



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2026 – 09:46 PM UTC

PDB ID : 6HKT / pdb_00006hkt
Title : Structure of an H1-bound 6-nucleosome array
Authors : Garcia-Saez, I.; Dimitrov, S.; Petosa, C.
Deposited on : 2018-09-08
Resolution : 9.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

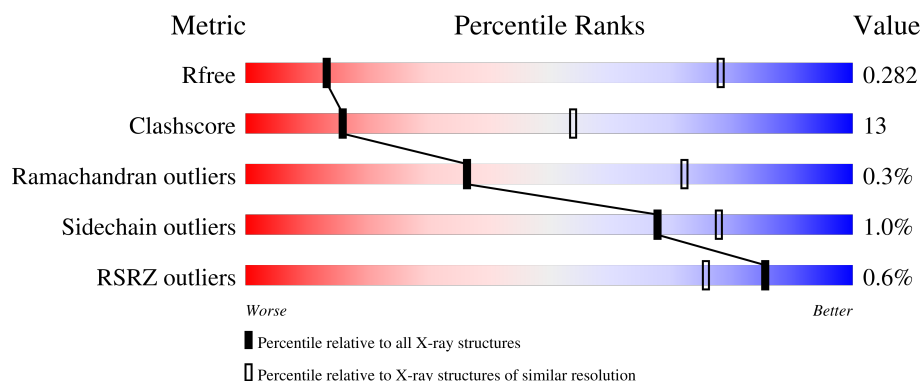
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 9.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1168 (11.50-4.00)
Clashscore	190562	1002 (15.00-4.06)
Ramachandran outliers	187476	1055 (11.50-4.00)
Sidechain outliers	187428	1018 (11.50-4.00)
RSRZ outliers	180081	1162 (11.50-4.00)

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

Mol	Chain	Length	Quality of chain
1	A	139	
1	E	139	
1	K	139	
1	O	139	
1	U	139	

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Mol	Chain	Length	Quality of chain
1	Y	139	
1	a	139	
1	e	139	
1	k	139	
1	o	139	
1	u	139	
1	y	139	
2	B	106	
2	F	106	
2	L	106	
2	P	106	
2	V	106	
2	Z	106	
2	b	106	
2	f	106	
2	l	106	
2	p	106	
2	v	106	
2	z	106	
3	0	133	
3	2	133	
3	C	133	
3	G	133	
3	M	133	
3	Q	133	

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Mol	Chain	Length	Quality of chain
3	W	133	
3	c	133	
3	g	133	
3	m	133	
3	q	133	
3	w	133	
4	1	129	
4	3	129	
4	D	129	
4	H	129	
4	N	129	
4	R	129	
4	X	129	
4	d	129	
4	h	129	
4	n	129	
4	r	129	
4	x	129	
5	I	1122	
6	J	1122	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 82122 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			
1	E	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	a	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	e	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			
1	K	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			
1	O	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	k	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	o	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			
1	U	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			
1	Y	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	u	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	y	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			

There are 36 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	HIS	-	expression tag	UNP P68431
a	-3	GLY	-	expression tag	UNP P68431
a	-2	SER	-	expression tag	UNP P68431
a	-1	HIS	-	expression tag	UNP P68431
e	-3	GLY	-	expression tag	UNP P68431
e	-2	SER	-	expression tag	UNP P68431
e	-1	HIS	-	expression tag	UNP P68431
K	-3	GLY	-	expression tag	UNP P68431
K	-2	SER	-	expression tag	UNP P68431
K	-1	HIS	-	expression tag	UNP P68431
O	-3	GLY	-	expression tag	UNP P68431
O	-2	SER	-	expression tag	UNP P68431
O	-1	HIS	-	expression tag	UNP P68431
k	-3	GLY	-	expression tag	UNP P68431
k	-2	SER	-	expression tag	UNP P68431
k	-1	HIS	-	expression tag	UNP P68431
o	-3	GLY	-	expression tag	UNP P68431
o	-2	SER	-	expression tag	UNP P68431
o	-1	HIS	-	expression tag	UNP P68431
U	-3	GLY	-	expression tag	UNP P68431
U	-2	SER	-	expression tag	UNP P68431
U	-1	HIS	-	expression tag	UNP P68431
Y	-3	GLY	-	expression tag	UNP P68431
Y	-2	SER	-	expression tag	UNP P68431
Y	-1	HIS	-	expression tag	UNP P68431
u	-3	GLY	-	expression tag	UNP P68431
u	-2	SER	-	expression tag	UNP P68431
u	-1	HIS	-	expression tag	UNP P68431
y	-3	GLY	-	expression tag	UNP P68431
y	-2	SER	-	expression tag	UNP P68431
y	-1	HIS	-	expression tag	UNP P68431

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	F	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	b	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	f	82	Total 653	C 412	N 127	O 113	S 1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	P	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	l	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	p	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	V	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	Z	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	v	82	Total 653	C 412	N 127	O 113	S 1	0	0	0
2	z	82	Total 653	C 412	N 127	O 113	S 1	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P62805
B	-2	SER	-	expression tag	UNP P62805
B	-1	HIS	-	expression tag	UNP P62805
F	-3	GLY	-	expression tag	UNP P62805
F	-2	SER	-	expression tag	UNP P62805
F	-1	HIS	-	expression tag	UNP P62805
b	-3	GLY	-	expression tag	UNP P62805
b	-2	SER	-	expression tag	UNP P62805
b	-1	HIS	-	expression tag	UNP P62805
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805
f	-1	HIS	-	expression tag	UNP P62805
L	-3	GLY	-	expression tag	UNP P62805
L	-2	SER	-	expression tag	UNP P62805
L	-1	HIS	-	expression tag	UNP P62805
P	-3	GLY	-	expression tag	UNP P62805
P	-2	SER	-	expression tag	UNP P62805
P	-1	HIS	-	expression tag	UNP P62805
l	-3	GLY	-	expression tag	UNP P62805
l	-2	SER	-	expression tag	UNP P62805
l	-1	HIS	-	expression tag	UNP P62805
p	-3	GLY	-	expression tag	UNP P62805
p	-2	SER	-	expression tag	UNP P62805

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Chain	Residue	Modelled	Actual	Comment	Reference
p	-1	HIS	-	expression tag	UNP P62805
V	-3	GLY	-	expression tag	UNP P62805
V	-2	SER	-	expression tag	UNP P62805
V	-1	HIS	-	expression tag	UNP P62805
Z	-3	GLY	-	expression tag	UNP P62805
Z	-2	SER	-	expression tag	UNP P62805
Z	-1	HIS	-	expression tag	UNP P62805
v	-3	GLY	-	expression tag	UNP P62805
v	-2	SER	-	expression tag	UNP P62805
v	-1	HIS	-	expression tag	UNP P62805
z	-3	GLY	-	expression tag	UNP P62805
z	-2	SER	-	expression tag	UNP P62805
z	-1	HIS	-	expression tag	UNP P62805

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	103	Total	C	N	O	0	0	0
			796	502	155	139			
3	G	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	c	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	g	103	Total	C	N	O	0	0	0
			796	502	155	139			
3	M	103	Total	C	N	O	0	0	0
			796	502	155	139			
3	Q	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	m	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	q	103	Total	C	N	O	0	0	0
			796	502	155	139			
3	W	103	Total	C	N	O	0	0	0
			796	502	155	139			
3	0	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	w	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	2	103	Total	C	N	O	0	0	0
			796	502	155	139			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP P04908
C	-2	SER	-	expression tag	UNP P04908
C	-1	HIS	-	expression tag	UNP P04908
G	-3	GLY	-	expression tag	UNP P04908
G	-2	SER	-	expression tag	UNP P04908
G	-1	HIS	-	expression tag	UNP P04908
c	-3	GLY	-	expression tag	UNP P04908
c	-2	SER	-	expression tag	UNP P04908
c	-1	HIS	-	expression tag	UNP P04908
g	-3	GLY	-	expression tag	UNP P04908
g	-2	SER	-	expression tag	UNP P04908
g	-1	HIS	-	expression tag	UNP P04908
M	-3	GLY	-	expression tag	UNP P04908
M	-2	SER	-	expression tag	UNP P04908
M	-1	HIS	-	expression tag	UNP P04908
Q	-3	GLY	-	expression tag	UNP P04908
Q	-2	SER	-	expression tag	UNP P04908
Q	-1	HIS	-	expression tag	UNP P04908
m	-3	GLY	-	expression tag	UNP P04908
m	-2	SER	-	expression tag	UNP P04908
m	-1	HIS	-	expression tag	UNP P04908
q	-3	GLY	-	expression tag	UNP P04908
q	-2	SER	-	expression tag	UNP P04908
q	-1	HIS	-	expression tag	UNP P04908
W	-3	GLY	-	expression tag	UNP P04908
W	-2	SER	-	expression tag	UNP P04908
W	-1	HIS	-	expression tag	UNP P04908
0	-3	GLY	-	expression tag	UNP P04908
0	-2	SER	-	expression tag	UNP P04908
0	-1	HIS	-	expression tag	UNP P04908
w	-3	GLY	-	expression tag	UNP P04908
w	-2	SER	-	expression tag	UNP P04908
w	-1	HIS	-	expression tag	UNP P04908
2	-3	GLY	-	expression tag	UNP P04908
2	-2	SER	-	expression tag	UNP P04908
2	-1	HIS	-	expression tag	UNP P04908

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	H	95	Total	C	N	O	S	0	0	0
			745	468	136	139	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	95	Total	C	N	O	S	0	0	0
			745	468	136	139	2			
4	h	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	95	Total	C	N	O	S	0	0	0
			745	468	136	139	2			
4	n	95	Total	C	N	O	S	0	0	0
			745	468	136	139	2			
4	r	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	X	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	1	95	Total	C	N	O	S	0	0	0
			745	468	136	139	2			
4	x	95	Total	C	N	O	S	0	0	0
			745	468	136	139	2			
4	3	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP P06899
D	-5	SER	-	expression tag	UNP P06899
D	-4	HIS	-	expression tag	UNP P06899
H	-6	GLY	-	expression tag	UNP P06899
H	-5	SER	-	expression tag	UNP P06899
H	-4	HIS	-	expression tag	UNP P06899
d	-6	GLY	-	expression tag	UNP P06899
d	-5	SER	-	expression tag	UNP P06899
d	-4	HIS	-	expression tag	UNP P06899
h	-6	GLY	-	expression tag	UNP P06899
h	-5	SER	-	expression tag	UNP P06899
h	-4	HIS	-	expression tag	UNP P06899
N	-6	GLY	-	expression tag	UNP P06899
N	-5	SER	-	expression tag	UNP P06899
N	-4	HIS	-	expression tag	UNP P06899
R	-6	GLY	-	expression tag	UNP P06899
R	-5	SER	-	expression tag	UNP P06899
R	-4	HIS	-	expression tag	UNP P06899
n	-6	GLY	-	expression tag	UNP P06899

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Chain	Residue	Modelled	Actual	Comment	Reference
n	-5	SER	-	expression tag	UNP P06899
n	-4	HIS	-	expression tag	UNP P06899
r	-6	GLY	-	expression tag	UNP P06899
r	-5	SER	-	expression tag	UNP P06899
r	-4	HIS	-	expression tag	UNP P06899
X	-6	GLY	-	expression tag	UNP P06899
X	-5	SER	-	expression tag	UNP P06899
X	-4	HIS	-	expression tag	UNP P06899
1	-6	GLY	-	expression tag	UNP P06899
1	-5	SER	-	expression tag	UNP P06899
1	-4	HIS	-	expression tag	UNP P06899
x	-6	GLY	-	expression tag	UNP P06899
x	-5	SER	-	expression tag	UNP P06899
x	-4	HIS	-	expression tag	UNP P06899
3	-6	GLY	-	expression tag	UNP P06899
3	-5	SER	-	expression tag	UNP P06899
3	-4	HIS	-	expression tag	UNP P06899

- Molecule 5 is a DNA chain called DNA (1122-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	1122	Total	C	N	O	P	0	0	0
			22861	10850	4162	6727	1122			

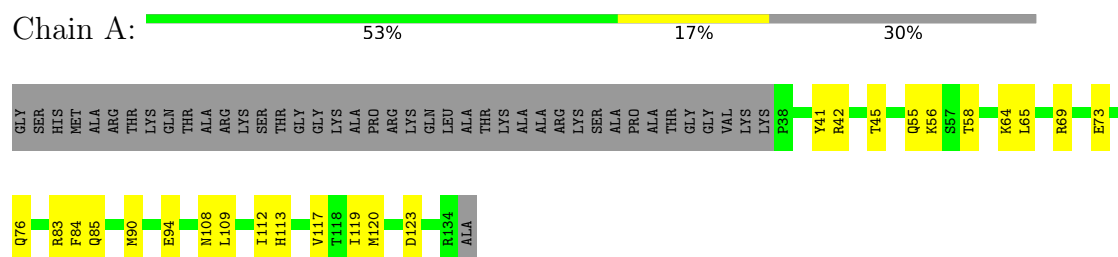
- Molecule 6 is a DNA chain called DNA (1122-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	1122	Total	C	N	O	P	0	0	0
			23141	10945	4337	6737	1122			

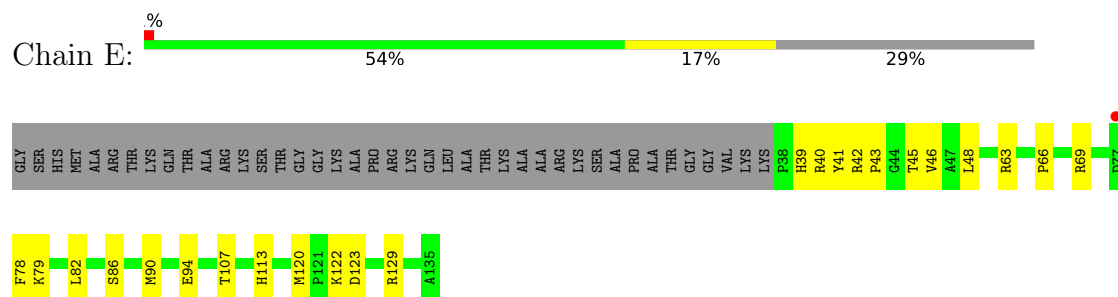
3 Residue-property plots [i](#)

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.

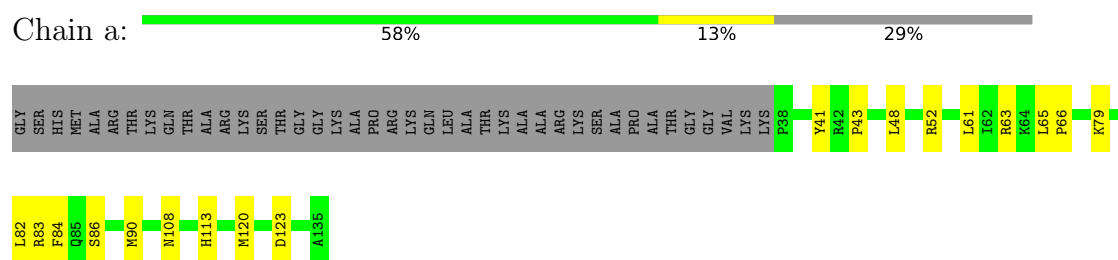
• Molecule 1: Histone H3.1



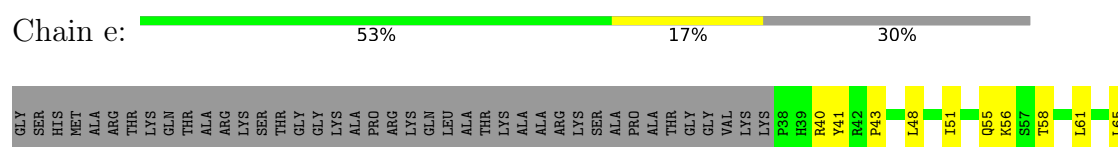
• Molecule 1: Histone H3.1

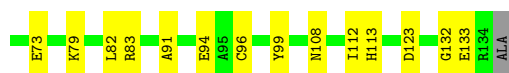


• Molecule 1: Histone H3.1

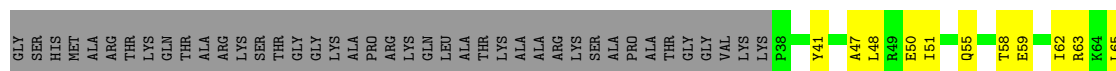


• Molecule 1: Histone H3.1

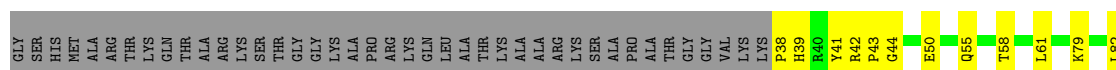




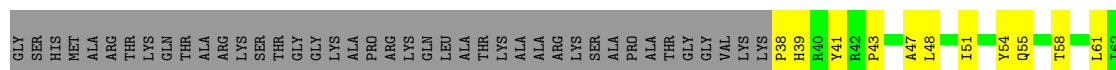
• Molecule 1: Histone H3.1



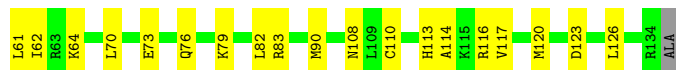
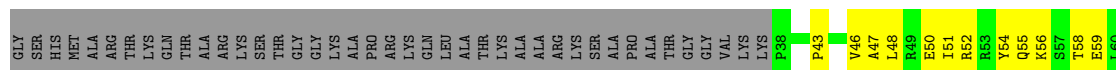
• Molecule 1: Histone H3.1



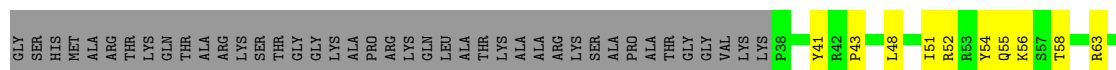
• Molecule 1: Histone H3.1



• Molecule 1: Histone H3.1



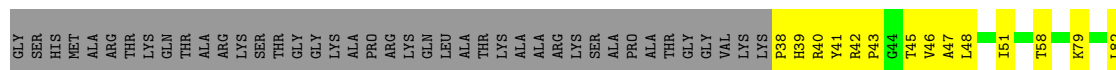
• Molecule 1: Histone H3.1





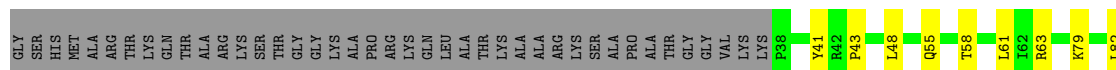
- Molecule 1: Histone H3.1

Chain Y: 48% 22% 29%



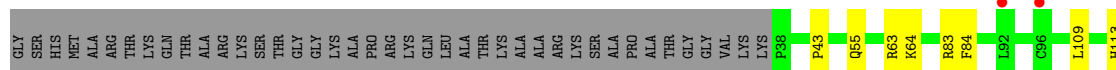
- Molecule 1: Histone H3.1

Chain u: 55% 15% 29%



- Molecule 1: Histone H3.1

Chain y: 64% 6% 30%



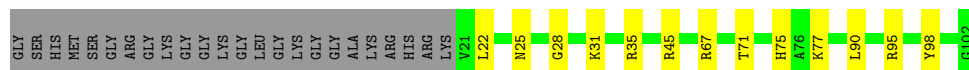
- Molecule 2: Histone H4

Chain B: 60% 17% 23%



- Molecule 2: Histone H4

Chain F: 65% 12% 23%



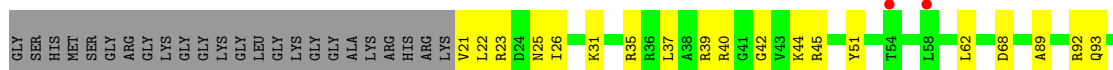
- Molecule 2: Histone H4



• Molecule 2: Histone H4



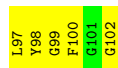
• Molecule 2: Histone H4



• Molecule 2: Histone H4



• Molecule 2: Histone H4



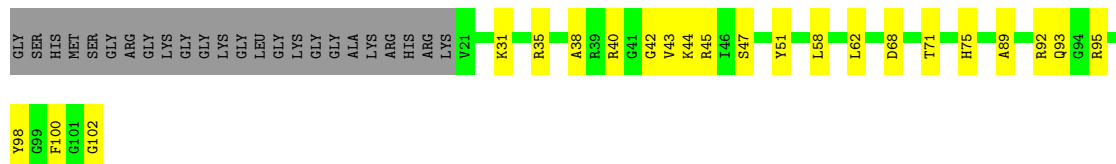
• Molecule 2: Histone H4





- Molecule 2: Histone H4

Chain V:



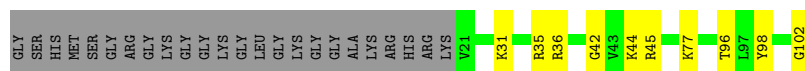
- Molecule 2: Histone H4

Chain Z:



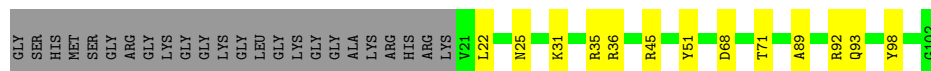
- Molecule 2: Histone H4

Chain v:



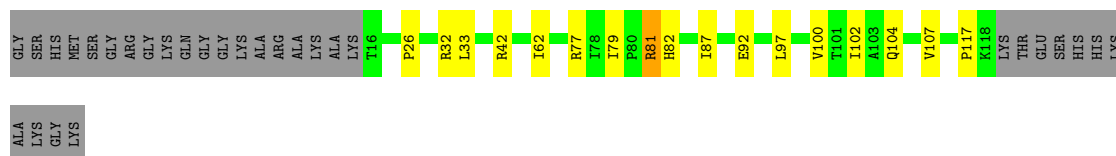
- Molecule 2: Histone H4

Chain z:



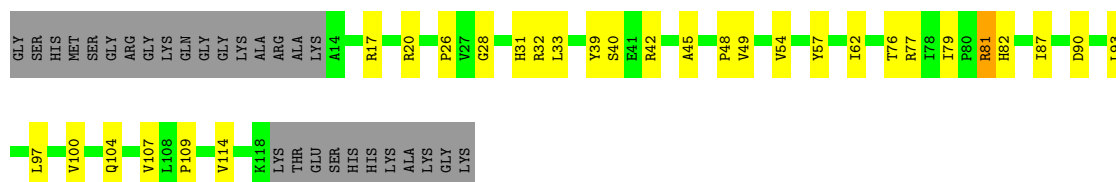
- Molecule 3: Histone H2A type 1-B/E

Chain C:

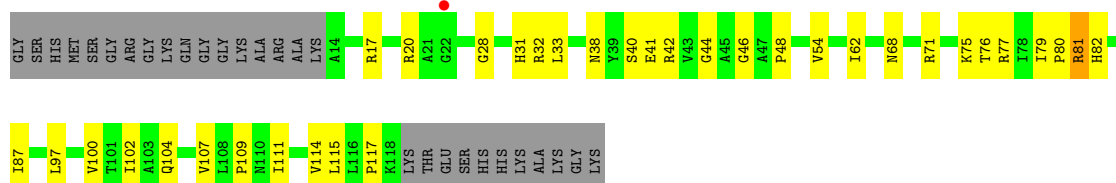


- Molecule 3: Histone H2A type 1-B/E

Chain G:



