



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 08:08 AM JST

PDB ID : 6LA8  
Title : 349 bp di-nucleosome harboring cohesive DNA termini assembled with linker histone H1.0  
Authors : Adhireksan, Z.; Lee, P.L.; Sharma, D.; Davey, C.A.  
Deposited on : 2019-11-12  
Resolution : 3.40 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](mailto: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>.

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

MolProbity : 4.02b-467  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

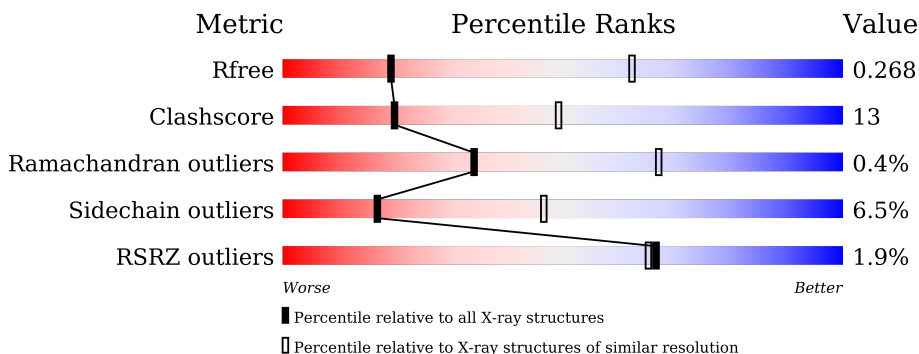
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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  $\geq 3$ , 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	136	
1	E	136	
1	K	136	
1	O	136	
2	B	103	
2	F	103	

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Mol	Chain	Length	Quality of chain
2	L	103	 70% 8% 22%
2	P	103	 68% 10% 22%
3	C	130	 75% 10% 15%
3	G	130	 72% 8% 19%
3	M	130	 69% 12% 18%
3	Q	130	 74% 7% 19%
4	D	126	 58% 17% 24%
4	H	126	 61% 13% 24%
4	N	126	 60% 15% 24%
4	R	126	 60% 15% 24%
5	I	349	 30% 67%
6	J	349	 42% 56%
7	S	194	 13% 23% 12% 62%

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 27058 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
			Total	C	N	O	S			
1	A	100	Total 825	C 520	N 160	O 141	S 4	0	0	0
1	E	99	Total 816	C 514	N 158	O 140	S 4	0	0	0
1	K	99	Total 816	C 514	N 158	O 140	S 4	0	0	0
1	O	98	Total 807	C 508	N 156	O 139	S 4	0	0	0

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	81	Total 646	C 407	N 126	O 112	S 1	0	0	0
2	F	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	L	80	Total 638	C 401	N 125	O 111	S 1	0	0	0
2	P	80	Total 638	C 401	N 125	O 111	S 1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	110	Total 849	C 535	N 168	O 146	0	0	0
3	G	105	Total 810	C 511	N 158	O 141	0	0	0
3	M	106	Total 819	C 517	N 160	O 142	0	0	0
3	Q	105	Total 812	C 512	N 158	O 142	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	H	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	N	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	R	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			

- Molecule 5 is a DNA chain called DNA (349-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	349	Total	C	N	O	P	0	0	0
			7149	3389	1357	2054	349			

- Molecule 6 is a DNA chain called DNA (349-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	349	Total	C	N	O	P	0	0	0
			7162	3407	1270	2136	349			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	S	74	Total	C	N	O	S	0	0	0
			568	354	107	106	1			

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	1	Total	Ca	0	0
			1	1		
8	I	11	Total	Ca	0	0
			11	11		
8	J	10	Total	Ca	0	0
			10	10		
8	M	1	Total	Ca	0	0
			1	1		

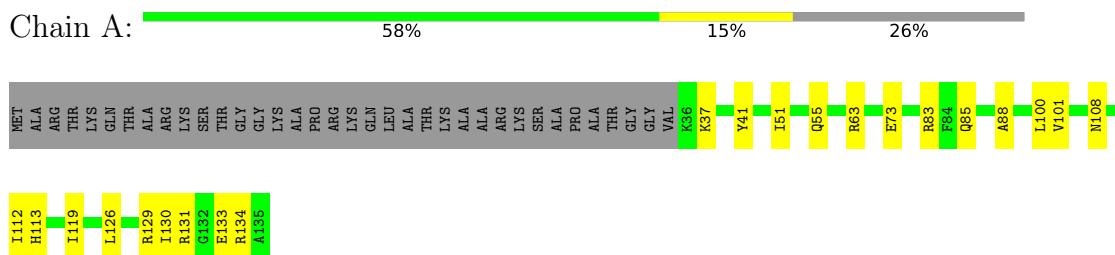
- Molecule 9 is POTASSIUM ION (three-letter code: K) (formula: K).

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
9	I	2	Total K 2 2	0	0
9	J	5	Total K 5 5	0	0

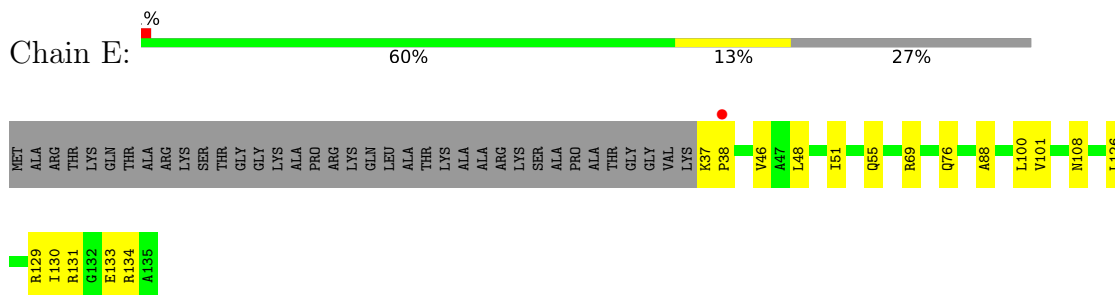
### 3 Residue-property plots [i](#)

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.

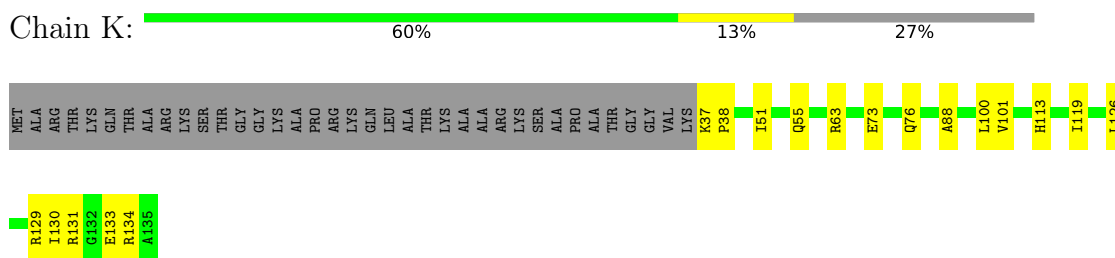
- Molecule 1: Histone H3.1



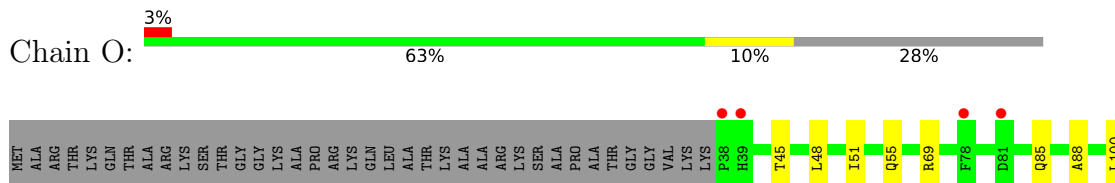
- Molecule 1: Histone H3.1



- Molecule 1: Histone H3.1

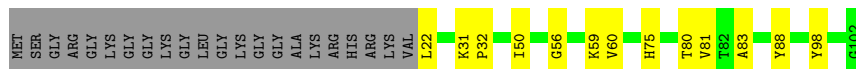


- Molecule 1: Histone H3.1

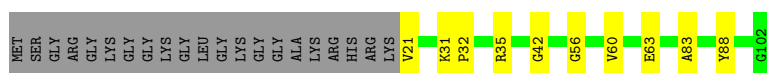




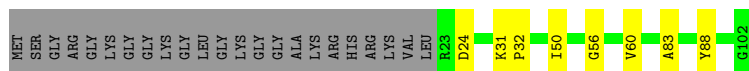
- Molecule 2: Histone H4



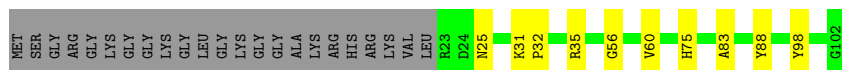
- Molecule 2: Histone H4



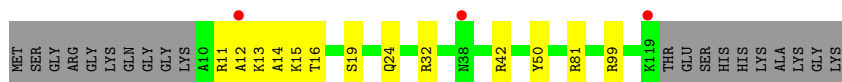
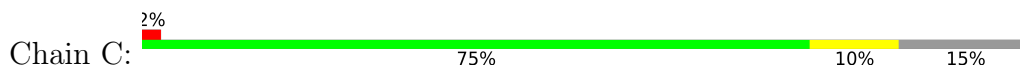
- Molecule 2: Histone H4



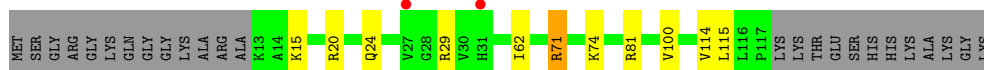
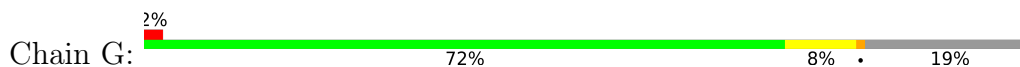
- Molecule 2: Histone H4



