



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:00 am BST

PDB ID : 3VD2  
Title : structure of p73 DNA binding domain tetramer modulates p73 transactivation  
Authors : Ethayathulla, A.S.; Tse, P.W.; Nguyen, S.; Viadiu, H.  
Deposited on : 2012-01-04  
Resolution : 4.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

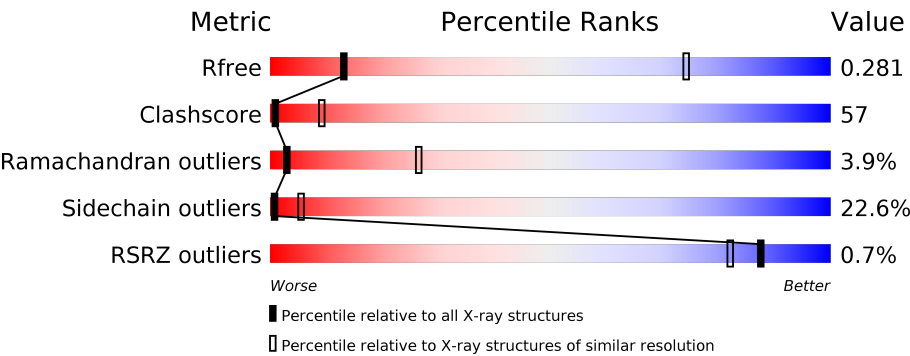
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	210	<div><div></div><div>29%51%15% . .</div></div>
1	B	210	<div><div></div><div>21%56%18% . 5%</div></div>
1	C	210	<div><div></div><div>32%50%13% .</div></div>
1	D	210	<div><div>%</div><div>31%50%14% 5%</div></div>
1	I	210	<div><div>%</div><div>20%56%19% . .</div></div>
1	J	210	<div><div></div><div>29%47%20% . .</div></div>

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Mol	Chain	Length	Quality of chain
2	E	14	<div><div></div><div>14%29%71%</div></div>
2	F	14	<div><div></div><div>14%79%7%</div></div>
2	G	14	<div><div></div><div>7%86%7%</div></div>
2	H	14	<div><div></div><div>21%79%</div></div>
2	K	14	<div><div></div><div>7%64%21%7%</div></div>
2	L	14	<div><div></div><div>7%21%50%21%7%</div></div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11152 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 Tumor protein p73.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1590	994	289	296	11			
1	B	200	Total	C	N	O	S	0	0	0
			1569	981	283	294	11			
1	C	203	Total	C	N	O	S	0	0	0
			1596	997	291	297	11			
1	D	199	Total	C	N	O	S	0	0	0
			1563	981	282	289	11			
1	I	202	Total	C	N	O	S	0	0	0
			1576	985	284	296	11			
1	J	202	Total	C	N	O	S	0	0	0
			1586	993	284	298	11			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	MET	-	INITIATING METHIONINE	UNP O15350
A	104	GLY	-	EXPRESSION TAG	UNP O15350
A	105	HIS	-	EXPRESSION TAG	UNP O15350
A	106	HIS	-	EXPRESSION TAG	UNP O15350
A	107	HIS	-	EXPRESSION TAG	UNP O15350
A	108	HIS	-	EXPRESSION TAG	UNP O15350
A	109	HIS	-	EXPRESSION TAG	UNP O15350
A	110	HIS	-	EXPRESSION TAG	UNP O15350
A	111	HIS	-	EXPRESSION TAG	UNP O15350
A	112	HIS	-	EXPRESSION TAG	UNP O15350
A	113	GLU	-	EXPRESSION TAG	UNP O15350
A	114	PHE	-	EXPRESSION TAG	UNP O15350
B	103	MET	-	INITIATING METHIONINE	UNP O15350
B	104	GLY	-	EXPRESSION TAG	UNP O15350
B	105	HIS	-	EXPRESSION TAG	UNP O15350
B	106	HIS	-	EXPRESSION TAG	UNP O15350
B	107	HIS	-	EXPRESSION TAG	UNP O15350

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Chain	Residue	Modelled	Actual	Comment	Reference
B	108	HIS	-	EXPRESSION TAG	UNP 015350
B	109	HIS	-	EXPRESSION TAG	UNP 015350
B	110	HIS	-	EXPRESSION TAG	UNP 015350
B	111	HIS	-	EXPRESSION TAG	UNP 015350
B	112	HIS	-	EXPRESSION TAG	UNP 015350
B	113	GLU	-	EXPRESSION TAG	UNP 015350
B	114	PHE	-	EXPRESSION TAG	UNP 015350
C	103	MET	-	INITIATING METHIONINE	UNP 015350
C	104	GLY	-	EXPRESSION TAG	UNP 015350
C	105	HIS	-	EXPRESSION TAG	UNP 015350
C	106	HIS	-	EXPRESSION TAG	UNP 015350
C	107	HIS	-	EXPRESSION TAG	UNP 015350
C	108	HIS	-	EXPRESSION TAG	UNP 015350
C	109	HIS	-	EXPRESSION TAG	UNP 015350
C	110	HIS	-	EXPRESSION TAG	UNP 015350
C	111	HIS	-	EXPRESSION TAG	UNP 015350
C	112	HIS	-	EXPRESSION TAG	UNP 015350
C	113	GLU	-	EXPRESSION TAG	UNP 015350
C	114	PHE	-	EXPRESSION TAG	UNP 015350
D	103	MET	-	INITIATING METHIONINE	UNP 015350
D	104	GLY	-	EXPRESSION TAG	UNP 015350
D	105	HIS	-	EXPRESSION TAG	UNP 015350
D	106	HIS	-	EXPRESSION TAG	UNP 015350
D	107	HIS	-	EXPRESSION TAG	UNP 015350
D	108	HIS	-	EXPRESSION TAG	UNP 015350
D	109	HIS	-	EXPRESSION TAG	UNP 015350
D	110	HIS	-	EXPRESSION TAG	UNP 015350
D	111	HIS	-	EXPRESSION TAG	UNP 015350
D	112	HIS	-	EXPRESSION TAG	UNP 015350
D	113	GLU	-	EXPRESSION TAG	UNP 015350
D	114	PHE	-	EXPRESSION TAG	UNP 015350
I	103	MET	-	INITIATING METHIONINE	UNP 015350
I	104	GLY	-	EXPRESSION TAG	UNP 015350
I	105	HIS	-	EXPRESSION TAG	UNP 015350
I	106	HIS	-	EXPRESSION TAG	UNP 015350
I	107	HIS	-	EXPRESSION TAG	UNP 015350
I	108	HIS	-	EXPRESSION TAG	UNP 015350
I	109	HIS	-	EXPRESSION TAG	UNP 015350
I	110	HIS	-	EXPRESSION TAG	UNP 015350
I	111	HIS	-	EXPRESSION TAG	UNP 015350
I	112	HIS	-	EXPRESSION TAG	UNP 015350
I	113	GLU	-	EXPRESSION TAG	UNP 015350

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Chain	Residue	Modelled	Actual	Comment	Reference
I	114	PHE	-	EXPRESSION TAG	UNP O15350
J	103	MET	-	INITIATING METHIONINE	UNP O15350
J	104	GLY	-	EXPRESSION TAG	UNP O15350
J	105	HIS	-	EXPRESSION TAG	UNP O15350
J	106	HIS	-	EXPRESSION TAG	UNP O15350
J	107	HIS	-	EXPRESSION TAG	UNP O15350
J	108	HIS	-	EXPRESSION TAG	UNP O15350
J	109	HIS	-	EXPRESSION TAG	UNP O15350
J	110	HIS	-	EXPRESSION TAG	UNP O15350
J	111	HIS	-	EXPRESSION TAG	UNP O15350
J	112	HIS	-	EXPRESSION TAG	UNP O15350
J	113	GLU	-	EXPRESSION TAG	UNP O15350
J	114	PHE	-	EXPRESSION TAG	UNP O15350

- Molecule 2 is a DNA chain called DNA (5'-D(\*AP\*TP\*GP\*GP\*AP\*CP\*AP\*TP\*GP\*TP\*CP\*CP\*AP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	P	0	0	0
			284	137	52	82	13			
2	F	14	Total	C	N	O	P	0	0	0
			284	137	52	82	13			
2	G	14	Total	C	N	O	P	0	0	0
			284	137	52	82	13			
2	H	14	Total	C	N	O	P	0	0	0
			284	137	52	82	13			
2	L	13	Total	C	N	O	P	0	0	0
			266	127	47	79	13			
2	K	13	Total	C	N	O	P	0	0	0
			264	127	50	75	12			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		

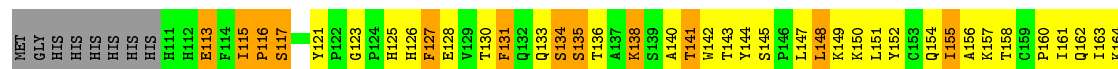
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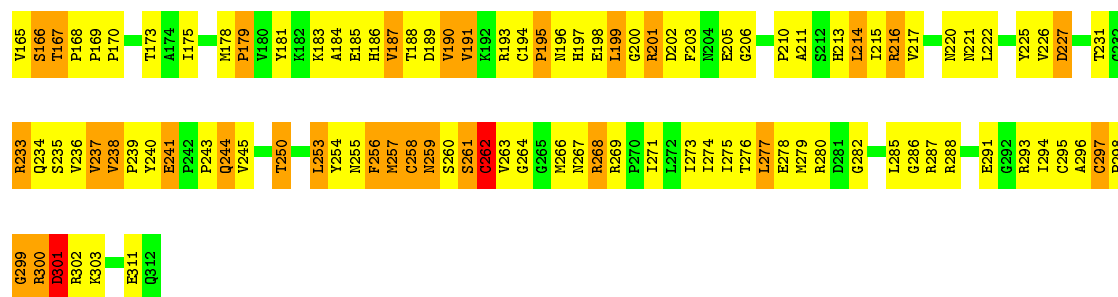
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Zn 1	0	0
3	A	1	Total 1	Zn 1	0	0

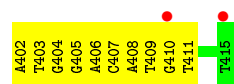








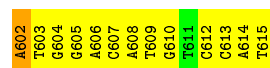
- Molecule 2: DNA (5'-D(\*AP\*TP\*GP\*GP\*AP\*CP\*AP\*TP\*GP\*TP\*CP\*CP\*AP\*T)-3')



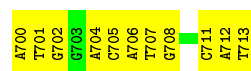
- Molecule 2: DNA (5'-D(\*AP\*TP\*GP\*GP\*AP\*CP\*AP\*TP\*GP\*TP\*CP\*CP\*AP\*T)-3')



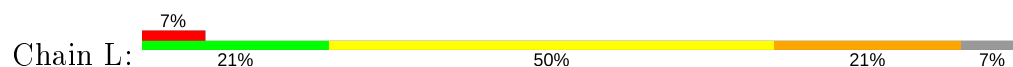
- Molecule 2: DNA (5'-D(\*AP\*TP\*GP\*GP\*AP\*CP\*AP\*TP\*GP\*TP\*CP\*CP\*AP\*T)-3')



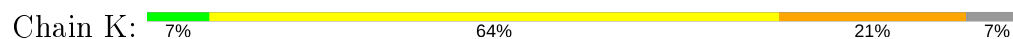
- Molecule 2: DNA (5'-D(\*AP\*TP\*GP\*GP\*AP\*CP\*AP\*TP\*GP\*TP\*CP\*CP\*AP\*T)-3')



- Molecule 2: DNA (5'-D(\*AP\*TP\*GP\*GP\*AP\*CP\*AP\*TP\*GP\*TP\*CP\*CP\*AP\*T)-3')



- Molecule 2: DNA (5'-D(\*AP\*TP\*GP\*GP\*AP\*CP\*AP\*TP\*GP\*TP\*CP\*CP\*AP\*T)-3')



A902	T903	G904	G905	A906	C907	A908	T909	G910	T911	C912	C913	A914	DT
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.40Å 91.13Å 137.47Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	45.69 – 4.00 45.69 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (45.69-4.00) 98.1 (45.69-4.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.59 (at 4.00Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.248 , 0.284 0.246 , 0.281	Depositor DCC
$R_{free}$ test set	350 reflections (2.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	91.2	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , -0.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.018 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.429 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.429 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.020 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	11152	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.53	0/1631	0.87	3/2218 (0.1%)
1	B	0.46	0/1609	0.93	2/2187 (0.1%)
1	C	0.49	0/1638	0.83	2/2226 (0.1%)
1	D	0.49	0/1604	0.81	0/2181
1	I	0.51	0/1615	0.86	5/2195 (0.2%)
1	J	0.49	0/1626	0.83	2/2209 (0.1%)
2	E	0.59	0/318	0.92	0/489
2	F	0.71	0/318	0.98	1/489 (0.2%)
2	G	0.71	0/318	1.01	2/489 (0.4%)
2	H	0.63	0/318	0.96	0/489
2	K	1.03	1/296 (0.3%)	1.29	2/455 (0.4%)
2	L	1.10	0/297	1.40	7/456 (1.5%)
All	All	0.56	1/11588 (0.0%)	0.91	26/16083 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1
2	K	0	1
2	L	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	905	DG	C2'-C1'	-5.78	1.46	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	PRO	C-N-CD	-12.21	93.73	120.60
1	J	115	ILE	C-N-CD	-10.49	97.52	120.60
2	L	810	DC	O5'-P-OP2	8.05	120.36	110.70
2	L	810	DC	OP2-P-O3'	7.14	120.90	105.20
2	G	602	DA	O3'-P-O5'	-6.97	90.77	104.00
2	L	806	DA	O5'-P-OP1	-6.97	99.43	105.70
2	L	810	DC	OP1-P-O3'	-5.99	92.02	105.20
1	A	112	HIS	N-CA-C	5.78	126.60	111.00
2	L	806	DA	C5'-C4'-O4'	5.68	120.09	109.30
1	I	245	VAL	N-CA-C	-5.62	95.83	111.00
1	A	219	GLY	N-CA-C	5.47	126.77	113.10
1	I	139	SER	N-CA-C	5.43	125.67	111.00
2	L	806	DA	C3'-C2'-C1'	-5.41	96.01	102.50
1	J	250	THR	N-CA-C	-5.41	96.41	111.00
2	K	906	DA	C3'-C2'-C1'	-5.35	96.08	102.50
1	I	219	GLY	N-CA-C	5.32	126.40	113.10
2	L	801	DT	OP1-P-OP2	-5.30	111.65	119.60
2	K	905	DG	O4'-C4'-C3'	-5.29	102.39	104.50
2	G	602	DA	O4'-C1'-N9	-5.19	104.37	108.00
1	I	202	ASP	N-CA-C	5.18	124.99	111.00
1	A	190	VAL	N-CA-C	5.17	124.96	111.00
2	F	503	DG	OP1-P-O3'	5.12	116.47	105.20
1	B	244	GLN	N-CA-C	-5.09	97.25	111.00
1	C	115	ILE	N-CA-C	-5.08	97.29	111.00
1	C	132	GLN	N-CA-C	-5.06	97.33	111.00
1	I	140	ALA	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	506	DA	Sidechain
2	K	904	DG	Sidechain
2	L	809	DT	Sidechain

## 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	1590	0	1549	192	0
1	B	1569	0	1535	233	0
1	C	1596	0	1554	152	0
1	D	1563	0	1533	194	0
1	I	1576	0	1537	202	0
1	J	1586	0	1548	175	0
2	E	284	0	160	12	0
2	F	284	0	160	18	0
2	G	284	0	160	19	0
2	H	284	0	160	16	0
2	K	264	0	148	14	0
2	L	266	0	148	16	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
All	All	11152	0	10192	1211	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 57.