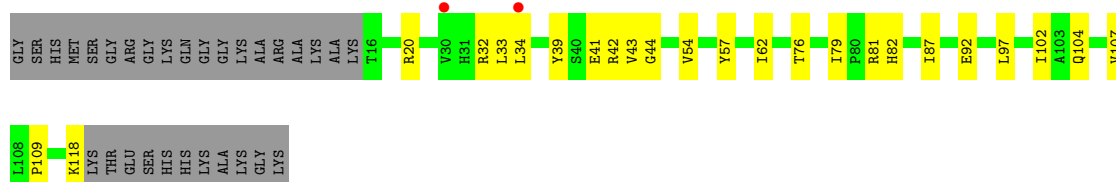
- Molecule 3: Histone H2A type 1-B/E



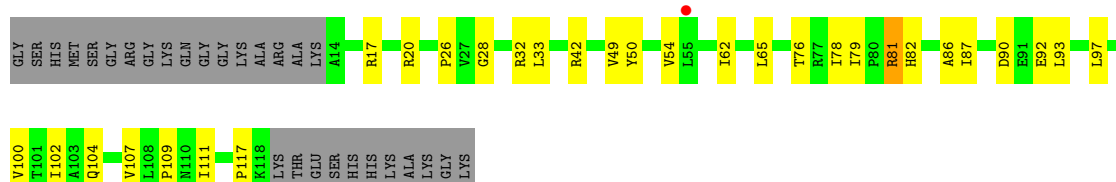
- Molecule 3: Histone H2A type 1-B/E



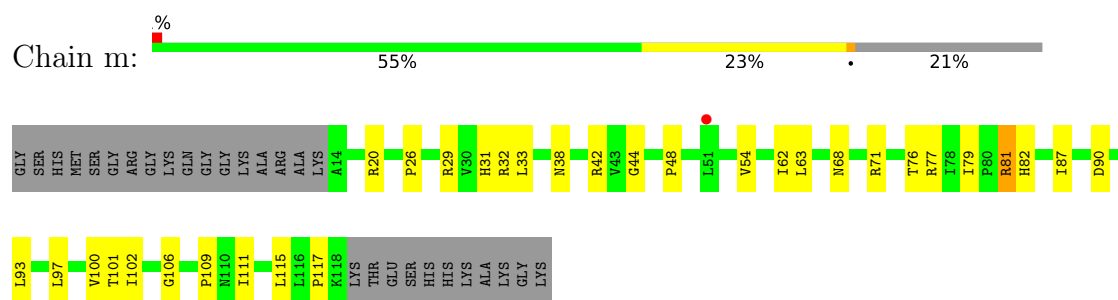
- Molecule 3: Histone H2A type 1-B/E



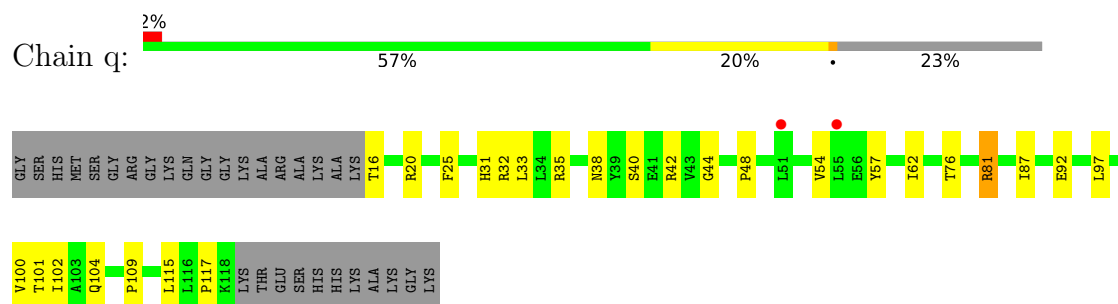
- Molecule 3: Histone H2A type 1-B/E



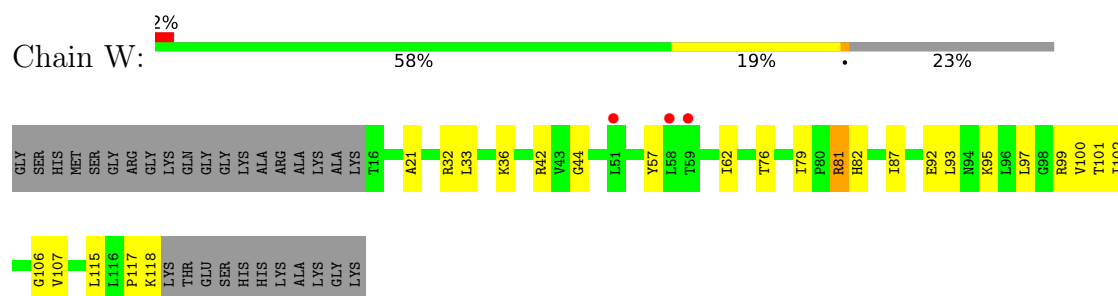
- Molecule 3: Histone H2A type 1-B/E



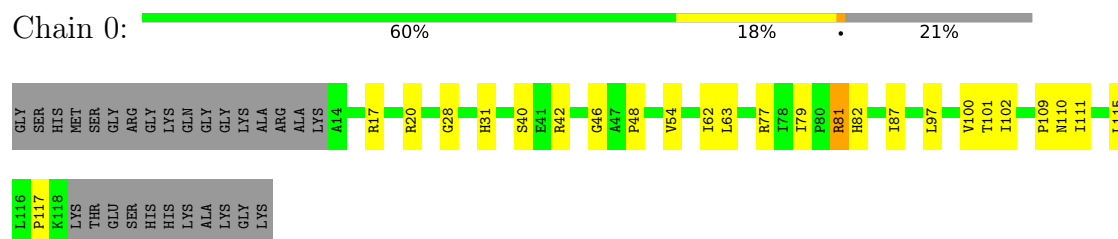
- Molecule 3: Histone H2A type 1-B/E



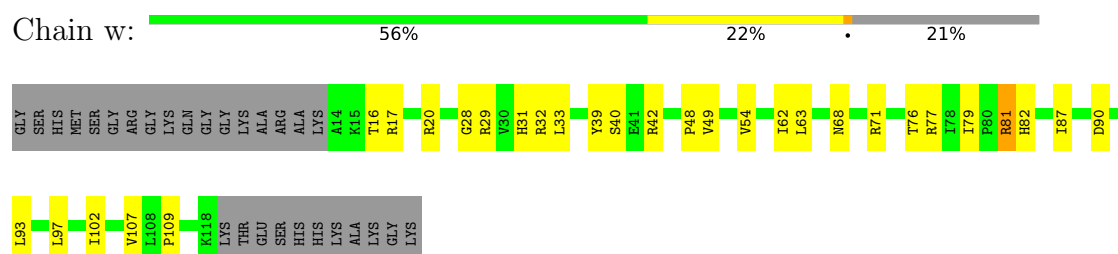
- Molecule 3: Histone H2A type 1-B/E



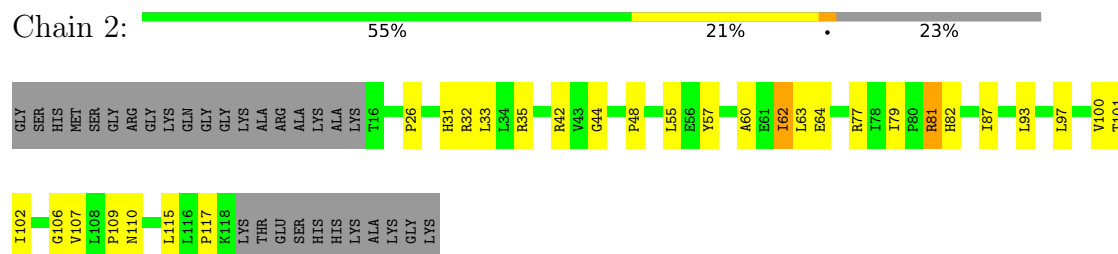
- Molecule 3: Histone H2A type 1-B/E



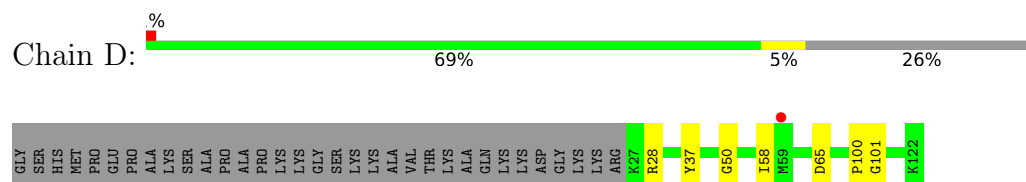
- Molecule 3: Histone H2A type 1-B/E



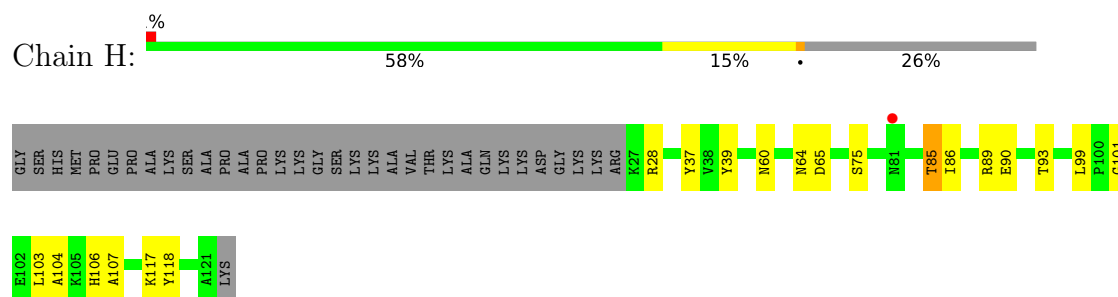
- Molecule 3: Histone H2A type 1-B/E



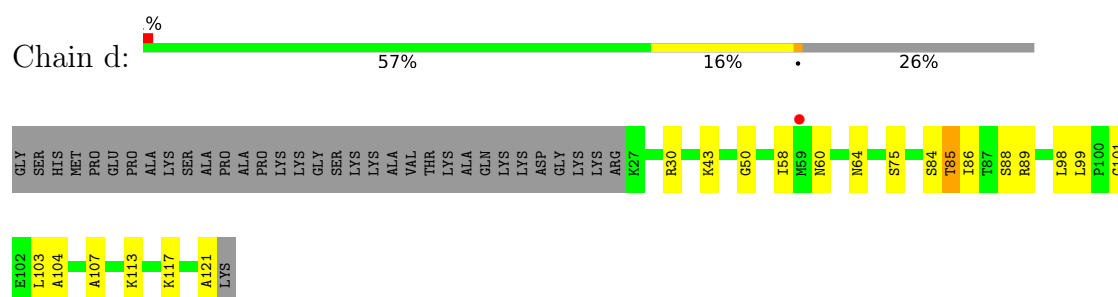
- Molecule 4: Histone H2B type 1-J



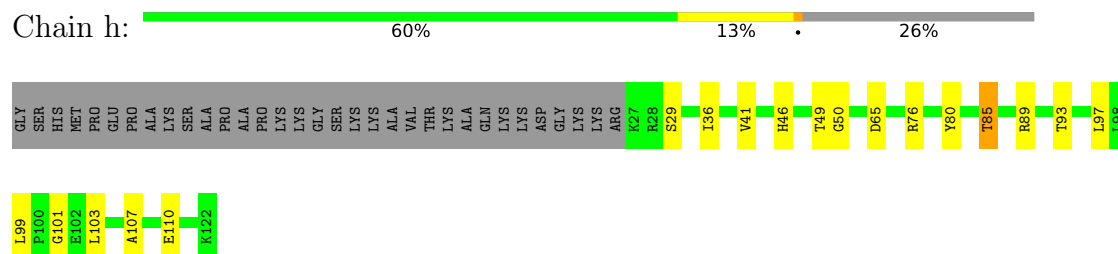
- Molecule 4: Histone H2B type 1-J



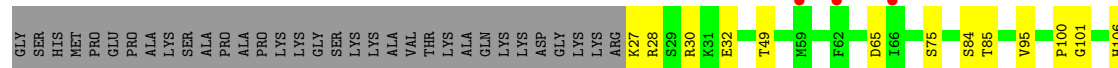
- Molecule 4: Histone H2B type 1-J



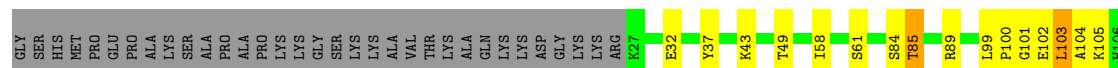
- Molecule 4: Histone H2B type 1-J



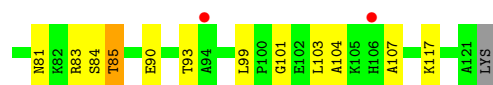
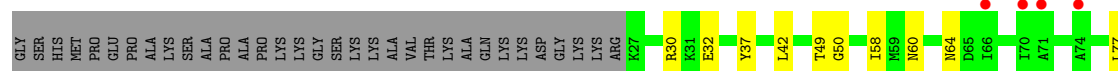
- Molecule 4: Histone H2B type 1-J



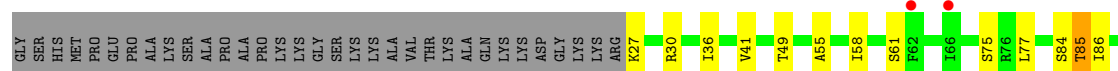
- Molecule 4: Histone H2B type 1-J



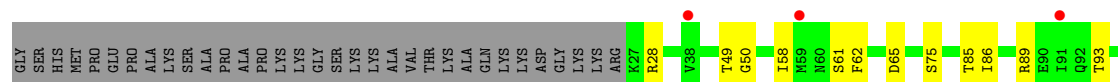
- Molecule 4: Histone H2B type 1-J



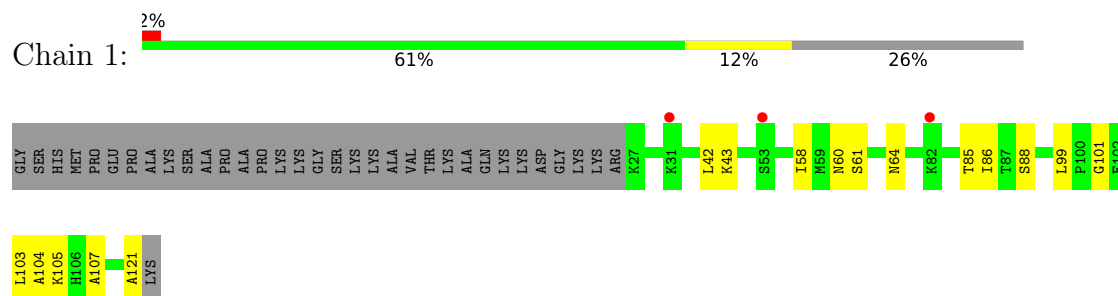
- Molecule 4: Histone H2B type 1-J



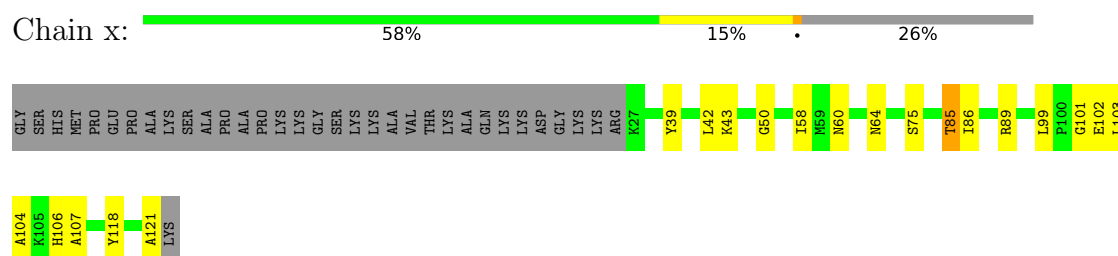
- Molecule 4: Histone H2B type 1-J



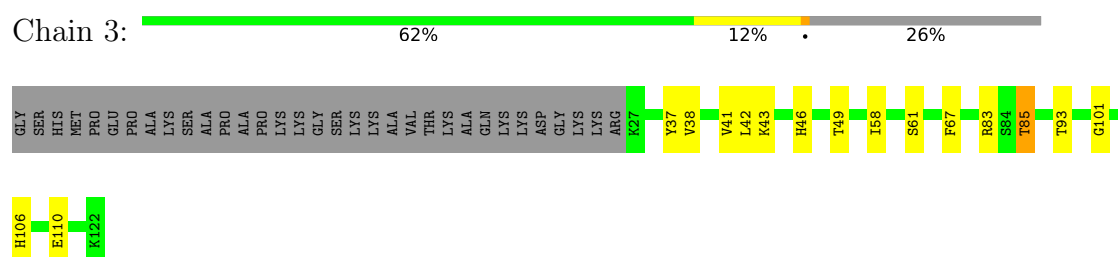
- Molecule 4: Histone H2B type 1-J



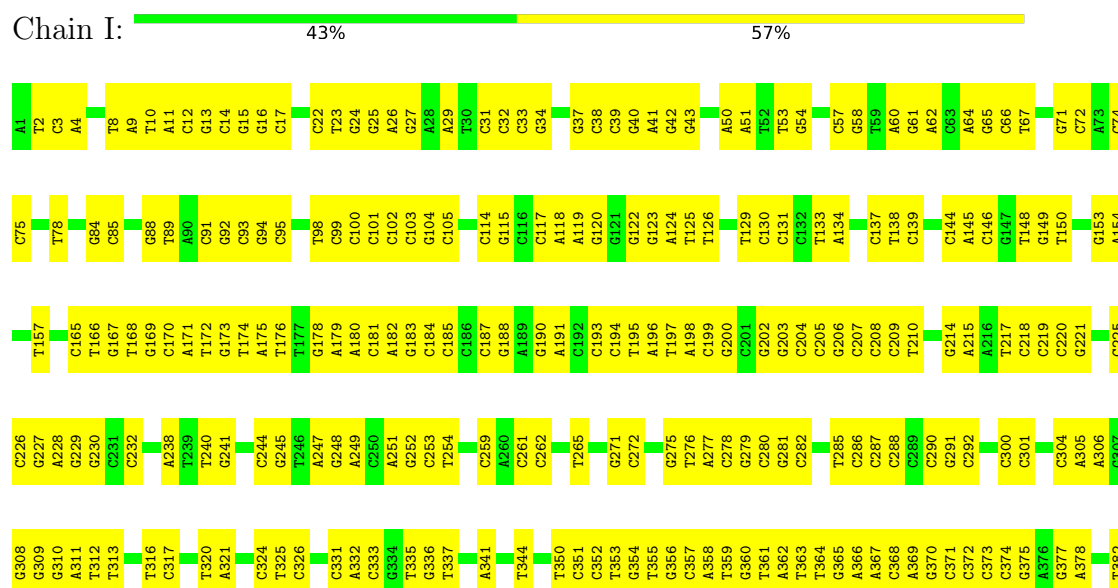
- Molecule 4: Histone H2B type 1-J

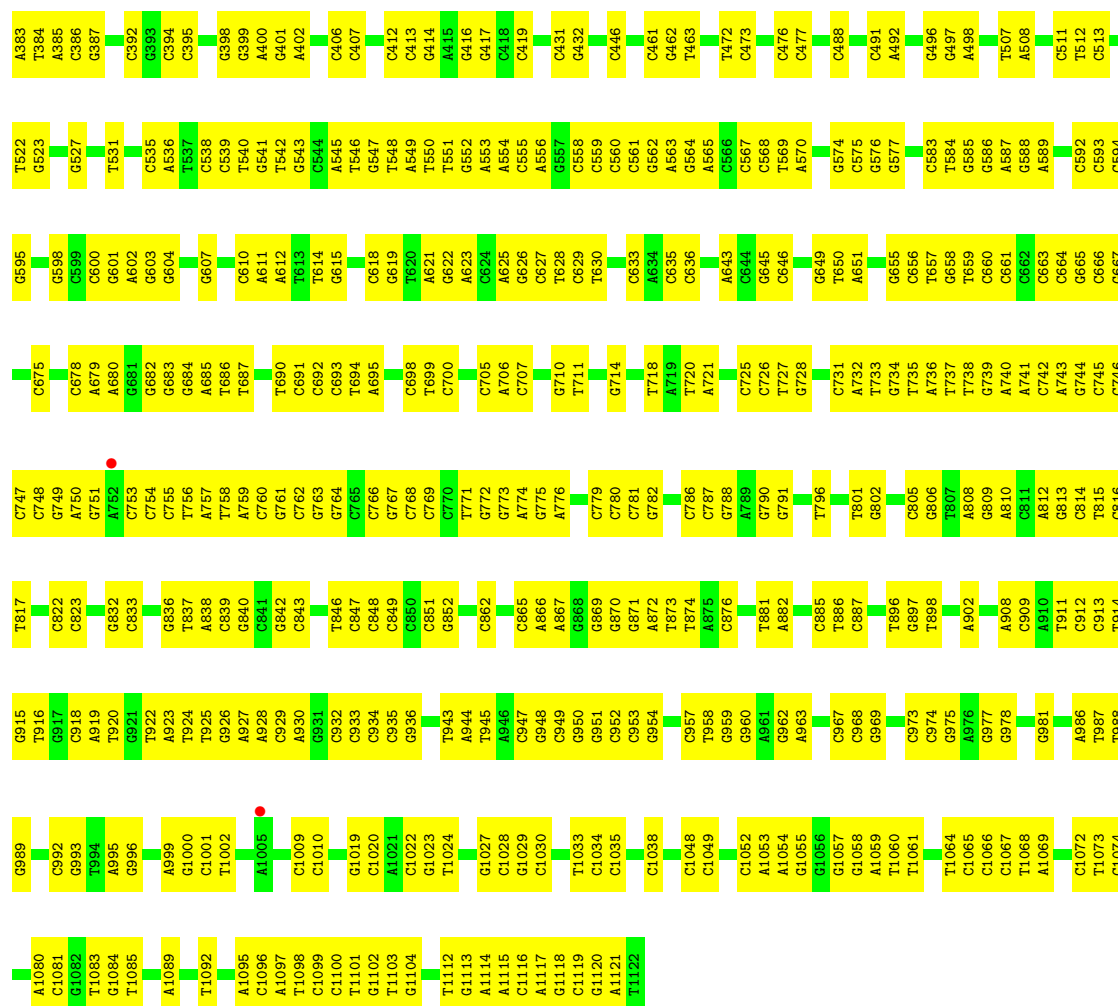


- Molecule 4: Histone H2B type 1-J



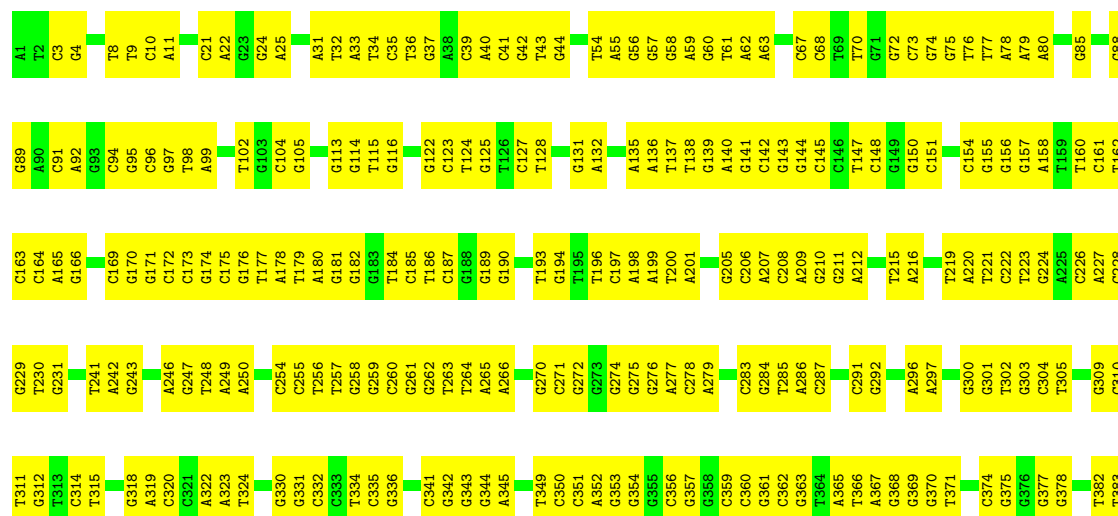
- Molecule 5: DNA (1122-MER)





• Molecule 6: DNA (1122-MER)

Chain J: 38% 62%



C384	G460	A532	C709	T784	T863	G938	G1010	
A385	G461	A620	G710	G785	G864	G939	T1011	C1086
A386	G462	G621				C940	T1012	
T387	G463	C535	C715	A788	G870	T941	A1013	C1089
A388	A464	C536	G716	G789	C871	T942	A1014	G1090
C389	C465	C537	G717	G790		T943		G1091
A390	A466	C538	G718	T791	C875	T944	C1019	G1092
T391	G467	A539	G719	G792	T876	C945	G1020	A1093
	C468	G541	T720	A798		A946	G1021	T1095
A394	C469	C542	T721		G879	A947	G1022	C1096
C395	C470	C543	T722	A802	A880	T948	G1023	
	G471	G550	T723	T802	C881	C950	A1024	C1099
A403	T472	T551	T724	A803	A883	A951	A1025	A1100
T404	A473	A552		G804	T885	T952	C1026	G1101
A406	G474	T553	C730	G805		G953	A1027	G1102
T407	C475	A554	G731	G806	C894	C954	G1028	G1103
A408		A555	G732	A807		A955	C1029	C1104
C409	C478	G556		G808	C890		G1030	G1105
T410	G479	G557	G737	T809	G891	G958	C1031	C1106
G411	A484	T598	T738	A810	G892	G959	G1032	C1107
A412	G487	G563	A739	A811	C893	A960	T1033	C1108
A413	G488	G564	T740		T895		A1034	G1109
A414	T489		A741	C814	C896		G1035	
C415	G490		G742	C815	G897	A964	C1039	T1122
G416			G743	C816	G898	T965	G1040	
T417			G744	T817	C899	A966		
			T745	T818	A900	T967	A1045	
G422	G496		C746	G819	A901	A968	G1046	
C423	C497		T747	G820	C901	T969	G1047	
A424	T498		C748	C821	G902	C970	G1048	
	G499		G749	G822	G903	T971	G1049	
	T500		G750	G823	G904	G972	T1050	
C501	T502		G751	T824	A906	A975	G1051	
T502			G752	T825		C976		
G505	A506		C753	A826	C909	T977	A1055	
			T754	A827	T910	G978	A1056	
A509	A510		G755		C911	T979	G1057	
T511	T512		T756	C832	C912		C1058	
C513	G513		T757	G833		G984	T1059	
	A514		C758	G834	G918		G1060	
C440	G515		T761	G835	G919	T989	T1061	
C441	C516		A762	G836	C920	A990	C1062	
G446	G517		C763	G837	C921	G991	T1063	
C447	G518		A764	A838	G922	G992	G1066	
G448	G519		T765	A840	C923	A993	A1067	
G449	C520		G766	G841	G924	A994		
T450	T521		C767	G842	T925	G995	A1070	
T451	G522		A768	G843	A926	T996	T1071	
A452	G523		C769	G844	A927	A997	T1072	
A453	C525		G770	G845	A928	A998	T1073	
A454			G771	T846	G929		G1074	
A455			A772	A847	G930	C1002	T1075	
C458	C528		A773	C848	G931	C1003	G1078	
G530	G529		A779	A858	T932	T1004	G1079	
G531	G530		T780	G859	C933	T1005	C1080	
			A781	C860	T934	G1006	C1081	
			T782	G861	C935	G1007	T1082	
			G783	G862	G936	G1008	C1083	

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	111.08 Å 238.76 Å 674.37 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.07 – 9.70 49.07 – 9.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.07-9.70) 98.8 (49.07-9.70)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 9.80 Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.254 , 0.286 0.256 , 0.282	Depositor DCC
R_{free} test set	573 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	339.6	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 306.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.21$, $\langle L^2 \rangle = 0.07$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	82122	wwPDB-VP
Average B, all atoms (Å ²)	544.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.14	0/813	0.34	0/1090
1	E	0.12	0/819	0.33	0/1097
1	K	0.16	0/813	0.38	0/1090
1	O	0.13	0/819	0.34	0/1097
1	U	0.13	0/813	0.34	0/1090
1	Y	0.13	0/819	0.35	0/1097
1	a	0.12	0/819	0.33	0/1097
1	e	0.17	0/813	0.36	0/1090
1	k	0.16	0/819	0.39	0/1097
1	o	0.13	0/813	0.36	0/1090
1	u	0.15	0/819	0.36	0/1097
1	y	0.14	0/813	0.34	0/1090
2	B	0.18	0/660	0.38	0/883
2	F	0.18	0/660	0.39	0/883
2	L	0.17	0/660	0.37	0/883
2	P	0.18	0/660	0.38	0/883
2	V	0.21	0/660	0.42	0/883
2	Z	0.19	0/660	0.42	0/883
2	b	0.20	0/660	0.39	0/883
2	f	0.21	0/660	0.40	0/883
2	l	0.31	0/660	0.56	1/883 (0.1%)
2	p	0.24	0/660	0.43	0/883
2	v	0.19	0/660	0.41	0/883
2	z	0.19	0/660	0.37	0/883
3	0	0.14	0/820	0.35	0/1107
3	2	0.13	0/806	0.35	0/1089
3	C	0.13	0/806	0.32	0/1089
3	G	0.20	0/820	0.33	0/1107
3	M	0.11	0/806	0.32	0/1089
3	Q	0.12	0/820	0.33	0/1107
3	W	0.11	0/806	0.33	0/1089
3	c	0.18	0/820	0.38	0/1107
3	g	0.11	0/806	0.32	0/1089
3	m	0.15	0/820	0.35	0/1107

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	q	0.15	0/806	0.37	0/1089
3	w	0.16	0/820	0.35	0/1107
4	1	0.14	0/756	0.33	0/1015
4	3	0.28	0/766	0.45	0/1026
4	D	0.11	0/766	0.37	0/1026
4	H	0.13	0/756	0.34	0/1015
4	N	0.11	0/766	0.34	0/1026
4	R	0.13	0/756	0.34	0/1015
4	X	0.11	0/766	0.35	0/1026
4	d	0.16	0/756	0.39	0/1015
4	h	0.11	0/766	0.34	0/1026
4	n	0.20	0/756	0.36	0/1015
4	r	0.18	0/766	0.40	0/1026
4	x	0.13	0/756	0.35	0/1015
5	I	0.22	0/25620	0.47	0/39502
6	J	0.22	0/25990	0.49	12/40152 (0.0%)
All	All	0.20	0/88210	0.44	13/128794 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	1048	DG	OP2-P-O3'	-9.36	79.92	108.00
6	J	300	DG	OP2-P-O3'	-9.30	80.10	108.00
6	J	861	DG	OP2-P-O3'	-9.30	80.10	108.00
6	J	487	DG	OP2-P-O3'	-9.29	80.14	108.00
6	J	674	DG	OP2-P-O3'	-9.25	80.25	108.00
6	J	113	DG	OP2-P-O3'	-9.20	80.39	108.00
6	J	300	DG	OP1-P-O3'	-5.53	91.41	108.00
6	J	861	DG	OP1-P-O3'	-5.52	91.45	108.00
6	J	113	DG	OP1-P-O3'	-5.52	91.45	108.00
6	J	674	DG	OP1-P-O3'	-5.50	91.51	108.00
6	J	487	DG	OP1-P-O3'	-5.49	91.54	108.00
6	J	1048	DG	OP1-P-O3'	-5.48	91.55	108.00
2	l	62	LEU	CB-CG-CD2	-5.45	94.36	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	801	0	839	34	0
1	E	807	0	844	27	0
1	K	801	0	839	36	0
1	O	807	0	844	23	0
1	U	801	0	839	33	0
1	Y	807	0	844	36	0
1	a	807	0	844	18	0
1	e	801	0	839	31	0
1	k	807	0	844	47	0
1	o	801	0	839	41	0
1	u	807	0	844	25	0
1	y	801	0	839	10	0
2	B	653	0	696	20	15
2	F	653	0	696	16	0
2	L	653	0	696	22	0
2	P	653	0	696	14	0
2	V	653	0	696	31	0
2	Z	653	0	696	26	4
2	b	653	0	696	15	15
2	f	653	0	696	22	0
2	l	653	0	696	43	0
2	p	653	0	696	39	0
2	v	653	0	696	10	0
2	z	653	0	696	10	0
3	0	810	0	866	38	0
3	2	796	0	848	37	1
3	C	796	0	848	15	0
3	G	810	0	866	28	0
3	M	796	0	848	21	0
3	Q	810	0	866	31	0
3	W	796	0	848	26	0
3	c	810	0	866	45	0
3	g	796	0	848	26	0
3	m	810	0	866	43	0
3	q	796	0	848	33	0
3	w	810	0	866	38	0
4	1	745	0	771	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	3	755	0	784	17	3
4	D	755	0	784	6	0
4	H	745	0	771	23	0
4	N	755	0	784	15	0
4	R	745	0	771	22	0
4	X	755	0	784	22	0
4	d	745	0	771	26	0
4	h	755	0	784	22	0
4	n	745	0	771	25	0
4	r	755	0	784	33	0
4	x	745	0	771	21	0
5	I	22861	0	12579	610	0
6	J	23141	0	12584	673	0
All	All	82122	0	63227	1824	19