- Molecule 3: Histone H2A type 1-B/E



- Molecule 3: Histone H2A type 1-B/E



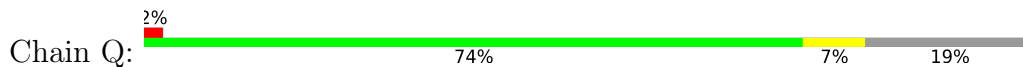
- Molecule 3: Histone H2A type 1-B/E



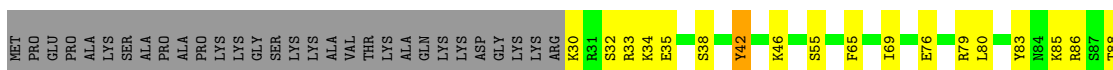




- Molecule 3: Histone H2A type 1-B/E



- Molecule 4: Histone H2B type 1-J



- Molecule 4: Histone H2B type 1-J



- Molecule 4: Histone H2B type 1-J

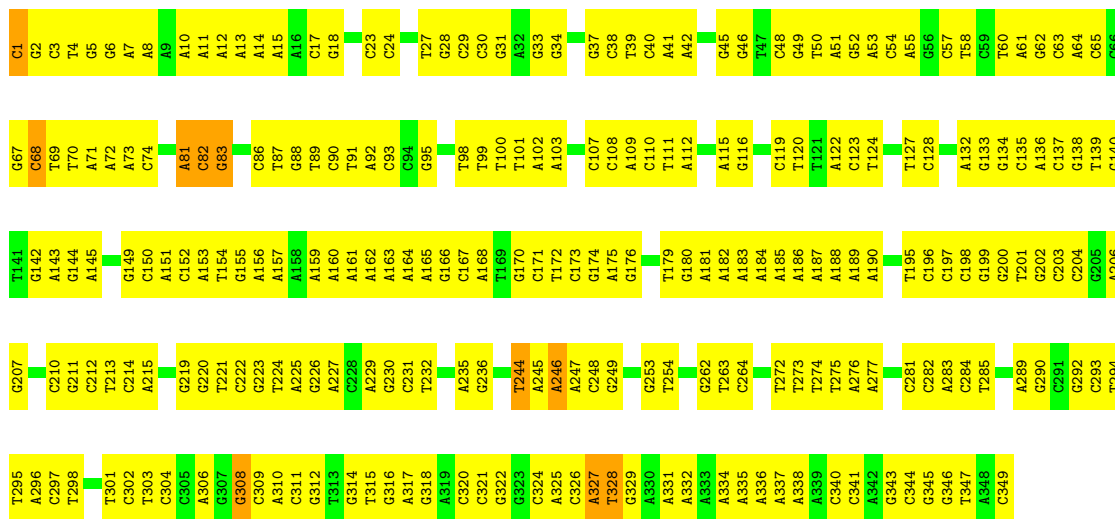
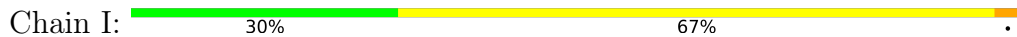


- Molecule 4: Histone H2B type 1-J





• Molecule 5: DNA (349-MER)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.06Å 184.07Å 223.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 3.40 49.32 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.32-3.40) 99.8 (49.32-3.40)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 3.40Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.206 , 0.265 0.212 , 0.268	Depositor DCC
$R_{free}$ test set	1381 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	126.8	Xtrriage
Anisotropy	0.222	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 89.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	27058	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	160.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

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

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	0.63	0/837	0.77	0/1120
1	E	0.62	0/828	0.77	0/1109
1	K	0.63	0/828	0.78	0/1109
1	O	0.63	0/819	0.77	0/1097
2	B	0.65	0/653	0.82	0/873
2	F	0.65	0/660	0.81	0/883
2	L	0.65	0/645	0.80	0/862
2	P	0.66	0/645	0.80	0/862
3	C	0.64	0/859	0.78	0/1157
3	G	0.64	0/820	0.78	0/1107
3	M	0.65	0/829	0.77	0/1118
3	Q	0.65	0/822	0.78	0/1110
4	D	0.65	0/766	0.76	0/1026
4	H	0.66	0/766	0.77	0/1026
4	N	0.66	0/766	0.76	0/1026
4	R	0.66	0/766	0.76	0/1026
5	I	0.57	10/8032 (0.1%)	0.85	5/12384 (0.0%)
6	J	0.54	3/8022 (0.0%)	0.85	4/12387 (0.0%)
7	S	0.72	0/574	0.85	0/765
All	All	0.60	13/28937 (0.0%)	0.82	9/42047 (0.0%)

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	1	DC	OP3-P	-10.47	1.48	1.61
5	I	1	DC	OP3-P	-10.20	1.49	1.61
5	I	306	DA	O3'-P	-7.53	1.52	1.61
5	I	327	DA	O3'-P	-5.72	1.54	1.61
5	I	328	DT	O3'-P	-5.52	1.54	1.61
5	I	111	DT	O3'-P	-5.43	1.54	1.61
6	J	141	DC	O3'-P	-5.32	1.54	1.61
5	I	244	DT	O3'-P	-5.32	1.54	1.61
5	I	298	DT	O3'-P	-5.30	1.54	1.61
6	J	254	DT	O3'-P	-5.12	1.55	1.61
5	I	68	DC	O3'-P	-5.12	1.55	1.61
5	I	83	DG	O3'-P	-5.07	1.55	1.61
5	I	246	DA	O3'-P	-5.06	1.55	1.61

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	343	DG	C1'-O4'-C4'	-6.93	103.17	110.10
6	J	335	DT	C1'-O4'-C4'	-6.41	103.69	110.10
5	I	82	DC	C1'-O4'-C4'	-6.35	103.75	110.10
5	I	308	DG	C1'-O4'-C4'	-6.32	103.78	110.10
6	J	346	DG	N9-C1'-C2'	5.54	123.12	112.60
5	I	81	DA	C1'-O4'-C4'	-5.45	104.65	110.10
5	I	46	DG	C1'-O4'-C4'	-5.11	105.00	110.10
5	I	115	DA	C1'-O4'-C4'	-5.09	105.00	110.10
6	J	16	DT	N1-C1'-C2'	5.09	122.27	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	14	ALA	Peptide

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	825	0	869	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	816	0	856	14	0
1	K	816	0	856	10	0
1	O	807	0	844	9	0
2	B	646	0	687	15	0
2	F	653	0	696	6	0
2	L	638	0	676	5	0
2	P	638	0	676	8	0
3	C	849	0	915	5	0
3	G	810	0	866	7	0
3	M	819	0	879	11	0
3	Q	812	0	868	4	0
4	D	755	0	784	13	0
4	H	755	0	784	15	0
4	N	755	0	784	13	0
4	R	755	0	784	15	0
5	I	7149	0	3902	245	1
6	J	7162	0	3943	242	1
7	S	568	0	597	22	1
8	G	1	0	0	0	0
8	I	11	0	0	0	0
8	J	10	0	0	0	0
8	M	1	0	0	0	0
9	I	2	0	0	0	0
9	J	5	0	0	0	0
All	All	27058	0	21266	598	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 13.

