103.83	111.50
2	J	211	DC	C4'-C3'-O3'	5.11	117.66	110.00
1	I	290	DG	C2'-C3'-O3'	-5.10	103.85	111.50
1	I	189	DA	N9-C1'-C2'	5.10	121.15	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	94	DC	C4'-C3'-O3'	5.10	117.65	110.00
5	C	100	VAL	CA-C-N	5.08	128.08	120.87
5	C	100	VAL	C-N-CA	5.08	128.08	120.87
2	J	55	DC	C4'-C3'-O3'	5.08	117.61	110.00
2	J	318	DC	C4'-C3'-O3'	5.06	117.60	110.00
2	J	124	DC	C2'-C3'-O3'	-5.06	103.91	111.50
2	J	269	DA	C2'-C3'-O3'	-5.06	103.91	111.50
7	S	25	HIS	CA-CB-CG	5.06	118.86	113.80
4	P	35	ARG	CB-CA-C	5.04	118.73	110.96
1	I	24	DC	C2'-C3'-O3'	-5.04	103.94	111.50
1	I	50	DG	C4'-C3'-O3'	5.04	117.56	110.00
2	J	71	DT	C2'-C3'-O3'	-5.04	103.94	111.50
2	J	205	DC	C2'-C3'-O3'	-5.04	103.94	111.50
2	J	144	DG	C2'-C3'-O3'	5.02	119.03	111.50
5	M	97	LEU	CA-C-N	5.02	125.66	119.99
5	M	97	LEU	C-N-CA	5.02	125.66	119.99
6	R	114	GLY	CA-C-N	5.01	127.00	120.28
6	R	114	GLY	C-N-CA	5.01	127.00	120.28
1	I	247	DT	C4'-C3'-O3'	-5.01	102.48	110.00

There are no chirality outliers.

There are no planarity outliers.

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	I	7230	0	3948	232	0
2	J	7245	0	3987	172	0
3	A	807	0	844	21	0
3	E	807	0	844	20	0
3	K	807	0	844	21	0
3	O	816	0	856	11	0
4	B	638	0	676	19	0
4	F	653	0	696	30	0
4	L	638	0	676	31	0
4	P	638	0	676	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	828	0	892	37	1
5	G	819	0	879	21	0
5	M	833	0	897	30	0
5	Q	824	0	884	35	1
6	D	755	0	784	39	0
6	H	766	0	797	23	1
6	N	755	0	784	29	1
6	R	755	0	784	50	0
7	S	575	0	604	33	0
7	T	575	0	604	30	0
8	I	2	0	0	0	0
8	J	1	0	0	0	0
9	I	2	0	0	0	0
9	J	3	0	0	0	0
10	C	1	0	0	2	0
10	G	1	0	0	0	0
10	M	1	0	0	1	0
10	Q	1	0	0	2	0
11	B	1	0	0	0	0
11	E	1	0	0	0	0
11	F	1	0	0	0	0
11	K	1	0	0	0	0
11	L	2	0	0	0	0
11	P	3	0	0	0	0
All	All	27785	0	21956	776	2

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 16.