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 (1824) 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:132:DA:H5'	3:w:42:ARG:HG2	1.32	1.08
1:o:76:GLN:OE1	2:p:22:LEU:HD12	1.55	1.05
2:l:98:TYR:HB3	4:r:58:ILE:HG13	1.40	1.03
2:V:92:ARG:HH21	4:X:98:LEU:HA	1.25	1.02
6:J:505:DG:H4'	3:m:42:ARG:HB3	1.43	0.98
1:K:58:THR:HG21	3:Q:81:ARG:HB2	1.54	0.90
3:c:117:PRO:HD3	1:e:48:LEU:HD11	1.52	0.89
5:I:977:DG:H2''	5:I:978:DG:OP2	1.71	0.89
3:c:104:GLN:NE2	1:e:94:GLU:OE1	2.06	0.88
5:I:603:DG:H2''	5:I:604:DG:OP2	1.71	0.87
5:I:42:DG:H2''	5:I:43:DG:OP2	1.75	0.86
5:I:229:DG:H2''	5:I:230:DG:OP2	1.73	0.86
1:U:123:ASP:OD1	1:Y:113:HIS:NE2	2.09	0.86
5:I:790:DG:H2''	5:I:791:DG:OP2	1.73	0.85
1:k:58:THR:HG21	3:q:81:ARG:HB2	1.58	0.85
5:I:538:DC:H4'	1:K:41:TYR:HE1	1.41	0.84
3:G:42:ARG:HB2	4:H:85:THR:HG23	1.57	0.84
5:I:851:DC:OP2	2:Z:35:ARG:NH1	2.10	0.84
1:K:73:GLU:HB2	2:L:25:ASN:HD22	1.41	0.84
5:I:610:DC:O2	6:J:513:DG:N2	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:42:ARG:HB2	4:1:85:THR:HG22	1.63	0.81
3:c:102:ILE:HG23	4:d:58:ILE:HD13	1.62	0.79
6:J:723:DT:H4'	1:O:41:TYR:HE1	1.47	0.79
5:I:664:DC:H42	6:J:459:DG:H1	1.31	0.79
1:K:123:ASP:OD1	1:O:113:HIS:NE2	2.14	0.79
5:I:100:DC:O2	6:J:1023:DG:N2	2.16	0.78
3:w:87:ILE:HD13	3:w:97:LEU:HD12	1.66	0.78
6:J:384:DC:H2''	6:J:385:DA:C8	2.20	0.77
5:I:27:DG:N2	6:J:1096:DC:O2	2.15	0.76
1:o:51:ILE:HG23	2:p:42:GLY:HA2	1.68	0.76
4:N:30:ARG:HH12	4:N:32:GLU:HG3	1.51	0.76
1:k:117:VAL:HG11	2:l:44:LYS:HE2	1.66	0.76
6:J:462:DG:H5'	1:o:43:PRO:HG2	1.66	0.76
1:K:113:HIS:NE2	1:O:123:ASP:OD1	2.19	0.76
1:E:46:VAL:N	5:I:104:DG:OP1	2.19	0.75
3:w:102:ILE:HG23	4:x:58:ILE:HD13	1.67	0.75
5:I:166:DT:H2'	5:I:167:DG:C8	2.22	0.74
5:I:852:DG:OP1	1:Y:46:VAL:N	2.20	0.74
5:I:352:DC:H2''	5:I:353:DT:C6	2.22	0.74
6:J:464:DA:OP1	1:o:117:VAL:N	2.21	0.74
1:U:113:HIS:NE2	1:Y:123:ASP:OD1	2.21	0.74
6:J:374:DC:H2''	6:J:375:DG:C8	2.22	0.74
6:J:1106:DG:H2''	6:J:1107:DC:C5	2.22	0.74
3:C:87:ILE:HD13	3:C:97:LEU:HD12	1.69	0.74
5:I:377:DG:H2''	5:I:378:DA:C8	2.22	0.73
2:l:75:HIS:HB2	4:n:93:THR:HG21	1.69	0.73
3:c:81:ARG:HB2	1:e:58:THR:HG21	1.69	0.73
5:I:757:DA:H2''	5:I:758:DT:H2'	1.71	0.73
6:J:275:DG:OP1	1:Y:42:ARG:NE	2.18	0.73
2:V:75:HIS:O	4:X:89:ARG:NH1	2.19	0.73
3:2:102:ILE:HG23	4:3:58:ILE:HD13	1.70	0.73
6:J:382:DT:H4'	6:J:383:DT:H5'	1.69	0.73
6:J:496:DG:H2''	6:J:497:DC:OP2	1.86	0.73
3:0:87:ILE:HD13	3:0:97:LEU:HD12	1.71	0.73
3:c:42:ARG:HB2	4:d:85:THR:HG23	1.70	0.73
1:k:94:GLU:OE2	3:q:104:GLN:NE2	2.19	0.73
6:J:862:DG:H2''	6:J:863:DT:OP2	1.89	0.73
5:I:1038:DC:H42	6:J:85:DG:H1	1.36	0.72
6:J:301:DG:H2''	6:J:302:DT:OP2	1.89	0.72
6:J:488:DG:H2''	6:J:489:DT:OP2	1.89	0.72
1:o:73:GLU:HG3	2:p:25:ASN:HD22	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:75:HIS:CE1	4:r:90:GLU:HG3	2.25	0.72
3:m:87:ILE:HD13	3:m:97:LEU:HD12	1.71	0.72
2:l:31:LYS:HE3	2:l:35:ARG:HH21	1.55	0.72
5:I:400:DA:N6	6:J:723:DT:O4	2.16	0.71
1:u:48:LEU:CD1	3:2:117:PRO:HD3	2.20	0.71
5:I:290:DC:H42	6:J:833:DG:H1	1.38	0.71
6:J:88:DG:H5'	1:y:43:PRO:HG2	1.72	0.71
4:N:65:ASP:OD2	2:P:98:TYR:OH	2.07	0.71
2:l:96:THR:O	3:q:101:THR:N	2.22	0.71
3:G:87:ILE:HD13	3:G:97:LEU:HD12	1.71	0.71
5:I:37:DG:N2	6:J:1086:DC:O2	2.18	0.71
5:I:1096:DC:H2''	5:I:1097:DA:OP2	1.89	0.71
3:g:42:ARG:NH1	4:h:85:THR:OG1	2.23	0.71
3:M:41:GLU:HB2	4:N:84:SER:HB3	1.70	0.71
1:A:42:ARG:HG3	5:I:165:DC:H3'	1.71	0.71
5:I:14:DC:H2''	5:I:15:DG:C8	2.24	0.71
5:I:705:DC:OP2	4:r:36:ILE:HG13	1.89	0.71
3:c:87:ILE:HD13	3:c:97:LEU:HD12	1.71	0.71
3:M:42:ARG:NH1	4:N:85:THR:OG1	2.23	0.71
6:J:141:DG:O3'	3:w:29:ARG:NH2	2.21	0.71
3:q:87:ILE:HD13	3:q:97:LEU:HD12	1.73	0.71
1:U:114:ALA:HA	1:Y:114:ALA:HA	1.72	0.70
3:c:111:ILE:HG12	1:e:51:ILE:HG21	1.72	0.70
2:f:75:HIS:O	4:h:89:ARG:NH1	2.22	0.70
6:J:945:DC:H2''	6:J:946:DA:C8	2.26	0.70
5:I:353:DT:H2''	5:I:354:DG:C8	2.26	0.70
6:J:156:DG:H2''	6:J:157:DG:OP2	1.91	0.70
5:I:183:DG:H2''	5:I:184:DC:C5	2.26	0.70
5:I:548:DT:H2''	5:I:549:DA:C8	2.26	0.70
5:I:598:DG:N2	6:J:525:DC:O2	2.19	0.70
3:g:87:ILE:HD13	3:g:97:LEU:HD12	1.72	0.70
5:I:100:DC:N3	6:J:1023:DG:N1	2.35	0.70
5:I:967:DC:H2''	5:I:968:DC:OP2	1.91	0.70
6:J:975:DA:H2''	6:J:976:DC:OP2	1.91	0.70
3:M:87:ILE:HD13	3:M:97:LEU:HD12	1.74	0.70
5:I:549:DA:H4'	5:I:550:DT:H5'	1.74	0.69
5:I:103:DC:H42	6:J:1020:DG:H1	1.41	0.69
5:I:694:DT:H4'	3:q:42:ARG:HB3	1.74	0.69
6:J:227:DA:H2''	6:J:228:DC:OP2	1.91	0.69
6:J:879:DG:H4'	3:c:42:ARG:HB3	1.74	0.69
2:p:68:ASP:OD2	2:p:93:GLN:NE2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:87:ILE:HD13	3:2:97:LEU:HD12	1.73	0.69
1:K:73:GLU:HB2	2:L:25:ASN:ND2	2.06	0.69
6:J:40:DA:H2''	6:J:41:DC:OP2	1.93	0.69
6:J:925:DT:H2''	6:J:926:DA:C8	2.27	0.69
2:l:98:TYR:HB3	4:r:58:ILE:CG1	2.21	0.69
5:I:885:DC:H2''	5:I:886:DT:OP2	1.93	0.69
6:J:114:DG:H2''	6:J:115:DT:OP2	1.93	0.69
6:J:1049:DG:H2''	6:J:1050:DT:OP2	1.91	0.69
3:Q:32:ARG:NH2	4:R:32:GLU:OE1	2.26	0.69
1:A:113:HIS:NE2	1:E:123:ASP:OD1	2.24	0.69
5:I:897:DG:H2''	5:I:898:DT:OP2	1.93	0.69
6:J:136:DA:H2''	6:J:137:DT:OP2	1.91	0.69
5:I:219:DC:H2''	5:I:220:DC:OP2	1.93	0.69
6:J:343:DG:H2''	6:J:344:DG:OP2	1.90	0.69
6:J:723:DT:H4'	1:O:41:TYR:CE1	2.27	0.69
5:I:324:DC:H2''	5:I:325:DT:OP2	1.92	0.68
6:J:414:DA:H2''	6:J:415:DC:OP2	1.93	0.68
2:b:31:LYS:HE3	2:b:35:ARG:HH21	1.59	0.68
3:Q:87:ILE:HD13	3:Q:97:LEU:HD12	1.75	0.68
1:o:59:GLU:O	2:p:40:ARG:NH1	2.17	0.68
1:U:120:MET:N	1:U:123:ASP:OD2	2.26	0.68
3:G:54:VAL:HG13	4:H:107:ALA:HB1	1.74	0.68
5:I:137:DC:H2''	5:I:138:DT:OP2	1.94	0.68
5:I:749:DG:H2''	5:I:750:DA:C8	2.29	0.68
6:J:151:DC:OP1	3:w:77:ARG:N	2.26	0.68
3:W:87:ILE:HD13	3:W:97:LEU:HD12	1.76	0.68
3:W:92:GLU:OE1	4:X:103:LEU:N	2.26	0.68
1:Y:120:MET:N	1:Y:123:ASP:OD2	2.24	0.68
2:F:75:HIS:O	4:H:89:ARG:NH1	2.22	0.68
6:J:524:DG:H3'	3:m:76:THR:HB	1.74	0.68
6:J:905:DG:H2''	6:J:906:DA:OP2	1.93	0.68
1:A:65:LEU:HB2	6:J:1045:DA:H3'	1.76	0.68
5:I:593:DC:H2''	5:I:594:DC:OP2	1.92	0.68
6:J:798:DA:OP1	3:g:17:ARG:N	2.23	0.68
5:I:488:DC:H42	6:J:635:DG:H22	1.39	0.67
5:I:780:DC:H2''	5:I:781:DC:OP2	1.93	0.67
6:J:788:DA:H2''	6:J:789:DC:OP2	1.94	0.67
6:J:936:DG:H2''	6:J:937:DG:C8	2.30	0.67
6:J:1082:DT:H2''	6:J:1083:DC:OP2	1.94	0.67
2:B:68:ASP:OD2	2:B:93:GLN:NE2	2.27	0.67
5:I:1072:DC:H2''	5:I:1073:DT:OP2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:68:ASP:OD2	2:V:93:GLN:NE2	2.26	0.67
6:J:334:DT:H2''	6:J:335:DC:OP2	1.94	0.67
2:v:31:LYS:HE3	2:v:35:ARG:HH21	1.60	0.67
4:D:65:ASP:OD2	2:F:98:TYR:OH	2.08	0.67
5:I:32:DC:H2''	5:I:33:DC:OP2	1.93	0.67
6:J:649:DG:H5'	1:O:43:PRO:HG2	1.75	0.67
2:F:31:LYS:HE3	2:F:35:ARG:HH21	1.60	0.67
5:I:416:DG:H2''	5:I:417:DG:OP2	1.94	0.67
6:J:131:DG:H4'	3:w:42:ARG:HD3	1.77	0.67
3:m:102:ILE:HG23	4:n:58:ILE:HD13	1.76	0.67
3:m:42:ARG:NH1	4:n:85:THR:OG1	2.28	0.67
5:I:149:DG:H2''	5:I:150:DT:OP2	1.95	0.67
5:I:805:DC:H2''	5:I:806:DG:OP2	1.94	0.67
5:I:665:DG:OP1	1:o:46:VAL:N	2.27	0.67
6:J:147:DT:H2''	6:J:148:DC:OP2	1.95	0.67
5:I:698:DC:H2''	5:I:699:DT:OP2	1.96	0.66
5:I:88:DG:H1	6:J:1035:DC:H42	1.43	0.66
5:I:259:DC:H5''	1:a:83:ARG:HG2	1.76	0.66
5:I:1057:DG:N2	6:J:67:DC:O2	2.28	0.66
3:M:54:VAL:HG21	4:N:95:VAL:HG21	1.76	0.66
1:A:58:THR:HG21	3:G:81:ARG:HB2	1.77	0.66
5:I:538:DC:H4'	1:K:41:TYR:CE1	2.28	0.66
6:J:530:DG:H2''	6:J:531:DG:OP2	1.94	0.66
1:u:55:GLN:HB3	3:2:109:PRO:HA	1.76	0.66
3:m:115:LEU:HD11	1:o:108:ASN:HD21	1.61	0.66
5:I:683:DG:N2	6:J:441:DC:O2	2.28	0.66
6:J:1092:DG:H2''	6:J:1093:DA:OP2	1.95	0.66
6:J:429:DA:H2''	6:J:430:DG:OP2	1.95	0.66
6:J:938:DG:H2''	6:J:939:DG:C8	2.31	0.66
5:I:244:DC:H2''	5:I:245:DG:OP2	1.96	0.66
6:J:895:DT:H2''	6:J:896:DC:OP2	1.95	0.66
5:I:539:DC:H2''	5:I:540:DT:C5	2.30	0.65
5:I:762:DC:H2''	5:I:763:DG:C8	2.31	0.65
3:G:39:TYR:HB3	4:H:86:ILE:HD12	1.77	0.65
6:J:242:DA:H2''	6:J:243:DG:OP2	1.96	0.65
6:J:323:DA:H2''	6:J:324:DT:OP2	1.95	0.65
2:L:21:VAL:O	2:L:22:LEU:HD12	1.97	0.65
2:P:31:LYS:HE3	2:P:35:ARG:HH21	1.62	0.65
6:J:933:DC:H2''	6:J:934:DT:C6	2.30	0.65
6:J:836:DG:H5'	1:e:43:PRO:HG2	1.77	0.65
3:c:42:ARG:NH1	4:d:85:THR:OG1	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:85:GLN:HG3	2:l:80:THR:CG2	2.27	0.65
1:A:109:LEU:HD13	1:E:129:ARG:HG2	1.77	0.65
6:J:59:DA:OP1	4:3:85:THR:OG1	2.12	0.65
1:o:76:GLN:OE1	2:p:22:LEU:CD1	2.39	0.65
3:2:57:TYR:O	3:2:60:ALA:HB3	1.96	0.65
6:J:58:DG:H4'	3:2:42:ARG:CD	2.27	0.65
2:L:98:TYR:HB3	4:R:58:ILE:HG23	1.79	0.65
2:l:102:GLY:OXT	4:r:61:SER:HA	1.96	0.65
2:B:80:THR:HG21	5:I:71:DG:H5''	1.79	0.65
5:I:1073:DT:H2''	5:I:1074:DC:OP2	1.97	0.65
5:I:992:DC:H2''	5:I:993:DG:OP2	1.98	0.64
5:I:1084:DG:H2''	5:I:1085:DT:OP2	1.94	0.64
3:M:20:ARG:NH2	4:N:122:LYS:O	2.26	0.64
5:I:1049:DC:H42	6:J:74:DG:H22	1.44	0.64
1:Y:108:ASN:ND2	2:Z:42:GLY:O	2.30	0.64
6:J:1091:DG:H2''	6:J:1092:DG:OP2	1.98	0.64
1:K:94:GLU:OE1	3:Q:104:GLN:NE2	2.24	0.64
1:u:48:LEU:HD11	3:2:117:PRO:HD3	1.78	0.64
2:v:96:THR:O	3:2:101:THR:N	2.30	0.64
5:I:336:DG:H2''	5:I:337:DT:OP2	1.96	0.64
1:k:120:MET:N	1:k:123:ASP:OD2	2.30	0.64
3:G:40:SER:HB3	4:H:86:ILE:HG13	1.79	0.64
5:I:305:DA:H2''	5:I:306:DA:OP2	1.96	0.64
6:J:518:DG:H2''	6:J:519:DC:OP2	1.98	0.64
3:m:101:THR:N	2:p:96:THR:O	2.30	0.64
5:I:710:DG:H2''	5:I:711:DT:OP2	1.97	0.64
3:Q:92:GLU:OE1	4:R:103:LEU:N	2.28	0.64
6:J:344:DG:H2''	6:J:345:DA:OP2	1.97	0.64
1:k:117:VAL:HG13	3:q:115:LEU:HD22	1.79	0.64
3:2:42:ARG:NH1	4:3:85:THR:OG1	2.30	0.64
6:J:127:DC:H2''	6:J:128:DT:OP2	1.98	0.64
5:I:291:DG:H5'	1:e:43:PRO:HA	1.78	0.63
5:I:618:DC:H2''	5:I:619:DG:OP2	1.96	0.63
6:J:531:DG:H2''	6:J:532:DA:OP2	1.96	0.63
5:I:57:DC:H2''	5:I:58:DG:OP2	1.97	0.63
2:b:75:HIS:CE1	4:d:89:ARG:HG2	2.32	0.63
5:I:790:DG:OP1	4:X:50:GLY:HA3	1.98	0.63
5:I:569:DT:H2''	5:I:570:DA:C8	2.33	0.63
6:J:157:DG:H2''	6:J:158:DA:OP2	1.98	0.63
6:J:554:DA:H2''	6:J:555:DG:C8	2.34	0.63
2:z:68:ASP:OD2	2:z:93:GLN:NE2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:175:DA:H2''	5:I:176:DT:C5	2.34	0.63
5:I:705:DC:OP2	4:r:36:ILE:CG1	2.46	0.63
3:c:38:ASN:O	3:g:38:ASN:HB3	1.98	0.63
3:2:57:TYR:HB2	4:3:110:GLU:HG3	1.81	0.63
5:I:66:DC:H2''	5:I:67:DT:OP2	1.97	0.63
6:J:781:DA:H2''	6:J:782:DT:OP2	1.99	0.63
6:J:879:DG:OP1	3:c:44:GLY:HA2	1.99	0.63
1:O:120:MET:N	1:O:123:ASP:OD2	2.25	0.63
3:q:42:ARG:NH1	4:r:85:THR:OG1	2.32	0.63
5:I:813:DG:H2''	5:I:814:DC:OP2	1.99	0.63
5:I:247:DA:H1'	5:I:248:DG:H5'	1.81	0.63
6:J:122:DG:H2''	6:J:123:DC:OP2	1.99	0.63
6:J:521:DT:H2''	6:J:522:DC:OP2	1.98	0.63
5:I:122:DG:N2	6:J:1002:DC:O2	2.32	0.62
6:J:229:DG:H2''	6:J:230:DT:OP2	1.98	0.62
6:J:510:DA:H2''	6:J:511:DT:OP2	1.98	0.62
6:J:845:DG:H2''	6:J:846:DT:OP2	1.99	0.62
1:o:59:GLU:OE1	2:p:40:ARG:NH2	2.30	0.62
5:I:394:DC:H2''	5:I:395:DC:C6	2.34	0.62
6:J:70:DT:OP1	1:y:84:PHE:N	2.29	0.62
6:J:891:DG:H2''	6:J:892:DG:OP2	1.98	0.62
1:k:119:ILE:HD13	2:l:43:VAL:HG21	1.81	0.62
1:A:69:ARG:NH2	6:J:1045:DA:OP1	2.32	0.62
6:J:990:DA:H2''	6:J:991:DG:OP2	1.99	0.62
6:J:314:DC:H2''	6:J:315:DT:OP2	1.98	0.62
6:J:870:DG:H2''	6:J:871:DC:OP2	1.99	0.62
1:E:40:ARG:NH2	5:I:104:DG:H21	1.98	0.62
5:I:699:DT:H2''	5:I:700:DC:OP2	1.99	0.62
6:J:55:DA:H2''	6:J:56:DG:OP2	1.98	0.62
1:E:43:PRO:HG2	6:J:1023:DG:H5'	1.79	0.62
5:I:65:DG:H2''	5:I:66:DC:OP2	2.00	0.62
5:I:238:DA:OP1	3:c:32:ARG:NH1	2.33	0.62
5:I:352:DC:H5''	1:a:41:TYR:CD1	2.34	0.62
6:J:97:DG:H2''	6:J:98:DT:OP2	2.00	0.62
5:I:531:DT:H3	6:J:592:DA:H61	1.48	0.62
5:I:563:DA:H2''	5:I:564:DG:C8	2.35	0.62
5:I:622:DG:OP1	4:n:84:SER:N	2.33	0.62
6:J:60:DG:OP1	4:3:83:ARG:NH2	2.33	0.62
5:I:918:DC:H2''	5:I:919:DA:C8	2.35	0.62
6:J:505:DG:C4'	3:m:42:ARG:HB3	2.27	0.62
6:J:884:DA:H2''	6:J:885:DT:OP2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:68:ASP:OD2	2:p:92:ARG:NH1	2.33	0.62
5:I:325:DT:H2"	5:I:326:DC:OP2	2.00	0.62
2:L:68:ASP:OD2	2:L:93:GLN:NE2	2.32	0.62
3:w:42:ARG:HB2	4:x:85:THR:HG23	1.82	0.61
6:J:1032:DG:H2"	6:J:1033:DT:OP2	1.99	0.61
3:G:45:ALA:HB1	4:H:118:TYR:HE2	1.65	0.61
4:n:58:ILE:HG23	2:p:98:TYR:CD2	2.35	0.61
1:u:126:LEU:HD22	1:y:113:HIS:CG	2.35	0.61
5:I:627:DC:H2"	5:I:628:DT:OP2	2.01	0.61
5:I:851:DC:H42	6:J:272:DG:H1	1.48	0.61
5:I:862:DC:H42	6:J:261:DG:H22	1.48	0.61
6:J:309:DG:H2"	6:J:310:DC:OP2	2.00	0.61
6:J:517:DG:H2"	6:J:518:DG:OP2	1.99	0.61
6:J:892:DG:H2"	6:J:893:DC:OP2	1.99	0.61
6:J:904:DG:H2"	6:J:905:DG:OP2	1.98	0.61
4:r:55:ALA:O	4:r:58:ILE:HG22	2.00	0.61
5:I:64:DA:H2"	5:I:65:DG:OP2	2.01	0.61
5:I:165:DC:H2"	5:I:166:DT:C6	2.36	0.61
5:I:773:DG:N2	6:J:351:DC:O2	2.34	0.61
6:J:928:DA:H2"	6:J:929:DG:C8	2.34	0.61
5:I:341:DA:H61	6:J:782:DT:H3	1.47	0.61
5:I:742:DC:H2"	5:I:743:DA:C8	2.36	0.61
6:J:143:DG:H2"	6:J:144:DG:OP2	2.00	0.61
6:J:144:DG:H2"	6:J:145:DC:OP2	2.01	0.61
6:J:1071:DA:H2"	6:J:1072:DT:OP2	1.99	0.61
5:I:114:DC:H42	6:J:1009:DG:H22	1.45	0.61
5:I:622:DG:P	4:n:84:SER:H	2.24	0.61
5:I:1000:DG:H2"	5:I:1001:DC:OP2	2.00	0.61
6:J:1062:DC:H2"	6:J:1063:DT:OP2	2.00	0.61
6:J:330:DG:H2"	6:J:331:DG:OP2	2.01	0.61
2:Z:84:MET:HE1	2:Z:102:GLY:HA2	1.83	0.61
3:0:102:ILE:HG23	4:1:58:ILE:HD13	1.82	0.61
5:I:251:DA:H2"	5:I:252:DG:OP2	2.01	0.61
5:I:1001:DC:H2"	5:I:1002:DT:OP2	2.01	0.61
6:J:1079:DG:H2"	6:J:1080:DC:OP2	2.01	0.61
3:c:46:GLY:C	4:d:88:SER:HB3	2.26	0.61
5:I:886:DT:H2"	5:I:887:DC:OP2	2.01	0.60
6:J:416:DG:H2"	6:J:417:DT:OP2	2.01	0.60
1:k:48:LEU:HD11	3:q:117:PRO:HD3	1.83	0.60
5:I:812:DA:H2"	5:I:813:DG:OP2	2.01	0.60
5:I:999:DA:H2"	5:I:1000:DG:OP2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:261:DC:H2''	5:I:262:DC:OP2	2.02	0.60
5:I:664:DC:OP1	2:p:45:ARG:HA	2.01	0.60
5:I:808:DA:H1'	5:I:809:DG:H5'	1.82	0.60
5:I:959:DG:H2''	5:I:960:DG:C8	2.36	0.60
6:J:465:DC:OP2	1:o:116:ARG:HD3	2.01	0.60
1:K:109:LEU:HD13	1:O:129:ARG:HG2	1.84	0.60
1:A:108:ASN:ND2	2:B:42:GLY:O	2.34	0.60
1:E:45:THR:N	5:I:104:DG:OP1	2.34	0.60
5:I:625:DA:H2''	5:I:626:DG:OP2	2.01	0.60
6:J:539:DA:H1'	6:J:540:DG:H5'	1.83	0.60
5:I:138:DT:H2''	5:I:139:DC:OP2	2.00	0.60
5:I:838:DA:H5'	1:U:43:PRO:HG2	1.82	0.60
5:I:953:DC:H2''	5:I:954:DG:C8	2.36	0.60
6:J:471:DG:H2''	6:J:472:DT:OP2	2.01	0.60
6:J:1108:DC:H2''	6:J:1109:DG:C8	2.36	0.60
3:q:25:PHE:HE1	4:r:41:VAL:HG21	1.66	0.60
2:Z:31:LYS:HE3	2:Z:35:ARG:HH21	1.67	0.60
6:J:35:DC:H2''	6:J:36:DT:OP2	2.02	0.60
1:k:109:LEU:HB3	1:o:126:LEU:HD11	1.84	0.60
2:v:98:TYR:HB3	4:3:58:ILE:HG23	1.84	0.60
5:I:576:DG:H2''	5:I:577:DG:C8	2.37	0.60
6:J:748:DC:H2''	6:J:749:DG:C8	2.37	0.60
3:w:42:ARG:CB	4:x:85:THR:HG23	2.31	0.60
6:J:802:DT:H2''	6:J:803:DA:C8	2.37	0.60
5:I:564:DG:H2''	5:I:565:DA:C8	2.36	0.60
5:I:814:DC:H2''	5:I:815:DT:OP2	2.01	0.60
6:J:535:DC:H2''	6:J:536:DT:H5'	1.83	0.60
6:J:705:DG:H5''	4:N:28:ARG:HD3	1.82	0.60
1:k:73:GLU:HB2	2:l:25:ASN:ND2	2.17	0.60
6:J:615:DT:H2''	6:J:616:DA:C8	2.37	0.60
6:J:875:DC:H2''	6:J:876:DT:OP2	2.02	0.60
2:p:35:ARG:NH2	2:p:51:TYR:OH	2.35	0.60
5:I:60:DA:H1'	5:I:61:DG:H5'	1.83	0.59
5:I:612:DA:P	3:m:32:ARG:HD3	2.41	0.59
5:I:822:DC:H2''	5:I:823:DC:OP2	2.02	0.59
5:I:902:DA:H61	6:J:221:DT:H3	1.48	0.59
6:J:223:DT:H2''	6:J:224:DG:C8	2.37	0.59
6:J:803:DA:H2''	6:J:804:DG:OP2	2.00	0.59
3:c:79:ILE:HG12	3:c:82:HIS:CE1	2.37	0.59
2:l:75:HIS:CD2	4:n:77:LEU:HB3	2.37	0.59
5:I:837:DT:H3	6:J:286:DA:H61	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:417:DT:H2''	6:J:418:DG:OP2	2.01	0.59
6:J:501:DC:H2''	6:J:502:DT:OP2	2.02	0.59
6:J:142:DC:P	3:w:29:ARG:HH22	2.25	0.59
2:P:75:HIS:CE1	4:R:89:ARG:HG2	2.37	0.59
2:B:79:LYS:N	6:J:1056:DA:OP1	2.30	0.59
5:I:309:DG:N2	6:J:815:DC:O2	2.36	0.59
6:J:331:DG:H2''	6:J:332:DC:OP2	2.02	0.59
1:k:51:ILE:HG12	2:l:39:ARG:O	2.01	0.59
5:I:118:DA:H2''	5:I:119:DA:OP2	2.03	0.59
5:I:247:DA:H4'	3:c:42:ARG:HD2	1.85	0.59
6:J:790:DG:H2''	6:J:791:DT:OP2	2.02	0.59
5:I:870:DG:N2	6:J:254:DC:O2	2.36	0.59
5:I:1009:DC:H2''	5:I:1010:DC:OP2	2.02	0.59
6:J:365:DA:H2''	6:J:366:DT:C6	2.36	0.59
1:o:50:GLU:HB2	2:p:39:ARG:HD2	1.84	0.59
1:U:48:LEU:CD1	3:0:117:PRO:HD3	2.33	0.59
4:X:58:ILE:HG23	2:Z:98:TYR:HB3	1.85	0.59
5:I:1059:DA:H2''	5:I:1060:DT:OP2	2.01	0.59
6:J:351:DC:H2''	6:J:352:DA:C8	2.38	0.59
2:f:92:ARG:NH2	4:h:97:LEU:O	2.36	0.59
5:I:612:DA:OP2	3:m:32:ARG:HD3	2.02	0.59
6:J:62:DA:H2''	6:J:63:DA:OP2	2.03	0.59
6:J:284:DG:H2''	6:J:285:DT:OP2	2.02	0.59
6:J:1057:DG:H2''	6:J:1058:DC:OP2	2.02	0.59
4:x:102:GLU:OE2	4:x:106:HIS:NE2	2.35	0.59
2:z:35:ARG:NH2	2:z:51:TYR:OH	2.35	0.59
1:E:66:PRO:HB3	2:F:28:GLY:HA3	1.85	0.59
5:I:771:DT:H2''	5:I:772:DG:C8	2.37	0.59
6:J:570:DT:H4'	6:J:571:DC:H5'	1.85	0.59
2:V:44:LYS:HB2	3:0:115:LEU:HD22	1.84	0.59
2:B:35:ARG:NH2	2:B:51:TYR:OH	2.36	0.58
5:I:157:DT:H3	6:J:966:DA:H61	1.51	0.58
5:I:1027:DG:OP1	1:u:117:VAL:N	2.35	0.58
2:L:35:ARG:NH2	2:L:51:TYR:OH	2.35	0.58
2:L:68:ASP:OD2	2:L:92:ARG:NH1	2.36	0.58
5:I:986:DA:P	3:w:32:ARG:HD3	2.43	0.58
5:I:995:DA:H1'	5:I:996:DG:H5'	1.85	0.58
5:I:1019:DG:H2''	5:I:1020:DC:OP2	2.03	0.58
6:J:791:DT:H2''	6:J:792:DG:OP2	2.03	0.58
5:I:228:DA:H4'	3:c:77:ARG:NE	2.17	0.58
5:I:252:DG:H2''	5:I:253:DC:OP2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:230:DT:H2''	6:J:231:DG:OP2	2.03	0.58
6:J:474:DC:OP1	2:l:47:SER:HA	2.02	0.58
5:I:476:DC:P	2:P:48:GLY:H	2.26	0.58
5:I:74:DC:H2''	5:I:75:DC:OP2	2.04	0.58
5:I:675:DC:H42	6:J:448:DG:H22	1.49	0.58
5:I:866:DA:H2''	5:I:867:DA:OP2	2.04	0.58
3:Q:92:GLU:OE2	4:R:102:GLU:N	2.32	0.58
5:I:275:DG:H1	6:J:848:DC:H42	1.51	0.58
5:I:750:DA:H1'	5:I:751:DG:C8	2.39	0.58
6:J:39:DC:H2''	6:J:40:DA:C8	2.39	0.58
6:J:671:DA:H3'	1:K:66:PRO:HD3	1.86	0.58
3:m:115:LEU:O	1:o:48:LEU:HD21	2.03	0.58
1:u:108:ASN:ND2	2:v:42:GLY:O	2.37	0.58
6:J:497:DC:OP2	6:J:497:DC:H6	1.87	0.58
6:J:741:DA:H2''	6:J:742:DG:C8	2.39	0.58
6:J:978:DT:H2''	6:J:979:DG:OP2	2.03	0.58
2:B:68:ASP:OD2	2:B:92:ARG:NH1	2.36	0.57
6:J:132:DA:H5'	3:w:42:ARG:CG	2.21	0.57
6:J:322:DA:H2''	6:J:323:DA:OP2	2.03	0.57
6:J:846:DT:H2''	6:J:847:DA:C8	2.39	0.57
6:J:989:DT:H2''	6:J:990:DA:C8	2.39	0.57
1:k:114:ALA:HB2	1:o:113:HIS:CD2	2.38	0.57
2:z:68:ASP:OD2	2:z:92:ARG:NH1	2.37	0.57
5:I:918:DC:H2''	5:I:919:DA:H8	1.68	0.57
3:w:40:SER:HB3	4:x:86:ILE:HG13	1.86	0.57
6:J:39:DC:H4'	3:2:77:ARG:HD2	1.86	0.57
6:J:948:DT:H2''	6:J:949:DA:C8	2.39	0.57
2:f:35:ARG:NH2	2:f:51:TYR:OH	2.37	0.57
1:k:100:LEU:HD11	2:l:58:LEU:HD13	1.85	0.57
4:n:58:ILE:HG12	2:p:98:TYR:HB3	1.86	0.57
2:F:75:HIS:CE1	4:H:89:ARG:HG2	2.39	0.57
5:I:253:DC:H2''	5:I:254:DT:OP2	2.04	0.57
6:J:498:DT:H5'	4:r:27:LYS:HD3	1.85	0.57
6:J:572:DA:H2''	6:J:573:DA:C8	2.39	0.57
3:q:32:ARG:HH21	3:q:33:LEU:HD21	1.70	0.57
5:I:607:DG:H1	6:J:516:DC:H42	1.52	0.57
5:I:99:DC:H2''	5:I:100:DC:OP2	2.03	0.57
5:I:301:DC:H42	6:J:822:DG:H22	1.53	0.57
5:I:685:DA:H2''	5:I:686:DT:OP2	2.04	0.57
6:J:54:DT:H2''	6:J:55:DA:C8	2.38	0.57
6:J:977:DG:H2''	6:J:978:DT:OP2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:41:GLU:HB2	4:d:84:SER:HB3	1.86	0.57
1:o:70:LEU:HD13	2:p:26:ILE:HA	1.86	0.57
2:p:75:HIS:CD2	4:r:77:LEU:HB3	2.39	0.57
6:J:631:DT:H5''	1:O:83:ARG:HG2	1.86	0.57
3:m:32:ARG:HH21	3:m:33:LEU:HD21	1.70	0.57
3:m:42:ARG:HB2	4:n:85:THR:HG23	1.87	0.57
1:A:65:LEU:HD22	6:J:1045:DA:H2'	1.86	0.57
5:I:350:DT:H2''	5:I:351:DC:C5	2.40	0.57
6:J:285:DT:H2''	6:J:286:DA:C8	2.40	0.57
6:J:428:DT:H2''	6:J:429:DA:C8	2.40	0.57
6:J:671:DA:H5''	1:K:66:PRO:HG3	1.87	0.57
6:J:738:DT:H2''	6:J:739:DA:N7	2.19	0.57
6:J:769:DC:H2''	6:J:770:DA:C8	2.39	0.57
1:a:61:LEU:O	2:b:36:ARG:NH2	2.27	0.57
2:l:75:HIS:NE2	4:n:77:LEU:HB3	2.20	0.57
4:H:60:ASN:O	4:H:64:ASN:ND2	2.38	0.57
6:J:620:DA:H2''	6:J:621:DG:C8	2.40	0.57
6:J:1050:DT:H2''	6:J:1051:DG:OP2	2.05	0.57
5:I:276:DT:H3	6:J:847:DA:H61	1.52	0.56
6:J:899:DC:P	3:c:76:THR:H	2.28	0.56
3:c:54:VAL:HG13	4:d:107:ALA:HB1	1.87	0.56
2:f:68:ASP:OD2	2:f:92:ARG:NH1	2.38	0.56
2:f:68:ASP:OD2	2:f:93:GLN:NE2	2.37	0.56
2:F:45:ARG:HA	5:I:103:DC:OP1	2.04	0.56
5:I:382:DT:H2''	5:I:383:DA:C8	2.40	0.56
5:I:796:DT:H5''	4:X:28:ARG:HH21	1.70	0.56
5:I:1002:DT:O2	6:J:122:DG:N2	2.38	0.56
6:J:175:DC:H2''	6:J:176:DG:C8	2.39	0.56
6:J:472:DT:H2''	6:J:473:DA:C8	2.40	0.56
6:J:756:DT:H4'	6:J:757:DT:H5'	1.86	0.56
5:I:651:DA:H5'	1:k:43:PRO:HG2	1.86	0.56
1:K:51:ILE:HG21	3:Q:111:ILE:HG12	1.87	0.56
5:I:372:DC:H2''	5:I:373:DC:C6	2.40	0.56
6:J:755:DG:H2''	6:J:756:DT:C6	2.40	0.56
6:J:757:DT:H4'	6:J:758:DC:H5'	1.88	0.56
1:a:52:ARG:NH1	3:g:111:ILE:HD13	2.19	0.56
6:J:362:DC:H2''	6:J:363:DG:C8	2.40	0.56
6:J:525:DC:P	3:m:76:THR:H	2.28	0.56
4:n:58:ILE:HG23	2:p:98:TYR:HD2	1.71	0.56
1:Y:79:LYS:HB3	1:Y:82:LEU:HD11	1.88	0.56
5:I:852:DG:OP2	1:Y:46:VAL:HB	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:1098:DT:H2''	5:I:1099:DC:C5	2.40	0.56
6:J:489:DT:H2''	6:J:490:DG:OP2	2.05	0.56
6:J:1033:DT:H2''	6:J:1034:DA:C8	2.40	0.56
3:M:87:ILE:HD12	3:M:102:ILE:HD11	1.88	0.56
3:m:117:PRO:HD3	1:o:48:LEU:HD13	1.87	0.56
4:D:50:GLY:HA3	5:I:42:DG:OP1	2.06	0.56
5:I:98:DT:H3	6:J:1025:DA:H61	1.54	0.56
5:I:734:DG:H1'	5:I:735:DT:H5'	1.86	0.56
6:J:359:DC:H2''	6:J:360:DC:C6	2.41	0.56
6:J:620:DA:OP1	4:R:84:SER:N	2.37	0.56
6:J:1083:DC:OP2	6:J:1083:DC:H2'	2.05	0.56
5:I:1053:DA:H2''	5:I:1054:DA:OP2	2.06	0.56
6:J:970:DC:H2''	6:J:971:DT:OP2	2.06	0.56
3:c:20:ARG:HD3	4:d:121:ALA:C	2.31	0.56
5:I:179:DA:H2''	5:I:180:DA:C8	2.41	0.56
5:I:626:DG:H2''	5:I:627:DC:OP2	2.04	0.56
6:J:131:DG:H2''	6:J:132:DA:OP2	2.05	0.56
6:J:863:DT:H2''	6:J:864:DG:OP2	2.06	0.56
6:J:935:DC:H2''	6:J:936:DG:C8	2.40	0.56
6:J:436:DA:H2''	6:J:437:DA:OP2	2.04	0.55
2:b:44:LYS:HD2	3:g:115:LEU:HD22	1.88	0.55
3:w:49:VAL:HG21	4:x:118:TYR:CG	2.41	0.55
3:w:54:VAL:HG13	4:x:107:ALA:HB1	1.87	0.55
5:I:84:DG:H2''	5:I:85:DC:OP2	2.06	0.55
5:I:352:DC:H2''	5:I:353:DT:C5	2.41	0.55
5:I:645:DG:H2''	5:I:646:DC:OP2	2.06	0.55
6:J:32:DT:H2'	6:J:33:DA:C8	2.41	0.55
6:J:368:DG:H2''	6:J:369:DG:C8	2.41	0.55
3:m:106:GLY:HA3	1:o:58:THR:HG22	1.86	0.55
5:I:271:DG:H2''	5:I:272:DC:OP2	2.06	0.55
3:q:57:TYR:HB2	4:r:110:GLU:HG3	1.88	0.55
3:0:40:SER:OG	4:1:86:ILE:HG13	2.06	0.55
1:A:41:TYR:HA	5:I:165:DC:H5''	1.88	0.55
5:I:173:DG:H1'	5:I:174:DT:H5'	1.87	0.55
5:I:1095:DA:H2''	5:I:1096:DC:OP2	2.06	0.55
6:J:42:DG:H2''	6:J:43:DT:OP2	2.04	0.55
6:J:241:DT:H2''	6:J:242:DA:C8	2.40	0.55
5:I:383:DA:H2''	5:I:384:DT:C6	2.41	0.55
6:J:810:DA:H2''	6:J:811:DA:OP2	2.07	0.55
2:p:75:HIS:HE1	4:r:90:GLU:HA	1.71	0.55
5:I:635:DC:H2''	5:I:636:DC:OP2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:774:DA:H1'	5:I:775:DG:H5'	1.89	0.55
6:J:161:DC:H2'	6:J:162:DT:H72	1.88	0.55
6:J:249:DA:H2''	6:J:250:DA:OP2	2.06	0.55
6:J:997:DA:H2''	6:J:998:DA:OP2	2.07	0.55
1:O:79:LYS:HB3	1:O:82:LEU:HD11	1.89	0.55
1:E:107:THR:HG23	1:E:123:ASP:HB2	1.89	0.55
1:E:120:MET:N	1:E:123:ASP:OD2	2.36	0.55
5:I:248:DG:OP1	4:d:85:THR:OG1	2.23	0.55
1:u:108:ASN:HD21	3:2:115:LEU:HD11	1.71	0.55
4:H:99:LEU:HB2	4:H:104:ALA:HB2	1.87	0.55
6:J:382:DT:H2''	6:J:383:DT:H72	1.89	0.55
1:K:73:GLU:CB	2:L:25:ASN:HD22	2.16	0.55
5:I:89:DT:H3	6:J:1034:DA:H61	1.54	0.55
6:J:752:DG:H2''	6:J:753:DC:C6	2.42	0.55
6:J:98:DT:H2''	6:J:99:DA:C8	2.42	0.55
6:J:211:DG:H2''	6:J:212:DA:C8	2.42	0.55
6:J:672:DG:OP2	1:K:65:LEU:N	2.30	0.55
1:o:62:ILE:HD11	2:p:37:LEU:HD11	1.88	0.55
4:H:75:SER:HA	4:H:86:ILE:HD11	1.89	0.54
5:I:199:DC:H2''	5:I:200:DG:C8	2.42	0.54
5:I:583:DC:H2''	5:I:584:DT:H72	1.88	0.54
3:C:87:ILE:HD12	3:C:102:ILE:HD11	1.87	0.54
5:I:286:DC:H2''	5:I:287:DC:OP2	2.08	0.54
5:I:852:DG:H21	1:Y:40:ARG:NH2	2.05	0.54
5:I:1052:DC:O2	6:J:72:DG:N2	2.41	0.54
6:J:222:DC:H2''	6:J:223:DT:OP2	2.06	0.54
6:J:271:DC:H2''	6:J:272:DG:OP2	2.07	0.54
3:q:42:ARG:HB2	4:r:85:THR:HG23	1.87	0.54
1:U:108:ASN:ND2	2:V:42:GLY:O	2.41	0.54
2:V:35:ARG:NH2	2:V:51:TYR:OH	2.39	0.54
1:Y:107:THR:HG23	1:Y:123:ASP:HB2	1.89	0.54
3:w:20:ARG:HD3	4:x:121:ALA:C	2.33	0.54
6:J:189:DG:H2''	6:J:190:DG:C8	2.42	0.54
6:J:410:DT:H2''	6:J:411:DG:C8	2.42	0.54
1:a:123:ASP:OD1	1:e:113:HIS:NE2	2.36	0.54
6:J:247:DG:H2''	6:J:248:DT:OP2	2.08	0.54
6:J:946:DA:H2''	6:J:947:DA:C8	2.43	0.54
6:J:954:DC:H2''	6:J:955:DA:C8	2.43	0.54
2:L:21:VAL:C	2:L:22:LEU:HD12	2.32	0.54
1:k:114:ALA:HA	1:o:114:ALA:HA	1.89	0.54
3:w:39:TYR:HB3	4:x:86:ILE:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:115:DT:H2''	6:J:116:DG:OP2	2.07	0.54
6:J:783:DC:H2''	6:J:784:DT:OP2	2.08	0.54
3:m:79:ILE:HG12	3:m:82:HIS:CE1	2.43	0.54
5:I:727:DT:H2''	5:I:728:DG:C8	2.43	0.54
6:J:302:DT:H2''	6:J:303:DG:OP2	2.08	0.54
6:J:356:DC:H1'	6:J:357:DG:H5'	1.89	0.54
1:u:120:MET:N	1:u:123:ASP:OD2	2.40	0.54
3:w:32:ARG:HH21	3:w:33:LEU:HD21	1.73	0.54
5:I:650:DT:H3	6:J:473:DA:H61	1.56	0.54
2:V:31:LYS:HE2	2:V:35:ARG:HH21	1.71	0.54
1:u:126:LEU:HD22	1:y:113:HIS:CB	2.38	0.54
6:J:36:DT:H2''	6:J:37:DG:C8	2.43	0.54
3:M:32:ARG:HH21	3:M:33:LEU:HD21	1.73	0.54
1:k:119:ILE:HG12	2:l:43:VAL:HG11	1.90	0.54
1:A:83:ARG:NH1	5:I:72:DC:H4'	2.22	0.54
5:I:232:DC:H42	6:J:891:DG:H1	1.55	0.54
6:J:210:DG:H2''	6:J:211:DG:C8	2.42	0.54
2:p:75:HIS:NE2	4:r:77:LEU:HB3	2.23	0.54
4:x:60:ASN:O	4:x:64:ASN:ND2	2.41	0.54
5:I:202:DG:H2''	5:I:203:DG:C8	2.43	0.54
5:I:958:DT:H2''	5:I:959:DG:C8	2.43	0.54
6:J:43:DT:H2''	6:J:44:DG:OP2	2.08	0.54
6:J:751:DG:H2''	6:J:752:DG:C8	2.43	0.54
5:I:594:DC:H2''	5:I:595:DG:C8	2.43	0.53
6:J:693:DA:H5'	3:M:42:ARG:HG2	1.90	0.53
4:R:99:LEU:HB2	4:R:104:ALA:HB2	1.89	0.53
2:l:75:HIS:HE1	4:n:90:GLU:HA	1.73	0.53
3:q:87:ILE:HD12	3:q:102:ILE:HD11	1.90	0.53
5:I:182:DA:H2''	5:I:183:DG:C8	2.44	0.53
5:I:218:DC:OP1	1:e:56:LYS:NZ	2.37	0.53
5:I:747:DC:H2''	5:I:748:DC:C6	2.42	0.53
6:J:784:DT:H2''	6:J:785:DG:C8	2.44	0.53
5:I:197:DT:H1'	5:I:198:DA:C8	2.43	0.53
5:I:311:DA:H2''	5:I:312:DT:OP2	2.09	0.53
5:I:369:DA:H2''	5:I:370:DG:C8	2.44	0.53
6:J:102:DT:H5'	1:u:43:PRO:HA	1.89	0.53
6:J:366:DT:H1'	6:J:367:DA:C8	2.43	0.53
6:J:394:DA:H2''	6:J:395:DC:C5	2.44	0.53
6:J:516:DC:H4'	4:n:30:ARG:HG3	1.91	0.53
6:J:971:DT:H2''	6:J:972:DG:C8	2.44	0.53
5:I:218:DC:H2''	5:I:219:DC:OP2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:292:DC:OP1	1:e:41:TYR:N	2.35	0.53
5:I:310:DG:H2''	5:I:311:DA:H8	1.73	0.53
5:I:538:DC:N4	6:J:584:DG:O6	2.41	0.53
5:I:660:DC:H2''	5:I:661:DC:OP2	2.09	0.53
6:J:301:DG:OP2	6:J:301:DG:H3'	2.08	0.53
2:f:31:LYS:HE2	2:f:35:ARG:HH21	1.73	0.53
1:E:78:PHE:CZ	2:F:67:ARG:HB2	2.43	0.53
5:I:204:DC:H2''	5:I:205:DC:C6	2.43	0.53
5:I:779:DC:H2''	5:I:780:DC:OP2	2.08	0.53
5:I:852:DG:H5''	1:Y:41:TYR:HB2	1.89	0.53
6:J:572:DA:H2''	6:J:573:DA:N7	2.24	0.53
2:b:98:TYR:OH	4:h:65:ASP:OD2	2.18	0.53
2:f:75:HIS:CE1	4:h:89:ARG:HG2	2.43	0.53
1:k:85:GLN:HG3	2:l:80:THR:HG22	1.90	0.53
5:I:308:DG:H4'	1:e:83:ARG:NH2	2.22	0.53
5:I:592:DC:H2''	5:I:593:DC:OP2	2.07	0.53
5:I:754:DC:H2''	5:I:755:DC:C6	2.44	0.53
5:I:914:DT:H2''	5:I:915:DG:C8	2.44	0.53
1:a:108:ASN:ND2	2:b:42:GLY:O	2.40	0.53
1:U:52:ARG:CG	3:0:111:ILE:HD11	2.38	0.53
3:0:40:SER:CB	4:1:86:ILE:HG13	2.39	0.53
1:A:55:GLN:OE1	3:G:109:PRO:HA	2.09	0.53
5:I:743:DA:H2''	5:I:744:DG:C8	2.44	0.53
6:J:1078:DG:H2''	6:J:1079:DG:OP2	2.09	0.53
3:c:81:ARG:NH2	3:c:107:VAL:O	2.39	0.53
6:J:806:DG:H4'	3:g:42:ARG:CZ	2.38	0.53
1:U:119:ILE:HD13	2:V:43:VAL:HG21	1.89	0.53
4:x:99:LEU:HB2	4:x:104:ALA:HB2	1.89	0.53
1:A:123:ASP:OD1	1:E:113:HIS:NE2	2.31	0.53
2:B:31:LYS:HE2	2:B:35:ARG:HH21	1.74	0.53
5:I:740:DA:H2''	5:I:741:DA:C8	2.43	0.53
5:I:832:DG:H2''	5:I:833:DC:OP2	2.09	0.53
6:J:390:DA:H2'	6:J:391:DT:H71	1.89	0.53
6:J:409:DC:H2''	6:J:410:DT:OP2	2.08	0.53
6:J:433:DA:OP1	4:r:84:SER:N	2.41	0.53
6:J:597:DT:H2''	6:J:598:DG:C8	2.44	0.53
6:J:671:DA:H3'	1:K:65:LEU:HB2	1.89	0.53
1:k:70:LEU:HA	2:l:25:ASN:HB3	1.91	0.53
1:E:69:ARG:NH1	2:F:25:ASN:OD1	2.38	0.53
5:I:488:DC:N4	6:J:635:DG:H22	2.07	0.53
6:J:200:DT:H2''	6:J:201:DA:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:434:DG:H2''	6:J:435:DT:OP2	2.08	0.53
6:J:692:DG:H5''	3:M:44:GLY:HA2	1.90	0.53
1:A:69:ARG:HH21	6:J:1045:DA:P	2.31	0.52
5:I:678:DC:H2''	5:I:679:DA:C8	2.44	0.52
6:J:583:DA:H2''	6:J:584:DG:N7	2.25	0.52
6:J:844:DC:H2''	6:J:845:DG:C8	2.45	0.52
3:m:20:ARG:O	4:n:117:LYS:HG3	2.09	0.52
5:I:943:DT:H2''	5:I:944:DA:H8	1.73	0.52
6:J:220:DA:H2''	6:J:221:DT:OP2	2.10	0.52
1:a:79:LYS:HB3	1:a:82:LEU:HD11	1.90	0.52
1:U:117:VAL:HG11	2:V:44:LYS:HD3	1.90	0.52
5:I:254:DT:O2	6:J:870:DG:N2	2.42	0.52
6:J:407:DA:H2''	6:J:408:DT:OP2	2.09	0.52
6:J:498:DT:H2''	6:J:499:DG:C8	2.44	0.52
5:I:15:DG:H2''	5:I:16:DG:C8	2.44	0.52
5:I:664:DC:N4	6:J:459:DG:H1	2.03	0.52
5:I:1080:DA:H2''	5:I:1081:DC:OP2	2.10	0.52
3:c:117:PRO:CD	1:e:48:LEU:HD11	2.34	0.52
5:I:370:DG:H4'	5:I:371:DC:H5'	1.92	0.52
6:J:80:DA:OP1	2:z:36:ARG:NH2	2.39	0.52
6:J:165:DA:H2''	6:J:166:DG:C8	2.45	0.52
6:J:883:DA:H2''	6:J:884:DA:OP2	2.09	0.52
3:g:54:VAL:HG13	4:h:107:ALA:HB1	1.90	0.52
1:K:47:ALA:HB3	2:L:44:LYS:HG3	1.91	0.52
1:U:94:GLU:HG3	2:V:100:PHE:CZ	2.45	0.52
1:U:126:LEU:CD1	1:Y:109:LEU:HB3	2.40	0.52
6:J:360:DC:H2''	6:J:361:DG:C8	2.45	0.52
6:J:390:DA:H2''	6:J:391:DT:H5'	1.90	0.52
1:a:113:HIS:NE2	1:e:123:ASP:OD1	2.37	0.52
3:m:63:LEU:HD13	4:n:42:LEU:HB2	1.91	0.52
1:E:42:ARG:NE	6:J:1023:DG:OP1	2.25	0.52
5:I:172:DT:H2''	5:I:173:DG:C8	2.45	0.52
5:I:847:DC:H2''	5:I:848:DC:OP2	2.10	0.52
5:I:977:DG:OP2	4:x:39:TYR:HE1	1.93	0.52
5:I:988:DT:H2''	5:I:989:DG:C8	2.45	0.52
5:I:927:DA:H2''	5:I:928:DA:C8	2.45	0.52
6:J:59:DA:H2''	6:J:60:DG:C8	2.45	0.52
6:J:170:DG:H2''	6:J:171:DG:C8	2.45	0.52
6:J:995:DG:H2''	6:J:996:DT:OP2	2.10	0.52
1:a:52:ARG:HG2	3:g:111:ILE:HD11	1.90	0.52
1:e:73:GLU:OE1	2:f:25:ASN:ND2	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:57:TYR:HB2	4:h:110:GLU:HG3	1.89	0.52
1:k:94:GLU:HG3	2:l:100:PHE:CZ	2.45	0.52
2:l:22:LEU:HB3	2:l:25:ASN:HD21	1.75	0.52
1:U:56:LYS:O	3:0:81:ARG:NH1	2.42	0.52
4:D:28:ARG:HD3	6:J:1079:DG:H5''	1.91	0.52
5:I:357:DC:C2	5:I:358:DA:N7	2.78	0.52
5:I:679:DA:H2''	5:I:680:DA:OP2	2.09	0.52
5:I:1092:DT:H3	6:J:31:DA:H61	1.57	0.52
6:J:942:DG:H2''	6:J:943:DT:C6	2.45	0.52
3:c:115:LEU:O	2:f:44:LYS:HD2	2.10	0.52
3:0:46:GLY:C	4:1:88:SER:HB3	2.35	0.52
3:2:32:ARG:HH21	3:2:33:LEU:HD21	1.74	0.52
3:2:87:ILE:HD12	3:2:102:ILE:HD11	1.91	0.52
5:I:173:DG:O6	6:J:949:DA:N6	2.43	0.52
5:I:869:DG:H4'	1:Y:83:ARG:NH2	2.25	0.52
6:J:219:DT:H2'	6:J:220:DA:C8	2.44	0.52
6:J:525:DC:OP1	3:m:77:ARG:N	2.35	0.52
6:J:573:DA:H2''	6:J:574:DT:C6	2.44	0.52
6:J:754:DT:H2''	6:J:755:DG:C8	2.45	0.52
2:f:92:ARG:NE	4:h:97:LEU:HB3	2.25	0.52
1:k:79:LYS:HB3	1:k:82:LEU:HD11	1.92	0.52
2:p:75:HIS:HE1	4:r:90:GLU:HG3	1.74	0.52
3:q:54:VAL:HG13	4:r:107:ALA:HB1	1.91	0.52
5:I:402:DA:H61	6:J:721:DT:H3	1.58	0.51
5:I:694:DT:OP1	3:q:44:GLY:HA2	2.10	0.51
5:I:725:DC:H4'	1:k:41:TYR:HE1	1.74	0.51
6:J:172:DC:H2''	6:J:173:DC:C6	2.46	0.51
6:J:209:DA:H2''	6:J:210:DG:C8	2.45	0.51
6:J:377:DG:C6	6:J:378:DG:C6	2.98	0.51
6:J:808:DG:H2''	6:J:809:DT:OP2	2.09	0.51
4:d:60:ASN:O	4:d:64:ASN:ND2	2.43	0.51
1:U:48:LEU:HD13	3:0:117:PRO:HD3	1.91	0.51
1:U:100:LEU:HD11	2:V:58:LEU:HD13	1.92	0.51
6:J:542:DG:H2''	6:J:543:DC:C6	2.45	0.51
3:q:20:ARG:O	4:r:117:LYS:HG2	2.11	0.51
6:J:1070:DA:H2''	6:J:1071:DA:OP2	2.10	0.51
2:z:31:LYS:HE2	2:z:35:ARG:HH21	1.75	0.51
3:m:109:PRO:HA	1:o:55:GLN:HB3	1.92	0.51
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.45	0.51
6:J:509:DA:H2''	6:J:510:DA:OP2	2.08	0.51
6:J:353:DG:H2''	6:J:354:DG:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:71:ARG:HB3	3:c:71:ARG:CZ	2.40	0.51
3:m:111:ILE:HD11	1:o:52:ARG:HG2	1.93	0.51
1:o:50:GLU:CB	2:p:39:ARG:HD2	2.41	0.51
1:U:51:ILE:CG2	3:0:111:ILE:HG12	2.41	0.51
2:V:92:ARG:NH2	4:X:98:LEU:HD12	2.25	0.51
1:Y:119:ILE:HG12	2:Z:43:VAL:HG11	1.93	0.51
3:0:79:ILE:HG12	3:0:82:HIS:CE1	2.45	0.51
5:I:187:DC:H2''	5:I:188:DG:C8	2.45	0.51
6:J:432:DG:H4'	3:q:42:ARG:CD	2.41	0.51
6:J:858:DA:OP2	1:a:65:LEU:HD23	2.10	0.51
6:J:919:DG:H2''	6:J:920:DC:C6	2.46	0.51
4:d:99:LEU:HB2	4:d:104:ALA:HB2	1.93	0.51
3:W:93:LEU:HD23	4:X:103:LEU:HD21	1.91	0.51
5:I:943:DT:H2''	5:I:944:DA:C8	2.45	0.51
6:J:169:DC:H2''	6:J:170:DG:C8	2.46	0.51
6:J:1100:DA:H2''	6:J:1101:DG:C8	2.46	0.51
3:c:17:ARG:NH2	3:c:28:GLY:HA2	2.26	0.51
3:c:17:ARG:HH21	3:c:28:GLY:HA2	1.76	0.51
1:O:61:LEU:HD12	2:P:37:LEU:HD23	1.92	0.51
1:u:55:GLN:OE1	3:2:110:ASN:N	2.44	0.51
5:I:545:DA:H1'	5:I:546:DT:H5'	1.92	0.51
5:I:574:DG:H2''	5:I:575:DC:C6	2.46	0.51
5:I:935:DC:H2''	5:I:936:DG:C8	2.46	0.51
3:W:101:THR:N	2:Z:96:THR:O	2.43	0.51
5:I:842:DG:H2''	5:I:843:DC:OP2	2.11	0.50
6:J:657:DC:H2''	6:J:658:DG:C8	2.46	0.50
6:J:954:DC:H2''	6:J:955:DA:H8	1.76	0.50
1:O:107:THR:HG23	1:O:123:ASP:HB2	1.91	0.50
3:0:17:ARG:HH21	3:0:28:GLY:HA2	1.76	0.50
4:1:99:LEU:HB2	4:1:104:ALA:HB2	1.94	0.50
1:A:83:ARG:HH11	5:I:72:DC:H4'	1.76	0.50
5:I:122:DG:H2''	5:I:123:DG:C8	2.46	0.50
6:J:8:DT:H4'	6:J:9:DT:H5'	1.94	0.50
6:J:335:DC:OP2	6:J:335:DC:H2'	2.11	0.50
5:I:124:DA:H2''	5:I:125:DT:OP2	2.10	0.50
5:I:181:DC:H2''	5:I:182:DA:C8	2.46	0.50
6:J:33:DA:H2''	6:J:34:DT:OP2	2.11	0.50
3:g:32:ARG:HH21	3:g:33:LEU:HD21	1.76	0.50
5:I:248:DG:H1'	5:I:249:DA:C8	2.46	0.50
5:I:849:DC:H42	6:J:274:DG:H1	1.59	0.50
5:I:1119:DC:H2''	5:I:1120:DG:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:96:DC:H2''	6:J:97:DG:C8	2.45	0.50
6:J:470:DC:H2''	6:J:471:DG:C8	2.46	0.50
1:K:48:LEU:HD11	3:Q:117:PRO:HD3	1.92	0.50
3:W:115:LEU:O	1:Y:48:LEU:HD11	2.11	0.50
3:w:79:ILE:HG12	3:w:82:HIS:CE1	2.46	0.50
5:I:26:DA:H2''	5:I:27:DG:OP2	2.11	0.50
5:I:929:DC:H2''	5:I:930:DA:H8	1.77	0.50
6:J:76:DT:H2''	6:J:77:DT:O5'	2.12	0.50
6:J:369:DG:C6	6:J:370:DG:C6	3.00	0.50
6:J:600:DC:H2''	6:J:601:DA:C8	2.47	0.50
1:u:79:LYS:HB3	1:u:82:LEU:HD11	1.93	0.50
5:I:31:DC:H2''	5:I:32:DC:OP2	2.10	0.50
5:I:911:DT:H2''	5:I:912:DC:C5	2.47	0.50
5:I:1057:DG:H2''	5:I:1058:DG:C8	2.47	0.50
6:J:177:DT:H2''	6:J:178:DA:C8	2.47	0.50
6:J:798:DA:H5''	3:g:16:THR:HA	1.93	0.50
3:M:104:GLN:NE2	1:O:58:THR:O	2.44	0.50
2:v:44:LYS:HB2	3:2:115:LEU:HB3	1.94	0.50
5:I:360:DG:C2	6:J:764:DA:C2	3.00	0.50
5:I:477:DC:H42	6:J:646:DG:H1	1.60	0.50
5:I:974:DC:H2''	5:I:975:DG:N7	2.27	0.50
5:I:1038:DC:N4	6:J:85:DG:H1	2.08	0.50
6:J:693:DA:C5'	3:M:42:ARG:HG2	2.42	0.50
6:J:738:DT:H2''	6:J:739:DA:C8	2.47	0.50
1:k:113:HIS:NE2	1:o:123:ASP:OD1	2.45	0.50
3:m:117:PRO:HD3	1:o:48:LEU:CD1	2.42	0.50
1:U:113:HIS:HE1	1:Y:122:LYS:HG3	1.77	0.50
5:I:173:DG:C2	6:J:951:DA:C2	3.00	0.50
5:I:882:DA:H5'	3:0:42:ARG:NH1	2.26	0.50
5:I:949:DC:H2''	5:I:950:DG:H8	1.77	0.50
5:I:952:DC:H2''	5:I:953:DC:C5	2.47	0.50
5:I:1058:DG:H2''	5:I:1059:DA:H8	1.76	0.50
6:J:556:DG:H2''	6:J:557:DG:C8	2.47	0.50
6:J:949:DA:C5	6:J:950:DC:C4	3.00	0.50
3:c:97:LEU:HB3	3:c:100:VAL:HB	1.93	0.50
1:e:48:LEU:HG	2:f:44:LYS:HE3	1.93	0.50
2:l:90:LEU:HB3	2:l:95:ARG:O	2.11	0.50
1:U:48:LEU:HD11	3:0:115:LEU:O	2.11	0.50
2:V:102:GLY:OXT	4:1:61:SER:HA	2.12	0.50
4:x:58:ILE:HG23	2:z:98:TYR:HD2	1.75	0.50
2:F:75:HIS:CE1	4:H:90:GLU:HA	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:820:DG:H2''	6:J:821:DC:OP2	2.11	0.50
2:V:71:THR:HG22	4:X:93:THR:HG23	1.93	0.50
3:0:20:ARG:HD3	4:1:121:ALA:C	2.36	0.50
2:B:79:LYS:HD3	6:J:1055:DG:P	2.51	0.49
5:I:1116:DC:H2''	5:I:1117:DA:C8	2.47	0.49
6:J:349:DT:H2''	6:J:350:DC:OP2	2.11	0.49
6:J:807:DA:OP1	4:h:85:THR:OG1	2.20	0.49
1:k:113:HIS:HB2	1:o:126:LEU:HD22	1.94	0.49
3:m:54:VAL:HG13	4:n:107:ALA:HB1	1.93	0.49
1:U:123:ASP:HA	1:Y:113:HIS:CE1	2.46	0.49
3:2:64:GLU:HA	4:3:46:HIS:HE1	1.77	0.49
5:I:558:DC:H2''	5:I:559:DC:C6	2.47	0.49
6:J:10:DC:H2''	6:J:11:DA:C8	2.47	0.49
6:J:387:DT:H2''	6:J:388:DA:C8	2.47	0.49
6:J:406:DT:H2'	6:J:407:DA:C8	2.47	0.49
6:J:637:DT:H2''	6:J:638:DT:O5'	2.12	0.49
6:J:1011:DT:H2''	6:J:1012:DT:O5'	2.12	0.49
3:g:87:ILE:HD12	3:g:102:ILE:HD11	1.93	0.49
5:I:301:DC:O2	6:J:823:DG:N2	2.45	0.49
5:I:733:DT:H2''	5:I:734:DG:H5'	1.94	0.49
6:J:208:DC:H2''	6:J:209:DA:C8	2.47	0.49
6:J:226:DC:H2''	6:J:227:DA:C8	2.47	0.49
6:J:659:DT:H2''	6:J:660:DA:C8	2.46	0.49
3:q:25:PHE:CE1	4:r:41:VAL:HG21	2.47	0.49
5:I:363:DT:H2''	5:I:364:DT:C6	2.48	0.49
5:I:1033:DT:H2''	5:I:1034:DC:C6	2.48	0.49
6:J:163:DC:H2''	6:J:164:DC:C6	2.47	0.49
1:k:54:TYR:O	2:l:40:ARG:NE	2.46	0.49
1:o:54:TYR:OH	2:p:36:ARG:NH1	2.45	0.49
1:U:55:GLN:OE1	3:0:110:ASN:N	2.36	0.49
1:A:83:ARG:HD3	5:I:72:DC:H5'	1.93	0.49
5:I:206:DG:C2	6:J:918:DG:C2	3.01	0.49
5:I:366:DA:H1'	5:I:367:DA:C8	2.47	0.49
6:J:131:DG:H4'	3:w:42:ARG:HB3	1.93	0.49
6:J:263:DT:H2''	6:J:264:DT:O5'	2.13	0.49
3:W:87:ILE:HD12	3:W:102:ILE:HD11	1.94	0.49
3:2:64:GLU:HA	4:3:46:HIS:CE1	2.47	0.49
6:J:3:DC:H2''	6:J:4:DG:C8	2.48	0.49
3:c:42:ARG:CB	4:d:85:THR:HG23	2.42	0.49
1:K:58:THR:CG2	3:Q:81:ARG:HB2	2.37	0.49
1:k:54:TYR:HB3	2:l:40:ARG:HE	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:20:ARG:O	4:H:117:LYS:HG3	2.13	0.49
5:I:240:DT:H2''	5:I:241:DG:C8	2.47	0.49
5:I:497:DG:H2''	5:I:498:DA:H8	1.78	0.49
5:I:718:DT:H3	6:J:405:DA:H61	1.59	0.49
1:K:62:ILE:HD11	2:L:37:LEU:HD11	1.94	0.49
1:A:58:THR:CG2	3:G:81:ARG:HB2	2.42	0.49
5:I:101:DC:H42	6:J:1022:DG:H1	1.61	0.49
5:I:173:DG:C5	5:I:174:DT:C4	3.01	0.49
5:I:1034:DC:H2''	5:I:1035:DC:OP2	2.11	0.49
6:J:1049:DG:OP2	6:J:1049:DG:H3'	2.13	0.49
3:O:54:VAL:HG13	4:1:107:ALA:HB1	1.93	0.49
4:1:60:ASN:O	4:1:64:ASN:ND2	2.46	0.49
5:I:78:DT:H3	6:J:1045:DA:H61	1.60	0.49
5:I:168:DT:C2	5:I:169:DG:C5	3.01	0.49
5:I:872:DA:H2''	5:I:873:DT:OP2	2.13	0.49
5:I:1024:DT:H3	6:J:99:DA:H61	1.61	0.49
6:J:135:DA:H2''	6:J:136:DA:OP2	2.12	0.49
3:Q:93:LEU:HD23	4:R:103:LEU:HD21	1.93	0.49
1:k:86:SER:O	1:k:90:MET:HG2	2.13	0.49
1:U:58:THR:HG21	3:O:81:ARG:HB2	1.95	0.49
5:I:166:DT:C2'	5:I:167:DG:C8	2.95	0.49
5:I:542:DT:H2''	5:I:543:DG:H8	1.77	0.49
5:I:846:DT:H2''	5:I:847:DC:C6	2.47	0.49
6:J:132:DA:O5'	6:J:132:DA:H8	1.96	0.49
6:J:433:DA:H2''	6:J:434:DG:C8	2.46	0.49
6:J:577:DA:C8	6:J:578:DT:H72	2.48	0.49
6:J:811:DA:OP2	6:J:811:DA:H2'	2.13	0.49
6:J:946:DA:H2''	6:J:947:DA:N7	2.27	0.49
1:O:100:LEU:HD11	2:P:58:LEU:HD13	1.94	0.49
5:I:720:DT:H3	6:J:403:DA:H61	1.61	0.48
6:J:197:DC:H2''	6:J:198:DA:C8	2.47	0.48
6:J:862:DG:H3'	6:J:862:DG:OP2	2.13	0.48
5:I:183:DG:H2''	5:I:184:DC:C6	2.48	0.48
5:I:344:DT:H3	6:J:779:DA:H61	1.62	0.48
5:I:400:DA:H1'	5:I:401:DG:H5'	1.94	0.48
5:I:603:DG:OP1	4:n:50:GLY:HA3	2.13	0.48
6:J:574:DT:H1'	6:J:575:DA:C8	2.48	0.48
6:J:1031:DC:H2''	6:J:1032:DG:C8	2.48	0.48
2:b:22:LEU:HB3	2:b:25:ASN:HD21	1.78	0.48
1:O:44:GLY:HA3	2:P:44:LYS:HE2	1.94	0.48
1:U:52:ARG:HG3	3:O:111:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:39:TYR:HB3	4:H:86:ILE:CD1	2.43	0.48
4:H:28:ARG:N	5:I:146:DC:OP1	2.45	0.48
5:I:33:DC:H2''	5:I:34:DG:C8	2.48	0.48
5:I:193:DC:H2''	5:I:194:DC:C6	2.48	0.48
5:I:205:DC:H2''	5:I:206:DG:H8	1.78	0.48
5:I:248:DG:OP1	4:d:84:SER:N	2.46	0.48
5:I:265:DT:H3	6:J:858:DA:H61	1.61	0.48
5:I:865:DC:H2''	5:I:866:DA:C8	2.47	0.48
6:J:446:DG:H2''	6:J:447:DC:OP2	2.12	0.48
3:W:32:ARG:HH21	3:W:33:LEU:HD21	1.78	0.48
1:Y:100:LEU:HD11	2:Z:58:LEU:HD13	1.94	0.48
3:w:17:ARG:HH21	3:w:28:GLY:HA2	1.78	0.48
5:I:10:DT:H2''	5:I:11:DA:C8	2.49	0.48
5:I:278:DC:H4'	2:b:45:ARG:CZ	2.43	0.48
5:I:550:DT:H2''	5:I:551:DT:C5	2.49	0.48
5:I:731:DC:H2''	5:I:732:DA:H8	1.78	0.48
6:J:58:DG:H4'	3:2:42:ARG:HD2	1.94	0.48
6:J:72:DG:H2''	6:J:73:DC:OP2	2.11	0.48
6:J:150:DG:H3'	3:w:76:THR:HB	1.94	0.48
6:J:270:DG:H2''	6:J:271:DC:OP2	2.12	0.48
2:f:88:TYR:CE2	4:h:80:TYR:HB3	2.48	0.48
3:g:25:PHE:HE1	4:h:41:VAL:HG21	1.79	0.48
2:v:44:LYS:HB3	3:2:115:LEU:HD22	1.94	0.48
5:I:170:DC:N3	5:I:171:DA:N6	2.61	0.48
5:I:353:DT:H2'	5:I:353:DT:OP2	2.13	0.48
6:J:154:DC:H2''	6:J:155:DG:N7	2.28	0.48
