



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:00 AM GMT

PDB ID : 1ZBB  
Title : Structure of the 4\_601\_167 Tetranucleosome  
Authors : Schalch, T.; Duda, S.; Sargent, D.F.; Richmond, T.J.  
Deposited on : 2005-04-08  
Resolution : 9.00 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

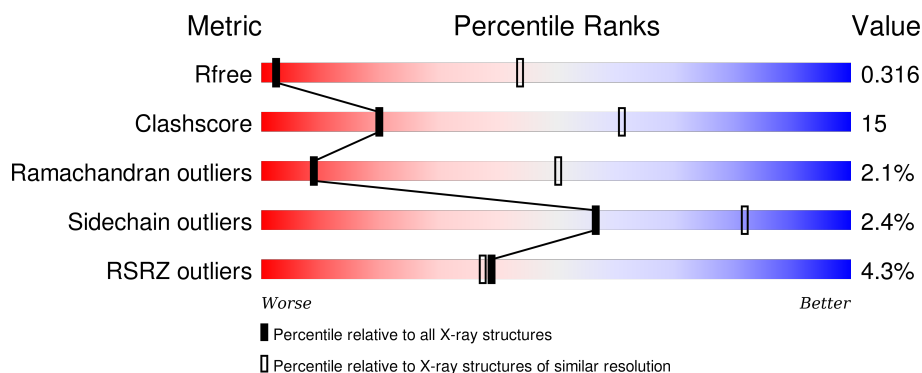
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 9.00 Å.

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








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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

Mol	Chain	Length	Quality of chain
1	I	347	<div> <div>4%</div> <div>48%</div> <div>52%</div> <div>.</div> </div>
2	J	347	<div> <div>4%</div> <div>40%</div> <div>60%</div> </div>
3	A	135	<div> <div>58%</div> <div>14%</div> <div>28%</div> </div>
3	E	135	<div> <div>67%</div> <div>.</div> <div>28%</div> </div>
3	a	135	<div> <div>%</div> <div>70%</div> <div>.</div> <div>28%</div> </div>

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Mol	Chain	Length	Quality of chain
3	e	135	
4	B	102	
4	F	102	
4	b	102	
4	f	102	
5	C	129	
5	G	129	
5	c	129	
5	g	129	
6	D	125	
6	H	125	
6	d	125	
6	h	125	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26851 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 STRAND 1 (ARBITRARY MODEL SEQUENCE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	347	Total	C	N	O	P	0	0	0
			7111	3394	1292	2079	346			

- Molecule 2 is a DNA chain called DNA STRAND 2 (ARBITRARY MODEL SEQUENCE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	347	Total	C	N	O	P	0	0	0
			7110	3394	1289	2081	346			

- Molecule 3 is a protein called HISTONE H3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	97	Total	C	N	O	S	0	0	0
			801	504	155	139	3			
3	E	97	Total	C	N	O	S	0	0	0
			801	504	155	139	3			
3	a	97	Total	C	N	O	S	0	0	0
			801	504	155	139	3			
3	e	97	Total	C	N	O	S	0	0	0
			801	504	155	139	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	CONFLICT	UNP P84233
E	102	ALA	GLY	CONFLICT	UNP P84233
a	102	ALA	GLY	CONFLICT	UNP P84233
e	102	ALA	GLY	CONFLICT	UNP P84233

- 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
			634	400	122	111	1			
4	F	94	Total	C	N	O	S	0	0	0
			750	469	154	126	1			
4	b	80	Total	C	N	O	S	0	0	0
			634	400	122	111	1			
4	f	94	Total	C	N	O	S	0	0	0
			750	469	154	126	1			

- Molecule 5 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	111	Total	C	N	O		0	0	0
			858	539	169	150				
5	G	109	Total	C	N	O		0	0	0
			843	531	164	148				
5	c	111	Total	C	N	O		0	0	0
			858	539	169	150				
5	g	109	Total	C	N	O		0	0	0
			843	531	164	148				

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	CONFLICT	UNP P06897
C	123	SER	ALA	CONFLICT	UNP P06897
G	99	ARG	GLY	CONFLICT	UNP P06897
G	123	SER	ALA	CONFLICT	UNP P06897
c	99	ARG	GLY	CONFLICT	UNP P06897
c	123	SER	ALA	CONFLICT	UNP P06897
g	99	ARG	GLY	CONFLICT	UNP P06897
g	123	SER	ALA	CONFLICT	UNP P06897

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	107	Total	C	N	O	S	0	0	0
			843	528	158	155	2			
6	H	99	Total	C	N	O	S	0	0	0
			785	493	146	144	2			
6	d	107	Total	C	N	O	S	0	0	0
			843	528	158	155	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	h	99	Total	C	N	O	S	0	0	0
			785	493	146	144	2			

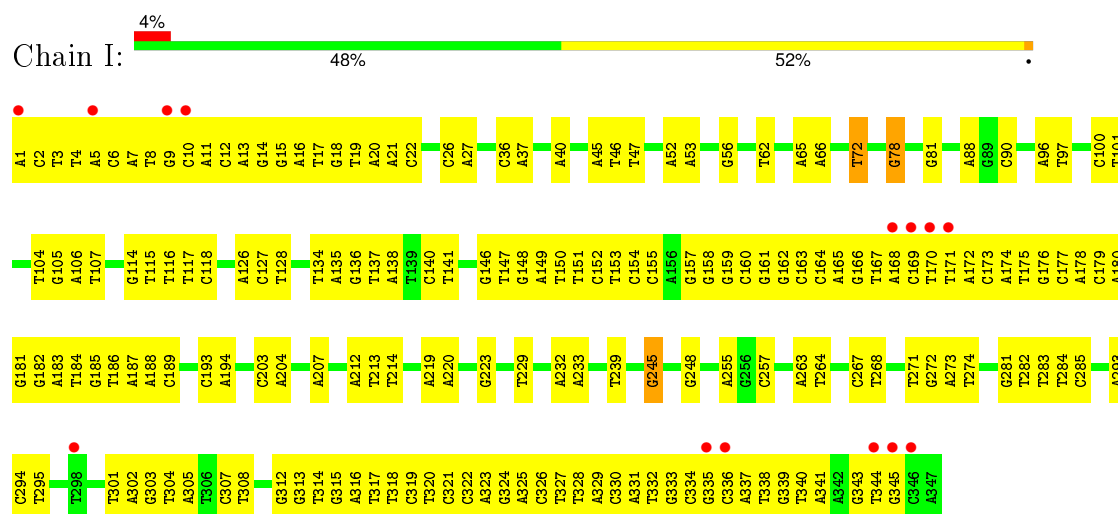
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	CONFLICT	UNP P02281
H	29	THR	SER	CONFLICT	UNP P02281
d	29	THR	SER	CONFLICT	UNP P02281
h	29	THR	SER	CONFLICT	UNP P02281

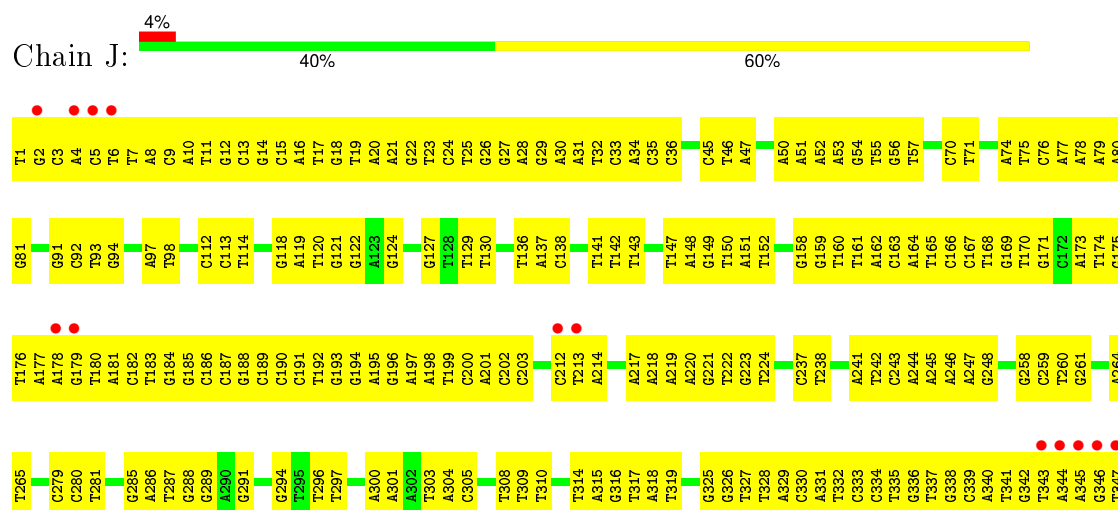
### 3 Residue-property plots

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

#### • Molecule 1: DNA STRAND 1 (ARBITRARY MODEL SEQUENCE)

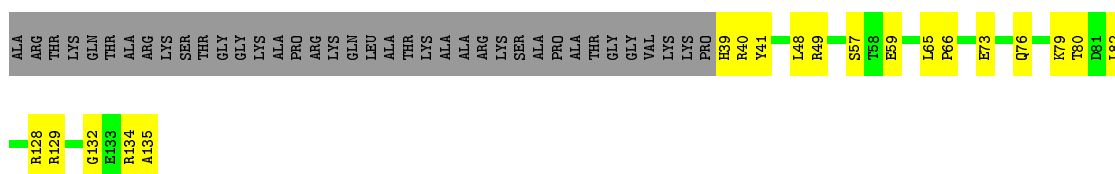


#### • Molecule 2: DNA STRAND 2 (ARBITRARY MODEL SEQUENCE)



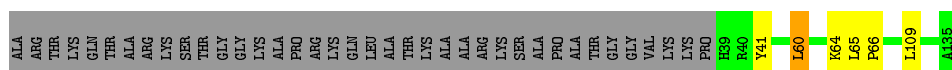
#### • Molecule 3: HISTONE H3





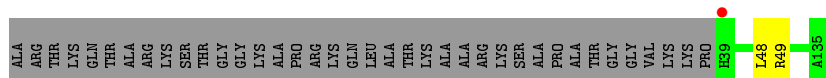
- Molecule 3: HISTONE H3

Chain E: 67% 28%



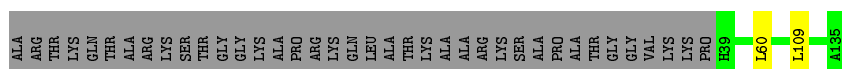
- Molecule 3: HISTONE H3

Chain a: 70% 28%



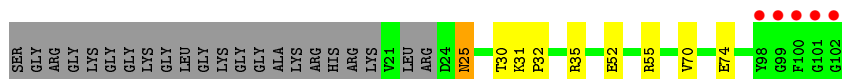
- Molecule 3: HISTONE H3

Chain e: 70% 28%



- Molecule 4: Histone H4

Chain B: 70% 22% 8% 5%



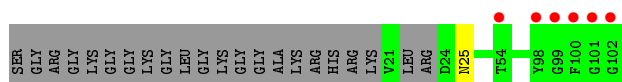
- Molecule 4: Histone H4

Chain F: 77% 12% 8% 4%



- Molecule 4: Histone H4

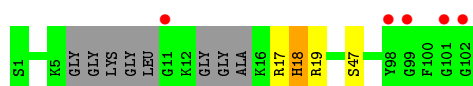
Chain b: 77% 22% 6% 5%



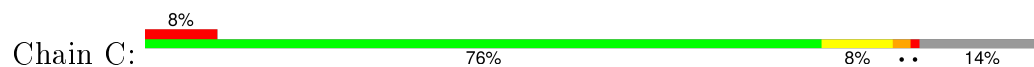
- Molecule 4: Histone H4

Chain f: 88% 8% 4% 5%





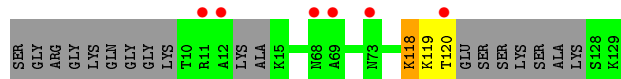
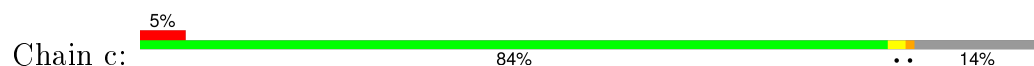
• Molecule 5: Histone H2A.1