All (1211) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ARG:HG3	1:B:237:VAL:HG22	1.32	1.10
1:B:163:ILE:O	1:B:249:PHE:HB2	1.56	1.06
1:I:243:PRO:HB2	1:I:246:GLY:HA2	1.36	1.04
1:I:215:ILE:HD13	1:I:215:ILE:H	1.17	1.03
1:J:214:LEU:HD23	1:J:215:ILE:HG13	1.39	1.03
1:B:310:ARG:HD3	1:B:311:GLU:H	1.21	1.02
1:J:145:SER:OG	1:J:302:ARG:HD3	1.59	1.02
1:A:193:ARG:HE	1:A:257:MET:CB	1.74	1.00
1:A:193:ARG:HE	1:A:257:MET:HB3	1.27	0.99
1:C:145:SER:HA	1:C:302:ARG:NH1	1.77	0.98
1:A:169:PRO:HB2	1:A:173:THR:HG21	1.44	0.98
1:I:220:ASN:ND2	1:I:222:LEU:H	1.60	0.98
1:J:141:THR:HA	1:J:154:GLN:HE21	1.26	0.98
1:A:279:MET:HG2	1:A:285:LEU:HD21	1.41	0.97
1:D:175:ILE:HG22	1:D:277:LEU:HA	1.46	0.96
1:A:259:ASN:HA	1:A:294:ILE:HB	1.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:GLU:CD	1:C:248:GLU:H	1.67	0.95
1:J:181:TYR:HA	1:J:271:ILE:HG22	1.48	0.94
1:C:306:GLU:O	1:C:310:ARG:HB2	1.68	0.93
1:I:152:TYR:HB3	1:I:298:PRO:HB3	1.47	0.93
1:B:179:PRO:O	1:B:191:VAL:HG21	1.69	0.92
1:I:201:ARG:HD3	1:I:201:ARG:H	1.35	0.92
1:I:218:GLU:HB2	1:I:255:ASN:ND2	1.84	0.92
1:I:243:PRO:HB2	1:I:246:GLY:CA	1.98	0.92
2:L:807:DT:H2''	2:L:808:DG:H5'	1.52	0.92
1:J:138:LYS:HA	1:J:299:GLY:HA3	1.50	0.91
1:I:220:ASN:HD22	1:I:222:LEU:H	1.10	0.91
1:A:307:ASP:HA	1:A:310:ARG:HG3	1.52	0.91
1:J:194:CYS:SG	1:J:262:CYS:HB3	2.11	0.91
1:I:278:GLU:HG2	1:I:284:VAL:HG22	1.52	0.90
1:A:196:ASN:HB2	1:B:196:ASN:HD21	1.35	0.89
2:H:706:DA:H2''	2:H:707:DT:H5'	1.52	0.88
1:B:179:PRO:HA	1:B:273:ILE:HG22	1.55	0.88
1:D:243:PRO:HB2	1:D:248:GLU:HB3	1.55	0.87
1:C:131:PHE:HE2	1:C:151:LEU:HD13	1.38	0.87
1:I:201:ARG:HG2	1:I:202:ASP:H	1.38	0.86
1:I:119:THR:O	1:I:287:ARG:HD2	1.76	0.86
1:I:226:VAL:O	1:I:234:GLN:HA	1.76	0.86
1:J:134:SER:HB2	1:J:143:THR:HA	1.58	0.85
1:I:224:GLN:O	1:I:226:VAL:HG23	1.76	0.84
1:B:310:ARG:HD3	1:B:311:GLU:N	1.91	0.84
1:I:215:ILE:H	1:I:215:ILE:CD1	1.89	0.84
1:B:121:TYR:HD1	1:B:122:PRO:HD2	1.43	0.84
1:I:161:ILE:HD11	1:I:254:TYR:CD1	2.13	0.83
1:C:145:SER:HA	1:C:302:ARG:HH11	1.43	0.83
2:F:506:DA:H2''	2:F:507:DT:H5'	1.61	0.82
1:I:143:THR:CG2	1:I:298:PRO:HB2	2.09	0.82
1:A:263:VAL:HG13	1:A:264:GLY:H	1.44	0.82
1:B:244:GLN:C	1:B:246:GLY:H	1.82	0.81
1:I:194:CYS:HB2	1:I:263:VAL:O	1.79	0.81
1:A:303:LYS:HG3	1:A:304:ALA:N	1.93	0.81
1:B:293:ARG:HG2	1:B:295:CYS:SG	2.19	0.81
1:J:279:MET:HG2	1:J:285:LEU:HD21	1.62	0.81
1:B:279:MET:HG3	1:B:283:GLN:HB3	1.61	0.81
2:L:812:DA:H2''	2:L:813:DT:OP2	1.79	0.81
1:A:179:PRO:O	1:A:191:VAL:HG21	1.81	0.81
1:C:259:ASN:HA	1:C:294:ILE:HG22	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:220:ASN:HD22	1:I:221:ASN:N	1.78	0.80
2:K:904:DG:H2"	2:K:905:DG:C8	2.16	0.80
1:B:272:LEU:HA	1:B:291:GLU:HA	1.63	0.80
1:B:129:VAL:HG21	1:B:288:ARG:HB3	1.64	0.80
1:D:283:GLN:NE2	1:J:245:VAL:HG11	1.96	0.80
1:J:193:ARG:HH21	1:J:257:MET:HB3	1.46	0.79
1:D:218:GLU:HG2	1:D:255:ASN:OD1	1.82	0.79
1:B:193:ARG:HD2	1:B:198:GLU:HA	1.64	0.79
1:J:186:HIS:CE1	1:J:269:ARG:HD3	2.18	0.79
1:D:126:HIS:HB3	1:D:166:SER:HB2	1.63	0.79
1:J:143:THR:HG22	1:J:298:PRO:HB3	1.63	0.79
1:B:179:PRO:HB2	1:B:191:VAL:HG11	1.65	0.79
1:B:303:LYS:HA	1:B:306:GLU:HB2	1.64	0.79
1:A:310:ARG:HD3	1:A:311:GLU:N	1.98	0.78
1:B:148:LEU:HD11	1:B:305:ASP:HB2	1.65	0.78
1:C:176:ARG:HB2	1:C:237:VAL:HG23	1.65	0.78
1:B:120:ASP:OD1	1:B:288:ARG:HD3	1.82	0.78
1:A:193:ARG:HD3	1:A:211:ALA:O	1.84	0.78
1:D:165:VAL:HG12	1:D:166:SER:H	1.47	0.78
1:C:201:ARG:HH21	1:C:202:ASP:HB2	1.49	0.77
1:B:258:CYS:HB3	1:B:262:CYS:SG	2.24	0.77
1:B:274:ILE:HG22	1:B:289:SER:HB3	1.66	0.77
1:C:193:ARG:NE	1:C:197:HIS:HB3	1.99	0.77
1:D:201:ARG:HD2	1:D:202:ASP:H	1.49	0.77
1:A:182:LYS:HG3	1:A:272:LEU:HD11	1.65	0.77
1:I:150:LYS:HD2	1:I:291:GLU:OE2	1.85	0.77
1:B:174:ALA:HA	1:B:239:PRO:HA	1.66	0.77
1:B:247:THR:O	1:B:249:PHE:HD2	1.68	0.77
1:D:117:SER:HB3	1:D:287:ARG:HH12	1.47	0.77
1:D:259:ASN:HA	1:D:294:ILE:HB	1.67	0.77
1:J:131:PHE:HD1	1:J:131:PHE:H	1.32	0.77
1:C:131:PHE:CE2	1:C:151:LEU:HD13	2.20	0.76
1:J:296:ALA:HB3	2:L:809:DT:H72	1.67	0.76
1:B:147:LEU:HB3	1:B:148:LEU:HD12	1.67	0.76
1:D:279:MET:HB2	1:D:283:GLN:HB3	1.67	0.76
1:B:119:THR:HG22	1:B:287:ARG:NH1	1.99	0.76
1:B:197:HIS:HB3	1:B:257:MET:SD	2.25	0.76
1:D:279:MET:HG3	1:D:280:ARG:H	1.50	0.76
1:B:285:LEU:N	1:B:285:LEU:HD12	2.00	0.76
1:D:225:TYR:CD2	1:D:236:VAL:HG12	2.20	0.76
1:J:193:ARG:HE	1:J:257:MET:HB3	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:511:DC:H2"	2:F:512:DA:OP2	1.86	0.76
1:J:259:ASN:O	1:J:262:CYS:HB2	1.86	0.76
1:I:293:ARG:HG2	1:I:295:CYS:SG	2.26	0.76
1:J:185:GLU:H	1:J:185:GLU:CD	1.89	0.76
1:D:174:ALA:HA	1:D:239:PRO:HA	1.68	0.75
1:A:201:ARG:NH1	1:A:202:ASP:HB2	2.01	0.75
1:C:120:ASP:HB2	1:C:287:ARG:O	1.87	0.75
2:F:512:DA:H8	2:F:512:DA:OP2	1.69	0.75
1:I:193:ARG:HD3	1:I:211:ALA:O	1.87	0.75
2:G:602:DA:H2"	2:G:603:DT:H5'	1.68	0.75
1:J:141:THR:HA	1:J:154:GLN:NE2	2.01	0.75
1:J:231:THR:OG1	1:J:233:ARG:HG2	1.86	0.74
1:D:193:ARG:HG3	1:D:213:HIS:O	1.88	0.74
1:J:150:LYS:HB2	1:J:291:GLU:HB3	1.68	0.74
1:A:196:ASN:HB2	1:B:196:ASN:ND2	2.03	0.74
1:A:303:LYS:HG3	1:A:304:ALA:H	1.52	0.74
1:I:218:GLU:HB2	1:I:255:ASN:HD22	1.52	0.74
1:A:218:GLU:HB2	1:A:255:ASN:ND2	2.03	0.74
1:B:266:MET:O	1:B:269:ARG:HG2	1.88	0.74
1:I:225:TYR:CD1	1:I:236:VAL:HG12	2.23	0.74
1:D:278:GLU:HG2	1:D:284:VAL:HG22	1.69	0.74
1:J:126:HIS:HB2	1:J:166:SER:HB2	1.70	0.74
1:J:193:ARG:NH2	1:J:257:MET:HB3	2.02	0.74
1:B:151:LEU:HD12	1:B:152:TYR:H	1.53	0.73
1:D:243:PRO:HB2	1:D:248:GLU:CB	2.17	0.73
1:D:256:PHE:N	1:D:256:PHE:HD1	1.85	0.73
1:A:263:VAL:HG13	1:A:264:GLY:N	2.02	0.73
1:B:301:ASP:OD1	1:B:304:ALA:HB2	1.88	0.73
1:A:263:VAL:O	1:A:267:ASN:ND2	2.20	0.73
1:B:176:ARG:HD2	1:B:278:GLU:OE1	1.87	0.73
1:D:121:TYR:HB3	1:D:286:GLY:HA2	1.70	0.73
1:B:186:HIS:CD2	1:B:269:ARG:HD2	2.23	0.73
2:L:806:DA:H2"	2:L:807:DT:H72	1.71	0.73
1:B:129:VAL:HG22	1:B:288:ARG:HD2	1.71	0.73
1:A:193:ARG:HE	1:A:257:MET:HB2	1.53	0.73
1:D:179:PRO:HG2	1:D:191:VAL:HG11	1.68	0.73
1:J:302:ARG:HH22	1:J:303:LYS:HE3	1.53	0.73
1:A:274:ILE:HG22	1:A:276:THR:HG22	1.70	0.73
1:A:280:ARG:HG3	1:A:280:ARG:HH11	1.54	0.73
1:C:184:ALA:O	1:C:187:VAL:HG12	1.89	0.72
1:J:155:ILE:HG23	1:J:156:ALA:N	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:GLN:HE21	1:D:209:ALA:H	1.37	0.72
1:D:186:HIS:ND1	1:D:269:ARG:HD3	2.04	0.72
2:H:707:DT:H2"	2:H:708:DG:OP2	1.88	0.72
1:B:148:LEU:N	1:B:148:LEU:HD12	2.05	0.72
1:B:131:PHE:HE2	1:B:151:LEU:HD22	1.54	0.72
1:D:186:HIS:CE1	1:D:269:ARG:HD3	2.24	0.72
1:J:190:VAL:HG12	1:J:233:ARG:HD2	1.72	0.72
1:B:252:ILE:HG22	1:B:253:LEU:N	2.04	0.72
1:B:150:LYS:HB3	1:B:291:GLU:HB3	1.71	0.72
1:B:243:PRO:HA	1:B:250:THR:H	1.54	0.72
1:I:163:ILE:O	1:I:249:PHE:HB3	1.89	0.72
1:I:196:ASN:OD1	1:J:196:ASN:HB2	1.90	0.72
1:A:231:THR:OG1	1:A:233:ARG:HG2	1.90	0.71
1:D:172:GLY:O	1:D:280:ARG:HA	1.90	0.71
1:C:201:ARG:NH2	1:C:202:ASP:HB2	2.05	0.71
1:I:129:VAL:HG23	1:I:288:ARG:HG3	1.72	0.71
1:A:117:SER:HB2	1:A:287:ARG:NH1	2.06	0.71
1:B:263:VAL:CG1	1:B:264:GLY:N	2.54	0.71
1:J:155:ILE:HD11	1:J:258:CYS:HA	1.71	0.71
1:A:130:THR:HB	1:A:162:GLN:HB2	1.73	0.71
1:D:193:ARG:HB2	1:D:212:SER:O	1.90	0.71
1:A:126:HIS:O	1:A:165:VAL:HA	1.91	0.70
1:A:193:ARG:NE	1:A:257:MET:HB3	2.03	0.70
1:A:178:MET:HB2	1:A:235:SER:HB3	1.72	0.70
1:B:307:ASP:O	1:B:310:ARG:HD2	1.90	0.70
1:D:121:TYR:HD1	1:D:122:PRO:HD2	1.55	0.70
1:B:125:HIS:HA	1:B:166:SER:OG	1.92	0.70
1:J:193:ARG:NE	1:J:257:MET:HB3	2.06	0.70
1:I:167:THR:HG22	1:I:168:PRO:HD2	1.71	0.70
1:J:143:THR:HG22	1:J:298:PRO:CB	2.21	0.70
1:J:186:HIS:ND1	1:J:269:ARG:HD3	2.06	0.70
1:B:119:THR:HG22	1:B:287:ARG:HH12	1.56	0.70
1:J:193:ARG:HG2	1:J:258:CYS:SG	2.31	0.70
1:A:142:TRP:HA	1:A:152:TYR:O	1.91	0.70
1:A:115:ILE:HD12	1:A:116:PRO:O	1.92	0.70
1:C:135:SER:O	1:C:140:ALA:HB2	1.91	0.70
1:B:131:PHE:CE2	1:B:151:LEU:HD22	2.27	0.69
1:C:200:GLY:O	1:C:204:ASN:ND2	2.24	0.69
1:C:307:ASP:O	1:C:311:GLU:HB2	1.91	0.69
2:H:700:DA:H2"	2:H:701:DT:H72	1.71	0.69
1:A:193:ARG:NH1	1:A:197:HIS:HB3	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:LYS:HG3	1:C:291:GLU:HB3	1.75	0.69
1:I:138:LYS:HE2	1:I:138:LYS:HA	1.73	0.69
1:I:150:LYS:HA	1:I:291:GLU:O	1.93	0.69
1:I:152:TYR:CB	1:I:298:PRO:HB3	2.21	0.69
1:B:259:ASN:HA	1:B:294:ILE:CG2	2.22	0.69
1:A:201:ARG:HH12	1:A:202:ASP:HB2	1.57	0.69
1:D:255:ASN:C	1:D:256:PHE:HD1	1.96	0.69
1:I:249:PHE:N	1:I:249:PHE:CD1	2.60	0.69
1:B:287:ARG:O	1:B:288:ARG:HG2	1.93	0.69
1:J:163:ILE:CG2	1:J:250:THR:HB	2.23	0.69
1:C:145:SER:HB2	1:C:302:ARG:CD	2.21	0.69
1:D:175:ILE:HD11	1:D:252:ILE:HD11	1.75	0.69
1:D:256:PHE:N	1:D:256:PHE:CD1	2.57	0.69
1:I:115:ILE:HD11	1:I:231:THR:HG21	1.75	0.69
1:A:182:LYS:HA	1:A:272:LEU:HD13	1.75	0.68
1:C:303:LYS:HE3	1:C:307:ASP:OD2	1.93	0.68
1:I:309:TYR:CD1	1:I:309:TYR:C	2.66	0.68
1:I:243:PRO:HG2	1:I:246:GLY:HA3	1.75	0.68
1:I:143:THR:HG22	1:I:298:PRO:HB2	1.74	0.68
1:D:138:LYS:HG3	1:D:139:SER:N	2.07	0.68
1:J:181:TYR:CE1	1:J:269:ARG:HD2	2.28	0.68
1:J:297:CYS:HB2	1:J:300:ARG:HB2	1.75	0.68
1:C:193:ARG:NH1	1:C:204:ASN:OD1	2.27	0.68
1:D:279:MET:CE	1:D:279:MET:HA	2.23	0.68
1:D:125:HIS:N	1:D:125:HIS:CD2	2.61	0.68
1:D:228:ASP:OD1	1:D:230:VAL:HB	1.94	0.68
1:J:256:PHE:HD1	1:J:256:PHE:N	1.91	0.68
1:D:179:PRO:HG2	1:D:191:VAL:CG1	2.23	0.68
2:G:614:DA:OP2	2:G:614:DA:H2'	1.94	0.68
1:I:118:ASN:HA	1:I:274:ILE:HD11	1.74	0.68
1:B:216:ARG:HA	1:B:225:TYR:HE2	1.58	0.67
1:B:178:MET:HE3	1:B:274:ILE:HD11	1.77	0.67
1:C:153:CYS:SG	1:C:159:CYS:HB2	2.34	0.67
1:I:215:ILE:HG12	1:I:236:VAL:HG13	1.75	0.67
2:L:808:DG:H2''	2:L:809:DT:H71	1.74	0.67
2:F:512:DA:C8	2:F:513:DT:H72	2.29	0.67
1:A:278:GLU:HB2	1:A:282:GLY:O	1.94	0.67
1:A:259:ASN:HB2	1:A:294:ILE:O	1.93	0.67
1:C:272:LEU:HD21	1:C:289:SER:HB2	1.77	0.67
1:J:302:ARG:NH2	1:J:303:LYS:HE3	2.10	0.67
1:A:167:THR:HB	1:A:168:PRO:HD2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:SER:HA	1:C:266:MET:SD	2.35	0.67
1:B:247:THR:O	1:B:249:PHE:CD2	2.48	0.67
1:J:256:PHE:CD1	1:J:256:PHE:N	2.58	0.67
1:D:114:PHE:CD2	1:D:231:THR:HG21	2.30	0.66
1:A:152:TYR:CB	1:A:298:PRO:HB3	2.25	0.66
1:I:280:ARG:HG3	1:I:281:ASP:H	1.59	0.66
1:J:131:PHE:CD1	1:J:131:PHE:N	2.59	0.66
1:J:214:LEU:CD2	1:J:215:ILE:HG13	2.21	0.66
1:D:218:GLU:HG3	1:D:218:GLU:O	1.94	0.66
1:D:123:GLY:HA2	1:D:285:LEU:O	1.95	0.66
2:E:403:DT:H2''	2:E:404:DG:C8	2.30	0.66
1:A:184:ALA:HA	1:A:187:VAL:HB	1.77	0.66
1:B:305:ASP:O	1:B:308:HIS:HB3	1.95	0.66
1:I:147:LEU:HG	1:I:148:LEU:CD2	2.26	0.66
2:K:902:DA:H1'	2:K:903:DT:H5'	1.77	0.66
1:I:193:ARG:HG2	1:I:258:CYS:SG	2.36	0.66
1:I:140:ALA:O	1:I:141:THR:C	2.34	0.66
1:J:151:LEU:HG	1:J:152:TYR:N	2.10	0.66
1:B:179:PRO:CA	1:B:273:ILE:HG22	2.25	0.66
1:I:201:ARG:HG2	1:I:202:ASP:N	2.11	0.66
1:A:140:ALA:O	1:A:298:PRO:HG2	1.95	0.66
1:I:169:PRO:HG3	1:I:240:TYR:CD2	2.31	0.66
1:A:216:ARG:HD2	1:A:257:MET:HE2	1.78	0.65
1:B:244:GLN:C	1:B:246:GLY:N	2.49	0.65
1:D:127:PHE:HE1	1:D:163:ILE:HG23	1.61	0.65
1:J:155:ILE:CG2	1:J:156:ALA:N	2.59	0.65
1:D:143:THR:HG23	1:D:152:TYR:HB2	1.77	0.65
1:C:193:ARG:HB2	1:C:213:HIS:O	1.95	0.65
1:A:121:TYR:CD2	1:A:286:GLY:HA2	2.31	0.65
1:I:215:ILE:N	1:I:215:ILE:HD13	2.00	0.65
1:I:177:ALA:HB3	1:I:254:TYR:HE2	1.61	0.65
1:A:150:LYS:HB2	1:A:291:GLU:O	1.97	0.65
1:A:259:ASN:HA	1:A:294:ILE:CB	2.22	0.65
1:C:247:THR:HG22	1:C:248:GLU:OE2	1.96	0.65
1:I:124:PRO:HG2	1:I:125:HIS:ND1	2.12	0.65
1:I:147:LEU:HG	1:I:148:LEU:HD21	1.79	0.65
1:B:122:PRO:HG2	1:B:123:GLY:H	1.62	0.65
1:B:186:HIS:NE2	1:B:269:ARG:HD2	2.11	0.65
2:H:713:DT:OP2	2:H:713:DT:H2'	1.96	0.65
1:I:123:GLY:HA3	1:I:285:LEU:O	1.97	0.65
1:A:152:TYR:HB3	1:A:298:PRO:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:220:ASN:HD22	1:I:222:LEU:N	1.91	0.65
1:J:257:MET:N	1:J:257:MET:SD	2.69	0.65
2:F:507:DT:H1'	2:F:508:DG:C8	2.32	0.65
1:B:193:ARG:HD3	1:B:257:MET:SD	2.36	0.65
1:C:187:VAL:HG13	1:C:188:THR:N	2.12	0.65
1:A:271:ILE:HG12	1:A:272:LEU:N	2.12	0.65
1:B:161:ILE:HG12	1:B:254:TYR:HD2	1.62	0.65
1:C:145:SER:HB2	1:C:302:ARG:HD3	1.79	0.65
1:C:218:GLU:O	1:C:253:LEU:HB2	1.97	0.64
1:B:131:PHE:HD2	1:B:142:TRP:HZ3	1.43	0.64
1:D:122:PRO:O	1:D:127:PHE:N	2.31	0.64
1:I:147:LEU:C	1:I:148:LEU:HD23	2.18	0.64
1:I:167:THR:CG2	1:I:168:PRO:HD2	2.27	0.64
1:C:279:MET:HB2	1:C:281:ASP:HB2	1.78	0.64
1:I:146:PRO:CD	1:I:147:LEU:H	2.10	0.64
1:C:163:ILE:O	1:C:250:THR:CG2	2.45	0.64
1:D:279:MET:HE3	1:D:279:MET:HA	1.80	0.64
1:A:216:ARG:HB3	1:A:225:TYR:OH	1.98	0.64
1:B:195:PRO:HG2	1:B:196:ASN:H	1.63	0.64
1:B:222:LEU:HD23	1:B:222:LEU:O	1.97	0.64
1:B:218:GLU:HB2	1:B:255:ASN:ND2	2.13	0.64
1:B:193:ARG:CZ	1:B:257:MET:HG3	2.28	0.64
1:C:161:ILE:O	1:C:161:ILE:HG13	1.97	0.64
1:D:121:TYR:CD1	1:D:122:PRO:HD2	2.33	0.63
1:D:119:THR:O	1:D:287:ARG:NE	2.31	0.63
1:D:198:GLU:O	1:D:204:ASN:ND2	2.30	0.63
1:A:271:ILE:HD11	1:A:273:ILE:CD1	2.28	0.63
1:C:148:LEU:O	1:C:149:LYS:HG2	1.98	0.63
2:K:902:DA:H2''	2:K:903:DT:OP2	1.98	0.63
1:A:125:HIS:CD2	1:A:169:PRO:HA	2.33	0.63
1:A:138:LYS:HB3	2:E:404:DG:OP2	1.98	0.63
1:A:196:ASN:CB	1:B:196:ASN:HD21	2.10	0.63
1:B:117:SER:HB3	1:B:287:ARG:CZ	2.28	0.63
1:D:300:ARG:O	1:D:300:ARG:HD2	1.98	0.63
1:A:117:SER:HB2	1:A:287:ARG:CZ	2.28	0.63
1:B:152:TYR:CZ	1:B:301:ASP:HB3	2.34	0.63
1:J:145:SER:HG	1:J:302:ARG:HD3	1.61	0.63
1:B:263:VAL:C	1:B:265:GLY:H	2.00	0.63
1:J:163:ILE:HG22	1:J:250:THR:HB	1.81	0.63