6:J:722:DC:H2'	6:J:723:DT:C6	2.49	0.48
6:J:958:DG:H2'	6:J:959:DG:C8	2.49	0.48
3:c:42:ARG:O	4:d:85:THR:HA	2.14	0.48
5:I:285:DT:H2''	5:I:286:DC:C6	2.48	0.48
5:I:1114:DA:H2''	5:I:1115:DA:N7	2.28	0.48
6:J:150:DG:O3'	3:w:77:ARG:HG3	2.14	0.48
6:J:283:DC:H2''	6:J:284:DG:C8	2.48	0.48
6:J:468:DC:H2''	6:J:469:DG:OP2	2.14	0.48
1:k:73:GLU:HB2	2:l:25:ASN:HD22	1.78	0.48
1:k:113:HIS:CG	1:o:126:LEU:HD22	2.48	0.48
2:v:77:LYS:HE3	4:x:89:ARG:CZ	2.43	0.48
5:I:23:DT:H2''	5:I:24:DG:C8	2.48	0.48
5:I:309:DG:H2''	5:I:310:DG:C8	2.48	0.48
5:I:332:DA:H2''	5:I:333:DC:OP2	2.14	0.48
5:I:585:DG:H2''	5:I:586:DG:OP2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:614:DT:H2''	5:I:615:DG:C8	2.49	0.48
5:I:808:DA:H4'	3:W:42:ARG:CZ	2.43	0.48
6:J:413:DC:H2''	6:J:414:DA:C8	2.48	0.48
3:G:31:HIS:HD1	3:G:48:PRO:HG3	1.78	0.48
5:I:622:DG:H1'	5:I:623:DA:C8	2.49	0.48
5:I:963:DA:H61	6:J:160:DT:H3	1.60	0.48
6:J:528:DC:H2''	6:J:529:DG:N7	2.29	0.48
6:J:563:DG:H2''	6:J:564:DG:C8	2.48	0.48
6:J:1007:DG:H2''	6:J:1008:DC:OP2	2.12	0.48
6:J:1102:DG:H2''	6:J:1103:DG:H8	1.78	0.48
3:G:49:VAL:HG21	4:H:118:TYR:CG	2.49	0.48
5:I:419:DC:H42	6:J:704:DG:H1	1.61	0.48
5:I:512:DT:H2''	5:I:513:DC:OP2	2.14	0.48
5:I:846:DT:H3	6:J:277:DA:H61	1.62	0.48
6:J:148:DC:OP2	6:J:148:DC:H2'	2.13	0.48
6:J:474:DC:H4'	2:l:45:ARG:CG	2.43	0.48
6:J:909:DC:H2'	6:J:910:DT:H72	1.96	0.48
6:J:911:DC:H2''	6:J:912:DC:C6	2.48	0.48
3:Q:54:VAL:HG13	4:R:107:ALA:HB1	1.95	0.48
3:Q:79:ILE:HG12	3:Q:82:HIS:CE1	2.49	0.48
4:X:61:SER:HA	2:Z:102:GLY:OXT	2.14	0.48
1:A:117:VAL:HG11	2:B:44:LYS:HD3	1.96	0.48
5:I:540:DT:H2''	5:I:541:DG:C8	2.49	0.48
6:J:94:DC:H2''	6:J:95:DG:OP2	2.14	0.48
6:J:498:DT:H2''	6:J:499:DG:H8	1.79	0.48
6:J:551:DT:H2''	6:J:552:DA:C8	2.48	0.48
6:J:650:DG:H4'	2:P:45:ARG:CZ	2.43	0.48
3:C:104:GLN:NE2	1:E:94:GLU:OE2	2.30	0.47
2:F:77:LYS:HE3	4:H:89:ARG:CZ	2.43	0.47
5:I:102:DC:H42	6:J:1021:DG:H1	1.62	0.47
5:I:171:DA:H2'	5:I:172:DT:H71	1.96	0.47
5:I:496:DG:H2''	5:I:497:DG:C8	2.49	0.47
5:I:655:DG:H2''	5:I:656:DC:OP2	2.14	0.47
6:J:780:DT:H2'	6:J:781:DA:C8	2.49	0.47
6:J:824:DT:H2''	6:J:825:DT:O5'	2.13	0.47
1:e:51:ILE:HD11	2:f:44:LYS:HA	1.95	0.47
1:K:55:GLN:OE1	3:Q:109:PRO:HA	2.14	0.47
1:u:122:LYS:C	1:y:113:HIS:HE1	2.22	0.47
4:3:46:HIS:HB3	4:3:49:THR:HB	1.95	0.47
5:I:744:DG:H2''	5:I:745:DC:C6	2.49	0.47
5:I:987:DT:P	3:w:17:ARG:HE	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:278:DC:H2''	6:J:279:DA:C8	2.49	0.47
6:J:688:DC:H2''	6:J:689:DT:OP2	2.14	0.47
4:d:113:LYS:HG2	4:d:117:LYS:HE2	1.95	0.47
5:I:167:DG:O6	6:J:955:DA:N6	2.47	0.47
5:I:172:DT:H2''	5:I:173:DG:H8	1.78	0.47
5:I:643:DA:P	2:l:36:ARG:HH12	2.37	0.47
6:J:383:DT:H2''	6:J:384:DC:C6	2.50	0.47
6:J:781:DA:H1'	6:J:782:DT:H5'	1.96	0.47
6:J:911:DC:H5''	1:e:41:TYR:CD1	2.49	0.47
6:J:931:DG:H2''	6:J:932:DT:C6	2.50	0.47
3:Q:97:LEU:HB3	3:Q:100:VAL:HB	1.96	0.47
3:W:115:LEU:HD22	2:Z:44:LYS:HB2	1.94	0.47
4:1:105:LYS:HB2	4:1:105:LYS:HE3	1.70	0.47
1:A:84:PHE:N	5:I:72:DC:OP1	2.36	0.47
1:A:113:HIS:HE1	1:E:122:LYS:HG3	1.78	0.47
3:C:42:ARG:HG2	6:J:1067:DA:H5'	1.96	0.47
6:J:450:DT:H2''	6:J:451:DT:O5'	2.14	0.47
6:J:941:DT:H2''	6:J:942:DG:C8	2.48	0.47
5:I:726:DC:H2''	5:I:727:DT:C5	2.49	0.47
5:I:839:DC:H4'	2:V:45:ARG:CD	2.45	0.47
3:W:81:ARG:NH2	3:W:107:VAL:O	2.44	0.47
3:G:76:THR:HB	5:I:153:DG:P	2.54	0.47
5:I:247:DA:H4'	3:c:42:ARG:CD	2.45	0.47
5:I:351:DC:C4	5:I:352:DC:N4	2.83	0.47
5:I:359:DT:C2	5:I:360:DG:C5	3.03	0.47
5:I:491:DC:H2''	5:I:492:DA:C8	2.50	0.47
5:I:561:DC:H2''	5:I:562:DG:C8	2.50	0.47
5:I:706:DA:H2''	5:I:707:DC:OP2	2.15	0.47
5:I:737:DT:H2''	5:I:738:DT:H5'	1.95	0.47
5:I:836:DG:H1	6:J:287:DC:H42	1.60	0.47
5:I:1029:DG:H2''	5:I:1030:DC:OP2	2.15	0.47
5:I:1048:DC:OP2	1:y:64:LYS:HB2	2.14	0.47
6:J:24:DG:H2''	6:J:25:DA:C8	2.50	0.47
6:J:193:DT:H2''	6:J:194:DG:C8	2.49	0.47
6:J:341:DC:H2''	6:J:342:DG:N7	2.30	0.47
2:b:24:ASP:OD1	2:b:27:GLN:HG2	2.14	0.47
2:b:77:LYS:HE3	4:d:89:ARG:CZ	2.44	0.47
1:A:56:LYS:NZ	6:J:964:DA:OP1	2.46	0.47
5:I:12:DC:H2''	5:I:13:DG:C8	2.49	0.47
5:I:53:DT:H2''	5:I:54:DG:C8	2.48	0.47
5:I:133:DT:H2''	5:I:134:DA:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:446:DC:P	1:K:72:ARG:HH12	2.38	0.47
5:I:462:DG:H2''	5:I:463:DT:C5	2.49	0.47
5:I:873:DT:H2''	5:I:874:DT:OP2	2.14	0.47
5:I:950:DG:C2	6:J:174:DG:C2	3.02	0.47
5:I:1052:DC:H2''	5:I:1053:DA:H8	1.79	0.47
6:J:350:DC:H1'	6:J:351:DC:C6	2.50	0.47
6:J:505:DG:H2''	6:J:506:DA:C8	2.49	0.47
6:J:660:DA:H2''	6:J:661:DC:C6	2.50	0.47
6:J:937:DG:H2''	6:J:938:DG:C8	2.49	0.47
1:K:59:GLU:OE1	2:L:40:ARG:NH2	2.47	0.47
3:Q:76:THR:O	4:R:49:THR:HA	2.15	0.47
3:W:92:GLU:HB3	4:X:100:PRO:HG2	1.97	0.47
5:I:89:DT:H3	6:J:1034:DA:N6	2.12	0.47
5:I:277:DA:H5'	1:a:43:PRO:HD2	1.96	0.47
5:I:603:DG:H1'	5:I:604:DG:H5'	1.95	0.47
5:I:870:DG:H2''	5:I:871:DG:C8	2.49	0.47
6:J:879:DG:H2''	6:J:880:DA:C8	2.49	0.47
6:J:1107:DC:H2''	6:J:1108:DC:OP2	2.15	0.47
3:c:32:ARG:HH21	3:c:33:LEU:HD21	1.77	0.47
2:L:31:LYS:HE2	2:L:35:ARG:HH21	1.80	0.47
3:Q:81:ARG:NH2	3:Q:107:VAL:O	2.42	0.47
2:B:45:ARG:CD	5:I:91:DC:H4'	2.44	0.47
3:C:117:PRO:HD3	1:E:48:LEU:HD11	1.97	0.47
5:I:280:DC:H1'	5:I:281:DG:C8	2.50	0.47
5:I:659:DT:H2''	5:I:660:DC:C6	2.50	0.47
5:I:683:DG:H2''	5:I:684:DG:C8	2.50	0.47
6:J:91:DC:H2''	6:J:92:DA:H8	1.80	0.47
6:J:181:DG:C6	6:J:182:DG:C6	3.02	0.47
6:J:537:DC:H2''	6:J:538:DC:C5	2.49	0.47
6:J:553:DT:H2''	6:J:554:DA:C8	2.50	0.47
6:J:581:DA:H2''	6:J:582:DC:C6	2.50	0.47
6:J:923:DC:H2''	6:J:924:DG:C8	2.50	0.47
2:l:24:ASP:OD1	2:l:27:GLN:HG2	2.15	0.47
3:m:76:THR:O	4:n:49:THR:HA	2.15	0.47
4:n:60:ASN:O	4:n:64:ASN:ND2	2.48	0.47
5:I:11:DA:H2''	5:I:12:DC:C6	2.50	0.47
5:I:220:DC:H2''	5:I:221:DG:C8	2.50	0.47
6:J:186:DT:H2''	6:J:187:DC:C6	2.50	0.47
6:J:763:DC:H2''	6:J:764:DA:H8	1.80	0.47
1:k:117:VAL:HG13	3:q:115:LEU:CD2	2.45	0.47
3:0:17:ARG:NH2	3:0:28:GLY:HA2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:63:LEU:HD13	4:1:42:LEU:HB2	1.96	0.47
1:A:120:MET:N	1:A:123:ASP:OD2	2.38	0.46
3:G:77:ARG:CZ	5:I:153:DG:H5'	2.45	0.46
3:G:81:ARG:NH2	3:G:107:VAL:O	2.45	0.46
5:I:60:DA:H2''	5:I:61:DG:OP2	2.15	0.46
5:I:949:DC:H2''	5:I:950:DG:C8	2.50	0.46
5:I:1117:DA:H2''	5:I:1118:DG:C8	2.50	0.46
6:J:91:DC:H2''	6:J:92:DA:C8	2.50	0.46
6:J:437:DA:OP2	6:J:437:DA:H2'	2.16	0.46
6:J:506:DA:H5'	3:m:42:ARG:HG2	1.97	0.46
6:J:675:DG:H2''	6:J:676:DT:OP2	2.14	0.46
6:J:743:DG:H2''	6:J:744:DG:C8	2.51	0.46
5:I:399:DG:H2'	5:I:400:DA:C8	2.50	0.46
5:I:908:DA:H2''	5:I:909:DC:OP2	2.15	0.46
2:f:71:THR:HG22	4:h:93:THR:HG23	1.97	0.46
4:R:105:LYS:HB2	4:R:105:LYS:HE3	1.72	0.46
3:m:90:ASP:HB3	3:m:93:LEU:HB2	1.97	0.46
1:U:99:TYR:HD1	2:V:95:ARG:CZ	2.28	0.46
3:0:40:SER:HB3	4:1:86:ILE:HG13	1.96	0.46
3:0:87:ILE:HD12	3:0:102:ILE:HD11	1.96	0.46
5:I:756:DT:H2''	5:I:757:DA:C8	2.50	0.46
6:J:433:DA:P	4:r:84:SER:H	2.38	0.46
6:J:555:DG:H2''	6:J:556:DG:C8	2.50	0.46
6:J:576:DC:H2''	6:J:577:DA:H8	1.79	0.46
6:J:584:DG:H2''	6:J:585:DG:C8	2.49	0.46
6:J:763:DC:H2''	6:J:764:DA:C8	2.51	0.46
6:J:837:DG:H4'	2:f:45:ARG:NH1	2.30	0.46
6:J:1099:DC:H2''	6:J:1100:DA:C8	2.49	0.46
2:l:99:GLY:HA2	4:r:58:ILE:HB	1.96	0.46
3:q:40:SER:HB3	4:r:86:ILE:HG13	1.97	0.46
4:x:75:SER:HA	4:x:86:ILE:HD11	1.97	0.46
5:I:1049:DC:N4	6:J:74:DG:H22	2.11	0.46
6:J:278:DC:H2''	6:J:279:DA:H8	1.80	0.46
6:J:579:DG:H1'	6:J:580:DC:H5'	1.97	0.46
6:J:692:DG:H2''	6:J:693:DA:C8	2.49	0.46
3:m:87:ILE:HD12	3:m:102:ILE:HD11	1.97	0.46
4:n:99:LEU:HB2	4:n:104:ALA:HB2	1.96	0.46
3:W:76:THR:O	4:X:49:THR:HA	2.16	0.46
3:2:63:LEU:HD11	4:3:38:VAL:HG13	1.96	0.46
5:I:16:DG:H2''	5:I:17:DC:C5	2.49	0.46
5:I:24:DG:H2''	5:I:25:DG:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:168:DT:H1'	5:I:169:DG:C8	2.50	0.46
5:I:1060:DT:H2''	5:I:1061:DT:OP2	2.16	0.46
6:J:248:DT:H2''	6:J:249:DA:C8	2.51	0.46
6:J:524:DG:C3'	3:m:76:THR:HB	2.43	0.46
6:J:927:DT:H2''	6:J:928:DA:C8	2.51	0.46
6:J:936:DG:H2''	6:J:937:DG:H8	1.79	0.46
6:J:940:DC:H2''	6:J:941:DT:H71	1.98	0.46
1:k:73:GLU:OE1	2:l:25:ASN:HB2	2.15	0.46
4:l:43:LYS:HA	4:l:43:LYS:HD3	1.74	0.46
1:u:101:VAL:HG11	3:2:107:VAL:HG11	1.96	0.46
5:I:607:DG:H1	6:J:516:DC:N4	2.13	0.46
6:J:114:DG:H3'	6:J:114:DG:OP2	2.16	0.46
6:J:151:DC:P	3:w:76:THR:HB	2.56	0.46
6:J:171:DG:H2''	6:J:172:DC:C5	2.51	0.46
6:J:842:DC:H2''	6:J:843:DG:OP2	2.16	0.46
6:J:996:DT:H2''	6:J:997:DA:C8	2.51	0.46
6:J:1005:DT:H2''	6:J:1006:DG:H5'	1.96	0.46
1:a:63:ARG:HD3	1:a:63:ARG:HA	1.66	0.46
1:k:113:HIS:CD2	1:o:110:CYS:O	2.68	0.46
4:r:75:SER:HA	4:r:86:ILE:HD11	1.97	0.46
3:G:26:PRO:HG3	4:H:37:TYR:CZ	2.50	0.46
5:I:285:DT:H3	6:J:838:DA:H61	1.63	0.46
5:I:386:DC:H2''	5:I:387:DG:C8	2.50	0.46
5:I:542:DT:H2''	5:I:543:DG:C8	2.50	0.46
5:I:926:DG:H2''	5:I:927:DA:C8	2.51	0.46
5:I:986:DA:OP1	3:w:29:ARG:HA	2.15	0.46
6:J:60:DG:H2''	6:J:61:DT:OP2	2.15	0.46
6:J:189:DG:H2''	6:J:190:DG:H8	1.80	0.46
6:J:319:DA:H1'	6:J:320:DC:H5'	1.98	0.46
6:J:909:DC:H2''	6:J:910:DT:H5'	1.98	0.46
3:m:100:VAL:HG11	2:p:98:TYR:CZ	2.51	0.46
3:G:31:HIS:ND1	3:G:48:PRO:HG3	2.31	0.46
5:I:61:DG:H1'	5:I:62:DA:C8	2.50	0.46
5:I:166:DT:C4	5:I:167:DG:C6	3.04	0.46
5:I:173:DG:C2	5:I:174:DT:C2	3.04	0.46
5:I:766:DC:H2''	5:I:767:DG:C8	2.51	0.46
5:I:1103:DT:H2''	5:I:1104:DG:C8	2.51	0.46
6:J:131:DG:H2''	6:J:132:DA:C8	2.50	0.46
1:k:47:ALA:O	1:k:51:ILE:HG13	2.16	0.46
3:w:63:LEU:HD13	4:x:42:LEU:HB2	1.98	0.46
1:E:41:TYR:HD2	5:I:105:DC:P	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:1120:DG:H2''	5:I:1121:DA:C8	2.51	0.46
2:b:44:LYS:HB2	3:g:115:LEU:HD13	1.98	0.46
1:e:99:TYR:OH	1:e:133:GLU:OE1	2.31	0.46
2:Z:22:LEU:HB3	2:Z:25:ASN:HD21	1.81	0.46
1:u:86:SER:O	1:u:90:MET:HG2	2.15	0.46
1:E:63:ARG:HA	1:E:63:ARG:HD3	1.66	0.46
5:I:172:DT:C2	5:I:173:DG:N7	2.84	0.46
5:I:720:DT:H2''	5:I:721:DA:OP2	2.16	0.46
5:I:1052:DC:H2''	5:I:1053:DA:C8	2.51	0.46
6:J:539:DA:H5'	6:J:539:DA:C8	2.51	0.46
6:J:788:DA:OP1	4:h:50:GLY:HA3	2.15	0.46
6:J:809:DT:H2''	6:J:810:DA:OP2	2.15	0.46
6:J:922:DG:H2''	6:J:923:DC:C6	2.51	0.46
3:c:80:PRO:HB3	4:d:58:ILE:CD1	2.46	0.46
3:g:79:ILE:HG12	3:g:82:HIS:CE1	2.51	0.46
5:I:357:DC:H2''	5:I:358:DA:H8	1.81	0.45
5:I:546:DT:H1'	5:I:547:DG:H5'	1.98	0.45
6:J:277:DA:H5'	2:Z:45:ARG:NH1	2.31	0.45
6:J:661:DC:H2''	6:J:662:DG:C8	2.51	0.45
3:Q:20:ARG:HE	3:Q:20:ARG:HB2	1.54	0.45
1:U:54:TYR:O	2:V:40:ARG:NE	2.50	0.45
2:V:71:THR:HG23	4:X:96:ARG:NH1	2.32	0.45
1:Y:118:THR:HA	2:Z:45:ARG:O	2.16	0.45
5:I:190:DG:H2''	5:I:191:DA:C8	2.51	0.45
5:I:371:DC:H2''	5:I:372:DC:OP2	2.16	0.45
6:J:627:DC:H4'	6:J:628:DC:H5'	1.98	0.45
6:J:754:DT:H2''	6:J:755:DG:H8	1.79	0.45
6:J:807:DA:H2''	6:J:808:DG:C8	2.52	0.45
3:c:80:PRO:HB3	4:d:58:ILE:HD12	1.99	0.45
1:K:120:MET:N	1:K:123:ASP:OD2	2.42	0.45
1:k:110:CYS:O	1:o:113:HIS:CD2	2.69	0.45
2:V:38:ALA:HB1	2:V:43:VAL:HB	1.98	0.45
2:V:89:ALA:O	2:V:93:GLN:HG2	2.17	0.45
5:I:29:DA:H61	6:J:1094:DT:H3	1.65	0.45
5:I:101:DC:N4	6:J:1022:DG:H1	2.14	0.45
5:I:678:DC:H2''	5:I:679:DA:H8	1.81	0.45
5:I:924:DT:H2''	5:I:925:DT:C6	2.51	0.45
5:I:932:DC:H2''	5:I:933:DC:C6	2.50	0.45
5:I:1112:DT:H2''	5:I:1113:DG:C8	2.52	0.45
6:J:205:DG:H2''	6:J:206:DC:C6	2.52	0.45
6:J:250:DA:OP2	6:J:250:DA:H2'	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:310:DC:OP2	6:J:310:DC:H6	1.98	0.45
4:R:43:LYS:HA	4:R:43:LYS:HD3	1.80	0.45
2:p:75:HIS:HB2	4:r:93:THR:HG21	1.97	0.45
1:A:76:GLN:OE1	2:B:22:LEU:HD12	2.15	0.45
1:E:79:LYS:HB3	1:E:82:LEU:HD11	1.98	0.45
5:I:209:DC:H2''	5:I:210:DT:C6	2.52	0.45
5:I:281:DG:H2''	5:I:282:DC:OP2	2.15	0.45
5:I:301:DC:N4	6:J:822:DG:H22	2.13	0.45
5:I:308:DG:N2	6:J:816:DC:O2	2.50	0.45
5:I:406:DC:H2''	5:I:407:DC:OP2	2.16	0.45
5:I:816:DC:H2''	5:I:817:DT:H72	1.98	0.45
5:I:915:DG:H2''	5:I:916:DT:C6	2.51	0.45
5:I:981:DG:H1	6:J:142:DC:H42	1.63	0.45
6:J:902:DC:H2''	6:J:903:DG:N7	2.31	0.45
6:J:967:DT:H2'	6:J:968:DA:C8	2.51	0.45
6:J:1029:DC:H2''	6:J:1030:DG:C8	2.51	0.45
2:b:92:ARG:NH2	4:d:98:LEU:HA	2.31	0.45
3:g:67:GLY:HA3	4:h:46:HIS:CE1	2.52	0.45
3:W:21:ALA:HB2	4:X:118:TYR:HB2	1.99	0.45
1:u:58:THR:HG21	3:2:81:ARG:HB2	1.98	0.45
2:z:22:LEU:HB3	2:z:25:ASN:HD21	1.81	0.45
2:B:45:ARG:NH1	5:I:92:DG:H5'	2.31	0.45
5:I:8:DT:H2''	5:I:9:DA:C8	2.52	0.45
5:I:431:DC:H2''	5:I:432:DG:OP2	2.16	0.45
5:I:1096:DC:H1'	5:I:1097:DA:H5'	1.98	0.45
6:J:505:DG:OP1	3:m:44:GLY:HA2	2.16	0.45
1:k:94:GLU:HG3	2:l:100:PHE:CE1	2.51	0.45
2:F:22:LEU:HB3	2:F:25:ASN:HD21	1.81	0.45
5:I:461:DC:H2''	5:I:462:DG:C8	2.51	0.45
6:J:226:DC:H4'	3:0:77:ARG:NE	2.31	0.45
6:J:394:DA:H2''	6:J:395:DC:C6	2.51	0.45
6:J:933:DC:H2''	6:J:934:DT:C5	2.51	0.45
6:J:994:DA:H2''	6:J:995:DG:C8	2.52	0.45
1:a:120:MET:N	1:a:123:ASP:OD2	2.45	0.45
1:k:63:ARG:HD3	1:k:63:ARG:HA	1.66	0.45
1:U:55:GLN:HB3	3:0:109:PRO:HA	1.98	0.45
1:U:63:ARG:HA	1:U:63:ARG:HD3	1.72	0.45
2:B:98:TYR:OH	4:H:65:ASP:OD2	2.28	0.45
3:C:97:LEU:HB3	3:C:100:VAL:HB	1.99	0.45
5:I:871:DG:H2''	5:I:872:DA:H8	1.82	0.45
6:J:737:DG:H2''	6:J:738:DT:C5	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:1066:DG:H2''	6:J:1067:DA:C8	2.52	0.45
3:m:68:ASN:OD1	3:m:71:ARG:NH2	2.49	0.45
2:p:31:LYS:HE2	2:p:35:ARG:HH21	1.81	0.45
1:A:94:GLU:HG3	2:B:100:PHE:CE1	2.52	0.45
5:I:123:DG:H2''	5:I:124:DA:H8	1.81	0.45
5:I:259:DC:OP1	1:a:84:PHE:N	2.46	0.45
5:I:535:DC:H2''	5:I:536:DA:OP2	2.17	0.45
5:I:758:DT:H1'	5:I:759:DA:C8	2.52	0.45
6:J:345:DA:OP2	6:J:345:DA:H8	2.00	0.45
6:J:697:DA:H2''	6:J:698:DT:OP2	2.16	0.45
6:J:718:DG:H2''	6:J:719:DA:OP2	2.15	0.45
1:a:86:SER:O	1:a:90:MET:HG2	2.16	0.45
1:k:113:HIS:NE2	1:o:110:CYS:HB3	2.32	0.45
5:I:169:DG:C2	6:J:955:DA:C2	3.05	0.45
5:I:686:DT:H2''	5:I:687:DT:OP2	2.16	0.45
5:I:775:DG:H2''	5:I:776:DA:H5''	1.99	0.45
5:I:1068:DT:OP1	3:2:44:GLY:HA2	2.17	0.45
6:J:138:DT:H2''	6:J:139:DG:C8	2.52	0.45
6:J:388:DA:H2''	6:J:389:DC:C6	2.52	0.45
6:J:539:DA:H5'	6:J:539:DA:H8	1.81	0.45
6:J:731:DG:H2''	6:J:732:DG:C8	2.52	0.45
6:J:748:DC:H2''	6:J:749:DG:H8	1.82	0.45
6:J:751:DG:H2''	6:J:752:DG:H8	1.81	0.45
2:f:22:LEU:HB3	2:f:25:ASN:HD21	1.81	0.45
1:K:47:ALA:O	1:K:51:ILE:HG13	2.17	0.45
3:Q:49:VAL:HG21	4:R:118:TYR:CG	2.52	0.45
1:Y:38:PRO:HB2	1:Y:39:HIS:H	1.65	0.45
2:Z:84:MET:HE1	2:Z:102:GLY:CA	2.46	0.45
3:G:20:ARG:HE	3:G:20:ARG:HB2	1.63	0.45
5:I:316:DT:H2''	5:I:317:DC:OP2	2.17	0.45
5:I:559:DC:H2''	5:I:560:DC:C5	2.52	0.45
5:I:766:DC:H2''	5:I:767:DG:H8	1.82	0.45
5:I:1067:DC:H42	6:J:56:DG:H1	1.63	0.45
6:J:61:DT:H2''	6:J:62:DA:OP2	2.17	0.45
6:J:124:DT:H2''	6:J:125:DG:C8	2.52	0.45
3:g:92:GLU:OE1	4:h:103:LEU:N	2.50	0.45
2:l:75:HIS:CE1	4:n:90:GLU:HG3	2.52	0.45
2:V:75:HIS:CE1	4:X:89:ARG:HG2	2.51	0.45
2:V:98:TYR:HB3	4:1:58:ILE:HG23	1.98	0.45
3:W:100:VAL:HA	2:Z:96:THR:O	2.17	0.45
3:C:102:ILE:HG23	4:D:58:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:549:DA:H2''	5:I:550:DT:C7	2.46	0.44
5:I:692:DC:H42	6:J:431:DG:H1	1.65	0.44
5:I:1027:DG:C3'	1:u:120:MET:HE1	2.48	0.44
6:J:593:DT:H2'	6:J:594:DA:C8	2.52	0.44
6:J:1029:DC:H2''	6:J:1030:DG:H8	1.83	0.44
6:J:1103:DG:H2''	6:J:1104:DC:C6	2.52	0.44
2:p:71:THR:HB	4:r:97:LEU:HD21	1.99	0.44
2:z:89:ALA:O	2:z:93:GLN:HG2	2.17	0.44
3:2:87:ILE:HD13	3:2:97:LEU:CD1	2.46	0.44
1:E:39:HIS:O	5:I:105:DC:H5''	2.16	0.44
5:I:154:DA:H61	6:J:969:DT:H3	1.65	0.44
5:I:206:DG:C2	5:I:207:DC:C2	3.05	0.44
5:I:304:DC:H2''	5:I:305:DA:C8	2.53	0.44
5:I:357:DC:C2	5:I:358:DA:C8	3.04	0.44
5:I:600:DC:H2''	5:I:601:DG:N7	2.32	0.44
6:J:452:DA:H2''	6:J:453:DA:H8	1.81	0.44
6:J:740:DT:H2''	6:J:741:DA:C8	2.52	0.44
6:J:750:DG:H2''	6:J:751:DG:C8	2.52	0.44
3:c:31:HIS:ND1	3:c:48:PRO:HG3	2.32	0.44
3:M:118:LYS:HB2	3:M:118:LYS:HE3	1.83	0.44
1:k:55:GLN:OE1	3:q:109:PRO:HA	2.18	0.44
1:o:120:MET:N	1:o:123:ASP:OD2	2.46	0.44
1:U:96:CYS:SG	2:V:62:LEU:HD21	2.57	0.44
1:A:45:THR:OG1	5:I:165:DC:OP1	2.14	0.44
5:I:3:DC:H2''	5:I:4:DA:C8	2.52	0.44
5:I:39:DC:H2''	5:I:40:DG:N7	2.32	0.44
5:I:117:DC:H2''	5:I:118:DA:C8	2.52	0.44
5:I:278:DC:H2''	5:I:279:DG:C8	2.52	0.44
5:I:373:DC:H2''	5:I:374:DC:C6	2.53	0.44
5:I:768:DC:H1'	5:I:769:DC:H5'	1.98	0.44
6:J:262:DG:H2''	6:J:263:DT:OP2	2.17	0.44
6:J:765:DT:H1'	6:J:766:DG:H5'	1.99	0.44
6:J:1039:DC:H2''	6:J:1040:DG:C8	2.52	0.44
3:M:76:THR:O	4:N:49:THR:HG23	2.17	0.44
1:o:47:ALA:O	1:o:51:ILE:HG13	2.16	0.44
2:p:22:LEU:HB3	2:p:25:ASN:HD21	1.81	0.44
3:G:57:TYR:CZ	4:H:106:HIS:HB2	2.52	0.44
5:I:309:DG:H5'	1:e:83:ARG:HE	1.82	0.44
5:I:968:DC:H2''	5:I:969:DG:C8	2.53	0.44
6:J:287:DC:OP1	2:V:47:SER:HA	2.17	0.44
6:J:839:DC:H2''	6:J:840:DA:H8	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:890:DC:H4'	4:d:30:ARG:HG3	1.98	0.44
6:J:932:DT:H2''	6:J:933:DC:C6	2.52	0.44
6:J:1059:DT:H2''	6:J:1060:DG:C8	2.53	0.44
3:W:99:ARG:O	2:Z:96:THR:N	2.49	0.44
4:X:58:ILE:HG12	2:Z:99:GLY:CA	2.48	0.44
5:I:168:DT:C2	5:I:169:DG:N7	2.86	0.44
5:I:552:DG:H2''	5:I:553:DA:C8	2.53	0.44
5:I:760:DC:H2''	5:I:761:DG:C8	2.52	0.44
6:J:89:DG:H4'	2:z:45:ARG:CZ	2.48	0.44
6:J:151:DC:P	3:w:76:THR:H	2.40	0.44
3:c:40:SER:HB3	4:d:86:ILE:HG13	1.99	0.44
1:O:50:GLU:HB2	2:P:39:ARG:HD2	2.00	0.44
1:k:117:VAL:CG1	2:l:44:LYS:HE2	2.44	0.44
3:W:106:GLY:HA3	1:Y:58:THR:HG22	1.99	0.44
2:z:71:THR:HG22	4:3:93:THR:HG23	1.98	0.44
3:2:63:LEU:HD12	4:3:41:VAL:HG12	1.99	0.44
5:I:175:DA:H1'	5:I:176:DT:C2	2.53	0.44
5:I:745:DC:H1'	5:I:746:DC:H5'	1.98	0.44
5:I:923:DA:H2''	5:I:924:DT:H71	2.00	0.44
6:J:140:DA:H5''	3:w:16:THR:HG22	1.99	0.44
6:J:826:DA:H2''	6:J:827:DA:H8	1.83	0.44
1:a:48:LEU:HD11	3:g:115:LEU:O	2.18	0.44
3:M:39:TYR:O	4:N:75:SER:OG	2.28	0.44
2:P:77:LYS:HE3	4:R:89:ARG:CZ	2.47	0.44
3:m:102:ILE:HA	2:p:98:TYR:HB2	2.00	0.44
3:C:81:ARG:NH2	3:C:107:VAL:O	2.49	0.44
5:I:731:DC:H2''	5:I:732:DA:C8	2.53	0.44
5:I:753:DC:H2''	5:I:754:DC:C6	2.53	0.44
5:I:1022:DC:H2''	5:I:1023:DG:C8	2.53	0.44
5:I:1069:DA:OP1	3:2:35:ARG:HD3	2.18	0.44
6:J:246:DA:H2''	6:J:247:DG:C8	2.53	0.44
6:J:522:DC:OP2	6:J:522:DC:H2'	2.17	0.44
2:b:75:HIS:O	4:d:89:ARG:NH1	2.45	0.44
1:k:107:THR:HG23	1:k:123:ASP:HB2	1.99	0.44
1:o:64:LYS:HD2	1:o:90:MET:HE1	1.99	0.44
3:W:92:GLU:OE2	4:X:102:GLU:N	2.42	0.44
1:Y:120:MET:C	2:Z:50:ILE:HD11	2.43	0.44
3:0:31:HIS:ND1	3:0:48:PRO:HG3	2.33	0.44
1:A:65:LEU:N	6:J:1046:DG:OP2	2.51	0.44
5:I:563:DA:H2''	5:I:564:DG:H8	1.82	0.44
5:I:567:DC:H2''	5:I:568:DC:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:695:DA:P	3:q:35:ARG:HD3	2.58	0.44
5:I:787:DC:H2''	5:I:788:DG:N7	2.33	0.44
6:J:78:DA:H2''	6:J:79:DA:H8	1.83	0.44
6:J:196:DT:H2''	6:J:197:DC:C6	2.53	0.44
6:J:761:DT:H4'	6:J:762:DA:H5'	2.00	0.44
6:J:839:DC:H2''	6:J:840:DA:C8	2.53	0.44
3:c:87:ILE:HD12	3:c:102:ILE:HD11	1.99	0.44
3:W:101:THR:O	2:Z:98:TYR:N	2.32	0.44
1:Y:86:SER:O	1:Y:90:MET:HG2	2.18	0.44
5:I:292:DC:H5''	1:e:40:ARG:HA	2.00	0.44
5:I:361:DT:C2	5:I:362:DA:C5	3.06	0.44
5:I:364:DT:H2''	5:I:365:DG:C8	2.53	0.44
5:I:369:DA:H2''	5:I:370:DG:H8	1.81	0.44
5:I:649:DG:H2''	5:I:650:DT:C5	2.53	0.44
5:I:690:DT:H2''	5:I:691:DC:OP2	2.18	0.44
5:I:951:DG:H2''	5:I:952:DC:C6	2.53	0.44
6:J:206:DC:H2''	6:J:207:DA:C8	2.53	0.44
6:J:215:DT:H2''	6:J:216:DA:H8	1.83	0.44
6:J:259:DG:H2''	6:J:260:DC:OP2	2.16	0.44
6:J:291:DC:H2''	6:J:292:DG:C8	2.52	0.44
6:J:661:DC:H4'	2:L:45:ARG:CZ	2.48	0.44
6:J:1010:DG:H2''	6:J:1011:DT:OP2	2.18	0.44
1:U:51:ILE:HG21	3:0:111:ILE:HG12	2.00	0.44
3:2:79:ILE:HG12	3:2:82:HIS:CE1	2.53	0.44
5:I:837:DT:H2''	5:I:838:DA:C8	2.53	0.43
6:J:21:DC:H2''	6:J:22:DA:C8	2.54	0.43
6:J:368:DG:H2''	6:J:369:DG:H8	1.81	0.43
6:J:896:DC:H2''	6:J:897:DG:C8	2.53	0.43
2:l:98:TYR:CE2	3:q:100:VAL:HG11	2.53	0.43
4:X:75:SER:HA	4:X:86:ILE:HD11	2.00	0.43
3:2:26:PRO:HD3	4:3:37:TYR:CD1	2.53	0.43
1:A:64:LYS:HD2	1:A:90:MET:HE1	1.99	0.43
1:A:94:GLU:OE1	3:G:104:GLN:NE2	2.48	0.43
3:C:32:ARG:HH21	3:C:33:LEU:HD21	1.82	0.43
5:I:401:DG:H2''	5:I:402:DA:H5''	1.99	0.43
5:I:633:DC:H5''	1:k:83:ARG:HG2	2.00	0.43
5:I:1064:DT:H2''	5:I:1065:DC:OP2	2.18	0.43
4:d:43:LYS:HA	4:d:43:LYS:HD3	1.76	0.43
2:P:22:LEU:HB3	2:P:25:ASN:HD21	1.81	0.43
3:m:38:ASN:HB3	3:q:38:ASN:HB3	2.01	0.43
3:q:76:THR:O	4:r:49:THR:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:98:TYR:N	3:O:101:THR:O	2.36	0.43
3:w:17:ARG:HD2	4:x:118:TYR:CE1	2.53	0.43
3:w:31:HIS:HD1	3:w:48:PRO:HG3	1.83	0.43
3:2:31:HIS:CD2	3:2:48:PRO:HG3	2.53	0.43
1:E:46:VAL:HB	5:I:104:DG:OP2	2.18	0.43
5:I:98:DT:H2''	5:I:99:DC:C6	2.54	0.43
5:I:184:DC:C2	5:I:185:DC:C5	3.06	0.43
5:I:226:DC:H2''	5:I:227:DG:N7	2.32	0.43
5:I:586:DG:H2''	5:I:587:DA:O4'	2.18	0.43
5:I:923:DA:C2'	5:I:924:DT:H71	2.48	0.43
5:I:977:DG:H1'	5:I:978:DG:H5'	2.00	0.43
6:J:8:DT:H2''	6:J:9:DT:C5	2.52	0.43
6:J:465:DC:H2''	6:J:466:DA:C8	2.53	0.43
6:J:744:DG:H2''	6:J:745:DT:H71	1.99	0.43
6:J:952:DT:C4	6:J:953:DG:C6	3.06	0.43
2:V:44:LYS:CB	3:O:115:LEU:HD22	2.48	0.43
1:u:118:THR:HA	2:v:45:ARG:HB3	1.99	0.43
3:w:87:ILE:HD12	3:w:102:ILE:HD11	1.99	0.43
1:y:63:ARG:HA	1:y:63:ARG:HD3	1.78	0.43
1:A:113:HIS:CE1	1:E:122:LYS:HG3	2.54	0.43
5:I:195:DT:H2''	5:I:196:DA:C8	2.53	0.43
6:J:179:DT:H2''	6:J:180:DA:C8	2.53	0.43
6:J:582:DC:H2''	6:J:583:DA:C8	2.53	0.43
6:J:844:DC:H2''	6:J:845:DG:H8	1.83	0.43
6:J:959:DG:H2''	6:J:960:DA:C8	2.53	0.43
1:e:79:LYS:HB3	1:e:82:LEU:HD11	2.00	0.43
1:Y:79:LYS:HD3	1:Y:82:LEU:HD21	2.00	0.43
3:O:31:HIS:HD1	3:O:48:PRO:HG3	1.83	0.43
3:O:97:LEU:HB3	3:O:100:VAL:HB	2.01	0.43
1:u:61:LEU:O	2:v:36:ARG:NH2	2.43	0.43
3:C:26:PRO:HD3	4:D:37:TYR:CD1	2.53	0.43
5:I:358:DA:C2	6:J:766:DG:C2	3.07	0.43
6:J:198:DA:H2''	6:J:199:DA:C8	2.53	0.43
6:J:435:DT:H2''	6:J:436:DA:OP2	2.19	0.43
6:J:455:DA:OP2	2:p:32:PRO:CD	2.67	0.43
6:J:505:DG:H4'	3:m:42:ARG:CB	2.31	0.43
6:J:515:DG:O3'	3:m:29:ARG:NH2	2.42	0.43
6:J:680:DA:H4'	1:K:83:ARG:NH2	2.33	0.43
6:J:772:DG:H2''	6:J:773:DA:C8	2.53	0.43
1:K:96:CYS:SG	2:L:62:LEU:HD21	2.59	0.43
1:k:38:PRO:HB2	1:k:39:HIS:H	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:26:PRO:HG3	4:n:37:TYR:CZ	2.53	0.43
3:W:118:LYS:HE3	3:W:118:LYS:HB2	1.84	0.43
2:Z:51:TYR:O	2:Z:55:ARG:HG3	2.19	0.43
1:E:42:ARG:HH21	6:J:1023:DG:P	2.42	0.43
2:F:75:HIS:HB2	4:H:93:THR:HG21	1.99	0.43
5:I:511:DC:H2''	5:I:512:DT:OP2	2.17	0.43
5:I:684:DG:H2''	5:I:685:DA:H8	1.84	0.43
5:I:977:DG:OP2	4:x:39:TYR:CE1	2.71	0.43
6:J:9:DT:H2''	6:J:10:DC:C6	2.54	0.43
6:J:255:DC:H2''	6:J:256:DT:OP2	2.18	0.43
6:J:708:DT:H2''	6:J:709:DC:OP2	2.17	0.43
6:J:715:DC:H2''	6:J:716:DG:N7	2.33	0.43
6:J:746:DC:H2''	6:J:747:DT:H71	2.01	0.43
1:e:91:ALA:HB2	2:f:100:PHE:CD2	2.53	0.43
4:h:76:ARG:HB3	4:h:80:TYR:CZ	2.54	0.43
1:K:51:ILE:HG23	2:L:42:GLY:HA2	2.00	0.43
1:K:94:GLU:OE1	3:Q:104:GLN:HG2	2.18	0.43
1:O:96:CYS:HG	2:P:61:PHE:HE2	1.62	0.43
2:V:42:GLY:O	3:O:115:LEU:HD11	2.17	0.43
5:I:120:DG:H1	6:J:1003:DC:H42	1.67	0.43
5:I:522:DT:H2''	5:I:523:DG:C8	2.54	0.43
5:I:1083:DT:H2''	5:I:1084:DG:C8	2.53	0.43
5:I:1100:DC:H5''	1:u:41:TYR:HA	2.00	0.43
6:J:132:DA:C5'	3:w:42:ARG:HG2	2.23	0.43
6:J:488:DG:H3'	6:J:488:DG:OP2	2.19	0.43
1:a:66:PRO:HB3	2:b:28:GLY:HA3	2.01	0.43
1:u:63:ARG:HD3	1:u:63:ARG:HA	1.58	0.43
5:I:148:DT:H2''	5:I:149:DG:C8	2.54	0.43
5:I:368:DC:C2	5:I:369:DA:C5	3.07	0.43
5:I:714:DG:P	3:q:76:THR:OG1	2.75	0.43
5:I:786:DC:H2''	5:I:787:DC:C5	2.54	0.43
5:I:896:DT:H2''	5:I:897:DG:C8	2.54	0.43
5:I:1028:DC:H1'	5:I:1029:DG:C8	2.54	0.43
6:J:449:DG:H2''	6:J:450:DT:OP2	2.18	0.43
6:J:452:DA:H2''	6:J:453:DA:C8	2.54	0.43
6:J:550:DG:H2'	6:J:551:DT:H71	1.99	0.43
2:p:89:ALA:O	2:p:93:GLN:HG2	2.18	0.43
3:G:32:ARG:HH21	3:G:33:LEU:HD21	1.83	0.43
5:I:131:DC:O2	6:J:993:DG:N2	2.52	0.43
5:I:208:DC:H2''	5:I:209:DC:C6	2.54	0.43
5:I:355:DT:H1'	5:I:356:DG:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:734:DG:H2''	5:I:735:DT:OP2	2.19	0.43
5:I:1101:DT:H2''	5:I:1102:DG:C8	2.53	0.43
6:J:36:DT:H2''	6:J:37:DG:N7	2.34	0.43
6:J:275:DG:H5'	1:Y:43:PRO:HD2	2.01	0.43
6:J:484:DA:OP2	1:k:65:LEU:HD23	2.19	0.43
6:J:768:DA:H4'	6:J:769:DC:H5'	2.01	0.43
3:Q:42:ARG:NH1	4:R:85:THR:OG1	2.52	0.43
3:W:79:ILE:HG12	3:W:82:HIS:CE1	2.54	0.43
4:X:65:ASP:OD1	2:Z:91:LYS:NZ	2.38	0.43
2:Z:90:LEU:HB3	2:Z:95:ARG:O	2.18	0.43
1:A:119:ILE:HD13	2:B:43:VAL:HG21	2.00	0.43
5:I:755:DC:H4'	5:I:756:DT:H5'	2.00	0.43
5:I:801:DT:H2''	5:I:802:DG:C8	2.54	0.43
5:I:852:DG:OP1	1:Y:45:THR:N	2.51	0.43
5:I:881:DT:H4'	3:O:42:ARG:HD3	2.01	0.43
6:J:248:DT:H2''	6:J:249:DA:OP2	2.19	0.43
6:J:788:DA:P	4:h:50:GLY:HA3	2.59	0.43
6:J:1100:DA:H2''	6:J:1101:DG:H8	1.83	0.43
1:e:96:CYS:SG	2:f:62:LEU:HD21	2.59	0.43
3:M:107:VAL:CG2	1:O:55:GLN:HG2	2.49	0.43
1:o:46:VAL:O	1:o:50:GLU:HG2	2.18	0.43
3:O:20:ARG:HE	3:O:20:ARG:HB2	1.64	0.43
1:u:129:ARG:HG2	1:y:109:LEU:HD13	2.01	0.43
2:B:31:LYS:HG3	2:B:51:TYR:CE1	2.54	0.42
5:I:202:DG:H2''	5:I:203:DG:H8	1.82	0.42
5:I:611:DA:H61	6:J:512:DT:H3	1.66	0.42
5:I:947:DC:H2''	5:I:948:DG:C8	2.54	0.42
5:I:1066:DC:H42	6:J:57:DG:H1	1.66	0.42
6:J:410:DT:H2''	6:J:411:DG:N7	2.34	0.42
6:J:752:DG:H2''	6:J:753:DC:H6	1.82	0.42
3:c:109:PRO:HG3	1:e:55:GLN:O	2.18	0.42
3:g:76:THR:O	4:h:49:THR:HG23	2.19	0.42
2:P:75:HIS:O	4:R:89:ARG:NH1	2.39	0.42
3:Q:90:ASP:HB3	3:Q:93:LEU:HB2	2.01	0.42
1:k:61:LEU:HD21	2:l:40:ARG:NH2	2.33	0.42
1:Y:83:ARG:O	2:Z:80:THR:HA	2.19	0.42
1:Y:119:ILE:HD13	2:Z:43:VAL:HG21	2.00	0.42
3:2:97:LEU:HB3	3:2:100:VAL:HB	2.01	0.42
5:I:125:DT:H2''	5:I:126:DT:OP2	2.16	0.42
5:I:312:DT:H2''	5:I:313:DT:OP2	2.19	0.42
5:I:392:DC:O2	6:J:732:DG:N2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:507:DT:H2''	5:I:508:DA:C8	2.54	0.42
5:I:550:DT:H2''	5:I:551:DT:C6	2.54	0.42
6:J:61:DT:H2''	6:J:62:DA:C8	2.54	0.42
6:J:903:DG:H2''	6:J:904:DG:OP2	2.19	0.42
6:J:919:DG:H2''	6:J:920:DC:C5	2.54	0.42
3:2:55:LEU:HD11	4:3:67:PHE:HD2	1.84	0.42
3:C:77:ARG:HD2	5:I:41:DA:H4'	2.01	0.42
1:E:41:TYR:O	5:I:104:DG:H4'	2.20	0.42
2:F:75:HIS:HE1	4:H:89:ARG:C	2.26	0.42
5:I:206:DG:C5	5:I:207:DC:C4	3.07	0.42
5:I:374:DC:C2	5:I:375:DG:C5	3.07	0.42
5:I:472:DT:H2''	5:I:473:DC:C6	2.54	0.42
6:J:350:DC:OP1	1:Y:41:TYR:HD1	2.02	0.42
6:J:353:DG:H2''	6:J:354:DG:H8	1.84	0.42
6:J:474:DC:H4'	2:l:45:ARG:HG2	2.01	0.42
6:J:639:DA:H2''	6:J:640:DA:C8	2.54	0.42
6:J:951:DA:C2	6:J:952:DT:C2	3.07	0.42
6:J:1089:DC:H2''	6:J:1090:DG:N7	2.35	0.42
3:g:58:LEU:HD11	4:h:99:LEU:HD11	2.01	0.42
3:g:93:LEU:HD23	4:h:103:LEU:HD21	2.01	0.42
2:L:102:GLY:OXT	4:R:61:SER:HA	2.19	0.42
1:A:109:LEU:HD11	1:E:129:ARG:CZ	2.49	0.42
5:I:181:DC:C2	5:I:182:DA:C5	3.08	0.42
5:I:288:DC:H42	6:J:835:DG:H1	1.67	0.42
5:I:300:DC:OP2	1:e:65:LEU:N	2.40	0.42
5:I:726:DC:H2''	5:I:727:DT:C7	2.49	0.42
6:J:311:DT:H2''	6:J:312:DG:C8	2.55	0.42
6:J:422:DG:H5''	4:r:30:ARG:NH2	2.35	0.42
6:J:742:DG:H1'	6:J:743:DG:C8	2.54	0.42
6:J:1102:DG:H2''	6:J:1103:DG:C8	2.54	0.42
3:Q:32:ARG:HH21	3:Q:33:LEU:HD21	1.83	0.42
1:k:118:THR:OG1	2:l:45:ARG:HB3	2.18	0.42
3:G:32:ARG:HD3	6:J:984:DG:OP1	2.20	0.42
5:I:178:DG:H2''	5:I:179:DA:C8	2.54	0.42
5:I:649:DG:H1	6:J:474:DC:H42	1.67	0.42
6:J:75:DG:H2''	6:J:76:DT:OP2	2.20	0.42
6:J:257:DT:H2''	6:J:258:DG:H5'	2.00	0.42
6:J:433:DA:OP1	4:r:85:THR:N	2.53	0.42
6:J:465:DC:H2''	6:J:466:DA:H8	1.84	0.42
6:J:585:DG:C5	6:J:586:DA:C6	3.08	0.42
2:B:89:ALA:O	2:B:93:GLN:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:26:DA:H1'	5:I:27:DG:H5'	2.00	0.42
5:I:94:DG:H2''	5:I:95:DC:OP2	2.19	0.42
5:I:129:DT:H2''	5:I:130:DC:OP2	2.19	0.42
5:I:214:DG:H2''	5:I:215:DA:H5''	2.01	0.42
5:I:446:DC:OP1	1:K:83:ARG:HA	2.20	0.42
5:I:549:DA:H2''	5:I:550:DT:C5	2.54	0.42
6:J:63:DA:OP2	6:J:63:DA:H2'	2.19	0.42
6:J:275:DG:P	1:Y:42:ARG:HE	2.39	0.42
6:J:880:DA:H1'	6:J:881:DC:H5'	2.01	0.42
6:J:951:DA:C5	6:J:952:DT:C4	3.07	0.42
3:Q:17:ARG:NH2	3:Q:28:GLY:HA2	2.35	0.42
2:p:71:THR:HG21	4:r:97:LEU:HG	2.02	0.42
2:p:75:HIS:CE1	4:r:90:GLU:HA	2.54	0.42
2:p:93:GLN:HG2	2:p:93:GLN:H	1.68	0.42
3:W:97:LEU:HB3	3:W:100:VAL:HB	2.01	0.42
1:E:86:SER:O	1:E:90:MET:HG2	2.20	0.42
5:I:23:DT:H2''	5:I:24:DG:H8	1.84	0.42
5:I:229:DG:OP1	4:d:50:GLY:HA3	2.20	0.42
5:I:368:DC:H2''	5:I:369:DA:C8	2.55	0.42
5:I:944:DA:H2'	5:I:945:DT:H71	2.01	0.42
6:J:180:DA:C6	6:J:181:DG:C6	3.06	0.42
6:J:818:DT:H2''	6:J:819:DG:H5'	2.02	0.42
3:c:107:VAL:HG21	2:f:40:ARG:O	2.20	0.42
1:K:50:GLU:OE1	2:L:39:ARG:NE	2.37	0.42
5:I:180:DA:H1'	5:I:181:DC:C6	2.54	0.42
5:I:365:DG:C2	5:I:366:DA:C2	3.07	0.42
5:I:735:DT:H2''	5:I:736:DA:C8	2.55	0.42
6:J:900:DA:OP2	3:c:75:LYS:HE2	2.19	0.42
6:J:950:DC:H1'	6:J:951:DA:C8	2.55	0.42
6:J:1026:DC:H2''	6:J:1027:DA:H8	1.83	0.42
1:a:48:LEU:HD21	3:g:115:LEU:HB3	2.02	0.42
1:e:132:GLY:HA3	3:g:99:ARG:NH2	2.34	0.42
1:K:79:LYS:HB3	1:K:82:LEU:HD11	2.01	0.42
3:Q:17:ARG:HH21	3:Q:28:GLY:HA2	1.84	0.42
3:Q:92:GLU:HB3	4:R:100:PRO:HG2	2.02	0.42
3:q:31:HIS:CD2	3:q:48:PRO:HG3	2.55	0.42
1:U:118:THR:OG1	2:V:45:ARG:HB3	2.20	0.42
1:Y:101:VAL:O	1:Y:105:GLU:HG3	2.19	0.42
4:x:43:LYS:HA	4:x:43:LYS:HD3	1.75	0.42
3:2:62:ILE:HD13	3:2:93:LEU:HD13	2.02	0.42
5:I:527:DG:H1	6:J:596:DC:H42	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:621:DA:H1'	5:I:622:DG:H5'	2.02	0.42
5:I:738:DT:H2''	5:I:739:DG:C8	2.55	0.42
5:I:934:DC:H2''	5:I:935:DC:C6	2.55	0.42
6:J:41:DC:H2''	6:J:42:DG:C8	2.54	0.42
6:J:70:DT:H5''	1:y:83:ARG:HD3	2.02	0.42
6:J:665:DC:H2''	6:J:666:DG:C8	2.55	0.42
6:J:809:DT:H2''	6:J:810:DA:C8	2.55	0.42
6:J:1073:DT:H2''	6:J:1074:DG:C8	2.55	0.42
3:c:114:VAL:CG2	1:e:112:ILE:HG12	2.50	0.42
1:k:61:LEU:HD12	2:l:37:LEU:HD23	2.01	0.42
1:o:61:LEU:HD13	2:p:36:ARG:O	2.20	0.42
5:I:354:DG:H1'	5:I:355:DT:C6	2.55	0.42
6:J:94:DC:H2''	6:J:95:DG:C8	2.55	0.42
6:J:435:DT:H2''	6:J:436:DA:C8	2.55	0.42
6:J:474:DC:H2''	6:J:475:DG:C8	2.54	0.42
6:J:705:DG:H5''	4:N:28:ARG:CD	2.49	0.42
6:J:924:DG:H2''	6:J:925:DT:C6	2.54	0.42
1:K:47:ALA:CB	2:L:44:LYS:HG3	2.49	0.42
1:U:52:ARG:HG2	3:O:111:ILE:HD11	2.01	0.42
5:I:93:DC:H1'	5:I:94:DG:C8	2.55	0.41
5:I:276:DT:H2''	5:I:277:DA:C8	2.56	0.41
5:I:695:DA:OP1	3:q:35:ARG:HD3	2.19	0.41
5:I:739:DG:C6	5:I:740:DA:C6	3.08	0.41
6:J:78:DA:H2''	6:J:79:DA:C8	2.55	0.41
6:J:196:DT:H2''	6:J:197:DC:C5	2.54	0.41
6:J:304:DC:H2''	6:J:305:DT:OP2	2.19	0.41
6:J:814:DC:H4'	6:J:815:DC:H5'	2.02	0.41
6:J:1101:DG:C6	6:J:1102:DG:C6	3.08	0.41
4:d:75:SER:HA	4:d:86:ILE:HD11	2.02	0.41
4:N:30:ARG:NH1	4:N:32:GLU:HG3	2.28	0.41
3:Q:87:ILE:HD12	3:Q:102:ILE:HD11	2.01	0.41
1:u:107:THR:HG23	1:u:123:ASP:HB2	2.01	0.41
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.55	0.41
5:I:91:DC:H2''	5:I:92:DG:C8	2.54	0.41
5:I:144:DC:H2'	5:I:145:DA:C8	2.56	0.41
5:I:278:DC:H4'	2:b:45:ARG:NE	2.36	0.41
5:I:657:DT:H2''	5:I:658:DG:C8	2.56	0.41
6:J:276:DG:H2''	6:J:277:DA:C8	2.55	0.41
6:J:318:DG:H5''	3:W:44:GLY:HA2	2.02	0.41
6:J:370:DG:C5	6:J:371:DT:C4	3.08	0.41
6:J:601:DA:H2''	6:J:602:DC:OP2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:86:SER:O	1:O:90:MET:HG2	2.19	0.41
1:k:51:ILE:HD13	2:l:42:GLY:HA2	2.02	0.41
1:u:58:THR:HG22	3:2:106:GLY:HA3	2.01	0.41
1:A:85:GLN:HG2	5:I:71:DG:OP1	2.20	0.41
5:I:398:DG:H2''	5:I:399:DG:H8	1.85	0.41
5:I:629:DC:H2''	5:I:630:DT:H72	2.03	0.41
5:I:741:DA:H2''	5:I:742:DC:C6	2.55	0.41
5:I:755:DC:C6	5:I:756:DT:H72	2.56	0.41
5:I:781:DC:H2''	5:I:782:DG:C8	2.56	0.41
5:I:912:DC:C4	5:I:913:DC:N4	2.88	0.41
6:J:296:DA:H1'	6:J:297:DA:C8	2.56	0.41
6:J:335:DC:H2''	6:J:336:DG:C8	2.56	0.41
6:J:602:DC:H2''	6:J:603:DG:C8	2.55	0.41
6:J:683:DG:H2''	6:J:684:DC:OP2	2.20	0.41
6:J:896:DC:OP2	6:J:896:DC:H2'	2.20	0.41
6:J:1013:DA:H2''	6:J:1014:DA:H8	1.85	0.41
2:L:23:ARG:HH11	2:L:23:ARG:HD2	1.74	0.41
1:Y:94:GLU:HG3	2:Z:100:PHE:CZ	2.56	0.41
2:v:102:GLY:OXT	4:3:61:SER:HA	2.20	0.41
5:I:38:DC:H2''	5:I:39:DC:C5	2.55	0.41
5:I:175:DA:H2''	5:I:176:DT:C7	2.50	0.41
5:I:320:DT:H2''	5:I:321:DA:C8	2.54	0.41
5:I:773:DG:H2'	5:I:774:DA:C8	2.56	0.41
5:I:836:DG:H2''	5:I:837:DT:C5	2.55	0.41
5:I:927:DA:H2''	5:I:928:DA:H8	1.85	0.41
6:J:382:DT:H1'	6:J:383:DT:C6	2.55	0.41
6:J:645:DC:H2''	6:J:646:DG:C8	2.55	0.41
6:J:858:DA:C6	6:J:859:DG:C6	3.08	0.41
6:J:1019:DC:H2''	6:J:1020:DG:OP2	2.20	0.41
6:J:1059:DT:H2''	6:J:1060:DG:H8	1.85	0.41
3:g:81:ARG:NH2	3:g:107:VAL:O	2.43	0.41
2:L:89:ALA:O	2:L:93:GLN:HG2	2.19	0.41
2:P:23:ARG:HH11	2:P:23:ARG:HD2	1.73	0.41
3:Q:65:LEU:HB2	3:Q:86:ALA:HB1	2.02	0.41
1:o:61:LEU:HD21	2:p:40:ARG:NH2	2.35	0.41
3:2:81:ARG:NH2	3:2:107:VAL:O	2.48	0.41
3:C:117:PRO:HD3	1:E:48:LEU:CD1	2.50	0.41
4:H:39:TYR:CE1	6:J:975:DA:OP2	2.73	0.41
5:I:37:DG:N1	6:J:1086:DC:N3	2.52	0.41
5:I:50:DA:H2''	5:I:51:DA:C8	2.56	0.41
5:I:377:DG:H2''	5:I:378:DA:H8	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:682:DG:H4'	1:o:83:ARG:NH2	2.36	0.41
5:I:809:DG:H1'	5:I:810:DA:C8	2.56	0.41
5:I:922:DT:H2''	5:I:923:DA:C8	2.55	0.41
5:I:1066:DC:O2	6:J:58:DG:N2	2.53	0.41
3:g:36:LYS:HE2	3:g:36:LYS:HB3	1.92	0.41
1:K:70:LEU:HD13	2:L:26:ILE:HA	2.01	0.41
3:m:32:ARG:NH2	4:n:32:GLU:OE1	2.42	0.41
3:W:95:LYS:HD2	4:X:100:PRO:HB3	2.01	0.41
1:A:73:GLU:OE1	2:B:25:ASN:ND2	2.37	0.41
3:G:17:ARG:HH21	3:G:28:GLY:HA2	1.85	0.41
5:I:384:DT:H1'	5:I:385:DA:C8	2.55	0.41
5:I:663:DC:H42	6:J:460:DG:H1	1.67	0.41
5:I:693:DC:H42	6:J:430:DG:H1	1.68	0.41
6:J:539:DA:H2''	6:J:540:DG:C8	2.56	0.41
6:J:552:DA:H2''	6:J:553:DT:C6	2.56	0.41
6:J:764:DA:C2	6:J:765:DT:C2	3.09	0.41
6:J:832:DC:H2''	6:J:833:DG:C8	2.55	0.41
6:J:871:DC:H5''	4:h:29:SER:HB3	2.03	0.41
4:n:58:ILE:HG23	2:p:98:TYR:HB3	2.02	0.41
3:q:92:GLU:OE1	4:r:103:LEU:N	2.53	0.41
3:w:68:ASN:OD1	3:w:71:ARG:NH2	2.54	0.41
1:A:112:ILE:HG23	3:G:114:VAL:HG21	2.03	0.41
1:A:119:ILE:HG12	2:B:43:VAL:HG11	2.03	0.41
3:C:92:GLU:HB3	4:D:100:PRO:HG2	2.03	0.41
3:G:90:ASP:HB3	3:G:93:LEU:HB2	2.03	0.41
5:I:2:DT:H2''	5:I:3:DC:C6	2.55	0.41
5:I:238:DA:P	3:c:32:ARG:HH11	2.44	0.41
5:I:275:DG:H2''	5:I:276:DT:C5	2.55	0.41
5:I:352:DC:H6	5:I:352:DC:H2'	1.58	0.41
5:I:753:DC:C2	5:I:754:DC:C4	3.09	0.41
5:I:840:DG:H5'	2:V:45:ARG:NH1	2.35	0.41
5:I:876:DC:H42	6:J:246:DA:N6	2.19	0.41
6:J:184:DT:H2''	6:J:185:DC:C5	2.55	0.41
3:c:20:ARG:HG3	4:d:121:ALA:HB3	2.03	0.41
3:c:111:ILE:HG12	1:e:51:ILE:CG2	2.46	0.41
5:I:290:DC:N4	6:J:833:DG:H1	2.12	0.41
6:J:155:DG:H2''	6:J:156:DG:OP2	2.21	0.41
6:J:275:DG:P	1:Y:42:ARG:HH21	2.44	0.41
6:J:998:DA:OP2	6:J:998:DA:H2'	2.20	0.41
3:M:109:PRO:HA	1:O:55:GLN:OE1	2.21	0.41
4:n:81:ASN:ND2	4:n:83:ARG:HD3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:36:LYS:HE2	3:W:36:LYS:HB3	1.95	0.41
4:3:43:LYS:HA	4:3:43:LYS:HD3	1.75	0.41
3:C:100:VAL:HG11	2:F:98:TYR:CE2	2.56	0.41
2:F:90:LEU:HB3	2:F:95:ARG:O	2.21	0.41
5:I:29:DA:N6	6:J:1094:DT:H3	2.19	0.41
5:I:166:DT:H2'	5:I:167:DG:H8	1.83	0.41
5:I:167:DG:C5	5:I:168:DT:C4	3.09	0.41
5:I:217:DT:H2''	5:I:218:DC:OP2	2.21	0.41
5:I:310:DG:H2''	5:I:311:DA:C8	2.55	0.41
5:I:335:DT:H2''	5:I:336:DG:C8	2.56	0.41
5:I:360:DG:O6	6:J:762:DA:N6	2.54	0.41
5:I:362:DA:C5	5:I:363:DT:C4	3.09	0.41
5:I:413:DC:H2''	5:I:414:DG:N7	2.36	0.41
5:I:556:DA:C2	6:J:568:DG:C2	3.08	0.41
5:I:574:DG:C2	6:J:550:DG:C2	3.09	0.41
5:I:643:DA:OP1	2:I:36:ARG:NH2	2.54	0.41
5:I:675:DC:O2	6:J:449:DG:N2	2.53	0.41
5:I:919:DA:H2''	5:I:920:DT:OP2	2.21	0.41
5:I:950:DG:H2''	5:I:951:DG:C8	2.56	0.41
5:I:1089:DA:H61	6:J:34:DT:H3	1.67	0.41
6:J:193:DT:H2''	6:J:194:DG:H8	1.85	0.41
6:J:318:DG:H2''	6:J:319:DA:C8	2.56	0.41
6:J:342:DG:H2''	6:J:343:DG:OP2	2.21	0.41
6:J:458:DC:H2''	6:J:459:DG:C8	2.56	0.41
6:J:464:DA:P	1:o:117:VAL:H	2.41	0.41
6:J:569:DT:H2''	6:J:570:DT:C6	2.56	0.41
6:J:639:DA:H2''	6:J:640:DA:H8	1.86	0.41
6:J:766:DG:C5	6:J:767:DC:C4	3.08	0.41
6:J:847:DA:H2''	6:J:848:DC:C6	2.56	0.41
6:J:911:DC:H5''	1:e:41:TYR:HD1	1.86	0.41
3:c:68:ASN:HA	3:c:71:ARG:NH2	2.36	0.41
3:c:114:VAL:HG21	1:e:112:ILE:HG12	2.03	0.41
1:K:113:HIS:CE1	1:O:123:ASP:HA	2.55	0.41
3:M:57:TYR:CZ	4:N:106:HIS:HB2	2.56	0.41
4:N:27:LYS:O	4:N:28:ARG:HG3	2.21	0.41
1:O:38:PRO:HB2	1:O:39:HIS:H	1.69	0.41
3:Q:50:TYR:HD2	4:R:115:VAL:HG21	1.86	0.41
3:Q:78:ILE:HG13	4:R:49:THR:HG21	2.02	0.41
2:I:97:LEU:HA	3:q:101:THR:O	2.21	0.41
2:V:98:TYR:CE2	3:0:100:VAL:HG11	2.56	0.41
2:B:93:GLN:HG2	2:B:93:GLN:H	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:602:DA:H4'	3:m:77:ARG:NE	2.36	0.41
5:I:763:DG:H2''	5:I:764:DG:C8	2.56	0.41
5:I:973:DC:H2''	5:I:974:DC:C5	2.56	0.41
6:J:529:DG:H2''	6:J:530:DG:OP2	2.21	0.41
6:J:730:DC:H2''	6:J:731:DG:H8	1.86	0.41
6:J:768:DA:H2''	6:J:769:DC:C5	2.56	0.41
1:K:63:ARG:HA	1:K:63:ARG:HD3	1.77	0.41
1:k:48:LEU:HD11	3:q:117:PRO:CD	2.50	0.41
2:l:31:LYS:HE3	2:l:35:ARG:NH2	2.30	0.41
4:X:62:PHE:HD1	2:Z:98:TYR:CE2	2.39	0.41
5:I:169:DG:C5	5:I:170:DC:C4	3.09	0.40
5:I:199:DC:H2''	5:I:200:DG:H8	1.85	0.40
5:I:928:DA:C4	5:I:929:DC:C4	3.09	0.40
5:I:957:DC:H2''	5:I:958:DT:H72	2.03	0.40
5:I:962:DG:H2''	5:I:963:DA:H5''	2.03	0.40
6:J:43:DT:H2''	6:J:44:DG:C8	2.57	0.40
2:f:38:ALA:HB1	2:f:43:VAL:HB	2.03	0.40
3:M:79:ILE:HG12	3:M:82:HIS:CE1	2.56	0.40
3:Q:26:PRO:HG3	4:R:37:TYR:CZ	2.56	0.40
1:o:79:LYS:HB3	1:o:82:LEU:HD11	2.02	0.40
1:U:119:ILE:HG12	2:V:43:VAL:HG11	2.03	0.40
3:W:117:PRO:HD3	1:Y:48:LEU:HD13	2.02	0.40
5:I:22:DC:H2''	5:I:23:DT:C6	2.56	0.40
5:I:412:DC:H2''	5:I:413:DC:C5	2.57	0.40
5:I:491:DC:H2''	5:I:492:DA:H8	1.86	0.40
5:I:554:DA:H1'	5:I:555:DC:C6	2.56	0.40
5:I:929:DC:H2''	5:I:930:DA:C8	2.55	0.40
5:I:977:DG:OP1	4:x:50:GLY:HA3	2.21	0.40
6:J:424:DA:H5''	3:q:16:THR:HA	2.03	0.40
6:J:652:DC:H2''	6:J:653:DA:C8	2.56	0.40
6:J:996:DT:H2''	6:J:997:DA:OP2	2.21	0.40
6:J:1090:DG:H2''	6:J:1091:DG:OP2	2.21	0.40
3:M:92:GLU:HB3	4:N:100:PRO:HG2	2.04	0.40
3:m:20:ARG:HE	3:m:20:ARG:HB2	1.60	0.40
3:m:100:VAL:HA	2:p:96:THR:HB	2.04	0.40
3:w:31:HIS:ND1	3:w:48:PRO:HG3	2.36	0.40
3:w:81:ARG:NH2	3:w:107:VAL:O	2.49	0.40
3:2:63:LEU:HD13	4:3:42:LEU:HB2	2.03	0.40
5:I:181:DC:H2''	5:I:182:DA:H8	1.86	0.40
5:I:555:DC:H1'	5:I:556:DA:H5'	2.04	0.40
5:I:588:DG:H2''	5:I:589:DA:H5''	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:913:DC:H5''	1:U:41:TYR:CD1	2.56	0.40
6:J:478:DC:H2''	6:J:479:DG:C8	2.57	0.40
6:J:581:DA:H2''	6:J:582:DC:C5	2.56	0.40
6:J:724:DC:OP1	1:O:42:ARG:N	2.52	0.40
1:e:61:LEU:HD13	2:f:36:ARG:HB3	2.03	0.40
3:M:39:TYR:HB3	4:N:75:SER:HB2	2.04	0.40
1:U:72:ARG:O	1:U:76:GLN:HB2	2.21	0.40
1:Y:47:ALA:O	1:Y:51:ILE:HG13	2.21	0.40
1:u:55:GLN:CD	3:2:110:ASN:H	2.26	0.40
3:w:90:ASP:HB3	3:w:93:LEU:HB2	2.03	0.40
2:F:71:THR:HG22	4:H:93:THR:HG23	2.02	0.40
3:G:97:LEU:HB3	3:G:100:VAL:HB	2.04	0.40
5:I:174:DT:C2	5:I:175:DA:C5	3.09	0.40
5:I:331:DC:OP2	4:h:36:ILE:HG13	2.21	0.40
6:J:104:DC:H2''	6:J:105:DG:C8	2.57	0.40
6:J:474:DC:H5''	2:l:45:ARG:HG2	2.04	0.40
6:J:557:DG:H2''	6:J:558:DT:C6	2.56	0.40
6:J:704:DG:H1'	6:J:705:DG:H5'	2.02	0.40
1:e:108:ASN:HD22	1:e:108:ASN:HA	1.70	0.40
2:f:92:ARG:NH1	2:f:92:ARG:HB3	2.36	0.40
3:W:57:TYR:HB2	4:X:110:GLU:HG3	2.04	0.40
5:I:57:DC:H6	5:I:57:DC:H2'	1.78	0.40
5:I:114:DC:H2''	5:I:115:DG:H8	1.86	0.40
5:I:178:DG:N2	6:J:946:DA:C2	2.90	0.40
5:I:225:DC:H2''	5:I:226:DC:C5	2.56	0.40
5:I:666:DC:H2''	5:I:667:DG:C8	2.56	0.40
5:I:926:DG:N2	6:J:198:DA:C2	2.90	0.40
5:I:1055:DG:H1	6:J:68:DC:H42	1.69	0.40
6:J:265:DA:H2''	6:J:266:DA:H8	1.86	0.40
6:J:440:DC:H4'	6:J:441:DC:H5'	2.04	0.40
6:J:709:DC:H2''	6:J:710:DG:C8	2.56	0.40
6:J:947:DA:C5	6:J:948:DT:C4	3.10	0.40
6:J:1013:DA:H2''	6:J:1014:DA:C8	2.56	0.40
1:K:113:HIS:CE1	1:O:122:LYS:HG3	2.57	0.40
3:M:34:LEU:HB3	3:M:43:VAL:HG21	2.04	0.40
3:Q:92:GLU:OE1	4:R:102:GLU:HB3	2.22	0.40
3:m:31:HIS:HD1	3:m:48:PRO:HG3	1.87	0.40
3:m:81:ARG:NH1	1:o:56:LYS:O	2.55	0.40
3:q:76:THR:O	4:r:49:THR:HA	2.21	0.40
3:w:39:TYR:HB3	4:x:86:ILE:CD1	2.51	0.40
3:w:109:PRO:HA	1:y:55:GLN:OE1	2.20	0.40