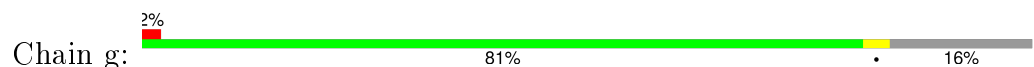
• Molecule 5: Histone H2A.1



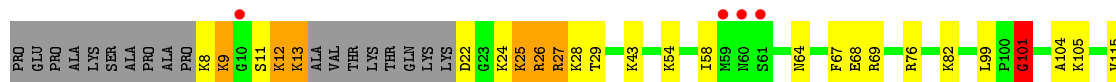
• Molecule 5: Histone H2A.1



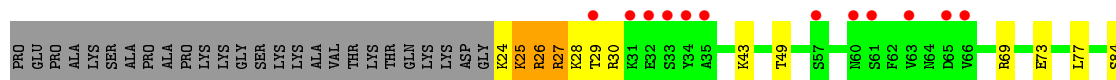
• Molecule 5: Histone H2A.1



• Molecule 6: Histone H2B.1

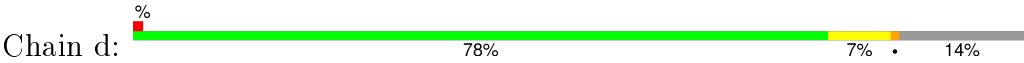


• Molecule 6: Histone H2B.1

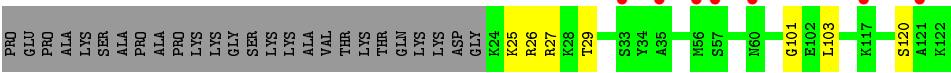




● Molecule 6: Histone H2B.1



● Molecule 6: Histone H2B.1



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.67Å 168.44Å 237.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 9.00 137.32 – 9.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (50.00-9.00) 97.0 (137.32-9.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.25 (at 8.44Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.386 , (Not available) 0.386 , 0.316	Depositor DCC
$R_{free}$ test set	91 reflections (4.78%)	DCC
Wilson B-factor (Å <sup>2</sup> )	749.9	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.02 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 2055 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	26851	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	234.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.81% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	I	0.46	0/7978	0.74	1/12312 (0.0%)
2	J	0.46	0/7976	0.73	0/12309
3	A	0.57	0/812	0.71	1/1088 (0.1%)
3	E	0.65	0/812	0.76	0/1088
3	a	0.57	0/812	0.71	1/1088 (0.1%)
3	e	0.65	0/812	0.75	0/1088
4	B	0.57	0/640	0.78	0/855
4	F	0.62	0/756	0.80	0/1001
4	b	0.57	0/640	0.78	0/855
4	f	0.62	0/756	0.80	0/1001
5	C	0.58	0/865	0.72	0/1161
5	G	0.46	0/853	0.67	0/1150
5	c	0.58	0/865	0.72	0/1161
5	g	0.46	0/853	0.67	0/1150
6	D	0.58	0/853	0.74	3/1135 (0.3%)
6	H	0.48	0/796	0.65	0/1065
6	d	0.58	0/853	0.74	3/1135 (0.3%)
6	h	0.48	0/796	0.65	0/1065
All	All	0.51	0/28728	0.73	9/41707 (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
1	I	0	10
2	J	0	2
All	All	0	12

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	d	76	ARG	NE-CZ-NH2	-5.35	117.62	120.30
6	D	69	ARG	NE-CZ-NH2	-5.32	117.64	120.30
3	A	49	ARG	NE-CZ-NH2	-5.27	117.66	120.30
6	D	76	ARG	NE-CZ-NH2	-5.22	117.69	120.30
3	a	49	ARG	NE-CZ-NH2	-5.20	117.70	120.30
6	d	101	GLY	N-CA-C	5.11	125.88	113.10
6	d	69	ARG	NE-CZ-NH2	-5.10	117.75	120.30
6	D	101	GLY	N-CA-C	5.08	125.79	113.10
1	I	72	DT	OP2-P-O3'	5.03	116.27	105.20