1:J:202:ASP:O	1:J:203:PHE:HB2	1.99	0.63
1:J:127:PHE:HD2	1:J:286:GLY:HA3	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:807:DT:C2'	2:L:808:DG:H5'	2.28	0.63
1:A:198:GLU:HG3	1:A:212:SER:HA	1.81	0.62
1:A:280:ARG:NH1	1:A:280:ARG:HG3	2.13	0.62
1:D:240:TYR:HE2	1:D:242:PRO:HG3	1.63	0.62
1:I:188:THR:HG23	1:I:189:ASP:N	2.13	0.62
1:A:182:LYS:HA	1:A:272:LEU:CD1	2.28	0.62
1:A:307:ASP:C	1:A:309:TYR:H	2.02	0.62
1:I:263:VAL:HG12	1:I:264:GLY:N	2.14	0.62
1:I:125:HIS:CD2	1:I:167:THR:HB	2.34	0.62
1:C:138:LYS:HA	1:C:299:GLY:HA3	1.81	0.62
1:A:278:GLU:OE1	1:A:282:GLY:HA2	2.00	0.62
1:D:188:THR:O	1:D:189:ASP:C	2.38	0.62
1:I:196:ASN:O	1:I:200:GLY:N	2.29	0.62
1:A:307:ASP:HA	1:A:310:ARG:CG	2.28	0.62
1:I:249:PHE:H	1:I:249:PHE:HD1	1.46	0.62
1:J:255:ASN:C	1:J:256:PHE:CD1	2.73	0.62
1:A:143:THR:HG22	1:A:298:PRO:HB2	1.82	0.62
2:H:700:DA:H2'	2:H:701:DT:C7	2.28	0.62
1:C:116:PRO:HB3	1:C:178:MET:CE	2.30	0.62
1:A:296:ALA:O	1:A:297:CYS:CB	2.45	0.61
1:A:271:ILE:HD11	1:A:273:ILE:HD11	1.82	0.61
1:D:193:ARG:HH21	1:D:197:HIS:HB3	1.64	0.61
1:I:204:ASN:HD22	1:I:211:ALA:HB2	1.65	0.61
1:B:263:VAL:HG13	1:B:264:GLY:H	1.65	0.61
1:D:277:LEU:HB3	1:D:286:GLY:O	1.99	0.61
1:B:138:LYS:HZ3	2:F:502:DG:H2'	1.64	0.61
1:C:259:ASN:N	1:C:262:CYS:SG	2.73	0.61
1:A:145:SER:HA	1:A:302:ARG:NH1	2.16	0.61
1:I:274:ILE:O	1:I:274:ILE:HG22	2.00	0.61
1:C:163:ILE:O	1:C:250:THR:HG22	2.00	0.61
1:I:193:ARG:HB2	1:I:212:SER:O	2.01	0.61
1:D:131:PHE:HE2	1:D:151:LEU:HD13	1.66	0.61
2:H:711:DC:OP2	2:H:711:DC:H2'	2.00	0.61
1:J:125:HIS:ND1	1:J:167:THR:HG23	2.16	0.61
1:D:240:TYR:CE2	1:D:242:PRO:HG3	2.36	0.60
1:A:135:SER:O	1:A:137:ALA:N	2.34	0.60
1:B:252:ILE:CG2	1:B:253:LEU:N	2.63	0.60
1:C:198:GLU:HG3	1:C:212:SER:HA	1.83	0.60
1:D:158:THR:HG22	1:D:218:GLU:OE1	2.01	0.60
1:I:214:LEU:HD23	1:I:215:ILE:HG23	1.81	0.60
1:D:225:TYR:CE2	1:D:236:VAL:HG12	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:ILE:HG21	1:D:259:ASN:OD1	2.02	0.60
2:H:700:DA:C2'	2:H:701:DT:H72	2.31	0.60
1:B:118:ASN:H	1:B:118:ASN:ND2	1.98	0.60
1:D:121:TYR:HB3	1:D:287:ARG:H	1.66	0.60
1:I:122:PRO:HD2	1:I:123:GLY:H	1.67	0.60
1:B:279:MET:HE2	1:B:280:ARG:H	1.66	0.60
1:C:193:ARG:CZ	1:C:197:HIS:HB3	2.32	0.60
1:I:222:LEU:O	1:I:222:LEU:HG	2.01	0.60
1:J:193:ARG:CZ	1:J:257:MET:HB3	2.32	0.60
1:A:197:HIS:O	1:A:200:GLY:N	2.31	0.60
1:B:147:LEU:HD23	1:B:147:LEU:O	2.01	0.60
1:J:134:SER:CB	1:J:143:THR:HA	2.30	0.60
1:J:255:ASN:C	1:J:256:PHE:HD1	2.04	0.60
1:D:175:ILE:CD1	1:D:252:ILE:HD11	2.31	0.60
2:K:913:DC:H2''	2:K:914:DA:C8	2.37	0.60
1:I:243:PRO:CG	1:I:246:GLY:HA3	2.31	0.60
1:I:280:ARG:HG3	1:I:281:ASP:N	2.16	0.60
1:J:170:PRO:HD2	1:J:173:THR:OG1	2.02	0.60
1:D:117:SER:CB	1:D:287:ARG:HH12	2.15	0.60
1:A:259:ASN:HB3	1:A:294:ILE:HG22	1.84	0.59
1:B:162:GLN:HE21	1:B:251:THR:HG21	1.66	0.59
1:B:213:HIS:CE1	1:B:235:SER:C	2.76	0.59
1:I:201:ARG:CD	1:I:201:ARG:H	2.11	0.59
1:A:216:ARG:HD2	1:A:257:MET:CE	2.32	0.59
1:C:173:THR:HG22	1:C:240:TYR:HB2	1.84	0.59
1:D:216:ARG:HD2	1:D:257:MET:CE	2.31	0.59
1:D:279:MET:HG2	1:D:281:ASP:OD2	2.03	0.59
1:J:164:LYS:HG2	1:J:165:VAL:O	2.03	0.59
1:A:121:TYR:CE1	1:A:123:GLY:HA2	2.37	0.59
1:I:215:ILE:N	1:I:215:ILE:CD1	2.63	0.59
1:B:213:HIS:HB2	1:B:234:GLN:OE1	2.03	0.59
1:A:124:PRO:HG2	1:A:125:HIS:H	1.67	0.59
1:A:218:GLU:HB2	1:A:255:ASN:HD21	1.68	0.59
1:D:259:ASN:HA	1:D:294:ILE:CB	2.32	0.59
1:I:293:ARG:NH2	2:K:909:DT:OP2	2.28	0.59
1:D:263:VAL:HG23	1:D:267:ASN:ND2	2.18	0.59
1:J:260:SER:O	1:J:268:ARG:N	2.27	0.59
1:B:266:MET:CE	1:B:271:ILE:HG21	2.32	0.59
2:L:808:DG:H2''	2:L:809:DT:OP2	2.02	0.59
1:D:185:GLU:HB2	1:D:186:HIS:ND1	2.18	0.59
1:I:174:ALA:HA	1:I:239:PRO:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:LYS:HD3	1:B:138:LYS:C	2.23	0.59
1:I:147:LEU:HD12	1:I:147:LEU:O	2.03	0.58
1:I:188:THR:HG23	1:I:189:ASP:H	1.68	0.58
2:L:806:DA:H2''	2:L:807:DT:C7	2.33	0.58
1:B:132:GLN:HB2	1:B:142:TRP:CH2	2.38	0.58
1:D:175:ILE:HA	1:D:276:THR:O	2.03	0.58
1:I:159:CYS:HB3	1:I:254:TYR:O	2.03	0.58
1:J:194:CYS:C	1:J:196:ASN:N	2.55	0.58
2:G:614:DA:H1'	2:G:615:DT:H5'	1.85	0.58
1:J:160:PRO:O	1:J:161:ILE:HG23	2.02	0.58
1:A:193:ARG:HB2	1:A:212:SER:O	2.03	0.58
1:D:126:HIS:CD2	1:D:126:HIS:O	2.57	0.58
1:I:119:THR:HG22	1:I:287:ARG:NH2	2.18	0.58
1:B:279:MET:HG2	1:B:285:LEU:HD11	1.86	0.58
1:D:201:ARG:HD2	1:D:202:ASP:N	2.19	0.58
1:A:303:LYS:CG	1:A:304:ALA:N	2.66	0.58
1:C:145:SER:HB2	1:C:302:ARG:HD2	1.84	0.58
1:D:155:ILE:HG12	1:D:256:PHE:O	2.04	0.58
1:I:216:ARG:HA	1:I:225:TYR:HE1	1.68	0.58
2:K:903:DT:H2''	2:K:904:DG:C8	2.39	0.58
1:D:215:ILE:O	1:D:236:VAL:CG1	2.52	0.58
1:I:220:ASN:ND2	1:I:222:LEU:N	2.43	0.58
1:J:121:TYR:O	1:J:286:GLY:HA2	2.04	0.58
1:A:220:ASN:ND2	1:A:238:VAL:HG23	2.19	0.58
1:C:266:MET:O	1:C:269:ARG:HB2	2.04	0.58
1:C:259:ASN:HA	1:C:294:ILE:CG2	2.32	0.58
2:G:602:DA:C2'	2:G:603:DT:H5'	2.34	0.58
1:J:188:THR:HG23	1:J:189:ASP:OD1	2.04	0.58
1:J:194:CYS:O	1:J:196:ASN:N	2.36	0.58
1:A:152:TYR:CZ	1:A:302:ARG:HA	2.39	0.58
1:I:259:ASN:N	1:I:262:CYS:SG	2.72	0.58
1:B:300:ARG:HH11	1:B:300:ARG:HG3	1.69	0.58
1:D:181:TYR:CE2	1:D:269:ARG:NH1	2.72	0.58
2:K:913:DC:H2''	2:K:914:DA:H8	1.69	0.58
1:D:279:MET:HG2	1:D:281:ASP:CG	2.23	0.57
1:D:293:ARG:HG2	1:D:295:CYS:SG	2.44	0.57
1:A:150:LYS:HE2	1:A:152:TYR:OH	2.04	0.57
1:C:248:GLU:CD	1:C:248:GLU:N	2.46	0.57
1:B:247:THR:O	1:B:249:PHE:N	2.37	0.57
1:C:154:GLN:HG2	1:C:295:CYS:O	2.03	0.57
1:I:186:HIS:CD2	1:I:269:ARG:HE	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:135:SER:HB2	1:J:140:ALA:CB	2.34	0.57
1:J:183:LYS:HB2	1:J:186:HIS:HD2	1.69	0.57
1:C:257:MET:N	1:C:257:MET:SD	2.77	0.57
1:C:307:ASP:HA	1:C:310:ARG:HB3	1.86	0.57
1:I:240:TYR:CE1	1:I:250:THR:HG21	2.40	0.57
1:J:175:ILE:HD11	1:J:240:TYR:HA	1.86	0.57
1:A:111:HIS:CD2	1:A:111:HIS:N	2.72	0.57
1:A:176:ARG:HB2	1:A:237:VAL:HG23	1.85	0.57
1:B:197:HIS:HB3	1:B:257:MET:CE	2.35	0.57
1:B:243:PRO:HA	1:B:250:THR:N	2.20	0.56
1:B:307:ASP:HA	1:B:310:ARG:HB3	1.86	0.56
1:D:155:ILE:HB	1:D:294:ILE:HG21	1.85	0.56
1:D:164:LYS:HG2	1:D:165:VAL:H	1.68	0.56
1:D:213:HIS:HA	1:D:234:GLN:NE2	2.21	0.56
1:C:277:LEU:HB3	1:C:286:GLY:H	1.70	0.56
1:J:193:ARG:HE	1:J:257:MET:CB	2.17	0.56
1:A:217:VAL:HG23	1:A:236:VAL:HG21	1.88	0.56
1:D:243:PRO:CB	1:D:248:GLU:HB3	2.33	0.56
1:I:138:LYS:NZ	1:I:139:SER:H	2.04	0.56
1:A:160:PRO:C	1:A:161:ILE:HD13	2.26	0.56
1:A:201:ARG:HD3	1:A:201:ARG:H	1.70	0.56
1:B:310:ARG:CD	1:B:311:GLU:N	2.67	0.56
1:D:276:THR:HG22	1:D:287:ARG:HB3	1.86	0.56
1:I:121:TYR:HB3	1:I:287:ARG:HB3	1.88	0.56
1:J:195:PRO:O	1:J:199:LEU:HB2	2.05	0.56
1:A:295:CYS:SG	1:A:298:PRO:HD3	2.46	0.56
1:B:125:HIS:ND1	1:B:125:HIS:N	2.54	0.56
1:D:216:ARG:HD2	1:D:257:MET:SD	2.46	0.56
1:I:164:LYS:C	1:I:165:VAL:HG22	2.25	0.56
1:A:248:GLU:N	1:A:248:GLU:OE1	2.39	0.56
1:B:193:ARG:CD	1:B:198:GLU:HA	2.35	0.56
1:B:252:ILE:CG2	1:B:253:LEU:H	2.19	0.56
2:F:506:DA:C2'	2:F:507:DT:H5'	2.34	0.56
2:G:613:DC:H2''	2:G:614:DA:C8	2.40	0.56
1:I:218:GLU:HB2	1:I:255:ASN:HD21	1.69	0.56
1:I:274:ILE:HD13	1:I:289:SER:HB3	1.88	0.56
1:A:209:ALA:HB2	1:A:225:TYR:CZ	2.41	0.55
1:B:163:ILE:HG22	1:B:164:LYS:N	2.21	0.55
1:B:263:VAL:HG13	1:B:267:ASN:ND2	2.20	0.55
1:D:198:GLU:HG3	1:D:212:SER:HA	1.87	0.55
1:C:263:VAL:HB	1:D:196:ASN:ND2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:152:TYR:HB3	1:I:298:PRO:CB	2.31	0.55
1:I:228:ASP:OD1	1:I:229:PRO:HD2	2.05	0.55
1:I:309:TYR:O	1:I:312:GLN:HG3	2.06	0.55
1:A:155:ILE:O	1:A:155:ILE:HG23	2.05	0.55
1:I:136:THR:HG22	1:I:137:ALA:N	2.21	0.55
1:A:160:PRO:O	1:A:161:ILE:HD13	2.06	0.55
1:C:279:MET:CB	1:C:281:ASP:HB2	2.36	0.55
1:I:186:HIS:CD2	1:I:269:ARG:HH11	2.24	0.55
1:J:217:VAL:HG22	1:J:254:TYR:CE1	2.42	0.55
1:A:296:ALA:O	1:A:297:CYS:SG	2.65	0.55
1:C:130:THR:OG1	1:C:162:GLN:HB2	2.07	0.55
1:C:179:PRO:HG2	1:C:191:VAL:CG2	2.37	0.55
1:C:146:PRO:HD2	1:C:302:ARG:HH12	1.71	0.55
1:J:236:VAL:HG13	1:J:236:VAL:O	2.07	0.55
1:C:145:SER:OG	1:C:306:GLU:OE2	2.24	0.55
1:C:179:PRO:O	1:C:191:VAL:HG21	2.07	0.55
2:H:711:DC:H2"	2:H:712:DA:C8	2.42	0.55
1:J:155:ILE:HD11	1:J:258:CYS:CA	2.37	0.55
1:B:199:LEU:HD12	1:B:199:LEU:O	2.06	0.55
1:C:127:PHE:HD2	1:C:286:GLY:HA3	1.71	0.55
1:A:236:VAL:HG13	1:A:236:VAL:O	2.06	0.55
1:B:132:GLN:HB2	1:B:142:TRP:HH2	1.72	0.55
1:B:271:ILE:HG12	1:B:272:LEU:N	2.19	0.55
1:C:138:LYS:CG	1:C:139:SER:N	2.70	0.55
1:D:155:ILE:HB	1:D:294:ILE:CG2	2.37	0.55
1:D:245:VAL:O	1:D:245:VAL:HG23	2.06	0.55
1:A:158:THR:HB	1:A:218:GLU:OE2	2.06	0.55
1:B:123:GLY:HA3	1:B:285:LEU:O	2.06	0.55
1:C:201:ARG:HE	1:C:202:ASP:N	2.05	0.55
1:D:152:TYR:HB3	1:D:298:PRO:HB2	1.89	0.55
2:K:906:DA:C2	2:K:907:DC:C2	2.94	0.55
1:D:179:PRO:CG	1:D:191:VAL:HG11	2.37	0.54
1:I:213:HIS:CD2	1:I:234:GLN:HB3	2.43	0.54
1:C:116:PRO:HB3	1:C:178:MET:HE1	1.89	0.54
1:D:112:HIS:C	1:D:114:PHE:H	2.11	0.54
1:D:155:ILE:HG12	1:D:156:ALA:N	2.23	0.54
1:D:237:VAL:HG12	1:D:238:VAL:N	2.21	0.54
1:I:212:SER:CB	1:I:234:GLN:HE22	2.20	0.54
1:B:241:GLU:O	1:B:250:THR:HB	2.07	0.54
1:I:145:SER:O	1:I:148:LEU:O	2.25	0.54
1:D:215:ILE:O	1:D:236:VAL:HG11	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:PRO:HG2	1:C:191:VAL:HG21	1.90	0.54
1:J:279:MET:O	1:J:282:GLY:N	2.34	0.54
1:B:147:LEU:HB3	1:B:148:LEU:CD1	2.37	0.54
1:C:152:TYR:HB3	1:C:298:PRO:HB3	1.89	0.54
1:D:279:MET:HG2	1:D:281:ASP:OD1	2.07	0.54
1:I:248:GLU:HB3	1:I:249:PHE:CD1	2.43	0.54
2:L:807:DT:H2''	2:L:808:DG:C5'	2.33	0.54
1:C:277:LEU:HB3	1:C:286:GLY:N	2.22	0.54
1:D:121:TYR:CE2	1:J:244:GLN:HB2	2.43	0.54
1:J:113:GLU:HA	1:J:113:GLU:OE2	2.07	0.54
1:B:115:ILE:HB	1:B:116:PRO:CD	2.37	0.54
1:B:263:VAL:HG13	1:B:264:GLY:N	2.22	0.54
1:C:144:TYR:CE2	1:C:146:PRO:HA	2.43	0.54
1:A:141:THR:OG1	1:A:142:TRP:N	2.38	0.53
1:B:188:THR:OG1	1:B:189:ASP:N	2.40	0.53
1:B:294:ILE:N	1:B:294:ILE:HD12	2.23	0.53
1:C:178:MET:HG3	1:C:179:PRO:HD2	1.91	0.53
1:D:156:ALA:HB1	1:D:203:PHE:CE2	2.43	0.53
1:D:276:THR:HG22	1:D:287:ARG:HG2	1.90	0.53
1:I:178:MET:HB2	1:I:235:SER:HB3	1.90	0.53
1:I:256:PHE:N	1:I:256:PHE:CD2	2.74	0.53
1:J:256:PHE:CD2	1:J:294:ILE:HD11	2.42	0.53
1:A:125:HIS:HB3	1:A:165:VAL:HG23	1.90	0.53
1:B:213:HIS:HE1	1:B:235:SER:C	2.12	0.53
1:B:274:ILE:O	1:B:274:ILE:HG13	2.08	0.53
1:B:285:LEU:N	1:B:285:LEU:CD1	2.69	0.53
1:D:263:VAL:C	1:D:265:GLY:H	2.10	0.53
1:J:198:GLU:C	1:J:200:GLY:H	2.10	0.53
1:B:301:ASP:OD1	1:B:304:ALA:CB	2.57	0.53
1:B:300:ARG:C	1:B:302:ARG:H	2.11	0.53
1:C:143:THR:HG22	1:C:298:PRO:HB2	1.91	0.53
1:A:152:TYR:HB2	1:A:298:PRO:HB3	1.90	0.53
1:A:266:MET:O	1:A:269:ARG:CD	2.57	0.53
1:B:272:LEU:HD23	1:B:272:LEU:O	2.08	0.53
1:C:263:VAL:HB	1:D:196:ASN:HD22	1.73	0.53
1:I:147:LEU:O	1:I:148:LEU:HD23	2.09	0.53
1:J:202:ASP:OD1	1:J:203:PHE:N	2.41	0.53
1:A:125:HIS:HB3	1:A:165:VAL:CG2	2.38	0.53
1:C:202:ASP:C	1:C:204:ASN:H	2.12	0.53
1:C:301:ASP:O	1:C:304:ALA:HB3	2.09	0.53
1:D:127:PHE:CE1	1:D:163:ILE:HG23	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:261:SER:HA	1:I:268:ARG:H	1.73	0.53
1:I:138:LYS:HG2	2:L:802:DG:C2'	2.39	0.53
1:A:266:MET:HA	1:A:269:ARG:HD3	1.90	0.53
1:B:122:PRO:HG2	1:B:123:GLY:N	2.24	0.53
2:G:612:DC:H2''	2:G:613:DC:OP2	2.09	0.53
1:I:146:PRO:HD2	1:I:147:LEU:H	1.73	0.53
1:D:127:PHE:CD2	1:D:277:LEU:HB2	2.44	0.53
2:E:410:DG:C8	2:E:411:DT:H72	2.43	0.53
1:B:142:TRP:C	1:B:143:THR:HG22	2.29	0.53
1:C:213:HIS:HA	1:C:234:GLN:OE1	2.09	0.53
1:I:128:GLU:HB2	1:I:164:LYS:HB2	1.91	0.53
1:I:210:PRO:HD2	1:I:225:TYR:CD2	2.43	0.53
1:J:201:ARG:HG2	1:J:202:ASP:N	2.23	0.53
1:J:279:MET:CG	1:J:285:LEU:HD21	2.38	0.53
1:A:279:MET:CG	1:A:285:LEU:HD21	2.29	0.52
1:B:310:ARG:HG2	1:B:311:GLU:O	2.09	0.52
1:D:121:TYR:HD1	1:D:122:PRO:CD	2.22	0.52
1:I:136:THR:HG22	1:I:137:ALA:H	1.74	0.52
1:I:141:THR:O	1:I:154:GLN:HB2	2.08	0.52
1:A:135:SER:HB2	1:A:140:ALA:HB1	1.91	0.52
1:B:240:TYR:HE1	1:B:250:THR:HG21	1.75	0.52
1:C:135:SER:C	1:C:137:ALA:H	2.12	0.52
1:C:190:VAL:HA	1:C:233:ARG:NH1	2.24	0.52
1:D:287:ARG:O	1:D:287:ARG:HD2	2.09	0.52
2:G:602:DA:H2'	2:G:603:DT:H71	1.90	0.52
1:B:244:GLN:HB2	1:B:248:GLU:HG2	1.92	0.52
1:C:144:TYR:CZ	1:C:146:PRO:HA	2.44	0.52
1:C:163:ILE:O	1:C:250:THR:HG23	2.10	0.52
1:D:193:ARG:HD3	1:D:257:MET:O	2.10	0.52
1:J:144:TYR:CG	1:J:145:SER:N	2.78	0.52
1:J:254:TYR:C	1:J:255:ASN:HD22	2.12	0.52
1:J:261:SER:O	1:J:262:CYS:C	2.47	0.52
1:B:179:PRO:C	1:B:191:VAL:HG21	2.30	0.52
1:C:306:GLU:O	1:C:310:ARG:CB	2.50	0.52
1:I:177:ALA:CB	1:I:254:TYR:HE2	2.23	0.52
1:J:158:THR:CG2	1:J:253:LEU:HB3	2.40	0.52
1:J:238:VAL:HG23	1:J:239:PRO:HD2	1.91	0.52
1:C:164:LYS:HD3	1:C:248:GLU:HB2	1.91	0.52
1:C:152:TYR:HB3	1:C:298:PRO:CB	2.39	0.52
1:D:172:GLY:HA3	1:D:280:ARG:CB	2.40	0.52
1:A:207:GLN:NE2	1:A:216:ARG:HH11	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:HIS:CG	1:D:126:HIS:O	2.62	0.52
1:J:193:ARG:NE	1:J:257:MET:O	2.42	0.52
1:A:186:HIS:ND1	1:A:269:ARG:NE	2.57	0.52
2:L:802:DG:H2"	2:L:803:DG:C8	2.45	0.52
1:C:210:PRO:HB2	1:C:213:HIS:HD2	1.75	0.51
1:D:125:HIS:C	1:D:166:SER:HB3	2.30	0.51
1:I:175:ILE:HD13	1:I:277:LEU:HA	1.91	0.51
1:A:155:ILE:O	1:A:155:ILE:CG2	2.58	0.51
1:B:207:GLN:C	1:B:209:ALA:N	2.64	0.51
1:B:198:GLU:HG3	1:B:211:ALA:O	2.10	0.51
1:C:210:PRO:HB2	1:C:213:HIS:CD2	2.44	0.51
1:D:145:SER:HB2	1:D:302:ARG:HD2	1.92	0.51
1:I:158:THR:HG23	1:I:218:GLU:OE1	2.10	0.51
1:I:309:TYR:HD1	1:I:309:TYR:C	2.14	0.51
1:J:150:LYS:HD3	1:J:291:GLU:CD	2.31	0.51
1:B:169:PRO:O	1:B:170:PRO:O	2.28	0.51