All (598) 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)
6:J:318:DC:H2''	6:J:319:DA:C8	1.60	1.35
5:I:346:DG:H2''	5:I:347:DT:OP2	1.41	1.14
5:I:153:DA:H2''	5:I:154:DT:OP2	1.51	1.08
4:H:49:HIS:HB3	4:H:52:THR:CG2	1.85	1.05
6:J:35:DG:H2'	6:J:36:DT:H72	1.34	1.04
6:J:202:DC:H2''	6:J:203:DT:OP2	1.58	1.02
4:R:49:HIS:HB3	4:R:52:THR:CG2	1.89	1.02
6:J:253:DG:H2''	6:J:254:DT:H72	1.38	1.02
6:J:345:DG:H4'	6:J:346:DG:OP1	1.59	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:73:GLU:O	1:K:76:GLN:HG2	1.61	1.00
5:I:262:DG:H2''	5:I:263:DT:OP2	1.64	0.95
6:J:318:DC:H2''	6:J:319:DA:N7	1.84	0.93
5:I:119:DC:H2''	5:I:120:DT:OP2	1.69	0.92
5:I:171:DC:H2''	5:I:172:DT:O5'	1.70	0.91
6:J:15:DT:H2'	6:J:16:DT:C6	2.05	0.91
5:I:230:DG:H2''	5:I:231:DC:OP2	1.68	0.91
6:J:23:DC:H2''	6:J:24:DC:OP2	1.72	0.90
6:J:162:DT:H2''	6:J:163:DT:C5'	2.02	0.89
6:J:346:DG:H4'	6:J:347:DT:OP1	1.69	0.89
4:H:49:HIS:HB3	4:H:52:THR:HG23	1.53	0.88
6:J:24:DC:H2''	6:J:25:DG:O5'	1.74	0.88
6:J:162:DT:H2''	6:J:163:DT:H5'	1.55	0.88
5:I:340:DC:H2''	5:I:341:DC:OP2	1.74	0.88
5:I:134:DG:H2''	5:I:135:DC:C6	2.09	0.88
6:J:193:DT:H2'	6:J:194:DG:C8	2.10	0.87
6:J:15:DT:H2''	6:J:16:DT:O5'	1.73	0.86
5:I:154:DT:H2''	5:I:155:DG:OP2	1.76	0.85
6:J:198:DC:H2''	6:J:199:DG:C8	2.11	0.85
5:I:303:DT:H2''	5:I:304:DC:OP2	1.76	0.85
4:R:49:HIS:HB3	4:R:52:THR:HG23	1.58	0.85
6:J:35:DG:H2'	6:J:36:DT:C7	2.06	0.84
6:J:339:DT:H4'	6:J:340:DC:OP1	1.76	0.84
6:J:253:DG:H2''	6:J:254:DT:C7	2.09	0.83
6:J:345:DG:C4'	6:J:346:DG:OP1	2.27	0.82
3:G:71:ARG:HH21	4:H:52:THR:HG22	1.43	0.82
5:I:28:DG:H2''	5:I:29:DC:OP2	1.77	0.82
6:J:15:DT:H2''	6:J:16:DT:C5'	2.10	0.81
6:J:163:DT:H2''	6:J:164:DT:O5'	1.80	0.81
6:J:24:DC:H2'	6:J:25:DG:C8	2.17	0.80
7:S:47:ARG:NH2	7:S:48:GLN:OE1	2.15	0.80
5:I:112:DA:H8	5:I:112:DA:P	2.03	0.80
5:I:175:DA:H2''	5:I:176:DG:OP2	1.82	0.79
6:J:192:DA:H2''	6:J:193:DT:O4'	1.84	0.78
6:J:162:DT:C2'	6:J:163:DT:H5'	2.14	0.78
6:J:175:DG:OP2	6:J:175:DG:H2'	1.83	0.77
5:I:346:DG:C2'	5:I:347:DT:OP2	2.29	0.77
7:S:36:ILE:HD11	7:S:95:LEU:HD11	1.67	0.76
5:I:165:DA:H2''	5:I:166:DG:OP2	1.84	0.76
1:E:76:GLN:HE22	2:F:21:VAL:HG12	1.50	0.76
6:J:14:DT:H2''	6:J:15:DT:OP2	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:340:DC:H2''	6:J:341:DC:OP2	1.87	0.75
6:J:264:DG:H2''	6:J:265:DT:OP2	1.84	0.75
6:J:313:DC:H2''	6:J:314:DT:OP2	1.85	0.75
6:J:347:DT:H4'	6:J:348:DA:OP1	1.87	0.74
5:I:37:DG:H2''	5:I:38:DC:OP2	1.87	0.74
5:I:134:DG:H2''	5:I:135:DC:H6	1.52	0.74
5:I:48:DC:H2''	5:I:49:DG:OP2	1.88	0.74
6:J:188:DT:H1'	6:J:189:DT:H5'	1.70	0.73
6:J:318:DC:C2'	6:J:319:DA:C8	2.56	0.73
6:J:52:DA:H1'	6:J:53:DG:C8	2.24	0.73
5:I:68:DC:C2'	5:I:69:DT:H5'	2.19	0.72
5:I:6:DG:H2''	5:I:7:DA:O5'	1.89	0.72
5:I:132:DA:N6	6:J:214:DT:O4	2.20	0.72
6:J:211:DG:H2''	6:J:212:DC:OP2	1.90	0.72
3:M:50:TYR:OH	4:N:95:GLN:NE2	2.22	0.72
6:J:15:DT:C2'	6:J:16:DT:C6	2.74	0.71
5:I:101:DT:H2''	5:I:102:DA:C8	2.26	0.71
7:S:43:ALA:O	7:S:84:THR:HG21	1.90	0.70
5:I:344:DC:H2''	5:I:345:DG:O4'	1.90	0.70
5:I:244:DT:H2''	5:I:245:DA:OP2	1.89	0.70
3:M:32:ARG:NH1	4:N:35:GLU:OE2	2.24	0.70
6:J:38:DC:H2''	6:J:39:DC:OP2	1.90	0.70
7:S:28:TYR:O	7:S:32:ILE:HG12	1.92	0.70
4:H:108:LYS:HA	4:H:108:LYS:HE2	1.74	0.70
5:I:309:DC:H2'	5:I:310:DA:C8	2.27	0.69
5:I:253:DG:H2''	5:I:254:DT:H72	1.74	0.69
6:J:253:DG:C2'	6:J:254:DT:H72	2.17	0.69
4:D:42:TYR:OH	5:I:33:DG:OP2	2.07	0.69
5:I:273:DT:H2''	5:I:274:DT:OP2	1.91	0.69
5:I:311:DC:H2''	5:I:312:DG:OP2	1.91	0.69
5:I:3:DC:H2''	5:I:4:DT:OP2	1.93	0.69
5:I:321:DC:H2''	5:I:322:DG:C8	2.28	0.69
5:I:30:DC:H2''	5:I:31:DG:OP2	1.93	0.68
5:I:226:DG:H1'	5:I:227:DA:C8	2.28	0.68
5:I:343:DG:H2''	5:I:344:DC:OP2	1.92	0.68
5:I:11:DA:H1'	5:I:12:DA:O5'	1.94	0.68
5:I:139:DT:H2''	5:I:140:DG:OP2	1.93	0.68
6:J:251:DC:H2''	6:J:252:DG:O5'	1.93	0.68
1:A:119:ILE:HG13	2:B:50:ILE:HD12	1.76	0.68
6:J:15:DT:H2'	6:J:16:DT:H6	1.55	0.68
6:J:318:DC:C2'	6:J:319:DA:N7	2.55	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:289:DA:H2''	5:I:290:DG:OP2	1.94	0.67
7:S:50:ILE:O	7:S:54:ILE:HG13	1.94	0.67
5:I:155:DG:OP2	5:I:155:DG:H8	1.77	0.67
5:I:164:DA:H2''	5:I:165:DA:OP2	1.92	0.67
6:J:186:DT:H2''	6:J:187:DT:OP2	1.92	0.67
5:I:292:DG:H2''	5:I:293:DC:OP2	1.94	0.67
5:I:13:DA:C8	5:I:13:DA:H5''	2.30	0.66
5:I:14:DA:C2'	5:I:15:DA:O5'	2.43	0.66
6:J:156:DT:OP1	1:O:45:THR:HG21	1.95	0.66
6:J:198:DC:H1'	6:J:199:DG:C8	2.30	0.66
5:I:207:DG:OP2	4:N:42:TYR:OH	2.14	0.66
1:E:37:LYS:NZ	6:J:332:DT:OP1	2.29	0.65
5:I:68:DC:H2''	5:I:69:DT:H5'	1.77	0.65
6:J:269:DT:H1'	6:J:270:DG:H5'	1.77	0.65
5:I:1:DC:H2''	5:I:2:DG:OP2	1.94	0.65
5:I:119:DC:C2'	5:I:120:DT:OP2	2.45	0.65
6:J:90:DG:H2''	6:J:91:DT:OP2	1.96	0.65
6:J:204:DC:H2''	6:J:205:DA:OP2	1.96	0.64
5:I:294:DT:H4'	5:I:295:DT:OP1	1.97	0.64
6:J:143:DG:H8	6:J:143:DG:OP2	1.81	0.64
5:I:29:DC:H2''	5:I:30:DC:OP2	1.96	0.64
5:I:2:DG:OP2	5:I:2:DG:H8	1.81	0.64
6:J:37:DG:H2''	6:J:38:DC:OP2	1.99	0.63
6:J:335:DT:H2''	6:J:336:DT:C5	2.33	0.63
6:J:188:DT:H4'	6:J:189:DT:OP1	1.99	0.63
5:I:134:DG:H2''	5:I:135:DC:C5	2.34	0.62
6:J:335:DT:H2''	6:J:336:DT:C6	2.33	0.62
4:H:49:HIS:CB	4:H:52:THR:HG23	2.28	0.62
5:I:174:DG:OP2	5:I:174:DG:H2'	1.98	0.62
6:J:175:DG:H4'	6:J:176:DC:OP1	1.99	0.62
6:J:344:DC:H2''	6:J:345:DG:O5'	1.98	0.62
5:I:272:DT:H2''	5:I:273:DT:OP2	1.98	0.62
5:I:274:DT:H2''	5:I:275:DT:OP2	2.00	0.62
5:I:334:DA:H2''	5:I:335:DA:OP2	1.99	0.62
6:J:188:DT:H1'	6:J:189:DT:C5'	2.29	0.62
3:C:32:ARG:NH1	4:D:35:GLU:OE2	2.32	0.61
5:I:127:DT:H2''	5:I:128:DC:C6	2.35	0.61
5:I:6:DG:C2'	5:I:7:DA:O5'	2.49	0.61
6:J:198:DC:C2'	6:J:199:DG:C8	2.83	0.61
3:G:15:LYS:HB2	6:J:218:DG:OP1	2.01	0.61
6:J:318:DC:H2''	6:J:319:DA:H8	1.54	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:87:VAL:HG22	7:S:88:GLY:H	1.64	0.61
5:I:153:DA:C2'	5:I:154:DT:OP2	2.30	0.61
4:H:108:LYS:HA	4:H:108:LYS:CE	2.31	0.61
6:J:183:DT:H4'	6:J:184:DT:OP1	2.00	0.61
6:J:98:DG:H2''	6:J:99:DT:OP2	2.00	0.60
6:J:223:DG:H1'	6:J:224:DT:H5'	1.83	0.60
6:J:347:DT:C4'	6:J:348:DA:OP1	2.49	0.60
6:J:191:DC:H2''	6:J:192:DA:O4'	2.01	0.60
6:J:253:DG:H2''	6:J:254:DT:OP2	2.01	0.60
6:J:24:DC:C2'	6:J:25:DG:C8	2.84	0.60
5:I:69:DT:H2''	5:I:70:DT:OP2	2.00	0.60
5:I:99:DT:H2''	5:I:100:DT:OP2	2.02	0.60
6:J:127:DC:H2''	6:J:128:DA:C8	2.37	0.60
6:J:6:DG:C8	6:J:7:DT:H72	2.37	0.60
5:I:276:DA:H1'	5:I:277:DA:C8	2.36	0.60
6:J:94:DG:H2''	6:J:95:DT:H5'	1.83	0.60
6:J:316:DG:H1'	6:J:317:DG:C5	2.37	0.60
1:A:108:ASN:HD21	3:G:115:LEU:HD11	1.66	0.60
5:I:156:DA:H2''	5:I:157:DA:OP2	2.02	0.60
5:I:149:DG:H2''	5:I:150:DC:OP2	2.02	0.59
6:J:202:DC:C2'	6:J:203:DT:OP2	2.37	0.59
7:S:95:LEU:N	7:S:95:LEU:HD22	2.17	0.59
5:I:13:DA:C8	5:I:13:DA:C5'	2.86	0.59
5:I:301:DT:H2''	5:I:302:DC:OP2	2.02	0.59
6:J:25:DG:H2''	6:J:26:DG:OP2	2.03	0.59
5:I:296:DA:H1'	5:I:297:DC:H5'	1.83	0.59
5:I:13:DA:C5'	5:I:13:DA:H8	2.15	0.59
5:I:248:DC:H1'	5:I:249:DG:H5'	1.85	0.58
6:J:194:DG:H2''	6:J:195:DT:H5'	1.84	0.58
6:J:187:DT:H2''	6:J:188:DT:OP2	2.02	0.58
5:I:52:DG:H1'	5:I:53:DA:C8	2.38	0.58
6:J:199:DG:C2'	6:J:200:DG:O5'	2.51	0.58
5:I:41:DA:H2''	5:I:42:DA:C8	2.39	0.58
1:K:37:LYS:HB3	1:K:38:PRO:HD2	1.85	0.58
5:I:281:DC:H2'	5:I:282:DC:C6	2.39	0.58
6:J:315:DC:OP2	6:J:315:DC:H6	1.87	0.58
5:I:180:DG:H2''	5:I:181:DA:OP2	2.03	0.58
4:R:49:HIS:CB	4:R:52:THR:HG23	2.32	0.58
1:E:69:ARG:NH2	5:I:103:DA:OP2	2.37	0.58
5:I:221:DT:H2''	5:I:222:DC:OP2	2.02	0.58
5:I:230:DG:C2'	5:I:231:DC:OP2	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:241:DG:OP2	6:J:241:DG:H2'	2.04	0.57
5:I:308:DG:H2''	5:I:309:DC:C6	2.39	0.57
6:J:30:DC:H2''	6:J:31:DA:OP2	2.04	0.57
1:A:73:GLU:CD	2:B:22:LEU:HB2	2.25	0.57
5:I:11:DA:H2''	5:I:12:DA:OP2	2.04	0.57
6:J:162:DT:H2''	6:J:163:DT:O4'	2.03	0.57
6:J:340:DC:C2'	6:J:341:DC:OP2	2.53	0.57
1:E:37:LYS:CG	1:E:38:PRO:HD2	2.34	0.57
1:A:119:ILE:HD12	2:B:50:ILE:HD13	1.87	0.57
6:J:1:DC:H2'	6:J:2:DG:C8	2.39	0.57
6:J:347:DT:H1'	6:J:348:DA:C8	2.39	0.57
5:I:235:DA:H1'	5:I:236:DG:C8	2.40	0.57
5:I:1:DC:H2''	5:I:2:DG:C8	2.40	0.56
6:J:198:DC:H2''	6:J:199:DG:N7	2.20	0.56
5:I:174:DG:H2'	5:I:174:DG:P	2.45	0.56
5:I:329:DG:C2	6:J:18:DA:C2	2.92	0.56
7:S:32:ILE:HD11	7:S:68:ILE:HG23	1.87	0.56
5:I:14:DA:H2''	5:I:15:DA:O5'	2.03	0.56
5:I:137:DC:H2''	5:I:138:DG:OP2	2.04	0.56
6:J:268:DG:H2''	6:J:269:DT:H5'	1.87	0.56
6:J:12:DT:H2''	6:J:13:DT:OP2	2.04	0.56
6:J:15:DT:H2''	6:J:16:DT:H5'	1.87	0.56
6:J:317:DG:H2''	6:J:318:DC:O4'	2.05	0.56
6:J:230:DC:H2''	6:J:231:DT:OP2	2.06	0.56
3:Q:42:ARG:O	4:R:88:THR:HA	2.06	0.56
3:Q:71:ARG:HH21	4:R:52:THR:HG22	1.71	0.56
1:A:119:ILE:HG13	2:B:50:ILE:CD1	2.36	0.56
6:J:117:DT:H2'	6:J:118:DG:C8	2.41	0.55
6:J:264:DG:C2'	6:J:265:DT:OP2	2.54	0.55
6:J:241:DG:H1'	6:J:242:DG:C8	2.41	0.55
6:J:15:DT:H2'	6:J:16:DT:H71	1.88	0.55
6:J:131:DT:H2''	6:J:132:DG:N7	2.21	0.55
5:I:244:DT:C2'	5:I:245:DA:OP2	2.55	0.55
5:I:263:DT:H2''	5:I:264:DC:OP2	2.07	0.55
6:J:275:DT:H2''	6:J:276:DA:C8	2.42	0.55
5:I:112:DA:P	5:I:112:DA:C8	2.94	0.55
7:S:32:ILE:HG23	7:S:50:ILE:HD12	1.88	0.55
6:J:193:DT:H2'	6:J:194:DG:N9	2.21	0.55
6:J:240:DC:H2''	6:J:241:DG:OP2	2.07	0.55
5:I:225:DA:H1'	5:I:226:DG:H5'	1.89	0.54
1:K:37:LYS:HB3	1:K:38:PRO:CD	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:36:ILE:CD1	7:S:95:LEU:HD11	2.37	0.54
5:I:253:DG:H2''	5:I:254:DT:C7	2.37	0.54
5:I:327:DA:N3	6:J:20:DG:N2	2.55	0.54
4:D:65:PHE:CE1	4:D:69:ILE:CD1	2.90	0.54
1:E:46:VAL:HB	5:I:95:DG:OP1	2.07	0.54
5:I:41:DA:C2	6:J:306:DG:N2	2.76	0.54
5:I:28:DG:C2'	5:I:29:DC:OP2	2.52	0.54
5:I:247:DA:H1'	5:I:248:DC:H5'	1.88	0.54
6:J:198:DC:C1'	6:J:199:DG:C8	2.90	0.54
6:J:336:DT:H2''	6:J:337:DT:OP2	2.07	0.54
5:I:122:DA:H2''	5:I:123:DC:OP2	2.08	0.54
6:J:162:DT:C3'	6:J:163:DT:H5'	2.38	0.54
6:J:346:DG:C4'	6:J:347:DT:OP1	2.48	0.54
6:J:136:DG:C6	6:J:137:DG:C6	2.96	0.54
5:I:90:DC:H2''	5:I:91:DT:OP2	2.08	0.53
5:I:58:DT:C2	6:J:289:DG:N2	2.76	0.53
5:I:331:DA:H2''	5:I:332:DA:OP2	2.08	0.53
5:I:82:DC:H2''	5:I:83:DG:C8	2.42	0.53
6:J:15:DT:C2'	6:J:16:DT:H6	2.20	0.53
5:I:185:DA:H2''	5:I:186:DA:OP2	2.08	0.53
4:R:65:PHE:CE1	4:R:69:ILE:CD1	2.91	0.53
5:I:273:DT:H1'	5:I:274:DT:O5'	2.09	0.53
6:J:262:DG:H8	6:J:262:DG:OP2	1.91	0.53
5:I:23:DC:H2''	5:I:24:DC:OP2	2.08	0.53
5:I:73:DA:C2	5:I:74:DC:C2	2.97	0.53
1:A:41:TYR:HA	5:I:156:DA:H5''	1.90	0.53
5:I:39:DT:H2''	5:I:40:DC:OP2	2.08	0.53
5:I:223:DG:H2''	5:I:224:DT:OP2	2.09	0.53
6:J:271:DC:H2''	6:J:272:DG:OP2	2.09	0.53
5:I:112:DA:H8	5:I:112:DA:O5'	1.92	0.53
5:I:138:DG:H2''	5:I:139:DT:OP2	2.09	0.53
6:J:143:DG:H2''	6:J:144:DC:C6	2.44	0.53
4:H:65:PHE:CE1	4:H:69:ILE:CD1	2.91	0.52
5:I:135:DC:H2'	5:I:136:DA:C8	2.45	0.52
4:N:65:PHE:CE1	4:N:69:ILE:CD1	2.91	0.52
5:I:245:DA:H2''	5:I:246:DA:OP2	2.08	0.52
5:I:54:DC:H2''	5:I:55:DA:C8	2.45	0.52
5:I:81:DA:H2''	5:I:82:DC:C6	2.44	0.52
5:I:174:DG:H2'	5:I:174:DG:O5'	2.09	0.52
5:I:317:DA:H2'	5:I:318:DG:C8	2.45	0.52
6:J:195:DT:H2''	6:J:196:DG:OP2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:231:DT:H2''	6:J:232:DT:OP2	2.09	0.52
5:I:160:DA:H2''	5:I:161:DA:OP2	2.08	0.52
5:I:174:DG:H4'	5:I:175:DA:OP1	2.09	0.52
6:J:82:DG:H2''	6:J:83:DA:C8	2.45	0.52
6:J:165:DT:H4'	6:J:166:DC:OP1	2.09	0.52
6:J:254:DT:OP2	6:J:254:DT:H73	2.09	0.52
6:J:337:DT:H2''	6:J:338:DT:OP2	2.09	0.52
5:I:38:DC:H2''	5:I:39:DT:OP2	2.09	0.52
5:I:92:DA:H2''	5:I:93:DC:C6	2.44	0.52
6:J:52:DA:H1'	6:J:53:DG:N7	2.24	0.52
5:I:87:DT:H2''	5:I:88:DG:OP2	2.08	0.52
5:I:202:DG:H2''	5:I:203:DC:OP2	2.09	0.52
6:J:319:DA:H2''	6:J:320:DC:C6	2.45	0.52
3:M:100:VAL:HG11	2:P:98:TYR:CE2	2.44	0.52
5:I:183:DA:H1'	5:I:184:DA:O5'	2.10	0.52
1:A:112:ILE:HG23	3:G:114:VAL:HG21	1.91	0.51
6:J:77:DC:H2''	6:J:78:DG:OP2	2.10	0.51
6:J:289:DG:H2''	6:J:290:DC:C6	2.45	0.51
5:I:109:DA:H2''	5:I:110:DC:OP2	2.10	0.51
5:I:151:DA:C2	6:J:196:DG:C2	2.98	0.51
5:I:154:DT:C2'	5:I:155:DG:OP2	2.53	0.51
5:I:180:DG:H1'	5:I:181:DA:OP2	2.11	0.51
6:J:62:DG:OP1	1:O:85:GLN:HA	2.10	0.51
1:K:119:ILE:HG13	2:L:50:ILE:HD12	1.93	0.51
5:I:183:DA:C1'	5:I:184:DA:O5'	2.58	0.51
2:B:98:TYR:CE2	3:G:100:VAL:HG11	2.45	0.51
6:J:35:DG:C2'	6:J:36:DT:H72	2.24	0.51
5:I:324:DC:H2''	5:I:325:DA:OP2	2.10	0.51
6:J:193:DT:C2'	6:J:194:DG:C8	2.91	0.51
6:J:23:DC:C2'	6:J:24:DC:OP2	2.53	0.51
6:J:223:DG:H2''	6:J:224:DT:OP2	2.10	0.51
3:C:11:ARG:HG3	3:C:12:ALA:N	2.26	0.50
4:H:49:HIS:CB	4:H:52:THR:CG2	2.76	0.50
6:J:15:DT:H2'	6:J:16:DT:C5	2.44	0.50
6:J:126:DC:H1'	6:J:127:DC:H5''	1.92	0.50
5:I:282:DC:H2'	5:I:283:DA:C8	2.46	0.50
5:I:327:DA:C2'	5:I:328:DT:O5'	2.60	0.50
6:J:251:DC:H2''	6:J:252:DG:C5'	2.42	0.50
6:J:272:DG:H2''	6:J:273:DT:OP2	2.11	0.50
5:I:231:DC:H2''	5:I:232:DT:OP2	2.12	0.50
7:S:83:GLN:HA	7:S:93:PHE:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:155:DG:C2	6:J:192:DA:C2	3.00	0.50