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	239	DT	Sidechain
1	I	245	DG	Sidechain
1	I	248	DG	Sidechain
1	I	255	DA	Sidechain
1	I	257	DC	Sidechain
1	I	72	DT	Sidechain
1	I	78	DG	Sidechain
1	I	81	DG	Sidechain
1	I	88	DA	Sidechain
1	I	90	DC	Sidechain
2	J	258	DG	Sidechain
2	J	91	DG	Sidechain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	7111	0	3916	266	0
2	J	7110	0	3917	309	0
3	A	801	0	838	26	0
3	E	801	0	838	7	0
3	a	801	0	838	0	0
3	e	801	0	838	0	0
4	B	634	0	671	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	750	0	809	29	0
4	b	634	0	671	0	0
4	f	750	0	809	0	0
5	C	858	0	919	31	0
5	G	843	0	903	25	0
5	c	858	0	919	0	0
5	g	843	0	903	0	0
6	D	843	0	891	48	0
6	H	785	0	825	48	0
6	d	843	0	891	0	0
6	h	785	0	825	0	0
All	All	26851	0	21221	707	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (707) 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:327:DT:H2''	2:J:328:DT:C6	1.67	1.27
2:J:30:DA:H5''	3:E:41:TYR:OH	120.42	1.26
2:J:30:DA:C5'	3:E:41:TYR:OH	121.14	1.14
5:C:12:ALA:HB1	5:C:15:LYS:HB3	1.29	1.14
2:J:337:DT:H2''	2:J:338:DG:H5''	1.14	1.11
6:D:13:LYS:HG3	6:D:25:LYS:HA	1.25	1.10
5:G:17:ARG:HH12	5:G:31:HIS:HD2	1.06	1.03
2:J:337:DT:C2'	2:J:338:DG:H5''	1.88	1.02
2:J:55:DT:OP1	5:C:12:ALA:HB3	232.24	1.02
2:J:222:DT:OP1	5:C:12:ALA:HB3	1.59	1.00
5:C:12:ALA:CB	5:C:15:LYS:HB3	1.92	0.99
5:C:118:LYS:HA	5:C:118:LYS:HE3	1.44	0.99
5:C:17:ARG:HH12	5:C:31:HIS:HD2	1.09	0.96
1:I:152:DC:H2''	1:I:153:DT:C5	2.03	0.93
2:J:335:DT:H5'	3:A:39:HIS:CD2	2.04	0.93
3:A:129:ARG:HD2	3:A:135:ALA:HB2	1.51	0.92
1:I:204:DA:H5''	6:H:25:LYS:HE3	220.23	0.92
1:I:37:DA:H5''	6:H:25:LYS:HE3	1.52	0.91
1:I:188:DA:H1'	1:I:189:DC:H5'	1.54	0.89
2:J:337:DT:H2''	2:J:338:DG:C5'	2.00	0.89
1:I:344:DT:H2''	1:I:345:DG:N7	1.88	0.89
2:J:1:DT:H2''	2:J:2:DG:C8	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:336:DC:H2''	1:I:337:DA:C8	2.11	0.86
5:C:17:ARG:HH12	5:C:31:HIS:CD2	1.95	0.84
5:G:17:ARG:HH12	5:G:31:HIS:CD2	1.95	0.84
2:J:195:DA:H2''	2:J:196:DG:C8	2.14	0.83
1:I:152:DC:H2''	1:I:153:DT:H72	1.59	0.83
2:J:327:DT:H2''	2:J:328:DT:C5	2.14	0.83
5:C:118:LYS:CE	5:C:118:LYS:HA	2.10	0.82
1:I:207:DA:N3	5:G:13:LYS:HE3	221.32	0.82
1:I:40:DA:N3	5:G:13:LYS:HE3	1.94	0.81
2:J:327:DT:C2'	2:J:328:DT:C6	2.59	0.81
4:F:16:LYS:HG2	4:F:17:ARG:HH11	1.46	0.81
2:J:70:DC:H2''	2:J:71:DT:H71	1.63	0.80
6:H:26:ARG:HD2	6:H:27:ARG:HH21	1.46	0.80
2:J:12:DG:H1'	2:J:13:DC:H5'	1.63	0.80
2:J:195:DA:H2''	2:J:196:DG:N7	1.97	0.80
2:J:160:DT:H2''	2:J:161:DT:H71	1.65	0.79
2:J:237:DC:H2''	2:J:238:DT:H71	1.63	0.79
2:J:11:DT:H2''	2:J:12:DG:C8	2.18	0.79
1:I:263:DA:H2''	1:I:264:DT:H5''	1.65	0.79
2:J:182:DC:C2'	2:J:183:DT:H72	2.13	0.79
1:I:136:DG:H5''	6:D:22:ASP:O	1.84	0.78
1:I:96:DA:H2''	1:I:97:DT:H5''	1.65	0.78
5:C:119:LYS:NZ	5:C:119:LYS:HA	1.98	0.78
1:I:152:DC:H2''	1:I:153:DT:C7	2.13	0.78
1:I:114:DG:H5''	6:H:27:ARG:HA	1.66	0.78
1:I:303:DG:H5''	6:D:22:ASP:O	215.39	0.77
1:I:335:DG:H1'	1:I:336:DC:H5'	1.65	0.77
1:I:281:DG:H5''	6:H:27:ARG:HA	203.98	0.77
2:J:315:DA:H4'	6:H:24:LYS:HD3	1.67	0.77
2:J:22:DG:H2''	2:J:23:DT:H71	1.65	0.77
2:J:23:DT:H2''	2:J:24:DC:C5	2.18	0.77
1:I:184:DT:H5''	3:A:41:TYR:OH	102.45	0.76
2:J:30:DA:C4'	3:E:41:TYR:OH	122.07	0.76
2:J:346:DG:H2''	2:J:347:DT:C7	2.16	0.76
2:J:30:DA:C5'	3:E:41:TYR:HH	121.18	0.75
2:J:335:DT:H5'	3:A:39:HIS:HD2	1.47	0.75
2:J:182:DC:H2''	2:J:183:DT:H72	1.68	0.75
5:C:12:ALA:HB1	5:C:15:LYS:CB	2.15	0.75
2:J:148:DA:H4'	6:H:24:LYS:HD3	207.68	0.75
6:D:13:LYS:HB2	6:D:26:ARG:H	1.52	0.74
4:F:12:LYS:HE2	4:F:12:LYS:HA	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:220:DA:OP2	5:C:32:ARG:NH1	2.20	0.74
2:J:314:DT:H2''	2:J:315:DA:H5'	1.69	0.74
2:J:53:DA:OP2	5:C:32:ARG:NH1	211.32	0.74
2:J:147:DT:H2''	2:J:148:DA:H5'	1.69	0.74
1:I:303:DG:H2''	1:I:304:DT:H5'	1.70	0.73
4:F:11:GLY:HA2	4:F:17:ARG:HG2	1.70	0.73
2:J:175:DG:C2'	2:J:176:DT:H72	2.18	0.73
2:J:327:DT:H2''	2:J:328:DT:N1	2.04	0.73
2:J:346:DG:C2'	2:J:347:DT:H72	2.18	0.73
2:J:182:DC:H2''	2:J:183:DT:C7	2.19	0.72
1:I:137:DT:H2''	1:I:138:DA:H5'	1.72	0.72
1:I:158:DG:H2''	1:I:159:DG:OP2	1.89	0.72
6:D:13:LYS:HG3	6:D:25:LYS:CA	2.14	0.72
1:I:168:DA:H2''	1:I:169:DC:OP2	1.90	0.71
1:I:174:DA:C2'	1:I:175:DT:H72	2.20	0.71
2:J:24:DC:H2''	2:J:25:DT:H71	1.70	0.71
1:I:344:DT:H2''	1:I:345:DG:C8	2.25	0.71
1:I:136:DG:H2''	1:I:137:DT:H5'	1.70	0.71
1:I:169:DC:H2'	1:I:170:DT:H72	1.71	0.71
2:J:30:DA:H4'	3:E:41:TYR:OH	121.51	0.71
1:I:304:DT:H2''	1:I:305:DA:H5'	1.72	0.71
2:J:327:DT:C2'	2:J:328:DT:C5	2.73	0.71
2:J:11:DT:H2''	2:J:12:DG:N7	2.06	0.71
2:J:242:DT:H1'	2:J:243:DC:H5''	1.74	0.70
2:J:289:DG:H8	4:F:1:SER:HA	1.57	0.69
1:I:169:DC:H2'	1:I:170:DT:C7	2.21	0.69
1:I:339:DG:C8	1:I:340:DT:H72	2.27	0.69
2:J:122:DG:H8	4:F:1:SER:HA	188.74	0.69
1:I:152:DC:C2'	1:I:153:DT:H72	2.22	0.69
2:J:75:DT:H1'	2:J:76:DC:H5''	1.74	0.69
6:H:26:ARG:C	6:H:28:LYS:H	1.97	0.69
1:I:170:DT:H1'	1:I:171:DT:H5''	1.73	0.68
4:F:12:LYS:HG3	4:F:16:LYS:HD3	1.75	0.68
1:I:336:DC:H2''	1:I:337:DA:N7	2.09	0.68
2:J:3:DC:H2''	2:J:4:DA:N7	2.09	0.68
2:J:25:DT:H2''	2:J:26:DG:OP2	1.94	0.68
2:J:22:DG:C2'	2:J:23:DT:H71	2.24	0.67
6:H:26:ARG:CD	6:H:27:ARG:HE	2.07	0.67
5:G:117:PRO:O	5:G:118:LYS:HG2	1.95	0.67
5:C:119:LYS:O	5:C:120:THR:HG22	1.95	0.67
3:E:60:LEU:HD23	3:E:64:LYS:HE2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:24:DC:C2'	2:J:25:DT:H71	2.24	0.67
1:I:170:DT:H2''	1:I:171:DT:C5'	2.25	0.67
6:H:43:LYS:HE2	6:H:43:LYS:HA	1.77	0.67
5:C:119:LYS:HZ1	5:C:119:LYS:HA	1.59	0.66
5:C:118:LYS:HE3	5:C:118:LYS:CA	2.24	0.66
3:A:79:LYS:HD3	3:A:82:LEU:HD21	1.78	0.66
2:J:18:DG:C2'	2:J:19:DT:H71	2.25	0.66
2:J:192:DT:H2''	2:J:193:DG:OP2	1.95	0.66
2:J:151:DA:H2''	2:J:152:DT:OP2	1.96	0.65
2:J:166:DC:H2''	2:J:167:DC:C5	2.31	0.65
1:I:37:DA:H5''	6:H:25:LYS:CE	2.26	0.65
1:I:325:DA:H2''	1:I:326:DC:OP2	1.95	0.65
1:I:343:DG:C8	1:I:344:DT:H72	2.31	0.65
5:G:17:ARG:NH1	5:G:31:HIS:HD2	1.89	0.65
2:J:245:DA:H1'	2:J:246:DA:C8	2.32	0.64
5:G:41:GLU:HG2	5:G:42:ARG:HG3	1.79	0.64
1:I:204:DA:H5''	6:H:25:LYS:CE	219.35	0.64
1:I:315:DG:H2''	1:I:316:DA:OP2	1.97	0.64
1:I:263:DA:C2'	1:I:264:DT:H5''	2.27	0.64
2:J:303:DT:OP2	5:G:35:ARG:NH2	2.31	0.64
1:I:171:DT:H2''	1:I:172:DA:OP2	1.98	0.64
1:I:96:DA:C2'	1:I:97:DT:H5''	2.27	0.64
5:G:114:VAL:HA	5:G:120:THR:HG23	1.80	0.64
2:J:136:DT:OP2	5:G:35:ARG:NH2	212.00	0.64
2:J:78:DA:H1'	2:J:79:DA:C8	2.31	0.64
2:J:318:DA:H2''	2:J:319:DT:OP2	1.96	0.64
2:J:334:DC:C4'	3:A:39:HIS:NE2	2.62	0.63
1:I:20:DA:H2''	1:I:21:DA:N7	2.12	0.63
2:J:50:DA:H2''	2:J:51:DA:OP2	1.98	0.63
2:J:217:DA:H2''	2:J:218:DA:OP2	1.98	0.63
1:I:282:DT:OP1	6:H:26:ARG:HA	214.24	0.63
1:I:335:DG:H1'	1:I:336:DC:C5'	2.28	0.63
5:G:20:ARG:CZ	6:H:122:LYS:OXT	2.47	0.63
1:I:2:DC:C2'	1:I:3:DT:H72	2.28	0.62
1:I:115:DT:OP1	6:H:26:ARG:HA	1.99	0.62
6:D:12:LYS:O	6:D:26:ARG:HA	2.00	0.62
2:J:52:DA:H3'	5:C:32:ARG:NH1	211.57	0.62
2:J:304:DA:H2''	2:J:305:DC:H5'	1.81	0.62
2:J:289:DG:C8	4:F:1:SER:HA	2.34	0.62
2:J:200:DC:H2''	2:J:201:DA:OP2	2.00	0.62
2:J:219:DA:H3'	5:C:32:ARG:NH1	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:137:DA:H2''	2:J:138:DC:H5'	1.81	0.62
2:J:334:DC:H4'	3:A:39:HIS:NE2	2.15	0.62
2:J:148:DA:H2''	2:J:149:DG:C5'	2.29	0.62
2:J:122:DG:C8	4:F:1:SER:HA	188.48	0.62
1:I:169:DC:C2'	1:I:170:DT:H72	2.30	0.61
2:J:326:DG:H1'	2:J:327:DT:H5'	1.82	0.61
6:D:121:ALA:O	6:D:122:LYS:HB2	2.01	0.61
6:H:28:LYS:HG2	6:H:28:LYS:O	2.01	0.61
4:F:12:LYS:HG3	4:F:16:LYS:HB3	1.82	0.61
2:J:12:DG:H1'	2:J:13:DC:C5'	2.31	0.61
2:J:315:DA:H2''	2:J:316:DG:C5'	2.29	0.61
2:J:346:DG:C2'	2:J:347:DT:C7	2.76	0.61
2:J:169:DG:C2'	2:J:170:DT:H72	2.31	0.61
2:J:46:DT:H2''	2:J:47:DA:H5'	1.83	0.60
2:J:346:DG:H2''	2:J:347:DT:H73	1.82	0.60
1:I:150:DT:C2'	1:I:151:DT:H72	2.31	0.60
2:J:56:DG:H2''	2:J:57:DT:C5'	2.31	0.60
2:J:223:DG:H2''	2:J:224:DT:C5'	2.32	0.60
1:I:169:DC:C2'	1:I:170:DT:C7	2.80	0.60
4:F:16:LYS:HG2	4:F:17:ARG:NH1	2.17	0.60
2:J:213:DT:H2''	2:J:214:DA:H5'	1.83	0.59
6:H:77:LEU:HD11	6:H:93:THR:CG2	2.32	0.59
6:D:115:VAL:O	6:D:119:THR:HG23	2.02	0.59
2:J:3:DC:H2''	2:J:4:DA:C8	2.37	0.59
2:J:175:DG:H2''	2:J:176:DT:C7	2.33	0.59
1:I:327:DT:C2'	1:I:328:DT:H72	2.32	0.59
2:J:173:DA:C2'	2:J:174:DT:H72	2.32	0.59
1:I:21:DA:H1'	1:I:22:DC:H5'	1.83	0.59
2:J:237:DC:H2''	2:J:238:DT:C7	2.32	0.59
6:H:119:THR:C	6:H:121:ALA:H	2.07	0.58
1:I:245:DG:OP2	5:C:129:LYS:NZ	81.99	0.58
2:J:70:DC:H2''	2:J:71:DT:C7	2.32	0.58
2:J:334:DC:C2'	2:J:335:DT:H72	2.33	0.58
1:I:324:DG:H2''	1:I:325:DA:H8	1.68	0.58
1:I:335:DG:H2''	1:I:336:DC:OP2	2.03	0.58
2:J:142:DT:O2	5:G:13:LYS:NZ	222.72	0.58
1:I:150:DT:H2''	1:I:151:DT:OP2	2.03	0.58
1:I:178:DA:H2''	1:I:179:DC:OP2	2.04	0.58
1:I:136:DG:H2''	1:I:137:DT:C5'	2.34	0.58
2:J:165:DT:H2''	2:J:166:DC:OP2	2.02	0.58
1:I:172:DA:H2''	1:I:173:DC:C6	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:324:DG:H2''	1:I:325:DA:C8	2.39	0.58
2:J:141:DT:H1'	2:J:142:DT:H5'	1.86	0.58
1:I:303:DG:H2''	1:I:304:DT:C5'	2.34	0.58
1:I:78:DG:OP2	5:C:129:LYS:NZ	2.36	0.58
1:I:187:DA:H2''	1:I:188:DA:C8	2.38	0.58
1:I:168:DA:P	1:I:168:DA:H8	2.28	0.57
5:C:119:LYS:HG3	5:C:119:LYS:O	2.05	0.57
2:J:327:DT:C6	2:J:328:DT:C4	2.93	0.57
6:D:12:LYS:HB2	6:D:27:ARG:H	1.69	0.57
2:J:308:DT:H1'	2:J:309:DT:H5'	1.86	0.57
1:I:185:DG:C2'	1:I:186:DT:H72	2.34	0.57
2:J:309:DT:O2	5:G:13:LYS:NZ	2.34	0.57
2:J:178:DA:H2''	2:J:179:DG:C8	2.40	0.57
1:I:106:DA:H2''	1:I:107:DT:OP2	2.05	0.57
1:I:3:DT:H2''	1:I:4:DT:OP2	2.05	0.57
1:I:184:DT:C5'	3:A:41:TYR:OH	102.91	0.56
1:I:169:DC:C6	1:I:170:DT:H72	2.40	0.56
2:J:169:DG:H2''	2:J:170:DT:OP2	2.05	0.56
1:I:273:DA:H2''	1:I:274:DT:OP2	2.04	0.56
2:J:122:DG:H2'	4:F:2:GLY:H	188.10	0.56
1:I:167:DT:O3'	1:I:168:DA:C8	2.59	0.56
1:I:170:DT:H2''	1:I:171:DT:H5'	1.85	0.56
1:I:149:DA:C2'	1:I:150:DT:H72	2.36	0.56
2:J:289:DG:H2'	4:F:2:GLY:H	1.70	0.56
2:J:16:DA:H2''	2:J:17:DT:OP2	2.05	0.56
1:I:327:DT:H2''	1:I:328:DT:OP2	2.05	0.56
1:I:186:DT:H2''	1:I:187:DA:OP2	2.05	0.56
2:J:175:DG:H2'	2:J:176:DT:H72	1.88	0.56
1:I:104:DT:H4'	1:I:105:DG:OP1	2.06	0.56
2:J:137:DA:H2''	2:J:138:DC:C5'	2.36	0.56
1:I:136:DG:H1'	1:I:137:DT:H5''	1.88	0.56
6:D:8:LYS:O	6:D:9:LYS:C	2.44	0.56
2:J:23:DT:C2'	2:J:24:DC:C5	2.90	0.55
1:I:9:DG:H2''	1:I:10:DC:OP2	2.04	0.55
2:J:6:DT:H2''	2:J:7:DT:OP2	2.07	0.55
1:I:303:DG:H1'	1:I:304:DT:H5''	1.88	0.55
3:A:79:LYS:HD2	4:B:74:GLU:HG2	1.88	0.55
2:J:35:DC:H1'	2:J:36:DC:H5'	1.89	0.55
2:J:340:DA:H2''	2:J:341:DT:OP2	2.05	0.55
1:I:18:DG:C2'	1:I:19:DT:H72	2.37	0.55
6:D:8:LYS:CG	6:D:11:SER:HB3	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:12:ALA:HB2	5:C:15:LYS:HB3	1.87	0.54