1:B:249:PHE:N	1:B:249:PHE:CD2	2.77	0.51
1:B:152:TYR:CE2	1:B:301:ASP:HB3	2.46	0.51
1:C:126:HIS:HD2	1:C:128:GLU:HG2	1.76	0.51
1:I:140:ALA:O	1:I:142:TRP:N	2.43	0.51
1:I:243:PRO:CB	1:I:246:GLY:HA3	2.40	0.51
1:J:266:MET:O	1:J:269:ARG:HG3	2.10	0.51
1:A:189:ASP:OD2	1:A:269:ARG:NH2	2.44	0.51
1:B:125:HIS:O	1:B:127:PHE:N	2.44	0.51
1:B:231:THR:OG1	1:B:233:ARG:HG2	2.10	0.51
2:G:603:DT:H2"	2:G:604:DG:C8	2.45	0.51
1:B:210:PRO:HD2	1:B:225:TYR:CD1	2.46	0.51
1:D:127:PHE:HB2	1:D:277:LEU:HD22	1.92	0.51
1:D:237:VAL:CG1	1:D:238:VAL:N	2.73	0.51
1:I:179:PRO:O	1:I:191:VAL:HG11	2.10	0.51
1:I:244:GLN:HG2	1:I:245:VAL:N	2.25	0.51
1:J:117:SER:O	1:J:287:ARG:HD2	2.11	0.51
1:A:217:VAL:HG23	1:A:236:VAL:CG2	2.39	0.51
1:A:310:ARG:HD3	1:A:310:ARG:C	2.31	0.51
1:C:117:SER:HB2	1:C:287:ARG:CZ	2.39	0.51
1:J:263:VAL:HG22	1:J:264:GLY:N	2.25	0.51
1:C:187:VAL:CG1	1:C:188:THR:N	2.74	0.51
1:C:238:VAL:HB	1:C:239:PRO:HD2	1.93	0.51
1:I:198:GLU:O	1:I:211:ALA:HB1	2.10	0.51
1:I:209:ALA:HB2	1:I:216:ARG:HE	1.75	0.51
1:I:243:PRO:CB	1:I:246:GLY:CA	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:278:GLU:OE1	1:J:282:GLY:HA2	2.11	0.51
1:B:240:TYR:CE2	1:B:242:PRO:HG3	2.46	0.51
1:C:259:ASN:ND2	1:C:295:CYS:HA	2.25	0.51
1:A:207:GLN:OE1	1:A:209:ALA:HB3	2.11	0.51
1:B:151:LEU:HD12	1:B:152:TYR:N	2.24	0.51
1:B:240:TYR:CE1	1:B:250:THR:HG21	2.46	0.51
1:J:127:PHE:CD2	1:J:286:GLY:HA3	2.43	0.51
1:A:220:ASN:HD22	1:A:238:VAL:CG2	2.23	0.50
1:A:118:ASN:HD21	1:A:272:LEU:HD22	1.74	0.50
1:J:274:ILE:HD12	1:J:274:ILE:N	2.26	0.50
1:B:163:ILE:O	1:B:249:PHE:O	2.30	0.50
1:D:241:GLU:O	1:D:250:THR:CG2	2.59	0.50
1:I:157:LYS:HE3	1:I:157:LYS:HA	1.93	0.50
1:I:213:HIS:HA	1:I:234:GLN:OE1	2.12	0.50
1:I:177:ALA:CB	1:I:254:TYR:CE2	2.94	0.50
1:J:179:PRO:O	1:J:191:VAL:HG21	2.12	0.50
1:C:121:TYR:CE1	1:C:123:GLY:HA2	2.47	0.50
1:C:167:THR:HB	1:C:168:PRO:HD2	1.93	0.50
1:D:222:LEU:O	1:D:224:GLN:HG3	2.12	0.50
1:I:142:TRP:HB3	1:I:153:CYS:HA	1.93	0.50
1:B:144:TYR:HE1	1:B:146:PRO:HA	1.76	0.50
1:D:214:LEU:O	1:D:214:LEU:HD22	2.10	0.50
2:F:512:DA:OP2	2:F:512:DA:C8	2.58	0.50
1:B:127:PHE:HE1	1:B:163:ILE:HG23	1.77	0.50
1:C:279:MET:O	1:C:282:GLY:N	2.43	0.50
1:C:216:ARG:NE	1:C:257:MET:HG2	2.26	0.50
1:I:214:LEU:HG	1:I:214:LEU:O	2.12	0.50
2:K:906:DA:H2"	2:K:907:DC:C6	2.47	0.50
1:A:135:SER:HB2	1:A:140:ALA:CB	2.41	0.50
1:A:263:VAL:CG1	1:A:264:GLY:H	2.21	0.50
1:D:138:LYS:HG2	2:H:702:DG:OP2	2.11	0.50
1:I:161:ILE:HD11	1:I:254:TYR:CG	2.46	0.50
1:A:253:LEU:HD23	1:A:253:LEU:N	2.26	0.50
1:B:216:ARG:HG3	1:B:225:TYR:CE2	2.46	0.50
1:B:129:VAL:CG2	1:B:288:ARG:HD2	2.42	0.50
1:D:173:THR:HG22	1:D:240:TYR:HB2	1.94	0.50
1:A:174:ALA:HB1	1:A:238:VAL:O	2.11	0.50
1:A:165:VAL:HG22	1:A:167:THR:O	2.12	0.49
1:A:195:PRO:HD2	1:A:264:GLY:HA3	1.94	0.49
1:B:148:LEU:N	1:B:148:LEU:CD1	2.74	0.49
1:B:173:THR:HG22	1:B:240:TYR:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ASN:HD22	1:B:204:ASN:C	2.14	0.49
1:C:135:SER:O	1:C:137:ALA:N	2.45	0.49
1:D:201:ARG:CD	1:D:201:ARG:N	2.74	0.49
1:I:122:PRO:HA	1:I:288:ARG:HH21	1.76	0.49
1:B:163:ILE:HD13	1:B:175:ILE:HD13	1.93	0.49
1:B:280:ARG:HG3	1:B:281:ASP:H	1.77	0.49
1:D:276:THR:HA	1:D:287:ARG:HB3	1.92	0.49
1:D:121:TYR:HB3	1:D:287:ARG:N	2.27	0.49
1:D:293:ARG:NE	1:D:295:CYS:SG	2.86	0.49
1:I:306:GLU:O	1:I:310:ARG:HB2	2.12	0.49
1:C:150:LYS:HE2	1:C:152:TYR:CZ	2.48	0.49
1:D:123:GLY:O	1:D:126:HIS:N	2.42	0.49
1:I:118:ASN:HA	1:I:274:ILE:CD1	2.42	0.49
1:I:279:MET:N	1:I:283:GLN:O	2.35	0.49
1:B:192:LYS:HG2	1:B:234:GLN:HE21	1.77	0.49
1:C:116:PRO:HB3	1:C:178:MET:HE3	1.94	0.49
1:I:146:PRO:CD	1:I:147:LEU:N	2.75	0.49
1:J:121:TYR:CE1	1:J:123:GLY:HA2	2.47	0.49
1:J:213:HIS:HA	1:J:234:GLN:OE1	2.13	0.49
1:D:259:ASN:CA	1:D:294:ILE:HB	2.40	0.49
1:J:194:CYS:O	1:J:195:PRO:C	2.49	0.49
1:J:240:TYR:OH	1:J:243:PRO:HD3	2.12	0.49
1:A:194:CYS:SG	1:A:196:ASN:HB3	2.52	0.49
1:B:266:MET:HE1	1:B:271:ILE:HG21	1.94	0.49
1:D:164:LYS:HG2	1:D:165:VAL:N	2.28	0.49
1:D:276:THR:HG22	1:D:287:ARG:CB	2.43	0.49
1:D:117:SER:HA	1:J:241:GLU:OE2	2.12	0.49
1:J:277:LEU:HD12	1:J:285:LEU:HD12	1.95	0.49
1:A:312:GLN:OE1	1:A:312:GLN:HA	2.13	0.49
1:D:259:ASN:HA	1:D:294:ILE:CG2	2.43	0.49
1:I:244:GLN:CD	1:I:245:VAL:HG23	2.33	0.49
1:A:263:VAL:CG1	1:A:264:GLY:N	2.74	0.49
1:B:204:ASN:C	1:B:204:ASN:ND2	2.66	0.49
1:B:266:MET:HE3	1:B:271:ILE:HG21	1.93	0.49
1:B:279:MET:CG	1:B:283:GLN:HB3	2.39	0.49
1:C:135:SER:C	1:C:137:ALA:N	2.66	0.49
1:C:277:LEU:HD12	1:C:285:LEU:HD12	1.95	0.49
1:C:121:TYR:CE2	1:C:285:LEU:O	2.65	0.49
1:D:279:MET:HG3	1:D:280:ARG:N	2.24	0.49
2:H:712:DA:H8	2:H:712:DA:OP2	1.96	0.49
1:J:237:VAL:HG13	1:J:238:VAL:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:902:DA:C2	2:K:903:DT:C2	3.01	0.49
1:A:134:SER:O	1:A:136:THR:N	2.44	0.48
1:A:160:PRO:HA	1:A:253:LEU:HA	1.94	0.48
1:B:280:ARG:HG3	1:B:281:ASP:N	2.27	0.48
1:D:154:GLN:HA	1:D:295:CYS:O	2.13	0.48
2:G:614:DA:H1'	2:G:615:DT:C5'	2.42	0.48
1:J:194:CYS:C	1:J:196:ASN:H	2.14	0.48
1:A:150:LYS:HB2	1:A:291:GLU:HB3	1.94	0.48
1:B:293:ARG:NH2	2:E:409:DT:P	2.86	0.48
1:I:164:LYS:O	1:I:165:VAL:HG22	2.13	0.48
1:A:112:HIS:C	1:A:112:HIS:CD2	2.85	0.48
1:A:121:TYR:O	1:A:286:GLY:HA2	2.13	0.48
1:D:299:GLY:O	1:D:303:LYS:HB2	2.14	0.48
1:I:203:PHE:O	1:I:207:GLN:HB2	2.13	0.48
1:B:209:ALA:HB3	1:B:216:ARG:HD2	1.96	0.48
1:D:256:PHE:HD2	1:D:294:ILE:HD11	1.79	0.48
1:A:142:TRP:HB3	1:A:153:CYS:HA	1.94	0.48
1:A:296:ALA:O	1:A:297:CYS:HB2	2.13	0.48
1:I:193:ARG:NE	1:I:197:HIS:HB3	2.28	0.48
2:K:904:DG:H2''	2:K:905:DG:H8	1.75	0.48
1:A:179:PRO:O	1:A:191:VAL:CG2	2.58	0.48
1:A:190:VAL:O	1:A:191:VAL:C	2.51	0.48
1:A:220:ASN:ND2	1:A:238:VAL:CG2	2.77	0.48
1:A:233:ARG:HA	1:A:233:ARG:HD3	1.60	0.48
1:C:146:PRO:HD2	1:C:302:ARG:NH1	2.28	0.48
1:C:197:HIS:O	1:C:198:GLU:C	2.52	0.48
1:J:226:VAL:HG12	1:J:227:ASP:N	2.29	0.48
1:A:216:ARG:HA	1:A:225:TYR:HE2	1.79	0.48
1:A:238:VAL:HG23	1:A:239:PRO:HD2	1.95	0.48
1:C:111:HIS:HB2	1:C:112:HIS:HD2	1.77	0.48
1:I:138:LYS:CE	1:I:299:GLY:HA3	2.43	0.48
1:J:210:PRO:HB2	1:J:213:HIS:HD2	1.78	0.48
1:A:167:THR:HB	1:A:168:PRO:CD	2.43	0.48
1:B:291:GLU:HG2	1:B:292:GLY:N	2.29	0.48
1:C:218:GLU:HB2	1:C:255:ASN:OD1	2.13	0.48
1:D:145:SER:O	1:D:149:LYS:N	2.46	0.48
1:D:272:LEU:HA	1:D:291:GLU:HA	1.96	0.48
2:G:602:DA:C2	2:H:713:DT:O2	2.67	0.48
1:I:115:ILE:N	1:I:116:PRO:HD3	2.28	0.48
1:I:125:HIS:N	1:I:125:HIS:ND1	2.61	0.48
1:I:195:PRO:HG2	1:I:196:ASN:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:225:TYR:O	1:J:226:VAL:HG23	2.13	0.48
1:J:277:LEU:HB3	1:J:286:GLY:H	1.79	0.48
1:A:214:LEU:O	1:A:257:MET:HG2	2.13	0.48
1:C:140:ALA:O	1:C:141:THR:C	2.52	0.48
1:D:123:GLY:C	1:D:125:HIS:N	2.66	0.48
1:D:125:HIS:HD2	1:D:125:HIS:N	2.09	0.48
1:D:220:ASN:OD1	1:D:222:LEU:HB3	2.14	0.48
1:B:244:GLN:HB2	1:B:248:GLU:CG	2.43	0.48
1:C:127:PHE:CD2	1:C:277:LEU:HD23	2.49	0.48
1:C:145:SER:CA	1:C:302:ARG:HH11	2.20	0.48
1:I:163:ILE:O	1:I:249:PHE:CB	2.61	0.48
1:J:142:TRP:HA	1:J:152:TYR:O	2.14	0.48
1:D:117:SER:HB3	1:J:241:GLU:HG3	1.96	0.47
1:D:259:ASN:N	1:D:262:CYS:SG	2.87	0.47
1:I:263:VAL:HG13	1:I:267:ASN:HD21	1.79	0.47
1:I:263:VAL:CG1	1:I:264:GLY:N	2.77	0.47
1:J:201:ARG:HE	1:J:202:ASP:H	1.62	0.47
1:B:115:ILE:N	1:B:115:ILE:HD13	2.29	0.47
1:B:179:PRO:HG2	1:B:191:VAL:HB	1.96	0.47
1:B:172:GLY:HA3	1:B:280:ARG:HB3	1.95	0.47
1:C:134:SER:O	1:C:136:THR:N	2.47	0.47
1:D:249:PHE:N	1:D:249:PHE:CD1	2.79	0.47
1:I:210:PRO:HD2	1:I:225:TYR:CG	2.49	0.47
1:A:151:LEU:HD12	1:A:290:PHE:CD2	2.49	0.47
1:A:220:ASN:C	1:A:222:LEU:H	2.16	0.47
1:C:193:ARG:NE	1:C:257:MET:HB3	2.29	0.47
1:J:298:PRO:O	1:J:300:ARG:N	2.48	0.47
1:D:160:PRO:HA	1:D:252:ILE:O	2.14	0.47
1:I:151:LEU:HG	1:I:152:TYR:N	2.29	0.47
1:I:209:ALA:CB	1:I:216:ARG:HE	2.27	0.47
1:D:284:VAL:O	1:J:245:VAL:HG23	2.14	0.47
1:C:228:ASP:HB3	1:C:233:ARG:H	1.80	0.47
1:D:227:ASP:O	1:D:228:ASP:C	2.52	0.47
1:I:195:PRO:O	1:I:198:GLU:HB3	2.15	0.47
1:I:311:GLU:O	1:I:312:GLN:OXT	2.32	0.47
1:J:280:ARG:C	1:J:282:GLY:H	2.18	0.47
1:B:187:VAL:HG12	1:B:188:THR:N	2.29	0.47
1:B:252:ILE:HG22	1:B:253:LEU:H	1.76	0.47
1:A:131:PHE:CZ	1:A:151:LEU:HG	2.49	0.47
1:B:163:ILE:CG2	1:B:164:LYS:N	2.77	0.47
1:B:263:VAL:HG12	1:B:264:GLY:N	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:LEU:H	1:B:272:LEU:HD23	1.80	0.47
1:B:305:ASP:OD1	1:B:305:ASP:C	2.53	0.47
1:D:190:VAL:CG2	1:D:191:VAL:N	2.77	0.47
2:G:602:DA:C2	2:G:603:DT:C2	3.03	0.47
1:J:127:PHE:CD1	1:J:128:GLU:N	2.83	0.47
1:B:272:LEU:CA	1:B:291:GLU:HA	2.40	0.47
1:C:138:LYS:HG2	1:C:139:SER:N	2.30	0.47
1:C:156:ALA:O	1:C:255:ASN:ND2	2.48	0.47
1:D:248:GLU:C	1:D:249:PHE:HD1	2.18	0.47
2:E:405:DG:H2"	2:E:406:DA:C8	2.50	0.47
1:J:259:ASN:HA	1:J:294:ILE:CG2	2.44	0.47
1:D:152:TYR:N	1:D:152:TYR:CD1	2.82	0.47
1:D:218:GLU:O	1:D:253:LEU:HB2	2.14	0.47
1:I:252:ILE:HG22	1:I:253:LEU:N	2.30	0.47
1:J:170:PRO:HG3	1:J:279:MET:SD	2.54	0.47
1:B:131:PHE:HD2	1:B:142:TRP:CZ3	2.27	0.47
1:B:259:ASN:HA	1:B:294:ILE:HB	1.97	0.47
1:C:214:LEU:CD1	1:C:258:CYS:HB2	2.45	0.47
1:D:151:LEU:HD22	1:D:290:PHE:CE1	2.50	0.47
1:D:191:VAL:O	1:D:191:VAL:HG13	2.13	0.47
1:D:248:GLU:C	1:D:249:PHE:CD1	2.89	0.47
1:J:181:TYR:CD1	1:J:269:ARG:HD2	2.50	0.46
1:A:118:ASN:ND2	1:A:272:LEU:HD22	2.31	0.46
1:B:226:VAL:HG12	1:B:227:ASP:N	2.30	0.46
1:B:263:VAL:C	1:B:265:GLY:N	2.63	0.46
1:D:179:PRO:O	1:D:191:VAL:HG11	2.15	0.46
1:D:291:GLU:HG2	1:D:292:GLY:H	1.79	0.46
1:D:310:ARG:HH21	1:J:206:GLY:H	1.62	0.46
1:I:125:HIS:CG	1:I:167:THR:HB	2.50	0.46
1:I:246:GLY:O	1:I:247:THR:C	2.54	0.46
1:J:184:ALA:HA	1:J:187:VAL:HG23	1.97	0.46
1:J:225:TYR:O	1:J:226:VAL:CG2	2.63	0.46
1:A:129:VAL:O	1:A:129:VAL:HG12	2.15	0.46
1:B:121:TYR:CD1	1:B:122:PRO:HD2	2.35	0.46
1:B:243:PRO:HB2	1:B:245:VAL:H	1.80	0.46
1:I:224:GLN:O	1:I:225:TYR:C	2.53	0.46
1:I:212:SER:OG	1:I:234:GLN:NE2	2.47	0.46
1:J:199:LEU:HA	1:J:199:LEU:HD23	1.52	0.46
1:A:178:MET:HB2	1:A:235:SER:CB	2.45	0.46
1:A:130:THR:HG21	1:A:249:PHE:CZ	2.50	0.46
1:D:125:HIS:H	1:D:125:HIS:CD2	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:ASN:OD1	1:D:195:PRO:HG2	2.14	0.46
2:F:507:DT:H2"	2:F:508:DG:OP2	2.15	0.46
1:A:240:TYR:OH	1:A:243:PRO:HD3	2.14	0.46
1:B:118:ASN:N	1:B:118:ASN:ND2	2.61	0.46
1:B:113:GLU:HG3	1:B:231:THR:HA	1.98	0.46
1:C:127:PHE:CE2	1:C:277:LEU:HB2	2.51	0.46
1:J:300:ARG:HB3	1:J:300:ARG:HE	1.32	0.46
1:I:122:PRO:CD	1:I:123:GLY:H	2.28	0.46
1:I:193:ARG:HE	1:I:197:HIS:HB3	1.80	0.46
1:J:217:VAL:HG22	1:J:254:TYR:HE1	1.80	0.46
1:J:259:ASN:ND2	1:J:294:ILE:HG22	2.30	0.46
1:A:266:MET:O	1:A:267:ASN:C	2.54	0.46
1:B:115:ILE:CD1	1:B:115:ILE:H	2.29	0.46
1:B:144:TYR:CE1	1:B:146:PRO:HA	2.50	0.46
1:C:228:ASP:OD1	1:C:230:VAL:HG23	2.15	0.46
2:H:706:DA:H2"	2:H:707:DT:C5'	2.35	0.46
1:J:169:PRO:HB2	1:J:170:PRO:HD2	1.98	0.46
1:A:170:PRO:HA	1:A:171:PRO:HD2	1.79	0.46
2:G:614:DA:H2"	2:G:615:DT:OP2	2.14	0.46
1:I:246:GLY:C	1:I:248:GLU:N	2.64	0.46
1:J:237:VAL:CG1	1:J:238:VAL:N	2.79	0.46
1:A:193:ARG:NE	1:A:257:MET:CB	2.59	0.46
1:A:151:LEU:HD12	1:A:290:PHE:HD2	1.81	0.46
1:A:152:TYR:OH	1:A:302:ARG:HA	2.16	0.46
1:B:284:VAL:C	1:B:285:LEU:HD12	2.36	0.46
1:B:294:ILE:HD12	1:B:294:ILE:H	1.81	0.46
1:D:127:PHE:CE2	1:D:277:LEU:HB2	2.51	0.46
1:J:131:PHE:CE1	1:J:144:TYR:CE2	3.03	0.46
1:B:127:PHE:HD2	1:B:286:GLY:HA3	1.81	0.46
1:D:122:PRO:HA	1:D:288:ARG:HH21	1.79	0.46
1:I:138:LYS:HZ3	1:I:139:SER:H	1.64	0.46
1:I:143:THR:HG22	1:I:298:PRO:CB	2.42	0.46
1:I:184:ALA:O	1:I:185:GLU:C	2.54	0.46
1:J:175:ILE:CD1	1:J:240:TYR:HA	2.46	0.46
2:K:907:DC:H1'	2:K:908:DA:C8	2.51	0.46
1:B:129:VAL:CG2	1:B:288:ARG:HB3	2.42	0.45
1:D:256:PHE:CD2	1:D:294:ILE:HD11	2.51	0.45
2:E:402:DA:N9	2:E:403:DT:H72	2.32	0.45
1:B:260:SER:HA	1:B:266:MET:HE2	1.97	0.45
1:C:202:ASP:OD1	1:C:203:PHE:N	2.49	0.45
1:C:279:MET:SD	1:C:285:LEU:HD21	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:GLN:HE21	1:J:245:VAL:HG21	1.79	0.45
1:I:172:GLY:HA3	1:I:280:ARG:HB3	1.98	0.45
1:J:193:ARG:HD2	1:J:211:ALA:O	2.16	0.45
1:B:115:ILE:HB	1:B:116:PRO:HD3	1.98	0.45
1:B:197:HIS:O	1:B:198:GLU:C	2.53	0.45
1:D:150:LYS:HA	1:D:291:GLU:O	2.15	0.45
1:J:198:GLU:C	1:J:200:GLY:N	2.70	0.45
1:J:170:PRO:CG	1:J:279:MET:SD	3.03	0.45
1:A:118:ASN:C	1:A:118:ASN:OD1	2.54	0.45
1:A:125:HIS:NE2	1:A:170:PRO:HD3	2.31	0.45
1:A:150:LYS:CB	1:A:291:GLU:HB3	2.46	0.45
1:B:176:ARG:HG3	1:B:237:VAL:CG2	2.23	0.45
1:B:228:ASP:HB3	1:B:231:THR:H	1.82	0.45
1:C:201:ARG:HH21	1:C:202:ASP:CB	2.24	0.45
1:D:121:TYR:CB	1:D:286:GLY:HA2	2.42	0.45
2:E:409:DT:H2"	2:E:410:DG:OP2	2.17	0.45
2:G:606:DA:H2"	2:G:607:DC:H6	1.82	0.45
1:J:148:LEU:C	1:J:149:LYS:HG3	2.36	0.45
1:J:198:GLU:O	1:J:200:GLY:N	2.50	0.45
1:A:273:ILE:O	1:A:289:SER:HA	2.16	0.45
1:B:258:CYS:CB	1:B:262:CYS:SG	2.95	0.45
1:C:179:PRO:HD3	1:C:215:ILE:HD12	1.99	0.45
1:C:259:ASN:HD22	1:C:295:CYS:HA	1.81	0.45
1:D:255:ASN:C	1:D:256:PHE:CD1	2.83	0.45
1:D:283:GLN:HG2	1:J:245:VAL:HG21	1.98	0.45
1:B:200:GLY:C	1:B:202:ASP:N	2.66	0.45
1:B:150:LYS:HD2	1:B:291:GLU:CD	2.37	0.45
1:C:154:GLN:HE21	1:C:296:ALA:HA	1.82	0.45
1:C:152:TYR:OH	1:C:305:ASP:OD2	2.25	0.45
1:I:236:VAL:O	1:I:236:VAL:HG23	2.16	0.45
1:J:150:LYS:HG2	1:J:152:TYR:CE1	2.52	0.45
1:A:140:ALA:O	1:A:141:THR:C	2.55	0.45
1:A:144:TYR:CZ	1:A:146:PRO:HA	2.51	0.45
1:B:197:HIS:HB3	1:B:257:MET:HE1	1.99	0.45
1:C:271:ILE:C	1:C:271:ILE:HD13	2.37	0.45
1:J:125:HIS:NE2	1:J:169:PRO:HA	2.32	0.45