5:I:175:DA:C4	5:I:176:DG:C8	2.99	0.50
5:I:340:DC:C2'	5:I:341:DC:OP2	2.49	0.50
6:J:87:DC:H2''	6:J:88:DG:OP2	2.12	0.50
6:J:224:DT:H2''	6:J:225:DA:C8	2.47	0.50
6:J:315:DC:H2''	6:J:316:DG:C8	2.46	0.50
7:S:27:LYS:HB3	7:S:30:ASP:HB2	1.94	0.50
4:N:80:LEU:CD1	4:N:96:THR:HB	2.42	0.50
1:A:88:ALA:HA	2:B:83:ALA:HA	1.93	0.50
5:I:67:DG:H2''	5:I:68:DC:O5'	2.12	0.50
5:I:98:DT:H2''	5:I:99:DT:OP2	2.12	0.50
6:J:223:DG:H1'	6:J:224:DT:C5'	2.42	0.50
5:I:180:DG:C2'	5:I:181:DA:OP2	2.59	0.49
6:J:61:DA:H2''	6:J:62:DG:C8	2.48	0.49
3:M:62:ILE:HD11	4:N:65:PHE:CE1	2.47	0.49
3:G:15:LYS:HD2	3:G:20:ARG:HE	1.76	0.49
5:I:64:DA:C2	5:I:65:DC:C2	3.00	0.49
5:I:289:DA:H1'	5:I:290:DG:H5'	1.95	0.49
6:J:155:DG:H4'	6:J:156:DT:OP1	2.12	0.49
4:D:80:LEU:CD1	4:D:96:THR:HB	2.41	0.49
5:I:61:DA:H2''	5:I:62:DG:C8	2.48	0.49
5:I:199:DG:H2''	5:I:200:DG:OP2	2.13	0.49
2:B:88:TYR:CE1	4:D:83:TYR:CE1	3.01	0.49
5:I:214:DC:H4'	5:I:215:DA:OP1	2.12	0.49
6:J:174:DA:H2''	6:J:175:DG:C8	2.47	0.49
5:I:1:DC:C2'	5:I:2:DG:OP2	2.61	0.49
6:J:35:DG:H2''	6:J:36:DT:C6	2.48	0.49
6:J:254:DT:H6	6:J:254:DT:O5'	1.95	0.49
1:A:85:GLN:HA	5:I:62:DG:OP1	2.13	0.49
5:I:143:DA:C2'	5:I:144:DG:C8	2.95	0.49
6:J:161:DT:H1'	6:J:162:DT:O5'	2.12	0.49
6:J:288:DA:C6	6:J:289:DG:C6	3.00	0.49
6:J:297:DC:H2''	6:J:298:DG:C8	2.48	0.49
3:M:71:ARG:HB3	3:M:71:ARG:HH11	1.76	0.49
5:I:229:DA:H2''	5:I:230:DG:OP2	2.12	0.49
6:J:64:DG:H1'	6:J:65:DG:H5'	1.95	0.49
4:D:76:GLU:OE2	4:D:79:ARG:NH1	2.46	0.48
5:I:170:DG:H2''	5:I:171:DC:OP2	2.13	0.48
5:I:132:DA:H2''	5:I:133:DG:N7	2.27	0.48
2:P:88:TYR:CD1	4:R:83:TYR:CZ	3.02	0.48
4:R:76:GLU:OE2	4:R:79:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:4:DT:H2''	5:I:5:DG:OP2	2.12	0.48
5:I:27:DT:H2''	5:I:28:DG:OP2	2.13	0.48
1:K:88:ALA:HA	2:L:83:ALA:HA	1.95	0.48
5:I:162:DA:H2''	5:I:163:DA:OP2	2.13	0.48
1:O:69:ARG:HB3	2:P:25:ASN:OD1	2.13	0.48
5:I:163:DA:H2''	5:I:164:DA:OP2	2.13	0.48
6:J:304:DT:H2''	6:J:305:DT:OP2	2.14	0.48
6:J:319:DA:C5	6:J:320:DC:N4	2.82	0.48
6:J:64:DG:H1'	6:J:65:DG:C5'	2.43	0.48
6:J:149:DG:H1'	6:J:150:DG:C8	2.49	0.48
6:J:302:DA:H2''	6:J:303:DA:OP2	2.13	0.48
1:O:88:ALA:HA	2:P:83:ALA:HA	1.95	0.48
5:I:337:DA:H2''	5:I:338:DA:OP2	2.13	0.48
5:I:3:DC:C2'	5:I:4:DT:OP2	2.61	0.48
5:I:317:DA:C2'	5:I:318:DG:C8	2.96	0.48
6:J:269:DT:H2''	6:J:270:DG:H5'	1.96	0.48
4:R:49:HIS:CB	4:R:52:THR:CG2	2.79	0.48
2:P:75:HIS:HB2	4:R:96:THR:HG21	1.96	0.47
6:J:167:DA:H2''	6:J:168:DT:OP2	2.13	0.47
6:J:194:DG:H2'	6:J:195:DT:C6	2.49	0.47
6:J:263:DC:H2''	6:J:264:DG:OP2	2.14	0.47
1:A:113:HIS:CG	1:E:126:LEU:HD22	2.49	0.47
5:I:10:DA:C2	6:J:337:DT:C2	3.02	0.47
5:I:314:DG:H4'	5:I:315:DT:OP1	2.14	0.47
5:I:325:DA:N3	5:I:326:DC:C6	2.83	0.47
6:J:188:DT:H2''	6:J:189:DT:H71	1.97	0.47
5:I:63:DC:H2''	5:I:64:DA:O5'	2.13	0.47
4:R:30:LYS:O	4:R:30:LYS:HG2	2.15	0.47
5:I:310:DA:H2''	5:I:311:DC:C6	2.49	0.47
1:E:37:LYS:HG2	1:E:38:PRO:HD2	1.95	0.47
5:I:316:DG:H2''	5:I:317:DA:N7	2.30	0.47
4:N:76:GLU:OE2	4:N:79:ARG:NH1	2.47	0.47
2:P:88:TYR:CE1	4:R:83:TYR:CE1	3.03	0.47
7:S:32:ILE:HD12	7:S:50:ILE:HD11	1.97	0.47
5:I:92:DA:N6	6:J:253:DG:C6	2.83	0.47
5:I:112:DA:H8	5:I:112:DA:OP2	1.97	0.47
5:I:69:DT:C2'	5:I:70:DT:OP2	2.63	0.47
5:I:72:DA:C2	5:I:73:DA:C4	3.02	0.47
6:J:163:DT:H2''	6:J:164:DT:C5'	2.44	0.47
6:J:319:DA:N7	6:J:320:DC:N4	2.62	0.47
4:D:65:PHE:CE1	4:D:69:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:134:DG:C2'	5:I:135:DC:C5	2.98	0.46
6:J:26:DG:H2''	6:J:27:DT:OP2	2.14	0.46
6:J:325:DA:H2''	6:J:326:DT:OP2	2.14	0.46
4:D:32:SER:OG	5:I:116:DG:OP1	2.27	0.46
5:I:179:DT:H2'	5:I:180:DG:C8	2.51	0.46
1:A:51:ILE:O	1:A:55:GLN:HG3	2.16	0.46
4:H:76:GLU:OE2	4:H:79:ARG:NH1	2.48	0.46
6:J:2:DG:H1'	6:J:3:DC:C6	2.50	0.46
6:J:101:DT:H2''	6:J:102:DA:C8	2.51	0.46
5:I:108:DC:H2''	5:I:109:DA:C5'	2.46	0.46
2:F:31:LYS:N	2:F:32:PRO:HD2	2.31	0.46
5:I:108:DC:H2''	5:I:109:DA:H5'	1.97	0.46
1:A:119:ILE:C	2:B:50:ILE:HD11	2.35	0.46
6:J:24:DC:OP2	6:J:24:DC:C6	2.68	0.46
6:J:309:DC:H2''	6:J:310:DG:C8	2.51	0.46
5:I:112:DA:C8	5:I:112:DA:OP2	2.69	0.46
5:I:281:DC:C2'	5:I:282:DC:C6	2.99	0.46
1:K:51:ILE:O	1:K:55:GLN:HG3	2.16	0.46
1:A:126:LEU:HD11	1:A:130:ILE:HD11	1.98	0.46
1:E:51:ILE:O	1:E:55:GLN:HG3	2.16	0.46
5:I:181:DA:OP2	5:I:181:DA:C8	2.69	0.46
5:I:201:DT:H2''	5:I:202:DG:OP2	2.16	0.46
2:B:80:THR:HB	6:J:288:DA:H5''	1.98	0.45
5:I:13:DA:H5''	5:I:13:DA:H8	1.73	0.45
6:J:36:DT:H2''	6:J:37:DG:O5'	2.17	0.45
6:J:57:DT:H2''	6:J:58:DT:OP2	2.16	0.45
2:L:31:LYS:N	2:L:32:PRO:HD2	2.31	0.45
1:O:51:ILE:O	1:O:55:GLN:HG3	2.17	0.45
2:B:31:LYS:N	2:B:32:PRO:HD2	2.32	0.45
5:I:136:DA:H2''	5:I:137:DC:OP2	2.16	0.45
5:I:159:DA:C6	5:I:160:DA:C6	3.05	0.45
4:H:49:HIS:HB3	4:H:52:THR:HG21	1.91	0.45
5:I:143:DA:H2'	5:I:144:DG:C8	2.51	0.45
5:I:173:DC:OP2	5:I:173:DC:C6	2.70	0.45
5:I:212:DC:H2''	5:I:213:DT:OP2	2.16	0.45
5:I:203:DC:H2''	5:I:204:DC:OP2	2.17	0.45
6:J:11:DT:C6	6:J:12:DT:C7	3.00	0.45
6:J:35:DG:C2'	6:J:36:DT:C7	2.87	0.45
3:M:16:THR:O	3:M:19:SER:OG	2.22	0.45
2:P:31:LYS:N	2:P:32:PRO:HD2	2.31	0.45
6:J:286:DA:H2''	6:J:287:DG:O5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:12:DT:C6	6:J:13:DT:C7	3.00	0.45
1:E:88:ALA:HA	2:F:83:ALA:HA	1.98	0.45
5:I:276:DA:C2	6:J:71:DA:C2	3.05	0.45
6:J:161:DT:H2''	6:J:162:DT:OP2	2.15	0.45
5:I:70:DT:H2''	5:I:71:DA:C8	2.52	0.45
6:J:24:DC:OP2	6:J:24:DC:H6	2.00	0.45
6:J:162:DT:H2''	6:J:163:DT:C4'	2.47	0.45
7:S:25:HIS:O	7:S:31:MET:HE2	2.17	0.45
5:I:167:DC:H2''	5:I:168:DA:OP2	2.16	0.45
6:J:29:DT:H2''	6:J:30:DC:OP2	2.17	0.45
6:J:185:DT:H2''	6:J:186:DT:OP2	2.17	0.45
6:J:12:DT:C5	6:J:13:DT:H73	2.52	0.45
5:I:57:DC:H2''	5:I:58:DT:OP2	2.16	0.44
5:I:197:DC:H2''	5:I:198:DC:H5'	1.98	0.44
6:J:15:DT:C2'	6:J:16:DT:O5'	2.51	0.44
6:J:12:DT:C6	6:J:13:DT:H71	2.52	0.44
4:R:65:PHE:CE1	4:R:69:ILE:HD11	2.53	0.44
2:B:88:TYR:CD1	4:D:83:TYR:CZ	3.06	0.44
1:E:126:LEU:HD11	1:E:130:ILE:HD11	2.00	0.44
5:I:108:DC:H2''	5:I:109:DA:O5'	2.18	0.44
5:I:144:DG:H1'	5:I:145:DA:C8	2.52	0.44
5:I:338:DA:C2	6:J:9:DT:O2	2.70	0.44
6:J:263:DC:C4	6:J:264:DG:O6	2.71	0.44
1:O:126:LEU:HD11	1:O:130:ILE:HD11	1.99	0.44
5:I:86:DC:H2''	5:I:87:DT:OP2	2.17	0.44
5:I:262:DG:C2'	5:I:263:DT:OP2	2.44	0.44
6:J:93:DC:H2'	6:J:94:DG:C8	2.52	0.44
6:J:324:DG:H2''	6:J:325:DA:OP2	2.17	0.44
5:I:12:DA:H2''	5:I:13:DA:O5'	2.17	0.44
5:I:91:DT:H4'	5:I:92:DA:OP1	2.17	0.44
4:N:65:PHE:CE1	4:N:69:ILE:HD11	2.53	0.44
6:J:261:DC:H2''	6:J:262:DG:OP2	2.17	0.44
1:E:108:ASN:ND2	2:F:42:GLY:O	2.50	0.43
5:I:150:DC:H2''	5:I:151:DA:OP2	2.18	0.43
5:I:310:DA:H2''	5:I:311:DC:OP2	2.17	0.43
3:M:71:ARG:HB3	3:M:71:ARG:NH1	2.33	0.43
3:G:62:ILE:HD11	4:H:65:PHE:CE1	2.52	0.43
6:J:11:DT:H1'	6:J:12:DT:C6	2.54	0.43
5:I:101:DT:C2'	5:I:102:DA:C8	3.00	0.43
5:I:284:DC:H2''	5:I:285:DT:OP2	2.18	0.43
6:J:247:DA:C4	6:J:248:DA:C8	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:LYS:HG3	1:E:38:PRO:HD2	2.00	0.43
2:F:56:GLY:O	2:F:60:VAL:HG23	2.19	0.43
5:I:17:DC:O2	5:I:18:DG:O4'	2.37	0.43
5:I:175:DA:H1'	5:I:176:DG:O5'	2.18	0.43
5:I:332:DA:C2	6:J:15:DT:C2	3.06	0.43
6:J:110:DC:H2''	6:J:111:DT:OP2	2.19	0.43
6:J:188:DT:C1'	6:J:189:DT:H5'	2.45	0.43
3:M:111:ILE:HG12	1:O:51:ILE:HG21	2.00	0.43
7:S:28:TYR:HA	7:S:31:MET:HB2	2.00	0.43
5:I:197:DC:H2'	5:I:198:DC:C6	2.54	0.43
5:I:6:DG:C2	5:I:7:DA:C2	3.07	0.43
5:I:161:DA:N6	6:J:184:DT:O4	2.52	0.43
6:J:39:DC:H2''	6:J:40:DT:C6	2.54	0.43
6:J:212:DC:H2''	6:J:213:DC:OP2	2.18	0.43
3:C:50:TYR:OH	4:D:95:GLN:NE2	2.40	0.43
5:I:281:DC:H2'	5:I:282:DC:C5	2.54	0.43
5:I:309:DC:H2''	5:I:310:DA:O5'	2.19	0.43
6:J:193:DT:H3'	6:J:194:DG:H8	1.84	0.43
6:J:210:DT:C4	6:J:211:DG:C6	3.07	0.43
2:L:56:GLY:O	2:L:60:VAL:HG23	2.19	0.43
1:A:41:TYR:OH	6:J:193:DT:H2''	2.18	0.42
5:I:2:DG:O6	6:J:343:DG:O6	2.36	0.42
6:J:44:DG:OP2	3:Q:20:ARG:NH2	2.51	0.42
6:J:205:DA:H1'	6:J:206:DC:C6	2.53	0.42
3:M:57:TYR:CZ	4:N:109:HIS:HB3	2.54	0.42
1:A:63:ARG:NH1	5:I:72:DA:H4'	2.34	0.42
3:C:16:THR:O	3:C:19:SER:OG	2.22	0.42
4:D:65:PHE:CZ	4:D:69:ILE:CD1	3.03	0.42
5:I:89:DT:H1'	5:I:90:DC:H5'	2.01	0.42
5:I:337:DA:H2'	5:I:337:DA:O5'	2.19	0.42
6:J:108:DT:H2''	6:J:109:DG:OP2	2.18	0.42
5:I:41:DA:C2	5:I:42:DA:C2	3.06	0.42
6:J:11:DT:O4'	6:J:12:DT:H5'	2.19	0.42
6:J:40:DT:H2''	6:J:41:DG:OP2	2.18	0.42
6:J:59:DC:H4'	6:J:60:DT:H5'	2.01	0.42
6:J:315:DC:OP2	6:J:315:DC:C6	2.69	0.42
1:K:113:HIS:CG	1:O:126:LEU:HD22	2.54	0.42
5:I:142:DG:H1'	5:I:143:DA:C8	2.54	0.42
6:J:14:DT:C5	6:J:15:DT:H73	2.54	0.42
6:J:107:DG:H2''	6:J:108:DT:OP2	2.20	0.42
1:K:131:ARG:HD3	1:K:133:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:O	1:A:101:VAL:C	2.58	0.42
4:H:30:LYS:O	4:H:30:LYS:HG2	2.19	0.42
4:H:65:PHE:CE1	4:H:69:ILE:HD11	2.54	0.42
5:I:327:DA:C2	6:J:20:DG:N2	2.87	0.42
1:K:126:LEU:HD11	1:K:130:ILE:HD11	2.02	0.42
4:N:80:LEU:HD13	4:N:96:THR:HB	2.02	0.42
1:A:119:ILE:CG1	2:B:50:ILE:CD1	2.98	0.42
5:I:107:DC:H2''	5:I:108:DC:O5'	2.19	0.42
5:I:142:DG:N2	6:J:205:DA:C2	2.87	0.42
5:I:165:DA:C2'	5:I:166:DG:OP2	2.62	0.42
5:I:187:DA:H1'	5:I:188:DA:O5'	2.19	0.42
6:J:210:DT:H2''	6:J:211:DG:OP2	2.19	0.42
6:J:312:DC:H2''	6:J:313:DC:OP2	2.20	0.42
5:I:316:DG:C2	5:I:317:DA:C2	3.07	0.42
5:I:320:DC:C4	5:I:321:DC:N4	2.88	0.42
6:J:248:DA:H2''	6:J:249:DC:C6	2.55	0.42
3:M:67:GLY:HA3	4:N:49:HIS:CD2	2.55	0.42
2:P:56:GLY:O	2:P:60:VAL:HG23	2.20	0.42
6:J:14:DT:C2	6:J:15:DT:C6	3.08	0.42
6:J:314:DT:H2''	6:J:315:DC:C5	2.54	0.42
6:J:335:DT:H2''	6:J:336:DT:C7	2.50	0.42
7:S:95:LEU:N	7:S:95:LEU:CD2	2.81	0.42
2:B:56:GLY:O	2:B:60:VAL:HG23	2.20	0.42
3:C:42:ARG:O	4:D:88:THR:HA	2.19	0.42
1:E:100:LEU:O	1:E:101:VAL:C	2.58	0.42
5:I:206:DA:H4'	3:M:77:ARG:CZ	2.49	0.42
6:J:51:DA:C5	6:J:52:DA:C6	3.08	0.42
5:I:30:DC:C2'	5:I:31:DG:OP2	2.64	0.41
5:I:33:DG:C6	5:I:34:DG:C6	3.08	0.41
5:I:186:DA:H2''	5:I:187:DA:OP2	2.19	0.41
5:I:302:DC:H2''	5:I:303:DT:OP2	2.19	0.41
6:J:193:DT:H2'	6:J:194:DG:C1'	2.50	0.41
6:J:203:DT:C2'	6:J:204:DC:OP2	2.68	0.41
6:J:307:DA:C5	6:J:308:DG:C6	3.08	0.41
5:I:171:DC:C2'	5:I:172:DT:O5'	2.53	0.41
5:I:181:DA:H2''	5:I:182:DA:OP2	2.19	0.41
5:I:184:DA:H2''	5:I:185:DA:OP2	2.20	0.41
1:O:100:LEU:O	1:O:101:VAL:C	2.58	0.41
7:S:46:SER:O	7:S:50:ILE:HG23	2.20	0.41
5:I:210:DC:H2''	5:I:211:DG:OP2	2.21	0.41
7:S:36:ILE:HD12	7:S:95:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:308:DG:H2''	5:I:309:DC:C5	2.55	0.41
1:K:100:LEU:O	1:K:101:VAL:C	2.58	0.41
4:R:65:PHE:CZ	4:R:69:ILE:CD1	3.04	0.41
7:S:24:ASP:N	7:S:59:LYS:HG2	2.35	0.41
5:I:60:DT:H2''	5:I:61:DA:C8	2.56	0.41
6:J:150:DG:H2''	6:J:151:DA:H5'	2.02	0.41
2:B:75:HIS:HB2	4:D:96:THR:HG21	2.02	0.41
5:I:325:DA:C4	5:I:326:DC:C6	3.09	0.41
6:J:34:DC:H2''	6:J:35:DG:O4'	2.21	0.41
6:J:81:DA:O5'	6:J:81:DA:H2'	2.21	0.41
4:H:65:PHE:CZ	4:H:69:ILE:CD1	3.03	0.41
5:I:23:DC:O2	6:J:324:DG:N2	2.54	0.41
6:J:199:DG:H2''	6:J:200:DG:O5'	2.19	0.41
6:J:273:DT:C6	6:J:274:DT:H72	2.55	0.41
5:I:189:DA:H2''	5:I:190:DA:OP2	2.20	0.41
5:I:337:DA:O5'	5:I:337:DA:C2'	2.69	0.41
6:J:289:DG:H2''	6:J:290:DC:H6	1.86	0.41
1:A:131:ARG:HD3	1:A:133:GLU:OE2	2.20	0.41
1:E:131:ARG:HD3	1:E:133:GLU:OE2	2.21	0.41
5:I:123:DC:H2''	5:I:124:DT:H71	2.03	0.41
6:J:11:DT:H1'	6:J:12:DT:O5'	2.21	0.41
6:J:47:DT:H2''	6:J:48:DA:H5'	2.03	0.41
6:J:136:DG:C5	6:J:137:DG:C5	3.09	0.41
6:J:147:DC:H2''	6:J:148:DG:C8	2.56	0.41
6:J:336:DT:H1'	6:J:337:DT:H5'	2.02	0.41
5:I:152:DC:H2''	5:I:153:DA:C5'	2.50	0.41
5:I:195:DT:H2''	5:I:196:DC:OP2	2.21	0.41
4:N:65:PHE:CZ	4:N:69:ILE:CD1	3.04	0.41
7:S:46:SER:O	7:S:49:SER:OG	2.28	0.41
5:I:197:DC:H42	6:J:149:DG:H1	1.68	0.40
5:I:219:DG:H2''	5:I:220:DG:OP2	2.21	0.40
6:J:14:DT:H1'	6:J:15:DT:O5'	2.21	0.40
6:J:183:DT:O2	6:J:184:DT:O4'	2.38	0.40
6:J:201:DT:H2''	6:J:202:DC:OP2	2.21	0.40
7:S:32:ILE:CD1	7:S:68:ILE:HG23	2.51	0.40
5:I:50:DT:H2''	5:I:51:DA:N7	2.36	0.40
5:I:345:DG:C2'	5:I:346:DG:C8	3.04	0.40
6:J:11:DT:H6	6:J:11:DT:H2'	1.77	0.40
7:S:25:HIS:HB2	7:S:31:MET:CE	2.51	0.40
5:I:31:DG:OP2	5:I:31:DG:H8	2.04	0.40
6:J:32:DC:H4'	3:Q:77:ARG:NE	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:262:DG:H2''	6:J:263:DC:OP2	2.21	0.40
2:F:88:TYR:CE1	4:H:83:TYR:CE1	3.09	0.40
5:I:8:DA:C2	6:J:339:DT:O2	2.74	0.40
5:I:335:DA:C6	5:I:336:DA:C6	3.08	0.40
6:J:14:DT:C6	6:J:15:DT:C7	3.04	0.40
6:J:68:DG:H2''	6:J:69:DT:OP2	2.20	0.40
6:J:225:DA:C6	6:J:226:DA:C6	3.09	0.40
4:R:70:PHE:CD1	4:R:70:PHE:C	2.95	0.40
1:A:83:ARG:O	2:B:81:VAL:N	2.47	0.40
5:I:6:DG:N1	5:I:7:DA:C2	2.90	0.40
5:I:10:DA:N6	6:J:335:DT:O4	2.54	0.40
5:I:17:DC:H1'	5:I:18:DG:H5'	2.03	0.40
5:I:45:DG:N2	6:J:302:DA:C2	2.90	0.40
5:I:161:DA:OP2	5:I:161:DA:H2'	2.21	0.40
2:L:88:TYR:CE1	4:N:83:TYR:CE1	3.09	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)
5:I:1:DC:O5'	5:I:349:DC:O3'[4_446]	1.84	0.36
6:J:112:DA:OP1	7:S:52:LYS:NZ[3_555]	2.09	0.11