All (776) 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)
2:J:210:DA:OP2	6:R:42:TYR:OH	1.76	1.02
7:S:62:GLU:O	7:S:64:ALA:N	1.98	0.96
2:J:318:DC:H4'	2:J:319:DG:OP1	1.65	0.96
1:I:167:DT:H5''	7:T:42:ARG:HD2	1.46	0.95
2:J:203:DG:H2''	2:J:204:DT:H5'	1.50	0.93
2:J:134:DA:H2''	2:J:135:DG:C8	2.04	0.92
2:J:162:DT:H2'	2:J:163:DT:H72	1.49	0.92
1:I:280:DA:OP1	3:A:69:ARG:NH2	2.03	0.92
1:I:221:DT:OP2	5:G:20:ARG:NH2	2.06	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:DT:H4'	1:I:225:DC:OP1	1.72	0.88
1:I:13:DA:H4'	1:I:14:DA:OP1	1.73	0.88
2:J:203:DG:H2''	2:J:204:DT:C5'	2.04	0.87
5:C:16:THR:HG22	5:C:19:SER:HB3	1.58	0.86
6:R:36:SER:HB2	6:R:63:ASN:HD21	1.40	0.84
5:M:81:ARG:NH2	5:M:107:VAL:O	2.11	0.83
5:Q:71:ARG:O	5:Q:74:LYS:N	2.11	0.83
5:Q:16:THR:HG23	5:Q:19:SER:HB2	1.61	0.82
2:J:58:DT:H2''	2:J:59:DT:OP2	1.79	0.81
1:I:318:DT:H4'	1:I:319:DG:OP1	1.82	0.80
4:P:72:TYR:OH	6:R:76:GLU:OE1	2.00	0.79
7:T:32:ILE:HG12	7:T:35:ALA:HB3	1.64	0.79
1:I:12:DA:H1'	1:I:13:DA:O4'	1.84	0.77
6:R:65:PHE:CE2	6:R:69:ILE:HD11	2.19	0.77
5:G:42:ARG:O	6:H:88:THR:HA	1.85	0.76
5:M:42:ARG:O	6:N:88:THR:HA	1.87	0.75
1:I:332:DG:H4'	1:I:333:DA:OP1	1.87	0.74
2:J:56:DG:H4'	2:J:57:DC:OP1	1.86	0.74
5:C:24:GLN:N	5:C:56:GLU:OE1	2.19	0.74
1:I:156:DG:H2''	1:I:157:DA:OP2	1.88	0.73
3:K:79:LYS:HB3	3:K:82:LEU:HD11	1.70	0.73
1:I:11:DA:H2''	1:I:12:DA:H5'	1.71	0.73
2:J:203:DG:C2'	2:J:204:DT:H5'	2.20	0.72
1:I:1:DC:H5''	1:I:353:DC:O3'	1.89	0.72
2:J:58:DT:H1'	2:J:59:DT:C5'	2.20	0.72
1:I:167:DT:H5''	7:T:42:ARG:CD	2.18	0.72
1:I:289:DA:H2''	1:I:290:DG:C8	2.24	0.72
7:T:81:LEU:HD11	7:T:95:LEU:HD23	1.72	0.71
5:C:71:ARG:O	5:C:74:LYS:N	2.20	0.71
4:P:68:ASP:OD2	4:P:92:ARG:NH1	2.21	0.71
2:J:217:DT:H2''	2:J:218:DG:C8	2.26	0.71
5:C:102:ILE:O	5:C:102:ILE:HG22	1.91	0.70
7:T:28:TYR:O	7:T:74:ARG:NH2	2.24	0.70
2:J:165:DT:H4'	7:S:67:GLN:HE22	1.57	0.70
2:J:58:DT:H1'	2:J:59:DT:H5'	1.73	0.70
7:T:34:ALA:HB3	7:T:58:TYR:OH	1.92	0.69
1:I:13:DA:H1'	1:I:14:DA:C5'	2.23	0.69
2:J:61:DT:H2''	2:J:62:DA:C8	2.28	0.69
2:J:236:DC:H2''	2:J:237:DT:OP2	1.92	0.68
6:N:49:HIS:HB3	6:N:52:THR:OG1	1.93	0.68
6:R:65:PHE:CZ	6:R:69:ILE:CD1	2.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:47:DC:H2''	2:J:48:DT:H71	1.76	0.68
6:N:65:PHE:CE2	6:N:69:ILE:CD1	2.76	0.68
2:J:22:DT:H2''	2:J:23:DG:C8	2.28	0.68
2:J:250:DA:OP1	4:P:36:ARG:NH2	2.25	0.68
2:J:324:DC:H2''	2:J:325:DG:C8	2.29	0.68
2:J:199:DG:H4'	2:J:200:DC:O5'	1.93	0.67
6:N:48:VAL:HG12	6:N:49:HIS:HD2	1.60	0.67
1:I:174:DT:H2''	1:I:175:DC:O5'	1.93	0.67
2:J:162:DT:H2'	2:J:163:DT:C7	2.24	0.67
6:H:65:PHE:CE2	6:H:69:ILE:CD1	2.78	0.67
6:R:65:PHE:CE2	6:R:69:ILE:CD1	2.78	0.67
7:T:47:ARG:NH1	7:T:48:GLN:OE1	2.27	0.67
4:L:68:ASP:OD2	4:L:92:ARG:NH1	2.27	0.67
5:C:66:ALA:O	5:C:69:ALA:HB3	1.96	0.66
2:J:148:DC:H2'	2:J:149:DG:C8	2.30	0.66
5:C:44:GLY:HA3	10:C:201:CL:CL	2.31	0.66
5:G:29:ARG:NH1	6:H:36:SER:O	2.29	0.66
2:J:270:DC:H2''	2:J:271:DG:C8	2.31	0.66
5:C:81:ARG:O	5:C:81:ARG:HG3	1.95	0.66
1:I:299:DA:H1'	1:I:300:DC:C6	2.30	0.66
2:J:301:DG:H1'	2:J:302:DA:C8	2.30	0.66
7:S:47:ARG:HD3	7:S:89:ALA:O	1.95	0.66
1:I:74:DA:H2''	1:I:75:DC:O5'	1.97	0.65
1:I:66:DC:H2''	1:I:67:DC:OP2	1.97	0.65
1:I:228:DA:H3'	6:H:87:SER:OG	1.97	0.65
2:J:202:DG:H2''	2:J:203:DG:O5'	1.97	0.65
1:I:247:DT:H2''	1:I:248:DA:C8	2.32	0.65
1:I:278:DT:H2''	1:I:279:DA:C8	2.32	0.64
2:J:250:DA:H1'	2:J:251:DA:H5'	1.79	0.64
1:I:153:DC:OP2	1:I:153:DC:H3'	1.98	0.64
2:J:200:DC:P	2:J:200:DC:H3'	2.38	0.64
1:I:150:DG:H2''	1:I:151:DC:OP2	1.98	0.63
2:J:144:DG:H2'	2:J:145:DC:C5	2.33	0.63
7:T:32:ILE:HD11	7:T:53:TYR:HB3	1.80	0.63
1:I:216:DT:H2''	1:I:217:DC:OP2	1.98	0.63
2:J:1:DC:O5'	2:J:353:DC:O3'	2.16	0.63
2:J:144:DG:H2'	2:J:145:DC:C6	2.34	0.63
1:I:301:DT:H2''	1:I:302:DA:C8	2.34	0.63
3:A:116:ARG:NH1	3:A:120:MET:SD	2.72	0.63
7:T:71:SER:O	7:T:75:LEU:HG	1.98	0.63
5:M:80:PRO:O	5:M:83:LEU:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:88:ARG:HD2	5:Q:94:ASN:OD1	1.98	0.63
2:J:234:DT:H2''	2:J:235:DT:OP2	1.99	0.62
2:J:57:DC:H4'	2:J:58:DT:OP1	1.99	0.62
3:E:99:TYR:OH	3:E:133:GLU:OE1	2.16	0.62
4:F:50:ILE:O	4:F:53:GLU:N	2.31	0.62
6:H:76:GLU:OE2	6:H:79:ARG:NH1	2.32	0.62
6:R:77:ALA:O	6:R:80:LEU:HB2	2.00	0.62
2:J:247:DT:H1'	2:J:248:DA:C8	2.34	0.62
7:T:81:LEU:HG	7:T:95:LEU:HA	1.81	0.62
5:M:37:GLY:HA3	5:M:39:TYR:CE2	2.35	0.62
4:P:88:TYR:CD1	6:R:83:TYR:CE2	2.87	0.61
7:T:25:HIS:ND1	7:T:31:MET:HE3	2.15	0.61
1:I:11:DA:C6	1:I:12:DA:C6	2.89	0.61
3:A:83:ARG:O	4:B:81:VAL:N	2.29	0.61
4:F:31:LYS:N	4:F:32:PRO:HD2	2.15	0.61
7:S:46:SER:O	7:S:49:SER:OG	2.13	0.61
1:I:99:DT:H2''	1:I:100:DT:OP2	2.01	0.61
5:M:29:ARG:O	5:M:33:LEU:HG	2.01	0.61
2:J:55:DC:H4'	2:J:56:DG:OP1	2.01	0.60
2:J:150:DG:H2''	2:J:151:DG:OP2	2.01	0.60
1:I:220:DT:H2'	1:I:221:DT:H72	1.84	0.60
1:I:13:DA:H1'	1:I:14:DA:H5'	1.84	0.60
2:J:335:DT:H2''	2:J:336:DT:H71	1.84	0.60
2:J:23:DG:H4'	2:J:24:DC:OP1	2.01	0.60
2:J:159:DT:H2''	2:J:160:DT:OP2	2.00	0.60
4:P:88:TYR:CE1	6:R:83:TYR:CE1	2.90	0.60
1:I:10:DA:C6	1:I:11:DA:C6	2.90	0.60
2:J:346:DA:H4'	2:J:347:DG:OP1	2.01	0.60
2:J:203:DG:H2''	2:J:204:DT:H5''	1.83	0.60
2:J:268:DT:H2''	2:J:269:DA:N7	2.17	0.60
6:R:37:TYR:CE2	6:R:66:VAL:HG11	2.37	0.59
1:I:45:DT:H2''	1:I:46:DG:O5'	2.02	0.59
4:P:88:TYR:CD1	6:R:83:TYR:CZ	2.90	0.59
1:I:145:DG:H2''	1:I:146:DA:C8	2.37	0.59
1:I:270:DC:H2''	1:I:271:DC:OP2	2.02	0.59
5:C:42:ARG:O	6:D:88:THR:HA	2.02	0.59
4:P:31:LYS:N	4:P:32:PRO:HD2	2.17	0.59
4:B:31:LYS:N	4:B:32:PRO:HD2	2.18	0.59
4:L:88:TYR:CE1	6:N:83:TYR:CE1	2.90	0.59
1:I:104:DA:H4'	3:O:63:ARG:CZ	2.32	0.59
3:A:51:ILE:HG21	5:G:111:ILE:HG12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:47:ARG:NE	7:S:89:ALA:O	2.36	0.59
3:E:126:LEU:HD11	3:E:130:ILE:HD11	1.85	0.58
1:I:218:DA:H1'	1:I:219:DA:C8	2.38	0.58
1:I:288:DT:H2''	1:I:289:DA:OP2	2.03	0.58
1:I:10:DA:OP2	1:I:10:DA:H2'	2.03	0.58
1:I:102:DT:H2''	1:I:103:DA:C8	2.39	0.58
2:J:145:DC:H2''	2:J:146:DA:C8	2.38	0.58
6:N:65:PHE:CZ	6:N:69:ILE:HD13	2.38	0.58
6:R:36:SER:HB2	6:R:63:ASN:ND2	2.14	0.58
5:Q:72:ASP:N	5:Q:72:ASP:OD1	2.36	0.58
1:I:154:DA:H4'	1:I:155:DT:H5'	1.86	0.58
1:I:272:DG:P	3:A:46:VAL:HB	2.44	0.58
5:C:29:ARG:NH2	6:D:36:SER:O	2.37	0.58
6:R:68:ASP:O	6:R:72:ARG:HG3	2.03	0.58
4:P:84:MET:HB3	4:P:88:TYR:CE2	2.39	0.58
1:I:93:DA:H2''	1:I:94:DC:C6	2.39	0.58
5:Q:29:ARG:NH2	6:R:36:SER:O	2.35	0.58
7:T:31:MET:SD	7:T:31:MET:C	2.87	0.58
2:J:17:DT:H4'	2:J:18:DC:OP1	2.02	0.58
3:A:118:THR:HA	4:B:45:ARG:HB3	1.84	0.58
3:K:65:LEU:O	3:K:66:PRO:C	2.46	0.58
5:Q:63:LEU:HD22	6:R:45:LEU:HD13	1.86	0.58
7:T:74:ARG:CZ	7:T:75:LEU:HD21	2.34	0.58
3:K:120:MET:O	3:K:121:PRO:C	2.47	0.57
6:N:77:ALA:O	6:N:80:LEU:HB2	2.03	0.57
5:Q:79:ILE:HD11	5:Q:81:ARG:HB3	1.86	0.57
1:I:13:DA:H2''	1:I:14:DA:H5'	1.85	0.57
4:B:88:TYR:CD1	6:D:83:TYR:CZ	2.91	0.57
3:K:128:ARG:HD2	3:K:133:GLU:OE1	2.04	0.57
1:I:13:DA:H1'	1:I:14:DA:H5''	1.85	0.57
1:I:150:DG:C2'	1:I:151:DC:OP2	2.53	0.57
6:N:65:PHE:CE2	6:N:69:ILE:HD13	2.40	0.57
2:J:333:DT:H2''	2:J:334:DT:C5'	2.34	0.57
4:L:60:VAL:HG12	4:L:64:ASN:ND2	2.19	0.57
6:R:62:MET:O	6:R:65:PHE:HB3	2.05	0.57
1:I:13:DA:C4'	1:I:14:DA:OP1	2.49	0.57
1:I:28:DT:H2''	1:I:29:DG:O5'	2.04	0.57
1:I:94:DC:H2''	1:I:95:DC:C6	2.39	0.57
5:Q:25:PHE:HB2	5:Q:56:GLU:HG3	1.86	0.57
7:S:53:TYR:O	7:S:56:SER:OG	2.15	0.57
7:S:47:ARG:CD	7:S:89:ALA:O	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:131:DC:H4'	1:I:131:DC:OP1	2.05	0.56
1:I:275:DT:H2''	1:I:276:DT:O5'	2.06	0.56
4:L:83:ALA:O	4:L:87:VAL:HG23	2.06	0.56
5:C:87:ILE:HD13	5:C:102:ILE:HD11	1.87	0.56
2:J:118:DT:H2''	2:J:119:DG:C8	2.41	0.56
5:C:71:ARG:O	5:C:72:ASP:C	2.49	0.56
1:I:4:DT:H1'	1:I:5:DG:C8	2.41	0.56
1:I:64:DC:H2''	1:I:65:DA:C5'	2.36	0.56
1:I:13:DA:C2'	1:I:14:DA:H5'	2.36	0.56
1:I:220:DT:H4'	1:I:221:DT:OP1	2.06	0.56
7:S:33:VAL:O	7:S:37:GLN:HB2	2.05	0.56
2:J:111:DC:H2'	2:J:112:DT:H72	1.87	0.56
2:J:186:DT:H4'	2:J:187:DT:OP1	2.05	0.56
4:F:29:ILE:HG13	4:F:58:LEU:CD2	2.36	0.56
1:I:212:DC:H2''	1:I:213:DC:O5'	2.05	0.56
1:I:219:DA:C8	1:I:220:DT:H72	2.41	0.56
1:I:323:DC:H2''	1:I:324:DC:OP2	2.05	0.56
2:J:22:DT:C2'	2:J:23:DG:C8	2.89	0.56
4:B:88:TYR:CD1	6:D:83:TYR:CE2	2.94	0.56
2:J:5:DG:H4'	2:J:6:DC:OP1	2.05	0.55
1:I:104:DA:H2''	1:I:105:DC:C6	2.42	0.55
5:G:13:LYS:C	5:G:13:LYS:HD2	2.31	0.55
6:R:49:HIS:HB3	6:R:52:THR:OG1	2.06	0.55
6:D:65:PHE:CE2	6:D:69:ILE:CD1	2.89	0.55
4:L:31:LYS:N	4:L:32:PRO:HD2	2.22	0.55
5:M:16:THR:O	5:M:16:THR:OG1	2.24	0.55
2:J:58:DT:H1'	2:J:59:DT:H5''	1.89	0.55
2:J:111:DC:H2''	2:J:112:DT:C6	2.42	0.55
2:J:333:DT:H2''	2:J:334:DT:H5'	1.89	0.55
1:I:135:DG:H2''	1:I:136:DC:OP2	2.06	0.55
2:J:20:DT:H2''	2:J:21:DG:C8	2.42	0.55
2:J:33:DC:H4'	2:J:34:DA:OP1	2.06	0.55
2:J:200:DC:H3'	2:J:200:DC:OP2	2.07	0.55
2:J:96:DT:O2	3:E:40:ARG:NH1	2.40	0.54
2:J:241:DG:H2''	2:J:242:DG:OP2	2.06	0.54
2:J:257:DT:H2''	2:J:258:DA:C8	2.42	0.54
7:S:85:LYS:O	7:S:91:GLY:HA3	2.06	0.54
1:I:104:DA:H2''	1:I:105:DC:H6	1.72	0.54
2:J:258:DA:H1'	2:J:259:DG:C8	2.42	0.54
2:J:136:DC:H2''	2:J:137:DG:C8	2.43	0.54
5:Q:16:THR:HG23	5:Q:19:SER:CB	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:150:DG:H1'	1:I:151:DC:OP2	2.08	0.54
1:I:243:DC:H2''	1:I:244:DG:OP2	2.07	0.54
1:I:1:DC:H2''	1:I:2:DG:C8	2.43	0.54
1:I:137:DA:C2	2:J:214:DG:N2	2.76	0.54
2:J:268:DT:H2''	2:J:269:DA:C8	2.43	0.54
4:B:90:LEU:HB3	4:B:95:ARG:O	2.08	0.54
1:I:274:DG:H2''	1:I:275:DT:H72	1.90	0.54
5:M:24:GLN:HG2	6:N:43:LYS:HB3	1.89	0.54
6:R:37:TYR:CD2	6:R:66:VAL:HG11	2.42	0.54
2:J:44:DA:OP1	5:C:17:ARG:HG3	2.08	0.54
2:J:65:DG:H4'	2:J:65:DG:OP1	2.08	0.54
2:J:110:DG:H2''	2:J:111:DC:OP2	2.08	0.54
1:I:23:DC:H2''	1:I:24:DC:OP2	2.07	0.53
1:I:114:DG:H2''	1:I:115:DA:C8	2.44	0.53
7:T:32:ILE:HG12	7:T:35:ALA:CB	2.36	0.53
1:I:226:DG:H1'	1:I:227:DT:H5'	1.90	0.53
5:C:17:ARG:HB3	6:D:121:TYR:HE2	1.72	0.53
4:F:26:ILE:HD11	4:F:55:ARG:O	2.08	0.53
5:Q:49:VAL:HG11	6:R:118:VAL:HA	1.91	0.53
2:J:130:DA:C8	2:J:131:DT:H72	2.44	0.53
2:J:298:DT:H2''	2:J:299:DA:OP2	2.08	0.53
1:I:237:DT:H2'	1:I:238:DA:C8	2.44	0.53
2:J:201:DC:OP2	2:J:201:DC:H3'	2.08	0.53
7:S:32:ILE:HG22	7:S:36:ILE:HD11	1.91	0.53
1:I:103:DA:H1'	1:I:104:DA:C8	2.43	0.53
4:B:88:TYR:CE1	6:D:83:TYR:CZ	2.96	0.53
1:I:26:DG:H4'	1:I:27:DG:OP1	2.08	0.53
1:I:234:DC:H2''	1:I:235:DT:OP2	2.09	0.53
6:D:68:ASP:O	6:D:72:ARG:HG3	2.09	0.53
5:Q:31:HIS:CD2	5:Q:48:PRO:HG3	2.44	0.53
3:A:55:GLN:OE1	5:G:109:PRO:HA	2.09	0.53
3:A:63:ARG:HB2	3:A:66:PRO:HG2	1.90	0.53
2:J:55:DC:C4'	2:J:56:DG:OP1	2.57	0.53
3:O:96:CYS:O	3:O:99:TYR:HB3	2.09	0.53
2:J:222:DA:H1'	2:J:223:DC:H5'	1.91	0.53
2:J:317:DT:H2''	2:J:318:DC:O5'	2.08	0.53
6:H:68:ASP:O	6:H:72:ARG:HG3	2.09	0.53
6:R:65:PHE:CZ	6:R:69:ILE:HD13	2.44	0.53
7:T:23:THR:HB	7:T:59:LYS:HG3	1.91	0.53
2:J:116:DG:H1'	2:J:117:DC:C6	2.44	0.53
3:K:59:GLU:N	3:K:59:GLU:OE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:50:TYR:OH	6:R:95:GLN:NE2	2.26	0.53
2:J:201:DC:H2''	2:J:202:DG:H5''	1.92	0.52