1:J:296:ALA:HB3	2:L:809:DT:C7	2.43	0.45
1:B:193:ARG:HD3	1:B:257:MET:HE3	1.99	0.45
1:C:145:SER:CB	1:C:302:ARG:HD2	2.46	0.45
1:D:187:VAL:HG13	1:D:188:THR:N	2.32	0.45
1:D:207:GLN:HG2	1:D:216:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:252:ILE:CG2	1:I:253:LEU:N	2.80	0.45
1:I:156:ALA:N	1:I:256:PHE:O	2.43	0.45
1:I:289:SER:O	1:I:290:PHE:HB3	2.16	0.45
1:J:194:CYS:N	1:J:258:CYS:SG	2.88	0.45
1:C:112:HIS:N	1:C:112:HIS:CD2	2.85	0.45
1:C:120:ASP:CB	1:C:288:ARG:HA	2.47	0.45
1:D:161:ILE:HG13	1:D:161:ILE:O	2.16	0.45
1:I:122:PRO:HB3	1:I:288:ARG:NH2	2.32	0.45
1:I:188:THR:CG2	1:I:189:ASP:H	2.29	0.45
1:A:135:SER:O	1:A:140:ALA:HB2	2.17	0.44
1:C:184:ALA:HA	1:C:187:VAL:HB	1.99	0.44
1:D:244:GLN:HA	1:D:244:GLN:OE1	2.17	0.44
2:G:605:DG:C6	2:G:606:DA:N6	2.85	0.44
1:A:307:ASP:C	1:A:309:TYR:N	2.69	0.44
1:B:194:CYS:HB2	1:B:263:VAL:O	2.17	0.44
1:B:122:PRO:HA	1:B:288:ARG:HH21	1.82	0.44
1:D:174:ALA:CA	1:D:239:PRO:HA	2.44	0.44
1:I:153:CYS:HB2	1:I:159:CYS:SG	2.58	0.44
1:A:202:ASP:O	1:A:204:ASN:N	2.51	0.44
1:B:228:ASP:HB3	1:B:232:GLY:H	1.83	0.44
1:B:244:GLN:HG3	1:B:244:GLN:O	2.17	0.44
1:C:150:LYS:HB3	1:C:152:TYR:CE1	2.51	0.44
1:D:131:PHE:CE2	1:D:151:LEU:HD13	2.51	0.44
2:L:801:DT:C2	2:L:802:DG:N7	2.85	0.44
1:B:195:PRO:HG2	1:B:196:ASN:ND2	2.32	0.44
1:D:161:ILE:C	1:D:161:ILE:HD12	2.38	0.44
1:J:197:HIS:O	1:J:200:GLY:N	2.42	0.44
1:B:300:ARG:HG3	1:B:300:ARG:NH1	2.32	0.44
1:C:259:ASN:C	1:C:261:SER:N	2.71	0.44
1:J:297:CYS:O	1:J:298:PRO:C	2.55	0.44
1:A:125:HIS:O	1:A:126:HIS:C	2.54	0.44
1:J:194:CYS:SG	1:J:262:CYS:CB	2.88	0.44
1:I:155:ILE:CG1	1:I:156:ALA:N	2.81	0.44
1:I:195:PRO:HG2	1:I:196:ASN:N	2.32	0.44
1:I:240:TYR:CE2	1:I:242:PRO:HA	2.53	0.44
1:I:139:SER:HB2	1:I:298:PRO:HG2	1.99	0.44
1:A:150:LYS:CE	1:A:152:TYR:CZ	3.01	0.44
1:A:220:ASN:HD22	1:A:238:VAL:HG21	1.82	0.44
1:B:192:LYS:HG2	1:B:234:GLN:NE2	2.32	0.44
1:J:178:MET:HB2	1:J:235:SER:HB3	1.99	0.44
1:B:207:GLN:C	1:B:209:ALA:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ASN:O	1:B:262:CYS:SG	2.76	0.44
1:D:310:ARG:HH21	1:J:205:GLU:HA	1.82	0.44
1:I:261:SER:O	1:I:262:CYS:C	2.56	0.44
1:I:298:PRO:O	1:I:299:GLY:C	2.56	0.44
1:J:210:PRO:O	1:J:213:HIS:HB2	2.18	0.44
2:F:500:DA:H2''	2:F:501:DT:H71	2.00	0.43
2:G:602:DA:H1'	2:G:603:DT:C5'	2.48	0.43
1:A:268:ARG:HE	1:A:268:ARG:HB2	1.46	0.43
1:B:138:LYS:HD3	1:B:139:SER:OG	2.18	0.43
2:F:507:DT:C1'	2:F:508:DG:C8	3.00	0.43
1:I:162:GLN:OE1	1:I:251:THR:HB	2.18	0.43
1:I:154:GLN:HA	1:I:295:CYS:O	2.18	0.43
1:D:165:VAL:HG12	1:D:166:SER:N	2.25	0.43
1:D:197:HIS:O	1:D:198:GLU:C	2.56	0.43
1:D:263:VAL:C	1:D:265:GLY:N	2.72	0.43
1:D:181:TYR:CZ	1:D:269:ARG:NH1	2.86	0.43
1:I:246:GLY:O	1:I:248:GLU:N	2.51	0.43
1:I:256:PHE:CD1	1:I:294:ILE:HD11	2.54	0.43
1:J:190:VAL:HG12	1:J:233:ARG:CD	2.46	0.43
1:A:289:SER:C	1:A:290:PHE:HD1	2.21	0.43
1:B:147:LEU:C	1:B:148:LEU:HD12	2.38	0.43
1:B:161:ILE:CG1	1:B:254:TYR:HD2	2.30	0.43
1:C:121:TYR:CZ	1:C:123:GLY:HA2	2.53	0.43
1:C:120:ASP:HB2	1:C:288:ARG:HA	2.00	0.43
1:I:138:LYS:HE2	1:I:299:GLY:HA3	1.99	0.43
1:A:183:LYS:HB3	1:A:185:GLU:HG3	2.00	0.43
1:A:271:ILE:HD11	1:A:273:ILE:HD12	2.00	0.43
1:B:120:ASP:OD1	1:B:288:ARG:CD	2.60	0.43
1:C:145:SER:O	1:C:149:LYS:N	2.50	0.43
1:D:277:LEU:O	1:D:284:VAL:HG13	2.19	0.43
1:I:131:PHE:CE1	1:I:144:TYR:CE1	3.07	0.43
1:I:259:ASN:HB2	1:I:262:CYS:SG	2.59	0.43
1:J:173:THR:HG22	1:J:240:TYR:HB2	1.99	0.43
1:J:296:ALA:CB	2:L:809:DT:H72	2.44	0.43
1:A:173:THR:HG23	1:A:240:TYR:HB3	1.99	0.43
1:A:220:ASN:C	1:A:222:LEU:N	2.72	0.43
1:A:281:ASP:C	1:A:281:ASP:OD1	2.57	0.43
1:A:297:CYS:N	1:A:298:PRO:CD	2.81	0.43
1:A:308:HIS:CD2	1:A:308:HIS:O	2.72	0.43
1:B:124:PRO:HG2	1:B:125:HIS:ND1	2.34	0.43
1:B:193:ARG:NH1	1:B:211:ALA:HA	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ARG:CD	1:B:257:MET:SD	3.05	0.43
1:B:259:ASN:HA	1:B:294:ILE:CB	2.48	0.43
1:B:300:ARG:C	1:B:302:ARG:N	2.72	0.43
1:C:302:ARG:O	1:C:306:GLU:HG3	2.19	0.43
1:D:237:VAL:O	1:D:238:VAL:HG12	2.18	0.43
1:I:130:THR:OG1	1:I:131:PHE:N	2.51	0.43
1:I:201:ARG:O	1:I:203:PHE:N	2.52	0.43
1:D:119:THR:OG1	1:J:241:GLU:OE1	2.31	0.43
1:J:260:SER:HA	1:J:266:MET:HE2	2.01	0.43
1:J:117:SER:HB2	1:J:287:ARG:CZ	2.49	0.43
1:B:162:GLN:HG3	1:B:251:THR:HG22	1.99	0.43
1:B:199:LEU:O	1:B:199:LEU:CD1	2.67	0.43
1:B:283:GLN:HB2	1:B:283:GLN:HE21	1.59	0.43
1:D:190:VAL:HG22	1:D:191:VAL:N	2.31	0.43
1:D:276:THR:HG22	1:D:287:ARG:CG	2.48	0.43
1:I:120:ASP:OD1	1:I:288:ARG:HA	2.18	0.43
1:J:150:LYS:HD3	1:J:291:GLU:HG2	2.01	0.43
1:J:128:GLU:HG3	1:J:288:ARG:CZ	2.48	0.43
1:A:228:ASP:HB3	1:A:233:ARG:H	1.84	0.43
1:B:178:MET:CE	1:B:274:ILE:HD11	2.44	0.43
1:C:216:ARG:HA	1:C:225:TYR:HE1	1.83	0.43
1:D:263:VAL:HG23	1:D:267:ASN:HD21	1.83	0.43
2:E:402:DA:C8	2:E:403:DT:H72	2.54	0.43
1:J:193:ARG:HB2	1:J:213:HIS:O	2.18	0.43
1:J:163:ILE:HG22	1:J:250:THR:O	2.19	0.43
1:B:240:TYR:OH	1:B:243:PRO:HD3	2.19	0.43
1:D:172:GLY:HA3	1:D:280:ARG:HB3	2.00	0.43
1:D:271:ILE:O	1:D:291:GLU:HG3	2.19	0.43
2:E:402:DA:H2"	2:E:403:DT:C7	2.49	0.43
1:A:116:PRO:HB2	1:A:180:VAL:HG21	2.00	0.43
1:C:170:PRO:O	1:C:171:PRO:C	2.56	0.43
1:D:186:HIS:CG	1:D:269:ARG:CD	3.02	0.43
1:I:280:ARG:C	1:I:282:GLY:H	2.22	0.43
1:J:135:SER:HB2	1:J:140:ALA:HB2	2.01	0.43
1:J:275:ILE:HD12	1:J:275:ILE:N	2.34	0.43
1:A:150:LYS:HE2	1:A:152:TYR:CZ	2.54	0.42
1:D:152:TYR:HB3	1:D:298:PRO:CB	2.49	0.42
1:D:202:ASP:C	1:D:204:ASN:N	2.70	0.42
1:D:279:MET:CG	1:D:281:ASP:OD1	2.67	0.42
1:I:242:PRO:O	1:I:243:PRO:C	2.57	0.42
1:J:127:PHE:CE1	1:J:163:ILE:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LYS:HD3	1:B:157:LYS:HA	1.62	0.42
1:B:263:VAL:HG13	1:B:267:ASN:HD21	1.83	0.42
1:D:291:GLU:HG2	1:D:292:GLY:N	2.34	0.42
1:J:302:ARG:HH22	1:J:303:LYS:CE	2.27	0.42
2:K:909:DT:H2''	2:K:910:DG:OP2	2.19	0.42
1:B:138:LYS:HG3	2:F:502:DG:C5'	2.49	0.42
1:C:170:PRO:HA	1:C:171:PRO:HD3	1.94	0.42
1:D:121:TYR:CG	1:D:286:GLY:HA2	2.54	0.42
1:D:237:VAL:C	1:D:238:VAL:HG12	2.39	0.42
2:F:504:DA:C2	2:F:505:DC:C2	3.08	0.42
2:G:605:DG:C6	2:G:606:DA:C6	3.06	0.42
1:I:122:PRO:HB3	1:I:288:ARG:HH21	1.84	0.42
1:I:220:ASN:HD22	1:I:220:ASN:C	2.21	0.42
1:J:154:GLN:HA	1:J:295:CYS:O	2.19	0.42
1:J:273:ILE:HG22	1:J:275:ILE:HD12	1.99	0.42
1:J:259:ASN:HA	1:J:294:ILE:HG22	2.01	0.42
1:B:240:TYR:CZ	1:B:242:PRO:HA	2.55	0.42
1:B:244:GLN:C	1:B:245:VAL:HG23	2.40	0.42
1:C:126:HIS:CD2	1:C:128:GLU:HG2	2.54	0.42
1:C:216:ARG:HD2	1:C:257:MET:CE	2.50	0.42
1:D:126:HIS:O	1:D:127:PHE:C	2.57	0.42
1:D:157:LYS:HD2	1:D:157:LYS:N	2.33	0.42
2:H:704:DA:C5	2:H:705:DC:C4	3.06	0.42
1:I:150:LYS:HE2	1:I:152:TYR:CZ	2.55	0.42
1:A:151:LEU:HD12	1:A:151:LEU:H	1.84	0.42
1:A:158:THR:HB	1:A:218:GLU:CD	2.40	0.42
1:B:149:LYS:HE3	1:B:149:LYS:HB3	1.84	0.42
1:C:145:SER:HA	1:C:146:PRO:HD2	1.75	0.42
1:D:241:GLU:O	1:D:250:THR:HG21	2.19	0.42
2:E:407:DC:H2''	2:E:408:DA:OP2	2.20	0.42
1:B:138:LYS:NZ	2:F:502:DG:H2'	2.33	0.42
1:I:150:LYS:CG	1:I:291:GLU:HB3	2.49	0.42
1:J:150:LYS:HB3	1:J:150:LYS:HE2	1.80	0.42
1:A:289:SER:C	1:A:290:PHE:CD1	2.92	0.42
1:B:115:ILE:HD13	1:B:115:ILE:H	1.84	0.42
1:B:171:PRO:O	1:B:173:THR:N	2.52	0.42
1:B:171:PRO:C	1:B:173:THR:H	2.22	0.42
1:I:129:VAL:HG21	1:I:288:ARG:HB2	2.02	0.42
1:J:128:GLU:HG3	1:J:288:ARG:HD2	2.01	0.42
1:A:140:ALA:O	1:A:298:PRO:CG	2.67	0.42
1:B:240:TYR:CE2	1:B:242:PRO:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:SER:OG	1:C:143:THR:HA	2.19	0.42
1:C:197:HIS:O	1:C:200:GLY:N	2.50	0.42
1:D:176:ARG:HB2	1:D:237:VAL:HG22	2.01	0.42
1:I:138:LYS:CE	1:I:139:SER:H	2.32	0.42
1:A:266:MET:O	1:A:269:ARG:HD2	2.20	0.42
1:A:296:ALA:C	1:A:297:CYS:SG	2.98	0.42
1:B:303:LYS:HE3	1:B:306:GLU:HG2	2.01	0.42
1:B:310:ARG:O	1:B:311:GLU:HB2	2.20	0.42
1:C:176:ARG:HB2	1:C:237:VAL:CG2	2.44	0.42
1:C:240:TYR:OH	1:C:242:PRO:HA	2.20	0.42
1:C:256:PHE:CB	1:C:294:ILE:HG12	2.50	0.42
1:D:151:LEU:HD23	1:D:151:LEU:H	1.85	0.42
1:J:239:PRO:O	1:J:240:TYR:C	2.57	0.42
1:J:273:ILE:HG22	1:J:275:ILE:CD1	2.50	0.42
1:J:121:TYR:CE2	1:J:285:LEU:O	2.72	0.42
1:A:154:GLN:HA	1:A:295:CYS:O	2.19	0.42
1:B:163:ILE:HB	1:B:250:THR:HG23	2.00	0.42
1:B:259:ASN:HA	1:B:294:ILE:HG21	2.00	0.42
1:C:144:TYR:O	1:C:302:ARG:CZ	2.68	0.42
1:D:127:PHE:CD2	1:D:277:LEU:CB	3.03	0.42
1:I:214:LEU:HD12	1:I:258:CYS:HB2	2.02	0.42
2:L:801:DT:H2"	2:L:802:DG:H8	1.84	0.42
1:A:216:ARG:HA	1:A:225:TYR:CE2	2.55	0.42
1:A:280:ARG:C	1:A:282:GLY:N	2.73	0.42
1:B:162:GLN:HG3	1:B:251:THR:CG2	2.50	0.42
1:I:220:ASN:ND2	1:I:221:ASN:N	2.58	0.42
1:A:111:HIS:HD2	1:A:111:HIS:N	2.17	0.41
1:I:257:MET:N	1:I:257:MET:SD	2.92	0.41
1:I:279:MET:SD	1:I:281:ASP:OD1	2.78	0.41
1:J:268:ARG:HG3	1:J:268:ARG:O	2.20	0.41
1:A:170:PRO:O	1:A:171:PRO:C	2.58	0.41
1:B:121:TYR:HD1	1:B:122:PRO:CD	2.23	0.41
1:B:252:ILE:O	1:B:253:LEU:HD23	2.20	0.41
1:B:150:LYS:HA	1:B:291:GLU:O	2.20	0.41
1:C:272:LEU:CD2	1:C:289:SER:HB2	2.49	0.41
2:H:712:DA:H2"	2:H:713:DT:OP2	2.20	0.41
1:I:195:PRO:HD3	1:I:264:GLY:HA3	2.02	0.41
1:A:272:LEU:HA	1:A:290:PHE:O	2.19	0.41
1:A:293:ARG:NE	1:A:301:ASP:OD2	2.52	0.41
1:B:181:TYR:CE2	1:B:269:ARG:NH1	2.88	0.41
1:C:207:GLN:HG3	1:C:216:ARG:HH12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:406:DA:H2''	2:E:407:DC:H6	1.85	0.41
1:I:180:VAL:O	1:I:271:ILE:HB	2.19	0.41
1:J:150:LYS:HD3	1:J:291:GLU:CG	2.49	0.41
1:J:178:MET:HG3	1:J:179:PRO:HD2	2.03	0.41
1:D:222:LEU:O	1:D:223:SER:C	2.58	0.41
2:F:500:DA:H1'	2:F:501:DT:C6	2.55	0.41
2:G:602:DA:H1'	2:G:603:DT:H5''	2.02	0.41
2:G:609:DT:H2''	2:G:610:DG:H8	1.86	0.41
1:J:131:PHE:CZ	1:J:144:TYR:CE1	3.08	0.41
2:K:912:DC:H2''	2:K:913:DC:C6	2.56	0.41
1:A:142:TRP:NE1	1:A:160:PRO:HD2	2.35	0.41
1:B:131:PHE:CD2	1:B:144:TYR:HB2	2.55	0.41
1:C:179:PRO:C	1:C:191:VAL:HG21	2.41	0.41
1:C:176:ARG:O	1:C:275:ILE:HA	2.19	0.41
1:D:261:SER:O	1:D:262:CYS:C	2.59	0.41
2:E:408:DA:H61	2:F:507:DT:H3	1.68	0.41
2:F:507:DT:C2	2:F:508:DG:N7	2.88	0.41
1:I:164:LYS:C	1:I:165:VAL:CG2	2.89	0.41
1:I:307:ASP:O	1:I:311:GLU:N	2.25	0.41
1:A:259:ASN:CB	1:A:294:ILE:O	2.64	0.41
1:B:122:PRO:CG	1:B:123:GLY:H	2.31	0.41
1:D:300:ARG:C	1:D:300:ARG:HD2	2.40	0.41
1:C:245:VAL:O	1:C:245:VAL:CG2	2.69	0.41
1:C:267:ASN:O	1:C:268:ARG:HB2	2.20	0.41
1:I:129:VAL:CG2	1:I:288:ARG:HB2	2.50	0.41
1:I:150:LYS:HG2	1:I:291:GLU:HB3	2.02	0.41
1:I:212:SER:HB2	1:I:234:GLN:HE22	1.84	0.41
1:J:300:ARG:O	1:J:301:ASP:C	2.59	0.41
1:A:202:ASP:C	1:A:204:ASN:N	2.74	0.41
1:A:257:MET:SD	1:A:257:MET:N	2.90	0.41
1:B:228:ASP:HA	1:B:229:PRO:HD3	1.87	0.41
1:B:261:SER:O	1:B:262:CYS:C	2.59	0.41
1:C:132:GLN:OE1	1:C:160:PRO:HG3	2.21	0.41
1:C:169:PRO:HB2	1:C:173:THR:OG1	2.21	0.41
1:I:214:LEU:HD13	1:I:266:MET:CE	2.51	0.41
1:I:119:THR:CG2	1:I:287:ARG:NH2	2.83	0.41
1:A:252:ILE:C	1:A:253:LEU:HD23	2.41	0.41
1:A:311:GLU:CG	1:A:312:GLN:H	2.34	0.41
1:B:300:ARG:O	1:B:302:ARG:N	2.54	0.41
1:C:202:ASP:C	1:C:204:ASN:N	2.74	0.41
1:C:216:ARG:HB2	1:C:255:ASN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:PRO:HG2	1:D:123:GLY:H	1.86	0.41
1:D:125:HIS:O	1:D:126:HIS:C	2.57	0.41
1:D:125:HIS:O	1:D:166:SER:N	2.53	0.41
1:J:214:LEU:O	1:J:256:PHE:HA	2.21	0.41
1:A:228:ASP:HB3	1:A:231:THR:OG1	2.21	0.41
1:A:193:ARG:NE	1:A:257:MET:HB2	2.29	0.41
1:B:171:PRO:HG2	1:B:172:GLY:H	1.86	0.41
1:B:276:THR:CG2	1:B:287:ARG:HG3	2.51	0.41
1:C:240:TYR:CG	1:C:241:GLU:N	2.89	0.41
1:I:193:ARG:CG	1:I:258:CYS:SG	3.08	0.41
1:A:197:HIS:O	1:A:198:GLU:C	2.59	0.41
1:A:176:ARG:HB3	1:A:276:THR:OG1	2.21	0.41
1:B:121:TYR:HB3	1:B:287:ARG:H	1.86	0.41
1:C:245:VAL:O	1:C:245:VAL:HG23	2.21	0.41
1:C:297:CYS:O	1:C:298:PRO:C	2.56	0.41
1:D:186:HIS:ND1	1:D:269:ARG:CD	2.81	0.41
1:D:288:ARG:HD3	1:D:288:ARG:HA	1.70	0.41
1:I:178:MET:HA	1:I:179:PRO:HD3	1.90	0.41
1:I:225:TYR:HD1	1:I:236:VAL:HG12	1.77	0.41
1:J:255:ASN:N	1:J:255:ASN:HD22	2.19	0.41
1:A:134:SER:CB	1:A:144:TYR:H	2.34	0.40
1:A:269:ARG:HA	1:A:270:PRO:HD3	1.94	0.40
1:J:167:THR:OG1	1:J:168:PRO:HD2	2.22	0.40
1:J:226:VAL:CG1	1:J:227:ASP:N	2.83	0.40
2:L:801:DT:C2	2:L:802:DG:C5	3.09	0.40
2:H:712:DA:C5	2:H:713:DT:C4	3.10	0.40
1:J:216:ARG:HG3	1:J:217:VAL:N	2.36	0.40
1:B:138:LYS:HG3	2:F:502:DG:H5"	2.03	0.40
1:C:126:HIS:HD2	1:C:128:GLU:CG	2.34	0.40
1:D:222:LEU:C	1:D:222:LEU:HD23	2.41	0.40
2:G:608:DA:C8	2:G:609:DT:C7	3.05	0.40
1:I:136:THR:HG22	1:I:138:LYS:H	1.87	0.40
1:B:224:GLN:HG2	1:I:229:PRO:HB3	2.02	0.40
1:J:220:ASN:C	1:J:222:LEU:H	2.24	0.40
1:A:297:CYS:N	1:A:298:PRO:HD2	2.36	0.40
1:B:119:THR:OG1	1:B:120:ASP:N	2.55	0.40
1:B:138:LYS:O	1:B:138:LYS:HD3	2.21	0.40
2:H:707:DT:C2'	2:H:708:DG:OP2	2.62	0.40
1:J:161:ILE:HD11	1:J:254:TYR:CE2	2.56	0.40
1:A:197:HIS:C	1:A:200:GLY:H	2.22	0.40
1:A:279:MET:O	1:A:282:GLY:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:PRO:HA	1:B:170:PRO:HD2	1.82	0.40
1:B:204:ASN:O	1:B:207:GLN:N	2.45	0.40
1:B:160:PRO:HA	1:B:252:ILE:O	2.22	0.40
1:I:244:GLN:CG	1:I:245:VAL:N	2.84	0.40
1:J:116:PRO:HG3	1:J:233:ARG:NH2	2.37	0.40
1:J:163:ILE:HG23	1:J:250:THR:HB	2.01	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	201/210 (96%)	162 (81%)	31 (15%)	8 (4%)	3	26
1	B	198/210 (94%)	150 (76%)	35 (18%)	13 (7%)	1	17
1	C	201/210 (96%)	158 (79%)	40 (20%)	3 (2%)	10	45
1	D	197/210 (94%)	152 (77%)	38 (19%)	7 (4%)	3	28
1	I	200/210 (95%)	159 (80%)	33 (16%)	8 (4%)	3	26
1	J	200/210 (95%)	161 (80%)	31 (16%)	8 (4%)	3	26
All	All	1197/1260 (95%)	942 (79%)	208 (17%)	47 (4%)	3	26