## 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	98/136 (72%)	92 (94%)	6 (6%)	0	100	100
1	E	97/136 (71%)	92 (95%)	5 (5%)	0	100	100
1	K	97/136 (71%)	92 (95%)	5 (5%)	0	100	100
1	O	96/136 (71%)	90 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	79/103 (77%)	74 (94%)	5 (6%)	0	100	100
2	F	80/103 (78%)	76 (95%)	4 (5%)	0	100	100
2	L	78/103 (76%)	74 (95%)	4 (5%)	0	100	100
2	P	78/103 (76%)	73 (94%)	5 (6%)	0	100	100
3	C	108/130 (83%)	100 (93%)	8 (7%)	0	100	100
3	G	103/130 (79%)	94 (91%)	9 (9%)	0	100	100
3	M	104/130 (80%)	96 (92%)	8 (8%)	0	100	100
3	Q	103/130 (79%)	95 (92%)	8 (8%)	0	100	100
4	D	94/126 (75%)	82 (87%)	10 (11%)	2 (2%)	7	30
4	H	94/126 (75%)	81 (86%)	12 (13%)	1 (1%)	14	44
4	N	94/126 (75%)	84 (89%)	9 (10%)	1 (1%)	14	44
4	R	94/126 (75%)	82 (87%)	11 (12%)	1 (1%)	14	44
7	S	72/194 (37%)	62 (86%)	9 (12%)	1 (1%)	11	37
All	All	1569/2174 (72%)	1439 (92%)	124 (8%)	6 (0%)	34	67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	104	GLY
4	H	104	GLY
4	N	104	GLY
4	R	104	GLY
4	D	33	ARG
7	S	26	PRO