4:P:64:ASN:N	4:P:64:ASN:HD22	2.07	0.52
7:T:31:MET:HE2	7:T:31:MET:HA	1.91	0.52
1:I:2:DG:H4'	1:I:3:DC:OP1	2.10	0.52
1:I:136:DC:H2''	1:I:137:DA:OP2	2.09	0.52
6:D:49:HIS:HB3	6:D:52:THR:HG23	1.90	0.52
7:S:81:LEU:HD11	7:S:95:LEU:HD23	1.91	0.52
1:I:265:DG:H2''	1:I:266:DT:H72	1.92	0.52
3:A:83:ARG:O	4:B:80:THR:HA	2.10	0.52
1:I:104:DA:OP1	3:O:69:ARG:NH2	2.43	0.52
5:C:100:VAL:HG11	4:F:98:TYR:CE2	2.44	0.52
6:D:32:SER:O	6:D:33:ARG:CB	2.57	0.52
5:Q:39:TYR:CE1	6:R:74:ALA:HB1	2.45	0.52
2:J:240:DT:H2''	2:J:241:DG:H5'	1.92	0.52
1:I:37:DC:H2''	1:I:38:DG:O5'	2.09	0.52
2:J:184:DT:H2''	2:J:185:DT:O5'	2.09	0.52
7:S:31:MET:HG3	7:S:54:ILE:HD12	1.92	0.52
4:L:25:ASN:O	4:L:28:GLY:N	2.34	0.51
4:L:75:HIS:HB2	6:N:96:THR:HG21	1.91	0.51
1:I:275:DT:H2''	1:I:276:DT:C5'	2.40	0.51
4:B:88:TYR:CE1	6:D:83:TYR:CE1	2.98	0.51
6:R:69:ILE:O	6:R:73:ILE:HG13	2.10	0.51
6:R:72:ARG:HB3	6:R:101:LEU:HD21	1.92	0.51
1:I:145:DG:OP2	5:Q:76:THR:N	2.30	0.51
1:I:174:DT:C2'	1:I:175:DC:O5'	2.58	0.51
2:J:78:DC:H2''	2:J:79:DG:O5'	2.11	0.51
1:I:11:DA:H2''	1:I:12:DA:C5'	2.38	0.51
1:I:12:DA:H1'	1:I:13:DA:H5'	1.93	0.51
1:I:26:DG:H1'	1:I:27:DG:C8	2.46	0.51
5:C:80:PRO:O	5:C:83:LEU:N	2.43	0.51
6:R:32:SER:O	6:R:33:ARG:HB2	2.11	0.51
1:I:124:DC:H2''	1:I:125:DT:C6	2.45	0.51
5:Q:26:PRO:HD3	6:R:40:TYR:CD1	2.46	0.51
7:T:75:LEU:HD13	7:T:81:LEU:HD13	1.93	0.51
1:I:223:DG:H2''	1:I:224:DT:OP2	2.11	0.51
3:K:107:THR:O	3:K:110:CYS:HB2	2.10	0.51
4:B:75:HIS:CD2	6:D:80:LEU:HD12	2.46	0.51
5:C:16:THR:O	5:C:19:SER:OG	2.19	0.51
6:H:65:PHE:CZ	6:H:69:ILE:HD13	2.46	0.51
6:R:123:SER:O	6:R:124:ALA:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:11:DA:C2'	1:I:12:DA:H5'	2.38	0.51
1:I:55:DC:H2''	1:I:56:DA:C8	2.46	0.51
1:I:330:DA:C2	2:J:21:DG:N2	2.80	0.51
2:J:17:DT:H2''	2:J:18:DC:C6	2.46	0.51
2:J:203:DG:C2'	2:J:204:DT:C5'	2.83	0.51
2:J:242:DG:OP2	2:J:242:DG:H8	1.93	0.51
1:I:89:DG:N2	2:J:262:DA:C2	2.79	0.50
1:I:151:DC:OP2	1:I:151:DC:H2'	2.10	0.50
1:I:229:DG:H1'	1:I:230:DA:C8	2.45	0.50
4:F:61:PHE:HE2	4:F:95:ARG:HD3	1.76	0.50
3:K:126:LEU:HD22	3:O:113:HIS:CG	2.47	0.50
5:M:81:ARG:O	5:M:81:ARG:HG3	2.10	0.50
7:S:62:GLU:C	7:S:64:ALA:N	2.70	0.50
1:I:168:DG:C2	2:J:183:DA:C2	2.98	0.50
1:I:236:DC:H2''	1:I:237:DT:H72	1.93	0.50
5:M:80:PRO:HD3	6:N:58:ALA:HB2	1.93	0.50
1:I:124:DC:H2''	1:I:125:DT:C5	2.46	0.50
2:J:269:DA:H2''	2:J:270:DC:C5	2.46	0.50
4:F:50:ILE:O	4:F:51:TYR:C	2.53	0.50
1:I:224:DT:H1'	1:I:225:DC:H5'	1.93	0.50
2:J:54:DG:C4'	2:J:55:DC:OP1	2.60	0.50
2:J:200:DC:C4	2:J:201:DC:N4	2.80	0.50
4:P:34:ILE:HG23	4:P:54:THR:HG21	1.93	0.50
5:Q:79:ILE:CD1	5:Q:81:ARG:HB3	2.42	0.50
1:I:146:DA:C5	1:I:147:DC:C4	3.00	0.50
1:I:42:DA:C2	1:I:43:DA:C5	2.99	0.50
1:I:160:DA:H4'	1:I:161:DA:OP1	2.12	0.50
5:C:100:VAL:HG11	4:F:98:TYR:CZ	2.47	0.50
7:S:25:HIS:HA	7:S:31:MET:CE	2.42	0.50
1:I:100:DT:H2''	1:I:101:DT:OP2	2.11	0.50
1:I:267:DC:H1'	1:I:268:DT:C6	2.46	0.50
7:T:26:PRO:HD2	7:T:31:MET:CE	2.41	0.50
1:I:66:DC:H1'	1:I:67:DC:H5'	1.94	0.49
2:J:111:DC:H2'	2:J:112:DT:C7	2.42	0.49
4:L:95:ARG:HB3	4:L:95:ARG:HH11	1.77	0.49
4:L:88:TYR:CE1	6:N:83:TYR:CD1	3.00	0.49
7:S:71:SER:O	7:S:75:LEU:HG	2.12	0.49
1:I:145:DG:H5'	5:Q:75:LYS:HD2	1.94	0.49
2:J:218:DG:H1'	2:J:219:DG:C8	2.46	0.49
2:J:338:DT:C2'	2:J:339:DT:H72	2.42	0.49
5:C:26:PRO:HD3	6:D:40:TYR:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:81:ARG:HD3	5:C:85:LEU:HD11	1.94	0.49
6:D:69:ILE:O	6:D:73:ILE:HG13	2.11	0.49
3:E:100:LEU:HD11	4:F:58:LEU:HD13	1.95	0.49
1:I:61:DT:H2''	1:I:62:DA:O5'	2.12	0.49
1:I:168:DG:N2	2:J:183:DA:C2	2.81	0.49
2:J:279:DA:H1'	2:J:280:DA:C8	2.47	0.49
4:L:78:ARG:NH1	4:L:82:THR:HG23	2.28	0.49
3:O:131:ARG:HD3	3:O:133:GLU:OE2	2.12	0.49
7:S:63:ASN:O	7:S:66:SER:N	2.40	0.49
1:I:328:DA:H2''	1:I:329:DC:O5'	2.13	0.49
3:K:83:ARG:O	4:L:80:THR:HA	2.12	0.49
1:I:209:DA:H4'	1:I:210:DG:OP1	2.13	0.49
2:J:215:DC:H2''	2:J:216:DC:C6	2.48	0.49
4:F:71:THR:HG21	6:H:100:LEU:HG	1.94	0.49
4:L:34:ILE:HG23	4:L:54:THR:HG21	1.94	0.49
1:I:230:DA:OP2	6:H:86:ARG:NH2	2.45	0.49
2:J:312:DC:H2''	2:J:313:DG:C8	2.47	0.49
1:I:15:DA:C6	1:I:16:DA:C6	3.01	0.49
1:I:154:DA:H4'	1:I:155:DT:OP1	2.13	0.49
2:J:18:DC:H2''	2:J:19:DA:C8	2.48	0.49
2:J:201:DC:H4'	2:J:202:DG:OP1	2.13	0.48
3:A:119:ILE:HD12	4:B:50:ILE:HD12	1.95	0.48
5:Q:39:TYR:O	6:R:78:SER:OG	2.30	0.48
1:I:11:DA:C2	1:I:12:DA:C4	3.01	0.48
1:I:244:DG:OP2	1:I:244:DG:H2'	2.13	0.48
2:J:199:DG:C4'	2:J:200:DC:O5'	2.59	0.48
2:J:201:DC:H1'	2:J:202:DG:H5''	1.95	0.48
2:J:204:DT:H2''	2:J:205:DC:C6	2.49	0.48
4:F:78:ARG:NH1	4:F:82:THR:HG23	2.28	0.48
1:I:114:DG:H2''	1:I:115:DA:N7	2.28	0.48
2:J:141:DT:H4'	2:J:142:DC:OP1	2.13	0.48
1:I:81:DT:H2''	1:I:82:DA:C8	2.49	0.48
1:I:5:DG:H2''	1:I:6:DC:O5'	2.14	0.48
1:I:161:DA:H4'	1:I:162:DA:OP1	2.13	0.48
1:I:345:DC:H4'	1:I:346:DA:OP1	2.14	0.48
2:J:129:DA:H2'	2:J:130:DA:C8	2.49	0.48
2:J:221:DG:OP1	5:Q:15:LYS:HD2	2.13	0.48
1:I:173:DC:H4'	1:I:174:DT:OP1	2.14	0.48
5:C:85:LEU:O	5:C:89:ASN:HB2	2.14	0.48
5:M:54:VAL:HG13	6:N:110:ALA:HB1	1.96	0.48
1:I:210:DG:P	6:H:42:TYR:HH	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:104:GLN:NE2	3:O:94:GLU:OE2	2.39	0.48
4:P:70:VAL:HA	4:P:73:THR:OG1	2.14	0.48
1:I:64:DC:H5'	3:K:83:ARG:HG2	1.95	0.47
1:I:156:DG:C2'	1:I:157:DA:OP2	2.60	0.47
5:C:24:GLN:HG2	6:D:43:LYS:HB3	1.96	0.47
1:I:275:DT:H2'	1:I:276:DT:C6	2.49	0.47
1:I:305:DC:H2''	1:I:306:DT:H5'	1.95	0.47
2:J:270:DC:H5''	2:J:270:DC:H6	1.79	0.47
2:J:278:DT:H2''	2:J:279:DA:C8	2.49	0.47
5:G:87:ILE:HD13	5:G:102:ILE:HD11	1.96	0.47
4:L:76:ALA:O	4:L:78:ARG:HG3	2.14	0.47
5:Q:39:TYR:CE1	6:R:74:ALA:CB	2.97	0.47
6:R:31:ARG:O	6:R:32:SER:C	2.57	0.47
1:I:24:DC:H1'	1:I:25:DC:C6	2.49	0.47
4:P:88:TYR:CE1	6:R:83:TYR:CZ	3.02	0.47
1:I:12:DA:OP1	7:T:63:ASN:ND2	2.48	0.47
1:I:147:DC:H2''	1:I:148:DC:OP2	2.14	0.47
1:I:300:DC:C2'	1:I:301:DT:H72	2.44	0.47
2:J:220:DA:H2''	2:J:221:DG:H8	1.80	0.47
2:J:267:DG:H2''	2:J:268:DT:OP2	2.15	0.47
2:J:297:DC:H2''	2:J:298:DT:H72	1.95	0.47
4:L:48:GLY:C	4:L:50:ILE:H	2.23	0.47
4:L:69:ALA:O	4:L:72:TYR:HB2	2.14	0.47
1:I:12:DA:C1'	1:I:13:DA:H5'	2.45	0.47
2:J:88:DC:H2''	2:J:89:DG:OP2	2.12	0.47
5:M:50:TYR:OH	6:N:95:GLN:NE2	2.47	0.47
4:P:78:ARG:NH1	4:P:82:THR:HG23	2.29	0.47
1:I:153:DC:H3'	1:I:153:DC:P	2.55	0.47
1:I:250:DA:H5''	3:E:63:ARG:HD3	1.97	0.47
1:I:331:DT:H2''	1:I:332:DG:C8	2.50	0.47
2:J:98:DC:H2''	2:J:99:DG:O5'	2.14	0.47
2:J:105:DG:H2''	2:J:106:DC:C6	2.50	0.47
4:B:30:THR:HB	4:B:32:PRO:HD2	1.96	0.47
4:F:68:ASP:OD2	4:F:92:ARG:NH1	2.48	0.47
5:C:24:GLN:CG	6:D:43:LYS:HB3	2.45	0.47
5:M:26:PRO:HD3	6:N:40:TYR:CD1	2.50	0.47
7:T:75:LEU:HD22	7:T:80:VAL:HG11	1.96	0.47
1:I:148:DC:H2''	1:I:149:DG:C8	2.50	0.47
1:I:217:DC:H4'	1:I:218:DA:OP1	2.15	0.47
1:I:274:DG:C2'	1:I:275:DT:H72	2.45	0.47
2:J:104:DA:H8	2:J:104:DA:OP2	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:216:DC:H2''	2:J:217:DT:OP2	2.14	0.47
5:C:102:ILE:O	5:C:103:ALA:C	2.58	0.47
4:F:83:ALA:O	4:F:87:VAL:HG23	2.14	0.47
1:I:50:DG:H2''	1:I:51:DT:H72	1.97	0.47
1:I:64:DC:H1'	1:I:65:DA:OP1	2.15	0.47
1:I:227:DT:H2''	1:I:228:DA:OP2	2.15	0.47
6:D:49:HIS:HB3	6:D:52:THR:CG2	2.44	0.47
6:D:123:SER:O	6:D:124:ALA:C	2.58	0.47
5:Q:26:PRO:HD3	6:R:40:TYR:CE1	2.50	0.47
7:S:81:LEU:HG	7:S:95:LEU:HA	1.97	0.47
1:I:102:DT:H6	1:I:102:DT:H5'	1.79	0.46
1:I:193:DT:H1'	1:I:194:DC:OP1	2.15	0.46
3:E:96:CYS:SG	4:F:62:LEU:HD21	2.56	0.46
6:H:38:SER:HB3	6:H:59:MET:CG	2.44	0.46
1:I:120:DC:H2''	1:I:121:DT:H5'	1.97	0.46
2:J:311:DG:C4	2:J:312:DC:C5	3.03	0.46
7:S:27:LYS:O	7:S:28:TYR:C	2.57	0.46
1:I:329:DC:H2''	1:I:330:DA:C8	2.51	0.46
2:J:209:DC:H1'	2:J:210:DA:C8	2.49	0.46
2:J:314:DG:OP1	6:N:30:LYS:HB3	2.15	0.46
4:L:88:TYR:CD1	6:N:83:TYR:CZ	3.04	0.46
4:P:61:PHE:HE2	4:P:95:ARG:HD3	1.80	0.46
1:I:12:DA:C6	1:I:13:DA:C6	3.04	0.46
1:I:244:DG:H4'	1:I:245:DC:OP1	2.16	0.46
6:D:32:SER:O	6:D:33:ARG:HB2	2.16	0.46
4:F:25:ASN:C	4:F:27:GLN:N	2.72	0.46
5:Q:16:THR:CG2	5:Q:19:SER:HB2	2.40	0.46
7:S:63:ASN:O	7:S:65:ASP:N	2.48	0.46
1:I:113:DA:H2''	1:I:114:DG:C8	2.50	0.46
1:I:124:DC:H2''	1:I:125:DT:H71	1.98	0.46
1:I:203:DG:H1'	1:I:204:DT:O5'	2.15	0.46
1:I:314:DC:C2'	1:I:315:DG:O5'	2.64	0.46
7:S:28:TYR:HB3	7:S:71:SER:CB	2.45	0.46
1:I:10:DA:H2''	1:I:11:DA:H5''	1.98	0.46
1:I:45:DT:OP1	5:M:20:ARG:NH2	2.48	0.46
1:I:240:DC:H2''	1:I:241:DA:OP2	2.16	0.46
2:J:95:DG:H2'	2:J:96:DT:H71	1.98	0.46
2:J:221:DG:H2''	2:J:222:DA:C8	2.51	0.46
3:E:42:ARG:O	3:E:43:PRO:C	2.59	0.46
5:Q:58:LEU:HD11	6:R:102:LEU:HD11	1.97	0.46
5:Q:90:ASP:OD1	5:Q:90:ASP:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:68:ILE:O	7:S:71:SER:OG	2.32	0.46
1:I:193:DT:C1'	1:I:194:DC:OP1	2.64	0.46
1:I:219:DA:N9	1:I:220:DT:H72	2.30	0.46
5:G:84:GLN:OE1	5:G:88:ARG:HG2	2.15	0.46
1:I:157:DA:H2''	1:I:158:DA:OP2	2.15	0.46
5:Q:70:ALA:O	5:Q:75:LYS:O	2.33	0.46
1:I:221:DT:OP1	5:G:14:ALA:HA	2.16	0.46
2:J:298:DT:H2''	2:J:299:DA:C8	2.51	0.46
3:A:44:GLY:O	3:A:47:ALA:HB3	2.16	0.46
6:H:71:GLU:O	6:H:72:ARG:C	2.58	0.46
1:I:141:DG:H4'	1:I:142:DT:OP1	2.16	0.45
6:D:31:ARG:O	6:D:32:SER:C	2.60	0.45
7:T:75:LEU:HD22	7:T:80:VAL:CG1	2.47	0.45
3:A:48:LEU:O	3:A:51:ILE:HB	2.16	0.45
4:B:34:ILE:HG23	4:B:54:THR:HG21	1.97	0.45
6:R:70:PHE:CD1	6:R:70:PHE:C	2.95	0.45
1:I:154:DA:C4'	1:I:155:DT:H5'	2.46	0.45
2:J:1:DC:C6	2:J:353:DC:H1'	2.51	0.45
2:J:228:DA:H2''	2:J:229:DA:O5'	2.17	0.45
3:K:88:ALA:HA	4:L:83:ALA:HA	1.98	0.45
6:R:32:SER:O	6:R:33:ARG:CB	2.64	0.45
1:I:275:DT:O5'	1:I:275:DT:H6	1.99	0.45
5:M:46:GLY:N	10:M:201:CL:CL	2.86	0.45
7:S:47:ARG:HB2	7:S:51:GLN:NE2	2.31	0.45
7:T:74:ARG:NH2	7:T:75:LEU:HD21	2.31	0.45
1:I:67:DC:H2''	1:I:68:DG:C8	2.52	0.45
1:I:236:DC:H4'	1:I:237:DT:OP1	2.16	0.45
3:A:100:LEU:HD11	4:B:58:LEU:HD13	1.99	0.45
5:M:39:TYR:CD1	6:N:74:ALA:HB1	2.52	0.45
1:I:42:DA:C2	1:I:43:DA:C6	3.05	0.45
1:I:71:DT:H2'	1:I:72:DA:C8	2.51	0.45
1:I:301:DT:OP1	5:C:44:GLY:HA2	2.16	0.45
1:I:333:DA:OP1	3:E:41:TYR:HD1	1.99	0.45
3:E:128:ARG:HD2	3:E:133:GLU:OE1	2.17	0.45
6:H:49:HIS:HB3	6:H:52:THR:OG1	2.17	0.45
6:H:41:VAL:CG1	6:H:59:MET:HE1	2.47	0.45
5:M:84:GLN:HG2	5:M:105:GLY:O	2.17	0.45
3:O:108:ASN:HB2	4:P:43:VAL:HG22	1.97	0.45
6:R:72:ARG:O	6:R:101:LEU:HD11	2.16	0.45
6:R:80:LEU:HD13	6:R:80:LEU:HA	1.80	0.45
7:T:63:ASN:O	7:T:65:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:59:DT:H2''	2:J:60:DC:O5'	2.17	0.45
2:J:98:DC:C2'	2:J:99:DG:O5'	2.65	0.45
2:J:331:DC:H2''	2:J:332:DG:OP2	2.17	0.45
5:M:50:TYR:O	5:M:54:VAL:HG23	2.17	0.45
7:T:72:ILE:O	7:T:76:VAL:HG23	2.17	0.45
2:J:11:DT:H2'	2:J:12:DT:H72	1.99	0.45
2:J:161:DT:C2'	2:J:162:DT:H72	2.47	0.45
5:G:56:GLU:O	5:G:57:TYR:C	2.59	0.45
1:I:152:DA:C6	1:I:153:DC:C4	3.05	0.45
1:I:210:DG:OP2	6:H:42:TYR:OH	2.30	0.45
1:I:13:DA:C1'	1:I:14:DA:H5'	2.46	0.44
1:I:312:DC:H2''	1:I:313:DA:C8	2.52	0.44
2:J:237:DT:C4	2:J:238:DA:C6	3.05	0.44
2:J:301:DG:N3	2:J:302:DA:C5	2.85	0.44
5:G:84:GLN:HG2	5:G:105:GLY:O	2.17	0.44
5:M:61:GLU:O	5:M:65:LEU:HD12	2.17	0.44