All (19) 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)
2:B:23:ARG:CG	2:b:23:ARG:CG[3_455]	0.58	1.62
2:B:23:ARG:CD	2:b:23:ARG:CG[3_455]	1.01	1.19
2:B:23:ARG:CG	2:b:23:ARG:CD[3_455]	1.01	1.19
2:B:23:ARG:CB	2:b:23:ARG:CD[3_455]	1.52	0.68
2:B:23:ARG:CD	2:b:23:ARG:CB[3_455]	1.53	0.67
2:B:23:ARG:CG	2:b:23:ARG:CB[3_455]	1.75	0.45
2:B:23:ARG:CB	2:b:23:ARG:CG[3_455]	1.76	0.44
2:Z:23:ARG:NH1	4:3:106:HIS:CG[2_655]	1.77	0.43
2:Z:23:ARG:NH1	4:3:106:HIS:CB[2_655]	1.85	0.35
2:B:23:ARG:NE	2:b:23:ARG:CG[3_455]	2.02	0.18
2:Z:23:ARG:NH1	4:3:106:HIS:CD2[2_655]	2.02	0.18
2:B:23:ARG:CG	2:b:23:ARG:NE[3_455]	2.03	0.17
2:Z:23:ARG:NH1	3:2:57:TYR:OH[2_655]	2.06	0.14
2:B:23:ARG:NH1	2:b:23:ARG:O[3_455]	2.09	0.11
2:B:23:ARG:O	2:b:23:ARG:NH1[3_455]	2.09	0.11
2:B:23:ARG:CA	2:b:23:ARG:CD[3_455]	2.10	0.10
2:B:23:ARG:CD	2:b:23:ARG:CA[3_455]	2.11	0.09
2:B:23:ARG:C	2:b:23:ARG:CD[3_455]	2.14	0.06
2:B:23:ARG:CD	2:b:23:ARG:C[3_455]	2.14	0.06