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	THR
1	B	170	PRO
1	B	243	PRO
1	B	245	VAL
1	B	248	GLU
1	I	202	ASP

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Mol	Chain	Res	Type
1	A	135	SER
1	A	137	ALA
1	B	172	GLY
1	B	189	ASP
1	C	135	SER
1	D	200	GLY
1	D	233	ARG
1	D	279	MET
1	I	165	VAL
1	J	116	PRO
1	A	171	PRO
1	A	203	PHE
1	A	297	CYS
1	B	126	HIS
1	B	233	ARG
1	B	282	GLY
1	B	301	ASP
1	C	136	THR
1	D	184	ALA
1	D	282	GLY
1	J	157	LYS
1	J	199	LEU
1	J	262	CYS
1	B	187	VAL
1	I	156	ALA
1	I	218	GLU
1	I	281	ASP
1	J	221	ASN
1	B	171	PRO
1	I	304	ALA
1	B	116	PRO
1	C	203	PHE
1	D	188	THR
1	J	301	ASP
1	I	230	VAL
1	I	155	ILE
1	A	191	VAL
1	A	190	VAL
1	D	160	PRO
1	J	187	VAL
1	J	299	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	177/186 (95%)	140 (79%)	37 (21%)	1	6
1	B	176/186 (95%)	137 (78%)	39 (22%)	1	6
1	C	178/186 (96%)	145 (82%)	33 (18%)	1	10
1	D	175/186 (94%)	139 (79%)	36 (21%)	1	7
1	I	175/186 (94%)	128 (73%)	47 (27%)	0	3
1	J	177/186 (95%)	130 (73%)	47 (27%)	0	3
All	All	1058/1116 (95%)	819 (77%)	239 (23%)	1	5