### 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	87/111 (78%)	84 (97%)	3 (3%)	37	65
1	E	86/111 (78%)	83 (96%)	3 (4%)	36	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	86/111 (78%)	83 (96%)	3 (4%)	36	65
1	O	85/111 (77%)	82 (96%)	3 (4%)	36	65
2	B	66/79 (84%)	65 (98%)	1 (2%)	65	82
2	F	67/79 (85%)	65 (97%)	2 (3%)	41	68
2	L	65/79 (82%)	64 (98%)	1 (2%)	65	82
2	P	65/79 (82%)	64 (98%)	1 (2%)	65	82
3	C	86/100 (86%)	81 (94%)	5 (6%)	20	50
3	G	83/100 (83%)	78 (94%)	5 (6%)	19	49
3	M	84/100 (84%)	78 (93%)	6 (7%)	14	44
3	Q	84/100 (84%)	79 (94%)	5 (6%)	19	49
4	D	82/105 (78%)	72 (88%)	10 (12%)	5	18
4	H	82/105 (78%)	71 (87%)	11 (13%)	4	15
4	N	82/105 (78%)	74 (90%)	8 (10%)	8	28
4	R	82/105 (78%)	73 (89%)	9 (11%)	6	23
7	S	61/158 (39%)	50 (82%)	11 (18%)	1	6
All	All	1333/1738 (77%)	1246 (94%)	87 (6%)	17	46