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	
1	A	95/139 (68%)	93 (98%)	2 (2%)	0	100	100
1	E	96/139 (69%)	93 (97%)	3 (3%)	0	100	100
1	K	95/139 (68%)	91 (96%)	4 (4%)	0	100	100
1	O	96/139 (69%)	93 (97%)	3 (3%)	0	100	100
1	U	95/139 (68%)	93 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	96/139 (69%)	93 (97%)	3 (3%)	0	100	100
1	a	96/139 (69%)	93 (97%)	3 (3%)	0	100	100
1	e	95/139 (68%)	93 (98%)	2 (2%)	0	100	100
1	k	96/139 (69%)	93 (97%)	3 (3%)	0	100	100
1	o	95/139 (68%)	94 (99%)	1 (1%)	0	100	100
1	u	96/139 (69%)	93 (97%)	3 (3%)	0	100	100
1	y	87/139 (63%)	85 (98%)	2 (2%)	0	100	100
2	B	80/106 (76%)	79 (99%)	1 (1%)	0	100	100
2	F	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	L	80/106 (76%)	79 (99%)	1 (1%)	0	100	100
2	P	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	V	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	Z	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	b	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	f	80/106 (76%)	79 (99%)	1 (1%)	0	100	100
2	l	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	p	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	v	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	z	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
3	0	103/133 (77%)	101 (98%)	2 (2%)	0	100	100
3	2	101/133 (76%)	99 (98%)	2 (2%)	0	100	100
3	C	101/133 (76%)	99 (98%)	2 (2%)	0	100	100
3	G	103/133 (77%)	101 (98%)	2 (2%)	0	100	100
3	M	101/133 (76%)	99 (98%)	2 (2%)	0	100	100
3	Q	103/133 (77%)	102 (99%)	1 (1%)	0	100	100
3	W	101/133 (76%)	100 (99%)	1 (1%)	0	100	100
3	c	103/133 (77%)	102 (99%)	1 (1%)	0	100	100
3	g	101/133 (76%)	99 (98%)	2 (2%)	0	100	100
3	m	103/133 (77%)	101 (98%)	2 (2%)	0	100	100
3	q	101/133 (76%)	100 (99%)	1 (1%)	0	100	100
3	w	103/133 (77%)	101 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	1	93/129 (72%)	91 (98%)	1 (1%)	1 (1%)	11	46
4	3	94/129 (73%)	91 (97%)	2 (2%)	1 (1%)	11	46
4	D	94/129 (73%)	89 (95%)	4 (4%)	1 (1%)	11	46
4	H	93/129 (72%)	91 (98%)	1 (1%)	1 (1%)	11	46
4	N	94/129 (73%)	91 (97%)	2 (2%)	1 (1%)	11	46
4	R	93/129 (72%)	92 (99%)	0	1 (1%)	11	46
4	X	94/129 (73%)	91 (97%)	2 (2%)	1 (1%)	11	46
4	d	93/129 (72%)	91 (98%)	1 (1%)	1 (1%)	11	46
4	h	94/129 (73%)	91 (97%)	2 (2%)	1 (1%)	11	46
4	n	93/129 (72%)	91 (98%)	1 (1%)	1 (1%)	11	46
4	r	94/129 (73%)	91 (97%)	2 (2%)	1 (1%)	11	46
4	x	93/129 (72%)	92 (99%)	0	1 (1%)	11	46
All	All	4444/6084 (73%)	4342 (98%)	90 (2%)	12 (0%)	36	72