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	HIS
1	A	112	HIS
1	A	131	PHE
1	A	133	GLN
1	A	135	SER
1	A	138	LYS
1	A	147	LEU
1	A	150	LYS
1	A	151	LEU
1	A	155	ILE
1	A	160	PRO
1	A	161	ILE
1	A	185	GLU
1	A	186	HIS
1	A	187	VAL
1	A	190	VAL
1	A	194	CYS
1	A	196	ASN
1	A	199	LEU
1	A	201	ARG
1	A	224	GLN
1	A	237	VAL

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Mol	Chain	Res	Type
1	A	238	VAL
1	A	248	GLU
1	A	253	LEU
1	A	259	ASN
1	A	268	ARG
1	A	269	ARG
1	A	271	ILE
1	A	276	THR
1	A	284	VAL
1	A	288	ARG
1	A	300	ARG
1	A	302	ARG
1	A	303	LYS
1	A	309	TYR
1	A	310	ARG
1	B	112	HIS
1	B	115	ILE
1	B	118	ASN
1	B	125	HIS
1	B	128	GLU
1	B	138	LYS
1	B	143	THR
1	B	145	SER
1	B	153	CYS
1	B	155	ILE
1	B	187	VAL
1	B	188	THR
1	B	190	VAL
1	B	191	VAL
1	B	194	CYS
1	B	204	ASN
1	B	205	GLU
1	B	216	ARG
1	B	228	ASP
1	B	230	VAL
1	B	235	SER
1	B	238	VAL
1	B	248	GLU
1	B	249	PHE
1	B	251	THR
1	B	257	MET
1	B	260	SER