1:I:146:DG:C2'	1:I:147:DT:H71	2.36	0.54
6:H:26:ARG:HD2	6:H:27:ARG:NH2	2.19	0.54
2:J:161:DT:H2''	2:J:162:DA:OP2	2.06	0.54
1:I:13:DA:H2''	1:I:14:DG:OP2	2.07	0.54
1:I:175:DT:H2''	1:I:176:DG:OP2	2.06	0.54
6:H:25:LYS:O	6:H:28:LYS:HB3	2.07	0.54
2:J:1:DT:H6	2:J:1:DT:HO5'	1.56	0.54
2:J:304:DA:H2''	2:J:305:DC:C5'	2.36	0.54
1:I:45:DA:H2''	1:I:46:DT:OP2	2.07	0.54
2:J:331:DA:C2'	2:J:332:DT:H72	2.36	0.54
1:I:317:DT:H2''	1:I:318:DT:OP2	2.06	0.54
2:J:242:DT:C2'	2:J:243:DC:H5''	2.37	0.54
3:A:79:LYS:HB3	3:A:82:LEU:HD11	1.89	0.54
1:I:2:DC:H2''	1:I:3:DT:C7	2.37	0.54
1:I:183:DA:C2'	1:I:184:DT:H72	2.38	0.54
2:J:18:DG:H2''	2:J:19:DT:H71	1.89	0.54
1:I:7:DA:C2'	1:I:8:DT:H72	2.37	0.54
4:F:18:HIS:O	4:F:19:ARG:HB2	2.08	0.54
1:I:322:DC:H2''	1:I:323:DA:OP2	2.07	0.54
2:J:12:DG:H2''	2:J:13:DC:OP2	2.06	0.54
2:J:162:DA:H2''	2:J:163:DC:OP2	2.07	0.54
1:I:271:DT:H4'	1:I:272:DG:OP1	2.06	0.54
1:I:174:DA:H2''	1:I:175:DT:H72	1.89	0.54
2:J:164:DA:H2''	2:J:165:DT:OP2	2.06	0.54
2:J:190:DC:C2	2:J:191:DC:C5	2.95	0.54
2:J:169:DG:H2''	2:J:170:DT:C7	2.38	0.54
2:J:75:DT:C2'	2:J:76:DC:H5''	2.37	0.54
1:I:170:DT:C1'	1:I:171:DT:H5''	2.38	0.54
2:J:193:DG:H2''	2:J:194:DG:OP2	2.07	0.54
1:I:182:DG:H2''	1:I:183:DA:OP2	2.07	0.53
2:J:148:DA:C2'	2:J:149:DG:H5''	2.38	0.53
1:I:271:DT:H1'	1:I:272:DG:C8	2.43	0.53
1:I:212:DA:H2''	1:I:213:DT:OP2	2.07	0.53
6:H:25:LYS:C	6:H:25:LYS:HD3	2.29	0.53
2:J:181:DA:H2''	2:J:182:DC:C5	2.44	0.53
1:I:3:DT:C2'	1:I:4:DT:H72	2.38	0.53
2:J:279:DC:H2''	2:J:280:DC:C5	2.43	0.53
1:I:149:DA:H2''	1:I:150:DT:OP2	2.08	0.53
1:I:331:DA:H2''	1:I:332:DT:OP2	2.07	0.53
4:F:11:GLY:CA	4:F:17:ARG:HG2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:DG:H2''	1:I:15:DG:OP2	2.07	0.53
1:I:16:DA:C2'	1:I:17:DT:H72	2.39	0.53
1:I:316:DA:H2''	1:I:317:DT:OP2	2.07	0.53
1:I:154:DC:H2''	1:I:155:DC:OP2	2.06	0.53
2:J:1:DT:H2''	2:J:2:DG:H8	1.71	0.53
1:I:337:DA:C8	1:I:338:DT:H72	2.44	0.53
2:J:315:DA:C2'	2:J:316:DG:H5''	2.38	0.53
2:J:112:DC:H2''	2:J:113:DC:C5	2.43	0.53
1:I:174:DA:H2''	1:I:175:DT:C7	2.38	0.53
1:I:104:DT:H1'	1:I:105:DG:C8	2.43	0.53
2:J:30:DA:H2''	2:J:31:DA:OP2	2.08	0.53
1:I:337:DA:H2''	1:I:338:DT:OP2	2.09	0.53
2:J:23:DT:H2''	2:J:24:DC:C6	2.44	0.52
2:J:342:DG:C2'	2:J:343:DT:H72	2.38	0.52
2:J:148:DA:H2''	2:J:149:DG:H5''	1.90	0.52
1:I:18:DG:H2''	1:I:19:DT:OP2	2.09	0.52
1:I:267:DC:H2''	1:I:268:DT:H71	1.91	0.52
2:J:342:DG:C8	2:J:343:DT:H72	2.43	0.52
2:J:202:DC:H1'	2:J:203:DC:H5'	1.91	0.52
2:J:241:DA:H2''	2:J:242:DT:H5'	1.91	0.52
4:F:30:THR:HB	4:F:32:PRO:HD2	1.92	0.52
1:I:170:DT:C2'	1:I:171:DT:H5''	2.39	0.52
1:I:317:DT:C2'	1:I:318:DT:H72	2.40	0.52
2:J:196:DG:H2''	2:J:197:DA:OP2	2.09	0.52
2:J:75:DT:C1'	2:J:76:DC:H5''	2.39	0.52
1:I:16:DA:H2''	1:I:17:DT:OP2	2.08	0.52
2:J:56:DG:H2''	2:J:57:DT:H5''	1.92	0.52
2:J:291:DG:OP1	4:F:79:LYS:NZ	2.39	0.52
1:I:185:DG:H2''	1:I:186:DT:OP2	2.09	0.52
1:I:96:DA:H2''	1:I:97:DT:C5'	2.39	0.52
2:J:75:DT:H2''	2:J:76:DC:C5'	2.39	0.52
5:G:41:GLU:HB3	6:H:84:SER:HB2	1.92	0.52
1:I:161:DG:H2''	1:I:162:DG:OP2	2.08	0.52
2:J:7:DT:H2''	2:J:8:DA:C8	2.45	0.52
1:I:17:DT:H2''	1:I:18:DG:OP2	2.09	0.52
1:I:100:DC:H2''	1:I:101:DT:H71	1.91	0.52
6:D:25:LYS:HD3	6:D:25:LYS:N	2.25	0.52
5:G:35:ARG:HH11	5:G:35:ARG:HG2	1.75	0.52
1:I:4:DT:H2''	1:I:5:DA:OP2	2.09	0.52
1:I:127:DC:H2'	1:I:128:DT:H71	1.92	0.52
1:I:169:DC:N1	1:I:170:DT:H72	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:198:DA:H2''	2:J:199:DT:OP2	2.10	0.52
2:J:315:DA:C4'	6:H:24:LYS:HD3	2.40	0.52
1:I:168:DA:P	1:I:168:DA:C8	3.03	0.51
2:J:341:DT:H2''	2:J:342:DG:OP2	2.10	0.51
2:J:166:DC:H2''	2:J:167:DC:C6	2.45	0.51
2:J:315:DA:H2''	2:J:316:DG:H5''	1.90	0.51
2:J:175:DG:C2'	2:J:176:DT:C7	2.87	0.51
1:I:294:DC:H2'	1:I:295:DT:H71	1.92	0.51
6:D:13:LYS:CB	6:D:26:ARG:H	2.20	0.51
1:I:114:DG:H4'	6:H:26:ARG:HG2	1.92	0.51
2:J:198:DA:C2'	2:J:199:DT:H72	2.40	0.51
2:J:242:DT:H2''	2:J:243:DC:C5'	2.40	0.51
1:I:10:DC:H2''	1:I:11:DA:OP2	2.09	0.51
2:J:223:DG:H2''	2:J:224:DT:H5''	1.92	0.51
2:J:158:DG:H2''	2:J:159:DG:OP2	2.09	0.51
2:J:242:DT:C1'	2:J:243:DC:H5''	2.39	0.51
2:J:31:DA:H2''	2:J:32:DT:OP2	2.09	0.51
2:J:74:DA:H2''	2:J:75:DT:H5'	1.92	0.51
1:I:18:DG:C8	1:I:19:DT:H72	2.45	0.51
4:F:31:LYS:HB3	4:F:32:PRO:HD3	1.93	0.51
2:J:143:DT:H4'	5:G:13:LYS:HB2	221.10	0.51
2:J:191:DC:C2'	2:J:192:DT:H71	2.40	0.51
2:J:310:DT:H4'	5:G:13:LYS:HB2	1.93	0.51
1:I:148:DG:H2''	1:I:149:DA:OP2	2.10	0.51
2:J:164:DA:C2'	2:J:165:DT:H72	2.41	0.51
1:I:263:DA:H2''	1:I:264:DT:C5'	2.39	0.51
6:H:118:TYR:O	6:H:121:ALA:HB3	2.11	0.51
2:J:16:DA:C8	2:J:17:DT:H72	2.46	0.51
2:J:331:DA:H2''	2:J:332:DT:OP2	2.10	0.51
6:H:28:LYS:HZ3	6:H:30:ARG:HG3	1.76	0.51
2:J:5:DC:C2'	2:J:6:DT:H72	2.41	0.51
1:I:284:DT:H2''	1:I:285:DC:O5'	2.11	0.51
2:J:342:DG:H2''	2:J:343:DT:OP2	2.11	0.51
5:G:118:LYS:O	5:G:118:LYS:HG3	2.11	0.51
1:I:273:DA:H2''	1:I:274:DT:H71	1.92	0.51
1:I:117:DT:H2''	1:I:118:DC:O5'	2.11	0.50
1:I:281:DG:H4'	6:H:26:ARG:HG2	208.14	0.50
2:J:160:DT:C2'	2:J:161:DT:H71	2.39	0.50
2:J:148:DA:C4'	6:H:24:LYS:HD3	206.91	0.50
4:B:31:LYS:N	4:B:32:PRO:HD2	2.26	0.50
2:J:340:DA:C2'	2:J:341:DT:H72	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:106:DA:H2''	1:I:107:DT:H71	1.92	0.50
1:I:159:DG:H2''	1:I:160:DC:OP2	2.11	0.50
6:H:26:ARG:HD2	6:H:27:ARG:HE	1.77	0.50
1:I:326:DC:H2''	1:I:327:DT:OP2	2.10	0.50
2:J:223:DG:H2''	2:J:224:DT:H5'	1.93	0.50
2:J:326:DG:H1'	2:J:327:DT:C5'	2.42	0.50
6:H:26:ARG:C	6:H:28:LYS:N	2.64	0.50
1:I:126:DA:H1'	1:I:127:DC:H5''	1.93	0.50
2:J:327:DT:H2'	2:J:328:DT:C5	2.47	0.50
5:C:17:ARG:NH1	5:C:31:HIS:HD2	1.93	0.50
2:J:166:DC:C2'	2:J:167:DC:C5	2.95	0.50
1:I:167:DT:H2''	1:I:168:DA:N7	2.27	0.50
2:J:335:DT:OP1	3:A:40:ARG:O	2.30	0.50
2:J:343:DT:H2''	2:J:344:DA:OP2	2.11	0.50
1:I:319:DC:C2'	1:I:320:DT:H72	2.41	0.50
1:I:7:DA:H2''	1:I:8:DT:OP2	2.11	0.50
4:F:20:LYS:HG2	4:F:21:VAL:N	2.27	0.50
2:J:18:DG:H2''	2:J:19:DT:OP2	2.11	0.49
2:J:21:DA:H2''	2:J:22:DG:OP2	2.12	0.49
6:D:13:LYS:CG	6:D:25:LYS:HA	2.18	0.49
1:I:321:DC:H2''	1:I:322:DC:OP2	2.12	0.49
1:I:162:DG:H2''	1:I:163:DC:OP2	2.12	0.49
1:I:164:DC:H2''	1:I:165:DA:OP2	2.12	0.49
2:J:336:DG:C2'	2:J:337:DT:H72	2.43	0.49
6:D:13:LYS:HB2	6:D:26:ARG:N	2.25	0.49
1:I:320:DT:H2''	1:I:321:DC:OP2	2.11	0.49
6:D:99:LEU:HB2	6:D:104:ALA:HB2	1.94	0.49
6:H:28:LYS:O	6:H:30:ARG:N	2.45	0.49
1:I:293:DA:H1'	1:I:294:DC:H5''	1.93	0.49
2:J:23:DT:H2''	2:J:24:DC:H5	1.71	0.49
2:J:28:DA:H2''	2:J:29:DG:OP2	2.11	0.49
2:J:6:DT:C2'	2:J:7:DT:H72	2.42	0.49
2:J:160:DT:H2''	2:J:161:DT:C7	2.36	0.49
2:J:168:DT:H2''	2:J:169:DG:OP2	2.11	0.49
1:I:163:DC:H2''	1:I:164:DC:OP2	2.12	0.49
2:J:29:DG:H2''	2:J:30:DA:OP2	2.12	0.49
1:I:318:DT:H2''	1:I:319:DC:OP2	2.12	0.49
2:J:188:DG:H2''	2:J:189:DC:OP2	2.12	0.49
2:J:325:DG:H2''	2:J:326:DG:OP2	2.11	0.49
1:I:116:DT:H2''	1:I:117:DT:H5''	1.94	0.49
2:J:344:DA:H2''	2:J:345:DA:OP2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:12:LYS:HD2	6:D:24:LYS:HB3	1.95	0.49
1:I:319:DC:H2''	1:I:320:DT:OP2	2.13	0.49
2:J:56:DG:H2''	2:J:57:DT:H5'	1.93	0.49
1:I:157:DG:H1'	1:I:158:DG:H5'	1.95	0.49
2:J:20:DA:H2''	2:J:21:DA:OP2	2.11	0.49
2:J:174:DT:H2''	2:J:175:DG:OP2	2.13	0.49
1:I:283:DT:H2''	1:I:284:DT:H5''	1.94	0.49
1:I:184:DT:H2''	1:I:185:DG:OP2	2.12	0.49
1:I:302:DA:H4'	6:D:24:LYS:H	213.44	0.49
6:D:43:LYS:HE2	6:D:43:LYS:HA	1.95	0.49
1:I:177:DC:H2''	1:I:178:DA:OP2	2.13	0.48
1:I:135:DA:H4'	6:D:24:LYS:H	1.78	0.48
3:A:128:ARG:CB	3:A:134:ARG:HG3	2.43	0.48
2:J:163:DC:H2''	2:J:164:DA:OP2	2.12	0.48
4:F:16:LYS:C	4:F:17:ARG:HD2	2.34	0.48
2:J:10:DA:C8	2:J:11:DT:H72	2.48	0.48
1:I:232:DA:H2''	1:I:233:DA:OP2	2.13	0.48
2:J:334:DC:C5'	3:A:41:TYR:HE2	2.25	0.48
1:I:2:DC:C2'	1:I:3:DT:C7	2.90	0.48
2:J:129:DT:H2''	2:J:130:DT:OP2	2.12	0.48
1:I:180:DA:H2''	1:I:181:DG:OP2	2.13	0.48
2:J:336:DG:H2''	2:J:337:DT:C7	2.44	0.48
6:D:25:LYS:O	6:D:26:ARG:C	2.51	0.48
6:D:8:LYS:HG2	6:D:11:SER:HB3	1.96	0.48
2:J:124:DG:OP1	4:F:79:LYS:NZ	173.73	0.48
2:J:247:DA:H2''	2:J:248:DG:OP2	2.13	0.48
4:B:52:GLU:OE1	4:B:55:ARG:NH1	2.47	0.48
1:I:183:DA:H2''	1:I:184:DT:OP2	2.13	0.48
2:J:346:DG:H2'	2:J:347:DT:H72	1.93	0.48
5:C:117:PRO:O	5:C:118:LYS:CB	2.61	0.48
1:I:344:DT:C2'	1:I:345:DG:N7	2.70	0.48
6:D:8:LYS:HG3	6:D:11:SER:HB3	1.96	0.48
3:A:57:SER:HB2	3:A:59:GLU:OE2	2.13	0.48
1:I:65:DA:H2''	1:I:66:DA:OP2	2.13	0.48
2:J:334:DC:H2'	2:J:335:DT:H72	1.94	0.48
1:I:329:DA:H2''	1:I:330:DC:OP2	2.14	0.48
2:J:169:DG:C2'	2:J:170:DT:C7	2.92	0.48
1:I:15:DG:H2''	1:I:16:DA:OP2	2.13	0.48
2:J:296:DT:H2''	2:J:297:DT:OP2	2.12	0.48
6:D:121:ALA:O	6:D:122:LYS:CB	2.62	0.48
1:I:149:DA:H2''	1:I:150:DT:C7	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:176:DG:H2''	1:I:177:DC:OP2	2.13	0.48
2:J:173:DA:H2'	2:J:174:DT:H72	1.94	0.48
1:I:160:DC:H2''	1:I:161:DG:OP2	2.14	0.47
2:J:80:DA:H2''	2:J:81:DG:OP2	2.13	0.47
5:C:11:ARG:HG3	6:D:122:LYS:HE2	1.96	0.47
1:I:316:DA:C2'	1:I:317:DT:H72	2.44	0.47
2:J:33:DC:H2''	2:J:34:DA:OP2	2.14	0.47
6:D:54:LYS:O	6:D:58:ILE:HG12	2.15	0.47
2:J:197:DA:H2''	2:J:198:DA:OP2	2.14	0.47
4:F:12:LYS:CG	4:F:16:LYS:HD3	2.44	0.47
2:J:5:DC:N1	2:J:6:DT:H72	2.30	0.47
2:J:187:DC:H2''	2:J:188:DG:OP2	2.14	0.47
2:J:26:DG:H2''	2:J:27:DG:OP2	2.14	0.47
2:J:27:DG:H2''	2:J:28:DA:OP2	2.15	0.47
2:J:167:DC:C2'	2:J:168:DT:H72	2.45	0.47
2:J:315:DA:H2''	2:J:316:DG:H5'	1.96	0.47
2:J:5:DC:C2'	2:J:6:DT:C7	2.92	0.47
1:I:219:DA:H2''	1:I:220:DA:O5'	2.14	0.47
2:J:336:DG:H2''	2:J:337:DT:OP2	2.15	0.47
6:D:13:LYS:HG3	6:D:26:ARG:H	1.80	0.47
2:J:5:DC:C6	2:J:6:DT:H72	2.50	0.47
1:I:137:DT:H2''	1:I:138:DA:C5'	2.43	0.47
2:J:149:DG:H2''	2:J:150:DT:O5'	2.15	0.47
2:J:316:DG:H2''	2:J:317:DT:O5'	2.15	0.47
1:I:340:DT:H2''	1:I:341:DA:C8	2.50	0.47
2:J:148:DA:H2''	2:J:149:DG:H5'	1.96	0.47
5:G:114:VAL:HG23	5:G:120:THR:CG2	2.45	0.47
6:H:26:ARG:O	6:H:28:LYS:N	2.48	0.47
4:F:12:LYS:HG2	4:F:17:ARG:HD3	1.97	0.47
2:J:14:DG:H2''	2:J:15:DC:C5	2.50	0.47
1:I:62:DT:OP1	4:F:19:ARG:HG3	2.15	0.47
6:D:13:LYS:HB3	6:D:13:LYS:HZ2	1.83	0.47
2:J:217:DA:OP2	6:D:8:LYS:HE3	2.15	0.47
2:J:19:DT:H2''	2:J:20:DA:OP2	2.14	0.46
1:I:8:DT:H2''	1:I:9:DG:OP2	2.15	0.46
5:C:11:ARG:O	5:C:12:ALA:HB2	2.15	0.46
6:D:25:LYS:H	6:D:25:LYS:HD3	1.80	0.46
1:I:153:DT:H2''	1:I:154:DC:OP2	2.15	0.46
1:I:5:DA:H2''	1:I:6:DC:OP2	2.14	0.46
1:I:229:DT:OP1	4:F:19:ARG:HG3	159.11	0.46
6:H:73:GLU:HB3	6:H:94:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:37:GLY:HA3	5:G:39:TYR:CE1	2.51	0.46
1:I:116:DT:H2''	1:I:117:DT:C5'	2.45	0.46
1:I:52:DA:H2''	1:I:53:DA:O5'	2.14	0.46