1:I:65:DA:H2''	1:I:66:DC:O5'	2.16	0.44
1:I:202:DG:C6	1:I:203:DG:C6	3.05	0.44
2:J:95:DG:OP1	4:F:46:ILE:N	2.40	0.44
2:J:338:DT:H2''	2:J:339:DT:C7	2.48	0.44
7:T:32:ILE:HG12	7:T:32:ILE:O	2.17	0.44
5:C:81:ARG:O	5:C:85:LEU:HG	2.17	0.44
3:K:118:THR:HA	4:L:45:ARG:O	2.17	0.44
1:I:64:DC:H2''	1:I:65:DA:H5''	2.00	0.44
1:I:214:DG:H4'	1:I:215:DC:OP1	2.16	0.44
5:M:26:PRO:HG3	6:N:40:TYR:CZ	2.53	0.44
6:N:105:GLU:OE1	6:N:105:GLU:HA	2.18	0.44
4:P:32:PRO:HB2	4:P:36:ARG:HH12	1.83	0.44
2:J:321:DC:H2''	2:J:322:DA:C8	2.51	0.44
4:F:90:LEU:HB3	4:F:95:ARG:O	2.18	0.44
4:F:101:GLY:O	4:F:102:GLY:C	2.60	0.44
3:K:42:ARG:O	3:K:43:PRO:C	2.60	0.44
3:K:128:ARG:HB3	3:K:133:GLU:HB2	2.00	0.44
4:L:72:TYR:OH	6:N:76:GLU:OE1	2.21	0.44
4:P:64:ASN:HD22	4:P:64:ASN:H	1.66	0.44
1:I:9:DA:C6	1:I:10:DA:C6	3.06	0.44
1:I:22:DT:H2''	1:I:23:DC:OP2	2.18	0.44
3:E:119:ILE:HD12	4:F:50:ILE:HD12	2.00	0.44
6:N:39:ILE:HD11	6:N:40:TYR:CZ	2.52	0.44
1:I:94:DC:H4'	4:P:45:ARG:CZ	2.48	0.44
1:I:217:DC:H2''	1:I:218:DA:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:343:DC:H2''	1:I:344:DG:C8	2.53	0.44
3:A:59:GLU:N	3:A:59:GLU:OE1	2.51	0.44
4:B:72:TYR:OH	6:D:76:GLU:OE1	2.31	0.44
4:F:32:PRO:O	4:F:35:ARG:HB2	2.18	0.44
6:H:42:TYR:O	6:H:43:LYS:C	2.61	0.44
5:M:63:LEU:HD11	6:N:41:VAL:HG13	1.98	0.44
6:R:105:GLU:HA	6:R:105:GLU:OE1	2.18	0.44
7:S:64:ALA:O	7:S:68:ILE:HG12	2.18	0.44
1:I:290:DG:H1'	1:I:291:DA:C8	2.52	0.44
2:J:109:DT:H2''	2:J:110:DG:OP2	2.18	0.44
4:B:76:ALA:O	4:B:77:LYS:HB2	2.17	0.44
6:D:80:LEU:HD13	6:D:80:LEU:HA	1.79	0.44
4:F:39:ARG:NH1	4:F:43:VAL:O	2.50	0.44
5:M:13:LYS:HE3	5:M:13:LYS:HA	1.99	0.44
1:I:74:DA:H3'	4:L:32:PRO:HG3	2.00	0.43
1:I:226:DG:H2''	1:I:227:DT:OP2	2.18	0.43
1:I:233:DG:H2''	1:I:234:DC:C6	2.53	0.43
2:J:95:DG:H2''	2:J:96:DT:C5'	2.47	0.43
2:J:141:DT:H2''	2:J:142:DC:C6	2.53	0.43
6:D:102:LEU:HA	6:D:103:PRO:HD3	1.89	0.43
3:E:118:THR:HA	4:F:45:ARG:O	2.18	0.43
4:L:60:VAL:HG12	4:L:64:ASN:HD21	1.80	0.43
4:L:95:ARG:HD2	4:L:95:ARG:HA	1.88	0.43
7:S:24:ASP:O	7:S:26:PRO:HD3	2.17	0.43
1:I:152:DA:H1'	1:I:153:DC:O5'	2.18	0.43
1:I:275:DT:C2'	1:I:276:DT:O5'	2.66	0.43
7:S:62:GLU:O	7:S:64:ALA:CB	2.66	0.43
1:I:89:DG:H2''	1:I:90:DT:OP2	2.18	0.43
1:I:225:DC:H2''	1:I:226:DG:OP2	2.17	0.43
1:I:282:DC:H2''	1:I:283:DG:OP1	2.18	0.43
2:J:3:DC:H2''	2:J:4:DT:C6	2.53	0.43
2:J:152:DA:C2'	2:J:153:DT:H71	2.48	0.43
1:I:152:DA:C5	1:I:153:DC:C4	3.07	0.43
3:O:42:ARG:O	3:O:43:PRO:C	2.60	0.43
7:S:28:TYR:HB3	7:S:71:SER:HB2	2.00	0.43
7:T:47:ARG:HE	7:T:90:SER:HA	1.82	0.43
1:I:181:DT:H2'	1:I:182:DG:C8	2.53	0.43
1:I:252:DG:H2''	1:I:253:DC:H5''	2.01	0.43
1:I:289:DA:H1'	1:I:290:DG:O4'	2.18	0.43
5:C:49:VAL:HG11	6:D:118:VAL:HA	2.01	0.43
6:R:62:MET:O	6:R:66:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:63:ASN:O	7:S:64:ALA:C	2.61	0.43
1:I:52:DA:C6	1:I:53:DG:C6	3.06	0.43
1:I:87:DC:H1'	1:I:88:DT:H5'	1.99	0.43
5:C:39:TYR:CE1	6:D:74:ALA:CB	3.02	0.43
5:C:47:ALA:N	5:C:48:PRO:HD2	2.34	0.43
5:C:80:PRO:O	5:C:83:LEU:HB2	2.18	0.43
6:H:62:MET:O	6:H:66:VAL:HG23	2.17	0.43
3:K:100:LEU:HD12	4:L:37:LEU:HD13	2.00	0.43
5:M:37:GLY:HA3	5:M:39:TYR:CD2	2.53	0.43
2:J:273:DG:C5'	3:K:40:ARG:HD2	2.49	0.43
6:D:79:ARG:O	6:D:80:LEU:C	2.61	0.43
1:I:209:DA:H4'	5:G:77:ARG:NE	2.34	0.43
2:J:101:DT:H2''	2:J:102:DT:OP2	2.18	0.43
2:J:210:DA:P	6:R:42:TYR:OH	2.73	0.43
6:N:72:ARG:O	6:N:101:LEU:HD11	2.19	0.43
2:J:223:DC:H2''	2:J:224:DT:OP2	2.18	0.43
2:J:241:DG:OP2	2:J:241:DG:H2'	2.19	0.43
3:E:51:ILE:O	3:E:52:ARG:C	2.62	0.43
3:E:120:MET:O	3:E:121:PRO:C	2.62	0.43
4:F:54:THR:O	4:F:57:VAL:N	2.52	0.43
3:K:76:GLN:O	3:K:77:ASP:C	2.62	0.43
5:Q:88:ARG:CD	5:Q:94:ASN:OD1	2.64	0.43
1:I:173:DC:H2''	1:I:174:DT:H72	2.00	0.43
2:J:95:DG:H2''	2:J:96:DT:H5''	2.00	0.43
2:J:192:DT:C6	2:J:193:DT:H72	2.54	0.43
2:J:272:DT:P	3:K:46:VAL:HB	2.59	0.43
6:D:95:GLN:HE21	6:D:95:GLN:HB2	1.68	0.43
3:K:73:GLU:O	3:K:76:GLN:HB2	2.19	0.43
5:Q:42:ARG:O	6:R:88:THR:HA	2.18	0.43
1:I:23:DC:C4	1:I:24:DC:N4	2.87	0.42
5:M:43:VAL:HG12	5:M:44:GLY:O	2.19	0.42
6:R:84:ASN:O	6:R:85:LYS:HB2	2.18	0.42
1:I:84:DG:C4	1:I:85:DC:C5	3.07	0.42
1:I:137:DA:H2''	1:I:138:DC:OP2	2.17	0.42
1:I:290:DG:H5''	3:A:83:ARG:CD	2.49	0.42
5:C:62:ILE:HD11	6:D:65:PHE:CE2	2.54	0.42
6:D:103:PRO:O	6:D:104:GLY:C	2.62	0.42
3:E:118:THR:HA	4:F:45:ARG:HB3	2.01	0.42
3:E:120:MET:N	3:E:123:ASP:OD2	2.48	0.42
5:G:46:GLY:O	5:G:49:VAL:HB	2.18	0.42
7:S:31:MET:SD	7:S:58:TYR:CD2	3.13	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:78:THR:OG1	7:S:80:VAL:HG23	2.19	0.42
7:T:34:ALA:O	7:T:38:ALA:HB3	2.19	0.42
4:L:66:ILE:HA	4:L:69:ALA:HB3	2.01	0.42
2:J:120:DT:H2'	2:J:121:DC:C5	2.54	0.42
2:J:162:DT:H2''	2:J:163:DT:OP1	2.17	0.42
4:F:31:LYS:N	4:F:32:PRO:CD	2.82	0.42
6:H:70:PHE:O	6:H:71:GLU:C	2.61	0.42
5:Q:26:PRO:HG3	6:R:40:TYR:CZ	2.55	0.42
5:Q:47:ALA:N	5:Q:48:PRO:HD2	2.35	0.42
6:R:41:VAL:HG11	6:R:59:MET:SD	2.59	0.42
7:T:63:ASN:O	7:T:66:SER:N	2.50	0.42
1:I:96:DG:H2''	1:I:97:DC:O5'	2.19	0.42
2:J:201:DC:C4	2:J:202:DG:C6	3.08	0.42
3:E:59:GLU:OE1	3:E:59:GLU:N	2.39	0.42
4:F:54:THR:O	4:F:55:ARG:C	2.62	0.42
2:J:242:DG:H2''	2:J:243:DC:OP2	2.19	0.42
5:C:84:GLN:OE1	5:C:84:GLN:HA	2.19	0.42
6:R:79:ARG:O	6:R:80:LEU:C	2.63	0.42
1:I:102:DT:H5'	1:I:102:DT:C6	2.54	0.42
1:I:124:DC:H2''	1:I:125:DT:C7	2.50	0.42
3:A:61:LEU:HD21	4:B:40:ARG:NH2	2.34	0.42
6:D:72:ARG:O	6:D:101:LEU:HD11	2.19	0.42
6:N:65:PHE:HA	4:P:98:TYR:CE2	2.55	0.42
7:S:40:LYS:HA	7:S:40:LYS:HD2	1.87	0.42
1:I:349:DG:H2''	1:I:350:DG:C8	2.55	0.42
2:J:62:DA:H1'	2:J:63:DG:C8	2.54	0.42
6:D:36:SER:OG	6:D:37:TYR:N	2.52	0.42
5:G:61:GLU:O	5:G:65:LEU:HD12	2.20	0.42
3:O:70:LEU:HD11	3:O:74:ILE:HD11	2.01	0.42
7:T:32:ILE:HD12	7:T:54:ILE:HA	2.00	0.42
1:I:209:DA:O3'	6:H:42:TYR:OH	2.38	0.42
1:I:332:DG:C4'	1:I:333:DA:OP1	2.63	0.42
2:J:293:DC:H4'	2:J:294:DT:OP1	2.20	0.42
2:J:313:DG:H2''	2:J:314:DG:O5'	2.20	0.42
3:A:48:LEU:HA	3:A:51:ILE:HD12	2.01	0.42
4:F:29:ILE:HG13	4:F:58:LEU:HD23	2.02	0.42
6:H:102:LEU:HA	6:H:103:PRO:HD3	1.94	0.42
3:K:51:ILE:HD11	4:L:43:VAL:O	2.20	0.42
7:S:32:ILE:HG22	7:S:36:ILE:CD1	2.50	0.42
1:I:75:DC:H1'	1:I:76:DG:H5'	2.02	0.42
1:I:212:DC:H4'	1:I:213:DC:OP1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:39:TYR:CD1	6:R:74:ALA:HB1	2.53	0.42
1:I:311:DG:H2''	1:I:312:DC:C6	2.55	0.41
2:J:34:DA:H4'	2:J:35:DC:OP1	2.19	0.41
2:J:68:DG:H2''	2:J:69:DG:C8	2.54	0.41
3:A:95:ALA:O	3:A:96:CYS:C	2.63	0.41
3:E:65:LEU:O	3:E:66:PRO:C	2.63	0.41
4:F:22:LEU:O	4:F:25:ASN:ND2	2.52	0.41
6:N:39:ILE:HG13	6:N:40:TYR:N	2.36	0.41
6:R:123:SER:O	6:R:125:LYS:N	2.53	0.41
1:I:322:DA:H4'	1:I:323:DC:OP1	2.20	0.41
2:J:104:DA:H2''	2:J:105:DG:H8	1.84	0.41
5:C:39:TYR:CE1	6:D:74:ALA:HB1	2.55	0.41
6:D:106:LEU:HD12	6:D:106:LEU:HA	1.95	0.41
4:L:66:ILE:O	4:L:69:ALA:HB3	2.20	0.41
4:P:83:ALA:O	4:P:87:VAL:HG23	2.20	0.41
5:Q:37:GLY:HA3	5:Q:39:TYR:CE2	2.55	0.41
1:I:12:DA:C6	1:I:13:DA:C5	3.08	0.41
1:I:281:DC:C2	1:I:282:DC:C5	3.09	0.41
2:J:1:DC:H2''	2:J:2:DG:C8	2.55	0.41
2:J:111:DC:C2'	2:J:112:DT:C6	3.03	0.41
5:G:31:HIS:HA	5:G:48:PRO:HB3	2.03	0.41
3:O:100:LEU:O	3:O:103:LEU:HB3	2.19	0.41
1:I:40:DT:H2''	1:I:41:DC:C5	2.56	0.41
1:I:42:DA:N3	1:I:43:DA:C5	2.88	0.41
2:J:152:DA:H2'	2:J:153:DT:H71	2.02	0.41
5:M:63:LEU:HD22	6:N:45:LEU:HD13	2.01	0.41
5:M:79:ILE:HG12	5:M:82:HIS:CE1	2.56	0.41
3:O:92:LEU:HG	4:P:86:VAL:HG11	2.02	0.41
5:Q:54:VAL:HG21	6:R:98:VAL:HG21	2.03	0.41
1:I:6:DC:H2''	1:I:7:DG:C8	2.56	0.41
1:I:308:DC:H2''	1:I:309:DA:C8	2.55	0.41
2:J:87:DG:C4	2:J:88:DC:C5	3.09	0.41
2:J:200:DC:P	2:J:200:DC:C3'	3.07	0.41
5:G:16:THR:O	5:G:19:SER:N	2.53	0.41
3:K:79:LYS:HD2	4:L:74:GLU:OE2	2.20	0.41
4:L:56:GLY:O	4:L:59:LYS:HB3	2.20	0.41
5:M:71:ARG:O	5:M:74:LYS:N	2.42	0.41
6:R:45:LEU:HD21	6:R:53:GLY:O	2.20	0.41
1:I:150:DG:C5	1:I:151:DC:C4	3.08	0.41
1:I:273:DC:H5'	3:A:40:ARG:HB2	2.02	0.41
2:J:145:DC:OP1	5:G:77:ARG:N	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:219:DG:H2''	2:J:220:DA:H8	1.84	0.41
3:A:47:ALA:O	3:A:48:LEU:C	2.63	0.41
3:E:51:ILE:HG22	3:E:52:ARG:N	2.34	0.41
4:F:50:ILE:HG22	4:F:51:TYR:N	2.36	0.41
7:S:69:LYS:HG3	7:S:89:ALA:HB2	2.01	0.41
3:A:121:PRO:C	3:A:123:ASP:H	2.29	0.41
3:K:99:TYR:HE2	4:L:57:VAL:HG12	1.86	0.41
1:I:214:DG:H1'	1:I:215:DC:C6	2.56	0.41
1:I:232:DA:H2''	1:I:233:DG:H5''	2.02	0.41
1:I:240:DC:H1'	1:I:241:DA:H5'	2.02	0.41
1:I:242:DC:H2''	1:I:243:DC:C6	2.55	0.41
2:J:129:DA:C2'	2:J:130:DA:C8	3.03	0.41
2:J:301:DG:H1'	2:J:302:DA:N7	2.35	0.41
4:B:88:TYR:CG	6:D:83:TYR:CE2	3.08	0.41
5:C:26:PRO:HG3	6:D:40:TYR:CZ	2.56	0.41
5:G:79:ILE:HB	5:G:80:PRO:HD2	2.02	0.41
1:I:14:DA:H1'	1:I:15:DA:H5'	2.03	0.41
1:I:192:DA:H4'	1:I:193:DT:OP1	2.21	0.41
1:I:210:DG:OP1	5:G:77:ARG:HD3	2.21	0.41
1:I:265:DG:C2'	1:I:266:DT:H72	2.51	0.41
2:J:25:DC:H5'	2:J:25:DC:H6	1.85	0.41
2:J:75:DA:C5	2:J:76:DC:C4	3.08	0.41
2:J:94:DC:C2'	2:J:95:DG:C8	3.04	0.41
2:J:232:DG:C4	2:J:233:DC:C5	3.09	0.41
4:B:78:ARG:NH1	4:B:82:THR:HG23	2.36	0.41
5:C:26:PRO:HD3	6:D:40:TYR:CE1	2.56	0.41
5:C:111:ILE:HG12	3:E:51:ILE:HG21	2.02	0.41
6:D:39:ILE:O	6:D:43:LYS:HG3	2.20	0.41
5:G:87:ILE:HG22	5:G:88:ARG:HD3	2.03	0.41
6:H:65:PHE:CE2	6:H:69:ILE:HD13	2.55	0.41
6:H:75:GLY:O	6:H:76:GLU:C	2.63	0.41
4:L:76:ALA:O	4:L:77:LYS:C	2.63	0.41
1:I:237:DT:C2'	1:I:238:DA:C8	3.03	0.41
5:Q:44:GLY:HA3	10:Q:201:CL:CL	2.58	0.41
3:E:60:LEU:HB3	3:E:93:GLN:NE2	2.36	0.40
6:H:68:ASP:OD1	6:H:72:ARG:NE	2.45	0.40
6:N:67:ASN:HB3	4:P:102:GLY:O	2.21	0.40
4:P:89:ALA:O	4:P:92:ARG:HB2	2.21	0.40
5:Q:46:GLY:N	10:Q:201:CL:CL	2.85	0.40
1:I:33:DA:H4'	5:M:77:ARG:NE	2.36	0.40
1:I:189:DA:H4'	1:I:190:DA:OP1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:219:DA:C2'	1:I:220:DT:H72	2.51	0.40
1:I:300:DC:H2''	1:I:301:DT:H72	2.03	0.40
2:J:143:DG:H1'	2:J:144:DG:C8	2.57	0.40
2:J:178:DC:OP2	7:T:97:LYS:CD	2.69	0.40
4:P:88:TYR:CE1	6:R:83:TYR:CD1	3.09	0.40
2:J:11:DT:H2''	2:J:12:DT:C6	2.57	0.40
2:J:56:DG:C2	2:J:57:DC:C2	3.09	0.40
2:J:187:DT:H2''	2:J:188:DT:C6	2.55	0.40
5:C:44:GLY:CA	10:C:201:CL:CL	3.03	0.40
4:F:76:ALA:O	4:F:77:LYS:C	2.64	0.40
7:S:75:LEU:HD13	7:S:81:LEU:HD13	2.02	0.40
1:I:11:DA:H1'	1:I:12:DA:H5'	2.02	0.40
1:I:267:DC:H2''	1:I:268:DT:H72	2.03	0.40
1:I:274:DG:H2''	1:I:275:DT:C7	2.51	0.40
1:I:289:DA:C2	1:I:290:DG:C2	3.10	0.40
2:J:302:DA:C4	2:J:303:DC:C5	3.10	0.40
5:G:57:TYR:CZ	5:G:61:GLU:OE1	2.74	0.40
4:L:89:ALA:O	4:L:90:LEU:C	2.64	0.40
5:M:68:ASN:O	5:M:71:ARG:N	2.54	0.40
5:M:108:LEU:HD23	5:M:108:LEU:HA	1.93	0.40
4:P:30:THR:HB	4:P:32:PRO:HD2	2.04	0.40
5:Q:87:ILE:HG23	5:Q:93:LEU:HB3	2.04	0.40
1:I:55:DC:H2''	1:I:56:DA:H8	1.84	0.40
1:I:101:DT:H2''	1:I:102:DT:OP2	2.21	0.40
2:J:117:DC:H2''	2:J:118:DT:O5'	2.21	0.40
2:J:219:DG:C2	2:J:220:DA:C5	3.09	0.40
5:C:50:TYR:CE2	6:D:95:GLN:NE2	2.90	0.40
6:D:65:PHE:CZ	6:D:69:ILE:HD13	2.56	0.40
6:N:46:LYS:O	6:N:50:PRO:HG3	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:51:ASP:OD2	5:Q:57:TYR:OH[1_455]	2.10	0.10
5:C:61:GLU:OE1	6:H:51:ASP:OD2[1_455]	2.17	0.03