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	101	GLY
4	H	101	GLY
4	d	101	GLY
4	h	101	GLY
4	N	101	GLY
4	R	101	GLY
4	n	101	GLY
4	r	101	GLY
4	X	101	GLY
4	1	101	GLY
4	x	101	GLY
4	3	101	GLY

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	
1	A	85/113 (75%)	85 (100%)	0	100	100
1	E	85/113 (75%)	85 (100%)	0	100	100
1	K	85/113 (75%)	85 (100%)	0	100	100
1	O	85/113 (75%)	85 (100%)	0	100	100
1	U	85/113 (75%)	85 (100%)	0	100	100
1	Y	85/113 (75%)	85 (100%)	0	100	100
1	a	85/113 (75%)	85 (100%)	0	100	100
1	e	85/113 (75%)	85 (100%)	0	100	100
1	k	85/113 (75%)	85 (100%)	0	100	100
1	o	85/113 (75%)	85 (100%)	0	100	100
1	u	85/113 (75%)	85 (100%)	0	100	100
1	y	85/113 (75%)	85 (100%)	0	100	100
2	B	67/81 (83%)	67 (100%)	0	100	100
2	F	67/81 (83%)	67 (100%)	0	100	100
2	L	67/81 (83%)	67 (100%)	0	100	100
2	P	67/81 (83%)	67 (100%)	0	100	100
2	V	67/81 (83%)	67 (100%)	0	100	100
2	Z	67/81 (83%)	67 (100%)	0	100	100
2	b	67/81 (83%)	67 (100%)	0	100	100
2	f	67/81 (83%)	67 (100%)	0	100	100
2	l	67/81 (83%)	67 (100%)	0	100	100
2	p	67/81 (83%)	67 (100%)	0	100	100
2	v	67/81 (83%)	67 (100%)	0	100	100
2	z	67/81 (83%)	67 (100%)	0	100	100
3	0	83/102 (81%)	81 (98%)	2 (2%)	43	64
3	2	82/102 (80%)	80 (98%)	2 (2%)	43	64
3	C	82/102 (80%)	80 (98%)	2 (2%)	43	64
3	G	83/102 (81%)	81 (98%)	2 (2%)	43	64
3	M	82/102 (80%)	80 (98%)	2 (2%)	43	64
3	Q	83/102 (81%)	81 (98%)	2 (2%)	43	64
3	W	82/102 (80%)	80 (98%)	2 (2%)	43	64
3	c	83/102 (81%)	81 (98%)	2 (2%)	43	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	g	82/102 (80%)	80 (98%)	2 (2%)	43	64
3	m	83/102 (81%)	81 (98%)	2 (2%)	43	64
3	q	82/102 (80%)	80 (98%)	2 (2%)	43	64
3	w	83/102 (81%)	81 (98%)	2 (2%)	43	64
4	1	81/107 (76%)	80 (99%)	1 (1%)	63	75
4	3	82/107 (77%)	81 (99%)	1 (1%)	63	75
4	D	82/107 (77%)	82 (100%)	0	100	100
4	H	81/107 (76%)	79 (98%)	2 (2%)	42	63
4	N	82/107 (77%)	82 (100%)	0	100	100
4	R	81/107 (76%)	79 (98%)	2 (2%)	42	63
4	X	82/107 (77%)	81 (99%)	1 (1%)	63	75
4	d	81/107 (76%)	79 (98%)	2 (2%)	42	63
4	h	82/107 (77%)	81 (99%)	1 (1%)	63	75
4	n	81/107 (76%)	79 (98%)	2 (2%)	42	63
4	r	82/107 (77%)	81 (99%)	1 (1%)	63	75
4	x	81/107 (76%)	79 (98%)	2 (2%)	42	63
All	All	3792/4836 (78%)	3753 (99%)	39 (1%)	68	78