2:J:334:DC:C5'	3:A:41:TYR:CE2	2.98	0.46
1:I:146:DG:H2''	1:I:147:DT:OP2	2.13	0.46
1:I:150:DT:H2''	1:I:151:DT:C7	2.46	0.46
2:J:189:DC:C2	2:J:190:DC:C5	3.03	0.46
2:J:243:DC:H2''	2:J:244:DA:O5'	2.16	0.46
2:J:76:DC:H2''	2:J:77:DA:O5'	2.16	0.46
2:J:97:DA:H2''	2:J:98:DT:H5'	1.97	0.46
5:C:15:LYS:HG3	5:C:19:SER:OG	2.16	0.46
6:D:64:ASN:O	6:D:68:GLU:HG3	2.16	0.46
1:I:170:DT:C2'	1:I:171:DT:C5'	2.93	0.46
2:J:31:DA:C8	2:J:32:DT:H72	2.51	0.46
2:J:50:DA:OP2	6:D:8:LYS:HE3	232.10	0.46
1:I:283:DT:H2''	1:I:284:DT:C5'	2.45	0.46
2:J:264:DA:H2''	2:J:265:DT:H5'	1.97	0.46
1:I:134:DT:H5'	6:D:27:ARG:NH2	2.31	0.46
2:J:10:DA:H2''	2:J:11:DT:OP2	2.14	0.46
1:I:339:DG:N9	1:I:340:DT:H72	2.30	0.46
1:I:18:DG:C2'	1:I:19:DT:C7	2.93	0.46
2:J:304:DA:H1'	2:J:305:DC:H5''	1.98	0.46
6:D:13:LYS:CG	6:D:26:ARG:H	2.29	0.45
2:J:195:DA:C2'	2:J:196:DG:N7	2.75	0.45
2:J:332:DT:H2''	2:J:333:DC:OP2	2.15	0.45
1:I:339:DG:H2''	1:I:340:DT:OP2	2.16	0.45
1:I:18:DG:H2''	1:I:19:DT:C7	2.46	0.45
1:I:1:DA:H2''	1:I:2:DC:C6	2.51	0.45
2:J:202:DC:H2''	2:J:203:DC:OP2	2.16	0.45
3:A:76:GLN:NE2	3:A:80:THR:HG22	2.31	0.45
2:J:185:DG:H2''	2:J:186:DC:OP2	2.17	0.45
6:H:102:GLU:OE2	6:H:106:HIS:NE2	2.49	0.45
1:I:301:DT:H5'	6:D:27:ARG:NH2	208.92	0.45
1:I:326:DC:C2'	1:I:327:DT:H72	2.47	0.45
2:J:169:DG:H2'	2:J:170:DT:H72	1.98	0.45
2:J:75:DT:H2''	2:J:76:DC:H5''	1.98	0.45
1:I:6:DC:H2''	1:I:7:DA:OP2	2.16	0.45
1:I:179:DC:H2''	1:I:180:DA:OP2	2.16	0.45
4:F:16:LYS:O	4:F:17:ARG:HD2	2.17	0.45
1:I:319:DC:C6	1:I:320:DT:H72	2.52	0.45
2:J:8:DA:H2''	2:J:9:DC:OP2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:137:DA:H1'	2:J:138:DC:H5''	1.98	0.45
1:I:78:DG:H2'	5:C:129:LYS:HZ2	1.81	0.45
2:J:329:DA:H2''	2:J:330:DC:OP2	2.16	0.45
2:J:334:DC:C2'	2:J:335:DT:C7	2.94	0.45
1:I:326:DC:C6	1:I:327:DT:H72	2.52	0.45
2:J:15:DC:H2''	2:J:16:DA:OP2	2.17	0.45
1:I:188:DA:C1'	1:I:189:DC:H5'	2.36	0.45
1:I:147:DT:H2''	1:I:148:DG:OP2	2.17	0.45
2:J:179:DG:H2''	2:J:180:DT:C7	2.47	0.45
1:I:162:DG:C4	1:I:163:DC:C5	3.05	0.45
1:I:304:DT:H2''	1:I:305:DA:C5'	2.43	0.45
2:J:92:DC:H2''	2:J:93:DT:H71	1.99	0.45
2:J:334:DC:O4'	3:A:39:HIS:NE2	2.49	0.45
2:J:4:DA:H2''	2:J:5:DC:OP2	2.17	0.45
1:I:2:DC:H2''	1:I:3:DT:OP2	2.16	0.45
2:J:328:DT:H2''	2:J:329:DA:OP2	2.18	0.44
3:A:65:LEU:HB3	3:A:66:PRO:HD3	2.00	0.44
1:I:169:DC:H2'	1:I:170:DT:H73	1.97	0.44
6:D:13:LYS:HZ3	6:D:13:LYS:HA	1.82	0.44
3:A:129:ARG:HB2	3:A:134:ARG:HE	1.83	0.44
2:J:54:DG:H5''	5:C:16:THR:HA	222.87	0.44
2:J:339:DC:H2''	2:J:340:DA:OP2	2.18	0.44
1:I:203:DC:H2''	1:I:204:DA:N7	2.32	0.44
2:J:166:DC:H2''	2:J:167:DC:H5	1.78	0.44
2:J:182:DC:H2'	2:J:183:DT:H72	1.93	0.44
1:I:185:DG:C8	1:I:186:DT:H72	2.52	0.44
1:I:326:DC:N1	1:I:327:DT:H72	2.32	0.44
2:J:6:DT:C6	2:J:7:DT:H72	2.53	0.44
1:I:327:DT:H2''	1:I:328:DT:C7	2.47	0.44
2:J:176:DT:H2''	2:J:177:DA:OP2	2.18	0.44
4:B:70:VAL:O	4:B:74:GLU:HG3	2.18	0.44
6:D:101:GLY:O	6:D:105:LYS:HG3	2.18	0.44
2:J:330:DC:H2''	2:J:331:DA:OP2	2.18	0.44
1:I:301:DT:OP1	6:D:28:LYS:NZ	199.32	0.44
1:I:146:DG:H2''	1:I:147:DT:H71	1.97	0.44
1:I:151:DT:H2''	1:I:152:DC:OP2	2.18	0.44
2:J:181:DA:H2''	2:J:182:DC:OP2	2.18	0.44
1:I:165:DA:H2''	1:I:166:DG:OP2	2.16	0.44
2:J:345:DA:H2''	2:J:346:DG:OP2	2.18	0.44
3:A:79:LYS:HD2	4:B:74:GLU:CG	2.48	0.44
1:I:140:DC:H2'	1:I:141:DT:H72	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:168:DA:H1'	1:I:169:DC:C6	2.53	0.44
5:C:117:PRO:O	5:C:118:LYS:HB2	2.18	0.44
1:I:147:DT:C2	1:I:148:DG:N7	2.86	0.44
1:I:36:DC:H2''	1:I:37:DA:N7	2.32	0.44
2:J:5:DC:H2'	2:J:6:DT:H72	1.99	0.44
4:B:30:THR:OG1	4:B:32:PRO:HG2	2.18	0.43
2:J:182:DC:H2''	2:J:183:DT:OP2	2.19	0.43
2:J:221:DG:H5''	5:C:16:THR:HA	2.00	0.43
2:J:242:DT:H2''	2:J:243:DC:H5''	1.98	0.43
1:I:116:DT:C2'	1:I:117:DT:H5''	2.49	0.43
2:J:335:DT:C5'	3:A:39:HIS:CD2	2.90	0.43
2:J:342:DG:C2'	2:J:343:DT:C7	2.96	0.43
1:I:96:DA:H1'	1:I:97:DT:H5''	2.00	0.43
2:J:237:DC:OP1	6:H:26:ARG:NH1	2.45	0.43
2:J:9:DC:H2''	2:J:10:DA:C8	2.53	0.43
2:J:259:DC:H2''	2:J:260:DT:H71	1.99	0.43
2:J:118:DG:H2''	2:J:119:DA:OP2	2.19	0.43
1:I:313:DG:H2''	1:I:314:DT:OP2	2.19	0.43
3:E:65:LEU:HB3	3:E:66:PRO:HD3	2.01	0.43
5:C:117:PRO:O	5:C:118:LYS:HG2	2.19	0.43
1:I:323:DA:H2''	1:I:324:DG:C8	2.54	0.43
2:J:188:DG:C4	2:J:189:DC:C5	3.06	0.43
1:I:100:DC:H2''	1:I:101:DT:C7	2.49	0.43
2:J:285:DG:H2''	2:J:286:DA:OP2	2.18	0.43
1:I:174:DA:H2'	1:I:175:DT:H72	1.99	0.43
1:I:185:DG:H2''	1:I:186:DT:C7	2.48	0.43
6:H:119:THR:C	6:H:121:ALA:N	2.73	0.43
1:I:267:DC:H2''	1:I:268:DT:C7	2.49	0.43
5:G:66:ALA:HB2	5:G:83:LEU:HD23	2.01	0.43
2:J:334:DC:H4'	3:A:39:HIS:CE1	2.54	0.43
3:A:132:GLY:HA2	3:A:135:ALA:HB3	2.01	0.43
4:F:12:LYS:CD	4:F:16:LYS:HD3	2.49	0.43
1:I:283:DT:C2'	1:I:284:DT:H5''	2.49	0.43
3:A:73:GLU:OE1	4:B:25:ASN:ND2	2.38	0.43
1:I:134:DT:O2	6:D:24:LYS:NZ	2.42	0.42
2:J:184:DG:H2''	2:J:185:DG:OP2	2.19	0.42
2:J:189:DC:H2''	2:J:190:DC:OP2	2.19	0.42
2:J:148:DA:H1'	2:J:149:DG:H5''	2.01	0.42
1:I:16:DA:H2''	1:I:17:DT:C7	2.49	0.42
1:I:185:DG:H2'	1:I:186:DT:H72	2.01	0.42
1:I:150:DT:H2'	1:I:151:DT:H72	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:122:DG:H2'	4:F:2:GLY:N	188.87	0.42
2:J:93:DT:H2''	2:J:94:DG:C8	2.55	0.42
2:J:342:DG:H2''	2:J:343:DT:C7	2.49	0.42
1:I:263:DA:H1'	1:I:264:DT:H5''	2.01	0.42
2:J:315:DA:H1'	2:J:316:DG:H5''	2.00	0.42
6:H:69:ARG:HD2	6:H:98:LEU:HD11	2.01	0.42
2:J:113:DC:H2''	2:J:114:DT:C7	2.50	0.42
1:I:193:DC:H2''	1:I:194:DA:N7	2.35	0.42
2:J:334:DC:H5'	3:A:41:TYR:HE2	1.85	0.42
1:I:181:DG:H2''	1:I:182:DG:OP2	2.18	0.42
1:I:2:DC:H2'	1:I:3:DT:H72	2.01	0.42
2:J:35:DC:H2''	2:J:36:DC:OP2	2.18	0.42
2:J:260:DT:H2''	2:J:261:DG:C8	2.55	0.42
1:I:307:DC:H2'	1:I:308:DT:H72	2.00	0.42
1:I:183:DA:H2'	1:I:184:DT:H72	2.01	0.42
2:J:186:DC:H2''	2:J:187:DC:OP2	2.17	0.42
2:J:326:DG:H2''	2:J:327:DT:OP2	2.18	0.42
2:J:31:DA:C2'	2:J:32:DT:H72	2.49	0.42
2:J:70:DC:OP1	6:H:26:ARG:NH1	209.61	0.42
1:I:330:DC:H2''	1:I:331:DA:C8	2.55	0.42
2:J:280:DC:H2''	2:J:281:DT:C7	2.50	0.42
1:I:159:DG:C4	1:I:160:DC:C5	3.08	0.42
3:A:129:ARG:CD	3:A:135:ALA:HB2	2.35	0.42
1:I:328:DT:H2''	1:I:329:DA:C8	2.55	0.42
1:I:333:DG:H2''	1:I:334:DC:C6	2.55	0.42
1:I:337:DA:N9	1:I:338:DT:H72	2.34	0.42
4:F:17:ARG:HD2	4:F:17:ARG:HA	1.73	0.42
5:G:93:LEU:HD23	6:H:103:LEU:HD21	2.01	0.42
1:I:166:DG:H2''	1:I:167:DT:OP2	2.19	0.42
1:I:134:DT:OP1	6:D:28:LYS:NZ	2.49	0.42
1:I:12:DC:H2''	1:I:13:DA:OP2	2.20	0.42
5:G:76:THR:O	6:H:49:THR:HG23	2.19	0.42
1:I:171:DT:H1'	1:I:172:DA:C8	2.55	0.41
1:I:174:DA:H2''	1:I:175:DT:OP2	2.19	0.41
2:J:24:DC:H2'	2:J:25:DT:H71	1.98	0.41
6:H:26:ARG:HE	6:H:27:ARG:HG2	1.85	0.41
2:J:11:DT:C2	2:J:12:DG:C6	3.08	0.41
2:J:11:DT:C2'	2:J:12:DG:N7	2.79	0.41
2:J:173:DA:H2''	2:J:174:DT:C7	2.50	0.41
1:I:1:DA:H2''	1:I:2:DC:C5	2.54	0.41
5:G:73:ASN:O	5:G:74:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:183:DA:H2''	1:I:184:DT:C7	2.51	0.41
6:H:28:LYS:HB3	6:H:28:LYS:HE3	1.93	0.41
1:I:343:DG:H2'	1:I:344:DT:H72	2.02	0.41
2:J:167:DC:H2''	2:J:168:DT:OP2	2.19	0.41
1:I:7:DA:H2''	1:I:8:DT:C7	2.50	0.41
1:I:26:DC:H2''	1:I:27:DA:N7	2.35	0.41
1:I:149:DA:C2'	1:I:150:DT:C7	2.98	0.41
1:I:317:DT:C6	1:I:318:DT:H72	2.56	0.41
2:J:244:DA:H2''	2:J:245:DA:O5'	2.19	0.41
1:I:183:DA:C2'	1:I:184:DT:C7	2.98	0.41
1:I:134:DT:H4'	6:D:27:ARG:CZ	2.51	0.41
2:J:183:DT:H2''	2:J:184:DG:OP2	2.20	0.41
2:J:173:DA:H2''	2:J:174:DT:OP2	2.21	0.41
2:J:179:DG:H2''	2:J:180:DT:H73	2.02	0.41
6:H:102:GLU:OE2	6:H:105:LYS:HE3	2.20	0.41
1:I:312:DG:H2''	1:I:313:DG:OP2	2.20	0.41
2:J:77:DA:H2''	2:J:78:DA:O5'	2.18	0.41
6:H:119:THR:O	6:H:121:ALA:N	2.52	0.41
6:D:12:LYS:HE3	6:D:24:LYS:HG2	2.03	0.41
1:I:301:DT:H4'	6:D:27:ARG:CZ	210.25	0.41
2:J:289:DG:H2'	4:F:2:GLY:N	2.34	0.41
1:I:171:DT:H1'	1:I:172:DA:H5'	2.03	0.41
1:I:173:DC:H2''	1:I:174:DA:OP2	2.20	0.41
1:I:223:DG:O4'	6:D:26:ARG:NH2	208.28	0.41
2:J:76:DC:H5'	2:J:76:DC:H6	1.84	0.41
1:I:19:DT:H2''	1:I:20:DA:OP2	2.21	0.41
2:J:340:DA:H2''	2:J:341:DT:C7	2.51	0.41
1:I:332:DT:H2''	1:I:333:DG:OP2	2.20	0.41
2:J:287:DT:H2''	2:J:288:DG:OP2	2.21	0.41
2:J:331:DA:H2''	2:J:332:DT:C7	2.50	0.41
1:I:185:DG:C2'	1:I:186:DT:C7	2.98	0.41
2:J:338:DG:C4	2:J:339:DC:C5	3.08	0.41
1:I:56:DG:O4'	6:D:26:ARG:NH2	2.54	0.41
6:H:26:ARG:CG	6:H:27:ARG:HE	2.34	0.41
2:J:181:DA:H2''	2:J:182:DC:H5	1.85	0.41
2:J:200:DC:H1'	2:J:201:DA:H5'	2.03	0.41
2:J:45:DC:H2'	2:J:46:DT:H72	2.02	0.41
2:J:212:DC:H2'	2:J:213:DT:H72	2.03	0.41
2:J:14:DG:H2''	2:J:15:DC:C6	2.56	0.41
1:I:46:DT:C2'	1:I:47:DT:H71	2.51	0.41
6:D:67:PHE:CD2	6:D:67:PHE:C	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:15:LYS:HE2	5:G:19:SER:OG	2.21	0.41
6:H:99:LEU:HA	6:H:100:PRO:HD3	1.94	0.41
1:I:331:DA:C8	1:I:332:DT:H72	2.56	0.41
2:J:243:DC:H5'	2:J:243:DC:H6	1.85	0.41
6:H:77:LEU:HD11	6:H:93:THR:HG22	2.03	0.41
1:I:213:DT:C2'	1:I:214:DT:H71	2.51	0.41
2:J:120:DT:H2''	2:J:121:DG:OP2	2.21	0.41
2:J:294:DG:OP1	6:D:29:THR:HG23	2.21	0.41
2:J:333:DC:C2	2:J:334:DC:C5	3.09	0.40
1:I:323:DA:H2''	1:I:324:DG:H8	1.86	0.40
6:H:26:ARG:HG2	6:H:27:ARG:HE	1.86	0.40
1:I:327:DT:H2'	1:I:328:DT:H72	2.02	0.40
1:I:16:DA:C2'	1:I:17:DT:C7	3.00	0.40
2:J:332:DT:C2	2:J:333:DC:C4	3.10	0.40
2:J:18:DG:H1'	2:J:19:DT:H5'	2.02	0.40
2:J:300:DA:C6	2:J:301:DA:C6	3.10	0.40
1:I:168:DA:H1'	1:I:169:DC:H5'	2.03	0.40
2:J:334:DC:H2''	2:J:335:DT:C7	2.51	0.40
2:J:342:DG:N9	2:J:343:DT:H72	2.36	0.40
1:I:334:DC:H2''	1:I:335:DG:OP2	2.20	0.40
1:I:340:DT:H2''	1:I:341:DA:OP2	2.21	0.40
2:J:16:DA:H1'	2:J:17:DT:H5'	2.04	0.40
2:J:127:DG:OP1	6:D:29:THR:HG23	203.57	0.40
4:B:35:ARG:NH1	4:B:35:ARG:HB2	2.37	0.40
1:I:181:DG:H2''	1:I:182:DG:C8	2.57	0.40
2:J:167:DC:C6	2:J:168:DT:H72	2.56	0.40
2:J:170:DT:H2''	2:J:171:DG:OP2	2.21	0.40
2:J:173:DA:C2'	2:J:174:DT:C7	2.99	0.40
1:I:18:DG:H2'	1:I:19:DT:H72	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	95/135 (70%)	95 (100%)	0	0	100	100
3	E	95/135 (70%)	95 (100%)	0	0	100	100
3	a	95/135 (70%)	95 (100%)	0	0	100	100
3	e	95/135 (70%)	95 (100%)	0	0	100	100
4	B	77/102 (76%)	76 (99%)	0	1 (1%)	15	60
4	F	88/102 (86%)	83 (94%)	3 (3%)	2 (2%)	8	48
4	b	77/102 (76%)	76 (99%)	0	1 (1%)	15	60
4	f	88/102 (86%)	83 (94%)	3 (3%)	2 (2%)	8	48
5	C	105/129 (81%)	103 (98%)	1 (1%)	1 (1%)	19	65
5	G	107/129 (83%)	101 (94%)	4 (4%)	2 (2%)	10	52
5	c	105/129 (81%)	103 (98%)	1 (1%)	1 (1%)	19	65
5	g	107/129 (83%)	101 (94%)	4 (4%)	2 (2%)	10	52
6	D	103/125 (82%)	95 (92%)	3 (3%)	5 (5%)	3	31
6	H	97/125 (78%)	91 (94%)	1 (1%)	5 (5%)	2	30
6	d	103/125 (82%)	95 (92%)	3 (3%)	5 (5%)	3	31
6	h	97/125 (78%)	91 (94%)	1 (1%)	5 (5%)	2	30
All	All	1534/1964 (78%)	1478 (96%)	24 (2%)	32 (2%)	9	50