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	96/138 (70%)	79 (82%)	16 (17%)	1 (1%)	12	25
3	E	96/138 (70%)	78 (81%)	16 (17%)	2 (2%)	5	13
3	K	96/138 (70%)	81 (84%)	14 (15%)	1 (1%)	12	25
3	O	97/138 (70%)	86 (89%)	10 (10%)	1 (1%)	12	25
4	B	78/105 (74%)	64 (82%)	12 (15%)	2 (3%)	4	9
4	F	80/105 (76%)	68 (85%)	9 (11%)	3 (4%)	2	5
4	L	78/105 (74%)	61 (78%)	16 (20%)	1 (1%)	9	21
4	P	78/105 (74%)	70 (90%)	7 (9%)	1 (1%)	9	21
5	C	105/132 (80%)	85 (81%)	14 (13%)	6 (6%)	1	2
5	G	104/132 (79%)	86 (83%)	15 (14%)	3 (3%)	3	8
5	M	106/132 (80%)	88 (83%)	14 (13%)	4 (4%)	2	5
5	Q	105/132 (80%)	89 (85%)	15 (14%)	1 (1%)	12	25
6	D	94/128 (73%)	77 (82%)	11 (12%)	6 (6%)	1	1
6	H	95/128 (74%)	76 (80%)	15 (16%)	4 (4%)	2	3
6	N	94/128 (73%)	80 (85%)	14 (15%)	0	100	100
6	R	94/128 (73%)	74 (79%)	16 (17%)	4 (4%)	2	4
7	S	73/195 (37%)	58 (80%)	8 (11%)	7 (10%)	0	0
7	T	73/195 (37%)	60 (82%)	10 (14%)	3 (4%)	2	4
All	All	1642/2402 (68%)	1360 (83%)	232 (14%)	50 (3%)	3	8