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	62	ILE
3	C	81	ARG
3	G	62	ILE
3	G	81	ARG
4	H	85	THR
4	H	103	LEU
3	c	62	ILE
3	c	81	ARG
4	d	85	THR
4	d	103	LEU
3	g	62	ILE
3	g	81	ARG
4	h	85	THR
3	M	62	ILE
3	M	81	ARG

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Mol	Chain	Res	Type
3	Q	62	ILE
3	Q	81	ARG
4	R	85	THR
4	R	103	LEU
3	m	62	ILE
3	m	81	ARG
4	n	85	THR
4	n	103	LEU
3	q	62	ILE
3	q	81	ARG
4	r	85	THR
3	W	62	ILE
3	W	81	ARG
4	X	85	THR
3	0	62	ILE
3	0	81	ARG
4	1	103	LEU
3	w	62	ILE
3	w	81	ARG
4	x	85	THR
4	x	103	LEU
3	2	62	ILE
3	2	81	ARG
4	3	85	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
4	D	81	ASN
4	D	92	GLN
1	E	39	HIS
4	H	92	GLN
4	d	46	HIS
3	g	38	ASN
2	L	25	ASN
3	M	38	ASN
3	M	104	GLN
3	Q	38	ASN
3	Q	94	ASN
4	R	46	HIS
4	R	64	ASN

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Mol	Chain	Res	Type
4	R	92	GLN
1	k	39	HIS
2	l	25	ASN
3	m	94	ASN
4	n	81	ASN
1	o	108	ASN
2	p	25	ASN
2	p	75	HIS
4	r	44	GLN
4	r	81	ASN
2	V	25	ASN
3	W	38	ASN
2	Z	25	ASN
1	u	108	ASN
3	w	104	GLN
3	2	31	HIS
3	2	112	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	97/139 (69%)	-0.79	0 100 100	321, 473, 538, 576	0
1	E	98/139 (70%)	-0.62	1 (1%) 79 68	379, 442, 554, 584	0
1	K	97/139 (69%)	-0.63	0 100 100	363, 424, 476, 499	0
1	O	98/139 (70%)	-0.52	0 100 100	403, 468, 528, 545	0
1	U	97/139 (69%)	-0.70	1 (1%) 79 68	382, 448, 493, 535	0
1	Y	98/139 (70%)	-0.57	0 100 100	400, 463, 530, 547	0
1	a	98/139 (70%)	-0.76	0 100 100	362, 467, 535, 568	0
1	e	97/139 (69%)	-0.76	0 100 100	404, 464, 549, 627	0
1	k	98/139 (70%)	-0.68	0 100 100	331, 420, 462, 473	0
1	o	97/139 (69%)	-0.84	0 100 100	336, 416, 471, 508	0
1	u	98/139 (70%)	-0.58	0 100 100	358, 445, 515, 546	0
1	y	97/139 (69%)	-0.67	2 (2%) 63 54	424, 502, 578, 608	0
2	B	82/106 (77%)	-0.69	0 100 100	392, 470, 528, 565	0
2	F	82/106 (77%)	-0.85	0 100 100	366, 429, 480, 492	0
2	L	82/106 (77%)	-0.58	2 (2%) 59 52	379, 427, 464, 472	0
2	P	82/106 (77%)	-0.53	2 (2%) 59 52	390, 469, 529, 597	0
2	V	82/106 (77%)	-0.50	0 100 100	349, 414, 457, 490	0
2	Z	82/106 (77%)	-0.56	0 100 100	353, 454, 504, 522	0
2	b	82/106 (77%)	-0.81	1 (1%) 76 65	385, 460, 501, 582	0
2	f	82/106 (77%)	-0.28	2 (2%) 59 52	369, 474, 538, 568	0
2	l	82/106 (77%)	-0.73	0 100 100	365, 408, 453, 463	0
2	p	82/106 (77%)	-0.82	0 100 100	323, 411, 488, 502	0
2	v	82/106 (77%)	-0.63	0 100 100	375, 440, 490, 512	0
2	z	82/106 (77%)	-0.78	0 100 100	415, 487, 533, 550	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	0	105/133 (78%)	-0.47	0 100 100	415, 471, 522, 539	0
3	2	103/133 (77%)	-0.54	0 100 100	386, 439, 519, 589	0
3	C	103/133 (77%)	-0.54	0 100 100	366, 456, 499, 562	0
3	G	105/133 (78%)	-0.71	0 100 100	284, 478, 544, 590	0
3	M	103/133 (77%)	-0.33	2 (1%) 66 56	355, 450, 510, 524	0
3	Q	105/133 (78%)	-0.41	1 (0%) 79 68	357, 430, 493, 512	0
3	W	103/133 (77%)	-0.12	3 (2%) 53 47	360, 451, 538, 596	0
3	c	105/133 (78%)	-0.16	1 (0%) 79 68	407, 479, 585, 614	0
3	g	103/133 (77%)	-0.71	0 100 100	328, 472, 527, 546	0
3	m	105/133 (78%)	-0.42	1 (0%) 79 68	339, 467, 515, 551	0
3	q	103/133 (77%)	-0.31	2 (1%) 66 56	343, 421, 472, 500	0
3	w	105/133 (78%)	-0.71	0 100 100	439, 512, 584, 603	0
4	1	95/129 (73%)	-0.15	3 (3%) 50 45	409, 471, 529, 551	0
4	3	96/129 (74%)	-0.34	0 100 100	371, 443, 518, 590	0
4	D	96/129 (74%)	-0.60	1 (1%) 79 68	366, 440, 512, 547	0
4	H	95/129 (73%)	-0.55	1 (1%) 78 67	405, 463, 569, 620	0
4	N	96/129 (74%)	-0.20	3 (3%) 51 46	365, 453, 518, 551	0
4	R	95/129 (73%)	-0.46	0 100 100	361, 433, 484, 539	0
4	X	96/129 (74%)	-0.10	3 (3%) 51 46	364, 430, 501, 538	0
4	d	95/129 (73%)	-0.09	1 (1%) 78 67	415, 475, 540, 557	0
4	h	96/129 (74%)	-0.55	0 100 100	397, 491, 554, 609	0
4	n	95/129 (73%)	-0.09	6 (6%) 26 31	410, 460, 514, 555	0
4	r	96/129 (74%)	-0.25	2 (2%) 63 54	349, 433, 493, 551	0
4	x	95/129 (73%)	-0.50	0 100 100	414, 523, 592, 636	0
5	I	1122/1122 (100%)	-0.42	2 (0%) 91 84	378, 585, 848, 1000	0
6	J	1122/1122 (100%)	-0.45	0 100 100	441, 585, 866, 1000	0
All	All	6792/8328 (81%)	-0.49	43 (0%) 85 76	284, 481, 718, 1000	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	n	70	ILE	5.7
4	N	59	MET	4.7

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Mol	Chain	Res	Type	RSRZ
4	X	59	MET	3.7
4	D	59	MET	3.6
4	X	38	VAL	3.3
4	N	62	PHE	3.2
3	q	55	LEU	3.2
3	W	59	THR	3.1
2	L	58	LEU	3.0
2	P	54	THR	2.9
4	r	66	ILE	2.8
3	q	51	LEU	2.8
1	y	96	CYS	2.8
4	X	91	ILE	2.6
4	H	81	ASN	2.6
4	n	66	ILE	2.6
3	W	51	LEU	2.6
4	n	71	ALA	2.5
3	W	58	LEU	2.5
4	n	94	ALA	2.5
1	E	77	ASP	2.5
4	d	59	MET	2.4
3	M	34	LEU	2.4
3	M	30	VAL	2.3
2	f	94	GLY	2.3
2	L	54	THR	2.2
4	l	53	SER	2.2
4	n	106	HIS	2.2
4	l	82	LYS	2.2
4	r	62	PHE	2.2
3	c	22	GLY	2.2
3	Q	55	LEU	2.2
1	U	77	ASP	2.2
4	l	31	LYS	2.2
2	P	34	ILE	2.1
3	m	51	LEU	2.1
4	N	66	ILE	2.1
2	f	102	GLY	2.1
1	y	92	LEU	2.1
2	b	58	LEU	2.1
4	n	74	ALA	2.1
5	I	752	DA	2.0
5	I	1005	DA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.