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	101	GLY
5	G	14	ALA
6	H	26	ARG
6	d	101	GLY
5	g	14	ALA
6	h	26	ARG
5	C	118	LYS
6	D	9	LYS
6	D	26	ARG
4	F	19	ARG
6	H	101	GLY
5	c	118	LYS
6	d	9	LYS
6	d	26	ARG
4	f	19	ARG
6	h	101	GLY

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Mol	Chain	Res	Type
6	D	12	LYS
6	D	27	ARG
4	F	18	HIS
5	G	119	LYS
6	H	27	ARG
6	H	120	SER
6	d	12	LYS
6	d	27	ARG
4	f	18	HIS
5	g	119	LYS
6	h	27	ARG
6	h	120	SER
6	H	29	THR
6	h	29	THR
4	B	25	ASN
4	b	25	ASN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	84/110 (76%)	83 (99%)	1 (1%)	78	90
3	E	84/110 (76%)	82 (98%)	2 (2%)	57	82
3	a	84/110 (76%)	83 (99%)	1 (1%)	78	90
3	e	84/110 (76%)	82 (98%)	2 (2%)	57	82
4	B	65/78 (83%)	65 (100%)	0	100	100
4	F	76/78 (97%)	73 (96%)	3 (4%)	39	72
4	b	65/78 (83%)	65 (100%)	0	100	100
4	f	76/78 (97%)	73 (96%)	3 (4%)	39	72
5	C	89/101 (88%)	86 (97%)	3 (3%)	44	75
5	G	87/101 (86%)	85 (98%)	2 (2%)	58	83
5	c	89/101 (88%)	86 (97%)	3 (3%)	44	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	g	87/101 (86%)	85 (98%)	2 (2%)	58	83
6	D	91/105 (87%)	88 (97%)	3 (3%)	45	76
6	H	85/105 (81%)	83 (98%)	2 (2%)	57	82
6	d	91/105 (87%)	88 (97%)	3 (3%)	45	76
6	h	85/105 (81%)	83 (98%)	2 (2%)	57	82
All	All	1322/1576 (84%)	1290 (98%)	32 (2%)	57	82