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	50	ILE
5	C	14	ALA
6	D	32	SER
6	D	33	ARG

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Mol	Chain	Res	Type
5	G	17	ARG
6	R	32	SER
6	R	33	ARG
7	S	39	GLU
7	S	63	ASN
7	S	64	ALA
7	T	30	ASP
7	T	64	ALA
5	C	44	GLY
5	C	72	ASP
6	D	104	GLY
4	F	50	ILE
5	G	14	ALA
6	H	104	GLY
5	M	64	GLU
5	Q	64	GLU
6	R	104	GLY
6	R	124	ALA
7	S	27	LYS
4	B	30	THR
5	C	71	ARG
6	D	79	ARG
6	D	80	LEU
3	E	117	VAL
4	F	51	TYR
7	S	62	GLU
7	T	26	PRO
5	C	49	VAL
5	C	98	GLY
3	E	51	ILE
6	H	54	ILE
6	H	120	LYS
3	K	43	PRO
4	L	26	ILE
5	M	44	GLY
5	M	69	ALA
4	P	67	ARG
6	D	124	ALA
5	G	49	VAL
7	S	28	TYR
7	S	58	TYR
6	H	75	GLY

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Mol	Chain	Res	Type
3	O	43	PRO
3	A	51	ILE
5	M	49	VAL
4	F	26	ILE