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	A	129	ARG
1	A	134	ARG
2	B	59	LYS
3	C	13	LYS
3	C	15	LYS
3	C	24	GLN
3	C	81	ARG
3	C	99	ARG
4	D	30	LYS
4	D	34	LYS
4	D	38	SER
4	D	42	TYR
4	D	46	LYS
4	D	55	SER
4	D	85	LYS
4	D	86	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	D	106	LEU
4	D	122	THR
1	E	48	LEU
1	E	129	ARG
1	E	134	ARG
2	F	35	ARG
2	F	63	GLU
3	G	24	GLN
3	G	29	ARG
3	G	71	ARG
3	G	74	LYS
3	G	81	ARG
4	H	31	ARG
4	H	38	SER
4	H	42	TYR
4	H	46	LYS
4	H	52	THR
4	H	55	SER
4	H	80	LEU
4	H	85	LYS
4	H	101	LEU
4	H	108	LYS
4	H	122	THR
1	K	63	ARG
1	K	129	ARG
1	K	134	ARG
2	L	24	ASP
3	M	24	GLN
3	M	36	LYS
3	M	71	ARG
3	M	74	LYS
3	M	81	ARG
3	M	118	LYS
4	N	31	ARG
4	N	38	SER
4	N	42	TYR
4	N	46	LYS
4	N	55	SER
4	N	85	LYS
4	N	86	ARG
4	N	122	THR
1	O	48	LEU