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	48	LEU
5	C	118	LYS
5	C	119	LYS
5	C	120	THR
6	D	13	LYS
6	D	25	LYS
6	D	82	LYS
3	E	60	LEU
3	E	109	LEU
4	F	17	ARG
4	F	18	HIS
4	F	47	SER
5	G	109	PRO
5	G	121	GLU
6	H	25	LYS
6	H	103	LEU
3	a	48	LEU
5	c	118	LYS
5	c	119	LYS
5	c	120	THR
6	d	13	LYS
6	d	25	LYS
6	d	82	LYS
3	e	60	LEU
3	e	109	LEU
4	f	17	ARG
4	f	18	HIS
4	f	47	SER
5	g	109	PRO
5	g	121	GLU

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Mol	Chain	Res	Type
6	h	25	LYS
6	h	103	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	93	GLN
5	C	31	HIS
6	D	92	GLN
3	E	125	GLN
5	G	31	HIS
5	G	110	ASN
3	a	39	HIS
4	b	93	GLN
5	c	31	HIS
6	d	92	GLN
3	e	125	GLN
5	g	31	HIS
5	g	110	ASN
6	h	92	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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, 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	I	347/347 (100%)	0.30	14 (4%) 42 40	238, 238, 238, 238	347 (100%)
2	J	347/347 (100%)	0.30	13 (3%) 45 42	238, 238, 238, 238	347 (100%)
3	A	97/135 (71%)	-0.40	0 100 100	230, 230, 230, 230	97 (100%)
3	E	97/135 (71%)	-0.54	0 100 100	230, 230, 230, 230	97 (100%)
3	a	97/135 (71%)	-0.23	1 (1%) 84 79	230, 230, 230, 230	97 (100%)
3	e	97/135 (71%)	-0.53	0 100 100	230, 230, 230, 230	97 (100%)
4	B	80/102 (78%)	0.15	5 (6%) 23 25	230, 230, 230, 230	80 (100%)
4	F	94/102 (92%)	-0.20	4 (4%) 39 37	230, 230, 230, 230	94 (100%)
4	b	80/102 (78%)	0.11	6 (7%) 17 21	230, 230, 230, 230	80 (100%)
4	f	94/102 (92%)	-0.11	5 (5%) 30 31	230, 230, 230, 230	94 (100%)
5	C	111/129 (86%)	0.23	10 (9%) 12 16	230, 230, 230, 230	111 (100%)
5	G	109/129 (84%)	-0.03	3 (2%) 56 52	230, 230, 230, 230	109 (100%)
5	c	111/129 (86%)	0.24	6 (5%) 29 30	230, 230, 230, 230	111 (100%)
5	g	109/129 (84%)	-0.07	2 (1%) 71 66	230, 230, 230, 230	109 (100%)
6	D	107/125 (85%)	-0.10	4 (3%) 45 42	230, 230, 230, 230	107 (100%)
6	H	99/125 (79%)	0.51	17 (17%) 2 8	230, 230, 230, 230	99 (100%)
6	d	107/125 (85%)	-0.15	1 (0%) 85 81	230, 230, 230, 230	107 (100%)
6	h	99/125 (79%)	0.28	7 (7%) 19 22	230, 230, 230, 230	99 (100%)
All	All	2282/2658 (85%)	0.05	98 (4%) 39 37	230, 230, 238, 238	2282 (100%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	101	GLY	6.3
4	b	101	GLY	6.2
6	H	121	ALA	6.1