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	85/113 (75%)	80 (94%)	5 (6%)	18	37
3	E	85/113 (75%)	81 (95%)	4 (5%)	23	47
3	K	85/113 (75%)	80 (94%)	5 (6%)	18	37
3	O	86/113 (76%)	80 (93%)	6 (7%)	14	29
4	B	65/81 (80%)	63 (97%)	2 (3%)	35	60
4	F	67/81 (83%)	65 (97%)	2 (3%)	36	61
4	L	65/81 (80%)	60 (92%)	5 (8%)	12	25
4	P	65/81 (80%)	62 (95%)	3 (5%)	24	48
5	C	85/102 (83%)	72 (85%)	13 (15%)	3	5
5	G	84/102 (82%)	78 (93%)	6 (7%)	13	28
5	M	85/102 (83%)	80 (94%)	5 (6%)	18	37
5	Q	84/102 (82%)	71 (84%)	13 (16%)	2	5
6	D	82/107 (77%)	68 (83%)	14 (17%)	2	3
6	H	83/107 (78%)	67 (81%)	16 (19%)	1	2
6	N	82/107 (77%)	71 (87%)	11 (13%)	4	7
6	R	82/107 (77%)	74 (90%)	8 (10%)	7	16
7	S	62/158 (39%)	49 (79%)	13 (21%)	1	1
7	T	62/158 (39%)	51 (82%)	11 (18%)	2	3
All	All	1394/1928 (72%)	1252 (90%)	142 (10%)	7	15