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Mol	Chain	Res	Type
1	O	129	ARG
1	O	134	ARG
2	P	35	ARG
3	Q	24	GLN
3	Q	29	ARG
3	Q	74	LYS
3	Q	81	ARG
3	Q	99	ARG
4	R	33	ARG
4	R	38	SER
4	R	42	TYR
4	R	46	LYS
4	R	52	THR
4	R	55	SER
4	R	80	LEU
4	R	85	LYS
4	R	122	THR
7	S	24	ASP
7	S	25	HIS
7	S	40	LYS
7	S	47	ARG
7	S	50	ILE
7	S	54	ILE
7	S	59	LYS
7	S	63	ASN
7	S	65	ASP
7	S	82	LYS
7	S	97	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
3	C	24	GLN
4	D	95	GLN
1	E	76	GLN
3	G	24	GLN
3	G	31	HIS
4	H	47	GLN
4	H	95	GLN
3	M	24	GLN
4	N	47	GLN

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Mol	Chain	Res	Type
4	N	49	HIS
4	N	95	GLN
1	O	108	ASN
3	Q	24	GLN
4	R	47	GLN
4	R	95	GLN
7	S	37	GLN
7	S	63	ASN
7	S	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 30 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

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	100/136 (73%)	-0.25	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	94, 119, 167, 210	0
1	E	99/136 (72%)	0.11	1 (1%) <span style="border: 1px solid blue; padding: 2px;">82</span> <span style="border: 1px solid blue; padding: 2px;">81</span>	94, 123, 168, 190	0
1	K	99/136 (72%)	-0.02	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	91, 116, 160, 215	0
1	O	98/136 (72%)	0.10	4 (4%) <span style="border: 1px solid red; padding: 2px;">37</span> <span style="border: 1px solid red; padding: 2px;">36</span>	97, 131, 179, 216	0
2	B	81/103 (78%)	-0.26	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	90, 114, 143, 190	0
2	F	82/103 (79%)	0.07	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	91, 117, 153, 221	0
2	L	80/103 (77%)	0.00	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	87, 111, 148, 220	0
2	P	80/103 (77%)	0.07	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	100, 126, 155, 211	0
3	C	110/130 (84%)	0.12	3 (2%) <span style="border: 1px solid blue; padding: 2px;">54</span> <span style="border: 1px solid blue; padding: 2px;">53</span>	101, 129, 198, 251	0
3	G	105/130 (80%)	0.13	2 (1%) <span style="border: 1px solid blue; padding: 2px;">66</span> <span style="border: 1px solid blue; padding: 2px;">65</span>	96, 127, 183, 202	0
3	M	106/130 (81%)	0.02	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	95, 127, 173, 227	0
3	Q	105/130 (80%)	0.03	2 (1%) <span style="border: 1px solid blue; padding: 2px;">66</span> <span style="border: 1px solid blue; padding: 2px;">65</span>	90, 127, 177, 196	0
4	D	96/126 (76%)	-0.18	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	93, 129, 182, 225	0
4	H	96/126 (76%)	0.19	2 (2%) <span style="border: 1px solid blue; padding: 2px;">63</span> <span style="border: 1px solid blue; padding: 2px;">62</span>	98, 135, 185, 245	0
4	N	96/126 (76%)	0.23	1 (1%) <span style="border: 1px solid blue; padding: 2px;">82</span> <span style="border: 1px solid blue; padding: 2px;">81</span>	99, 130, 196, 241	0
4	R	96/126 (76%)	0.02	2 (2%) <span style="border: 1px solid blue; padding: 2px;">63</span> <span style="border: 1px solid blue; padding: 2px;">62</span>	96, 132, 190, 231	0
5	I	349/349 (100%)	-0.97	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	115, 177, 263, 321	0
6	J	349/349 (100%)	-0.96	1 (0%) <span style="border: 1px solid blue; padding: 2px;">94</span> <span style="border: 1px solid blue; padding: 2px;">93</span>	112, 179, 267, 315	0
7	S	74/194 (38%)	1.75	26 (35%) <span style="border: 1px solid red; padding: 2px;">0</span> <span style="border: 1px solid red; padding: 2px;">0</span>	155, 197, 234, 256	1 (1%)
All	All	2301/2872 (80%)	-0.22	44 (1%) <span style="border: 1px solid blue; padding: 2px;">66</span> <span style="border: 1px solid blue; padding: 2px;">65</span>	87, 139, 221, 321	1 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	S	55	LYS	5.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	N	125	LYS	5.0
4	R	125	LYS	4.5
7	S	93	PHE	4.5
7	S	58	TYR	4.4
1	O	38	PRO	4.3
7	S	54	ILE	4.2
7	S	26	PRO	3.8
7	S	87	VAL	3.7
7	S	57	HIS	3.7
7	S	41	ASN	3.6
7	S	88	GLY	3.6
4	R	30	LYS	3.5
3	C	119	LYS	3.5
7	S	63	ASN	3.4
4	H	31	ARG	3.3
7	S	83	GLN	3.2
4	H	32	SER	3.1
1	O	39	HIS	3.0
7	S	29	SER	2.9
7	S	90	SER	2.9
1	O	81	ASP	2.8
1	E	38	PRO	2.8
3	C	38	ASN	2.8
3	Q	120	THR	2.8
7	S	92	SER	2.7
7	S	72	ILE	2.6
7	S	53	TYR	2.6
7	S	71	SER	2.4
3	C	12	ALA	2.3
3	Q	38	ASN	2.3
7	S	43	ALA	2.3
7	S	33	VAL	2.2
7	S	75	LEU	2.2
7	S	38	ALA	2.2
1	O	78	PHE	2.2
7	S	56	SER	2.2
7	S	89	ALA	2.1
7	S	32	ILE	2.1
7	S	25	HIS	2.1
3	G	31	HIS	2.1
7	S	69	LYS	2.1
3	G	27	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
6	J	349	DC	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
9	K	J	415	1/1	0.51	0.09	156,156,156,156	0
8	CA	J	409	1/1	0.66	0.11	173,173,173,173	0
8	CA	I	411	1/1	0.67	0.12	153,153,153,153	0
8	CA	I	409	1/1	0.71	0.18	190,190,190,190	0
9	K	J	411	1/1	0.73	0.28	146,146,146,146	0
8	CA	J	405	1/1	0.74	0.19	145,145,145,145	0
8	CA	J	410	1/1	0.76	0.15	181,181,181,181	0
8	CA	I	407	1/1	0.84	0.17	145,145,145,145	0
8	CA	I	403	1/1	0.85	0.08	124,124,124,124	0
8	CA	I	405	1/1	0.86	0.10	174,174,174,174	0
8	CA	J	406	1/1	0.86	0.15	159,159,159,159	0
8	CA	G	201	1/1	0.87	0.29	140,140,140,140	0
8	CA	J	401	1/1	0.87	0.07	126,126,126,126	0
9	K	I	412	1/1	0.87	0.18	153,153,153,153	0
9	K	I	413	1/1	0.87	0.18	130,130,130,130	0
8	CA	I	408	1/1	0.87	0.14	191,191,191,191	0
8	CA	I	402	1/1	0.87	0.14	126,126,126,126	0
9	K	J	412	1/1	0.89	0.17	147,147,147,147	0
8	CA	J	407	1/1	0.89	0.06	150,150,150,150	0
8	CA	I	401	1/1	0.90	0.17	148,148,148,148	0
8	CA	J	404	1/1	0.90	0.69	177,177,177,177	0
8	CA	I	406	1/1	0.90	0.25	175,175,175,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	K	J	413	1/1	0.92	0.15	154,154,154,154	0
9	K	J	414	1/1	0.93	0.12	157,157,157,157	0
8	CA	J	408	1/1	0.94	0.10	160,160,160,160	0
8	CA	M	201	1/1	0.94	0.25	155,155,155,155	0
8	CA	I	404	1/1	0.94	0.22	139,139,139,139	0
8	CA	J	403	1/1	0.95	0.08	135,135,135,135	0
8	CA	J	402	1/1	0.96	0.07	137,137,137,137	0
8	CA	I	410	1/1	0.98	0.09	151,151,151,151	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.