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Mol	Chain	Res	Type	RSRZ
2	J	5	DC	6.1
6	H	29	THR	5.5
4	b	99	GLY	5.2
4	f	101	GLY	4.3
1	I	345	DG	4.3
4	B	102	GLY	4.2
6	H	33	SER	4.1
6	h	33	SER	4.1
2	J	346	DG	4.0
6	D	10	GLY	4.0
1	I	170	DT	3.9
6	h	57	SER	3.8
1	I	346	DC	3.8
5	C	12	ALA	3.7
4	F	101	GLY	3.7
4	F	99	GLY	3.7
2	J	345	DA	3.7
5	C	10	THR	3.6
4	b	102	GLY	3.5
4	b	98	TYR	3.5
4	f	99	GLY	3.4
6	H	119	THR	3.4
2	J	4	DA	3.4
4	f	102	GLY	3.3
4	f	98	TYR	3.2
6	h	60	ASN	3.1
2	J	178	DA	3.1
5	C	128	SER	3.1
6	H	60	ASN	3.1
1	I	5	DA	3.0
4	B	99	GLY	3.0
4	f	11	GLY	3.0
2	J	179	DG	2.9
6	H	66	VAL	2.9
2	J	344	DA	2.9
4	F	98	TYR	2.9
2	J	6	DT	2.9
5	C	103	ALA	2.8
6	h	121	ALA	2.8
1	I	336	DC	2.8
5	c	69	ALA	2.7
6	H	31	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
6	H	120	SER	2.7
2	J	213	DT	2.7
6	H	34	TYR	2.7
1	I	169	DC	2.6
6	H	32	GLU	2.6
4	F	102	GLY	2.6
6	H	61	SER	2.6
2	J	343	DT	2.6
6	H	57	SER	2.6
6	h	35	ALA	2.6
6	H	35	ALA	2.5
1	I	171	DT	2.5
5	G	117	PRO	2.5
1	I	1	DA	2.5
4	b	100	PHE	2.5
2	J	347	DT	2.5
2	J	2	DG	2.4
4	b	54	THR	2.4
5	g	103	ALA	2.4
6	D	59	MET	2.4
5	C	73	ASN	2.4
1	I	344	DT	2.3
6	H	65	ASP	2.3
6	H	122	LYS	2.3
4	B	98	TYR	2.3
6	d	59	MET	2.2
5	C	68	ASN	2.2
5	c	11	ARG	2.2
6	h	56	MET	2.2
5	c	73	ASN	2.2
6	D	61	SER	2.2
1	I	9	DG	2.2
5	g	20	ARG	2.2
5	C	72	ASP	2.2
1	I	298	DT	2.2
5	G	115	LEU	2.2
1	I	10	DC	2.2
1	I	335	DG	2.2
1	I	168	DA	2.2
4	B	100	PHE	2.1
5	c	120	THR	2.1
5	C	63	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
5	G	20	ARG	2.1
6	H	63	VAL	2.1
3	a	39	HIS	2.1
5	C	101	THR	2.1
6	H	118	TYR	2.1
5	c	12	ALA	2.1
6	D	60	ASN	2.0
6	h	117	LYS	2.0
5	C	59	THR	2.0
5	c	68	ASN	2.0
2	J	212	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.