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	39	HIS
3	A	40	ARG
3	A	87	SER
3	A	118	THR
3	A	129	ARG
4	B	71	THR
4	B	82	THR
5	C	13	LYS
5	C	15	LYS
5	C	16	THR
5	C	18	SER
5	C	24	GLN
5	C	29	ARG
5	C	71	ARG
5	C	72	ASP
5	C	73	ASN
5	C	74	LYS
5	C	81	ARG
5	C	101	THR
5	C	119	LYS
6	D	36	SER
6	D	42	TYR
6	D	80	LEU
6	D	85	LYS
6	D	87	SER
6	D	90	THR
6	D	91	SER
6	D	93	GLU
6	D	99	ARG
6	D	101	LEU
6	D	113	GLU
6	D	118	VAL
6	D	123	SER
6	D	125	LYS
3	E	48	LEU
3	E	87	SER
3	E	117	VAL
3	E	122	LYS
4	F	47	SER
4	F	95	ARG
5	G	13	LYS
5	G	24	GLN
5	G	71	ARG

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Mol	Chain	Res	Type
5	G	74	LYS
5	G	81	ARG
5	G	101	THR
6	H	31	ARG
6	H	36	SER
6	H	38	SER
6	H	48	VAL
6	H	52	THR
6	H	56	SER
6	H	63	ASN
6	H	69	ILE
6	H	78	SER
6	H	85	LYS
6	H	87	SER
6	H	88	THR
6	H	101	LEU
6	H	105	GLU
6	H	106	LEU
6	H	122	THR
3	K	48	LEU
3	K	68	GLN
3	K	77	ASP
3	K	129	ARG
3	K	134	ARG
4	L	30	THR
4	L	80	THR
4	L	82	THR
4	L	92	ARG
4	L	95	ARG
5	M	24	GLN
5	M	71	ARG
5	M	74	LYS
5	M	81	ARG
5	M	107	VAL
6	N	31	ARG
6	N	52	THR
6	N	55	SER
6	N	63	ASN
6	N	78	SER
6	N	85	LYS
6	N	91	SER
6	N	101	LEU

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Mol	Chain	Res	Type
6	N	113	GLU
6	N	118	VAL
6	N	122	THR
3	O	43	PRO
3	O	48	LEU
3	O	59	GLU
3	O	87	SER
3	O	129	ARG
3	O	134	ARG
4	P	47	SER
4	P	64	ASN
4	P	73	THR
5	Q	13	LYS
5	Q	15	LYS
5	Q	16	THR
5	Q	19	SER
5	Q	24	GLN
5	Q	29	ARG
5	Q	30	VAL
5	Q	56	GLU
5	Q	62	ILE
5	Q	72	ASP
5	Q	74	LYS
5	Q	76	THR
5	Q	81	ARG
6	R	78	SER
6	R	80	LEU
6	R	88	THR
6	R	99	ARG
6	R	101	LEU
6	R	106	LEU
6	R	118	VAL
6	R	125	LYS
7	S	23	THR
7	S	32	ILE
7	S	33	VAL
7	S	45	SER
7	S	49	SER
7	S	52	LYS
7	S	59	LYS
7	S	60	VAL
7	S	68	ILE

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Mol	Chain	Res	Type
7	S	84	THR
7	S	90	SER
7	S	92	SER
7	S	97	LYS
7	T	24	ASP
7	T	25	HIS
7	T	31	MET
7	T	33	VAL
7	T	40	LYS
7	T	50	ILE
7	T	52	LYS
7	T	60	VAL
7	T	67	GLN
7	T	68	ILE
7	T	84	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	76	GLN
3	A	108	ASN
4	B	64	ASN
5	C	24	GLN
5	C	89	ASN
6	D	47	GLN
6	D	63	ASN
6	D	95	GLN
3	E	68	GLN
3	E	93	GLN
3	E	108	ASN
3	E	125	GLN
4	F	64	ASN
5	G	24	GLN
5	G	89	ASN
6	H	49	HIS
4	L	64	ASN
4	L	93	GLN
5	M	24	GLN
6	N	47	GLN
6	N	49	HIS
6	N	63	ASN
6	N	82	HIS

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Mol	Chain	Res	Type
6	N	95	GLN
4	P	64	ASN
4	P	75	HIS
6	R	47	GLN
6	R	49	HIS
6	R	63	ASN
6	R	95	GLN
7	S	51	GLN
7	S	67	GLN
7	T	51	GLN
7	T	67	GLN
7	T	83	GLN

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](#)

Of 12 ligands modelled in this entry, 12 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	I	353/353 (100%)	-0.56	0 100 100	69, 146, 265, 317	0
2	J	353/353 (100%)	-0.51	0 100 100	83, 145, 263, 358	0
3	A	98/138 (71%)	-0.37	0 100 100	58, 85, 134, 163	0
3	E	98/138 (71%)	-0.35	0 100 100	39, 72, 117, 171	0
3	K	98/138 (71%)	-0.29	0 100 100	59, 85, 137, 167	0
3	O	99/138 (71%)	-0.32	0 100 100	53, 81, 134, 184	0
4	B	80/105 (76%)	-0.36	0 100 100	51, 79, 117, 169	0
4	F	82/105 (78%)	-0.41	3 (3%) 45 35	42, 65, 107, 242	0
4	L	80/105 (76%)	-0.27	0 100 100	55, 83, 123, 169	0
4	P	80/105 (76%)	-0.38	1 (1%) 75 68	46, 75, 113, 172	0
5	C	107/132 (81%)	-0.26	0 100 100	41, 70, 117, 202	0
5	G	106/132 (80%)	-0.39	0 100 100	40, 78, 120, 152	0
5	M	108/132 (81%)	-0.34	1 (0%) 81 76	50, 77, 123, 176	0
5	Q	107/132 (81%)	-0.15	2 (1%) 66 59	42, 78, 148, 208	0
6	D	96/128 (75%)	-0.33	0 100 100	45, 71, 140, 167	0
6	H	97/128 (75%)	-0.34	0 100 100	50, 76, 169, 219	0
6	N	96/128 (75%)	-0.25	0 100 100	56, 81, 143, 196	0
6	R	96/128 (75%)	-0.31	1 (1%) 79 74	54, 76, 148, 170	0
7	S	75/195 (38%)	0.40	1 (1%) 75 68	104, 167, 213, 284	1 (1%)
7	T	75/195 (38%)	0.45	1 (1%) 75 68	181, 240, 294, 319	1 (1%)
All	All	2384/3108 (76%)	-0.34	10 (0%) 88 87	39, 93, 235, 358	2 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	P	102	GLY	3.1
4	F	21	VAL	3.1
7	T	54	ILE	3.0
5	Q	14	ALA	2.8
4	F	22	LEU	2.7
5	M	12	ALA	2.7
5	Q	12	ALA	2.6
4	F	102	GLY	2.5
6	R	30	LYS	2.4
7	S	29	SER	2.3

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(Å ²)	Q<0.9
9	K	I	403	1/1	0.85	0.09	116,116,116,116	0
9	K	J	404	1/1	0.85	0.15	134,134,134,134	0
8	CA	J	401	1/1	0.86	0.07	125,125,125,125	0
9	K	I	404	1/1	0.93	0.05	110,110,110,110	0
8	CA	I	402	1/1	0.93	0.06	116,116,116,116	0
9	K	J	402	1/1	0.94	0.06	101,101,101,101	0
9	K	J	403	1/1	0.95	0.08	97,97,97,97	0
10	CL	M	201	1/1	0.95	0.05	83,83,83,83	0
8	CA	I	401	1/1	0.96	0.05	119,119,119,119	0
10	CL	Q	201	1/1	0.97	0.05	69,69,69,69	0
10	CL	C	201	1/1	0.98	0.07	72,72,72,72	0
10	CL	G	201	1/1	0.98	0.04	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.