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Mol	Chain	Res	Type
1	B	269	ARG
1	B	271	ILE
1	B	279	MET
1	B	280	ARG
1	B	283	GLN
1	B	285	LEU
1	B	297	CYS
1	B	303	LYS
1	B	305	ASP
1	B	306	GLU
1	B	309	TYR
1	B	310	ARG
1	C	111	HIS
1	C	115	ILE
1	C	117	SER
1	C	122	PRO
1	C	135	SER
1	C	139	SER
1	C	147	LEU
1	C	148	LEU
1	C	150	LYS
1	C	160	PRO
1	C	164	LYS
1	C	188	THR
1	C	191	VAL
1	C	201	ARG
1	C	227	ASP
1	C	230	VAL
1	C	237	VAL
1	C	244	GLN
1	C	245	VAL
1	C	247	THR
1	C	248	GLU
1	C	250	THR
1	C	257	MET
1	C	258	CYS
1	C	260	SER
1	C	271	ILE
1	C	276	THR
1	C	277	LEU
1	C	283	GLN
1	C	285	LEU

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Mol	Chain	Res	Type
1	C	301	ASP
1	C	302	ARG
1	C	312	GLN
1	D	121	TYR
1	D	125	HIS
1	D	127	PHE
1	D	141	THR
1	D	143	THR
1	D	147	LEU
1	D	152	TYR
1	D	154	GLN
1	D	155	ILE
1	D	157	LYS
1	D	160	PRO
1	D	161	ILE
1	D	183	LYS
1	D	192	LYS
1	D	193	ARG
1	D	194	CYS
1	D	198	GLU
1	D	201	ARG
1	D	212	SER
1	D	214	LEU
1	D	224	GLN
1	D	238	VAL
1	D	244	GLN
1	D	249	PHE
1	D	255	ASN
1	D	256	PHE
1	D	271	ILE
1	D	272	LEU
1	D	276	THR
1	D	281	ASP
1	D	285	LEU
1	D	287	ARG
1	D	301	ASP
1	D	303	LYS
1	D	305	ASP
1	D	308	HIS
1	I	115	ILE
1	I	125	HIS
1	I	134	SER

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Mol	Chain	Res	Type
1	I	135	SER
1	I	138	LYS
1	I	148	LEU
1	I	151	LEU
1	I	153	CYS
1	I	157	LYS
1	I	158	THR
1	I	161	ILE
1	I	165	VAL
1	I	173	THR
1	I	180	VAL
1	I	182	LYS
1	I	190	VAL
1	I	194	CYS
1	I	199	LEU
1	I	201	ARG
1	I	202	ASP
1	I	205	GLU
1	I	207	GLN
1	I	214	LEU
1	I	215	ILE
1	I	220	ASN
1	I	221	ASN
1	I	222	LEU
1	I	227	ASP
1	I	235	SER
1	I	245	VAL
1	I	249	PHE
1	I	250	THR
1	I	251	THR
1	I	256	PHE
1	I	258	CYS
1	I	266	MET
1	I	268	ARG
1	I	269	ARG
1	I	271	ILE
1	I	276	THR
1	I	277	LEU
1	I	283	GLN
1	I	285	LEU
1	I	297	CYS
1	I	300	ARG

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Mol	Chain	Res	Type
1	I	309	TYR
1	I	311	GLU
1	J	113	GLU
1	J	115	ILE
1	J	117	SER
1	J	127	PHE
1	J	130	THR
1	J	131	PHE
1	J	133	GLN
1	J	134	SER
1	J	135	SER
1	J	136	THR
1	J	138	LYS
1	J	141	THR
1	J	147	LEU
1	J	148	LEU
1	J	155	ILE
1	J	162	GLN
1	J	166	SER
1	J	167	THR
1	J	179	PRO
1	J	190	VAL
1	J	191	VAL
1	J	195	PRO
1	J	201	ARG
1	J	214	LEU
1	J	216	ARG
1	J	227	ASP
1	J	233	ARG
1	J	237	VAL
1	J	238	VAL
1	J	241	GLU
1	J	244	GLN
1	J	253	LEU
1	J	256	PHE
1	J	257	MET
1	J	258	CYS
1	J	259	ASN
1	J	261	SER
1	J	262	CYS
1	J	267	ASN
1	J	268	ARG

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Mol	Chain	Res	Type
1	J	276	THR
1	J	277	LEU
1	J	293	ARG
1	J	297	CYS
1	J	300	ARG
1	J	301	ASP
1	J	311	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	196	ASN
1	A	255	ASN
1	A	259	ASN
1	A	308	HIS
1	B	118	ASN
1	B	162	GLN
1	B	196	ASN
1	B	204	ASN
1	B	244	GLN
1	B	267	ASN
1	B	283	GLN
1	C	111	HIS
1	C	112	HIS
1	C	126	HIS
1	C	154	GLN
1	C	186	HIS
1	C	213	HIS
1	C	259	ASN
1	C	308	HIS
1	D	125	HIS
1	D	207	GLN
1	D	224	GLN
1	D	267	ASN
1	D	283	GLN
1	I	204	ASN
1	I	220	ASN
1	I	255	ASN
1	J	154	GLN
1	J	186	HIS
1	J	213	HIS

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Mol	Chain	Res	Type
1	J	255	ASN
1	J	259	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	203/210 (96%)	-0.38	0 100 100	45, 74, 104, 125	3 (1%)
1	B	200/210 (95%)	-0.33	0 100 100	67, 88, 112, 123	1 (0%)
1	C	203/210 (96%)	-0.33	1 (0%) 91 85	50, 77, 103, 123	2 (0%)
1	D	199/210 (94%)	-0.20	3 (1%) 73 64	60, 87, 118, 127	2 (1%)
1	I	202/210 (96%)	-0.33	2 (0%) 82 74	57, 84, 111, 125	2 (0%)
1	J	202/210 (96%)	-0.35	0 100 100	54, 78, 108, 132	2 (0%)
2	E	14/14 (100%)	0.41	2 (14%) 2 3	76, 98, 132, 142	0
2	F	14/14 (100%)	-0.25	0 100 100	76, 104, 126, 137	0
2	G	14/14 (100%)	-0.31	0 100 100	74, 102, 142, 159	0
2	H	14/14 (100%)	-0.15	0 100 100	76, 100, 140, 151	0
2	K	13/14 (92%)	0.20	0 100 100	81, 103, 122, 137	0
2	L	13/14 (92%)	0.20	1 (7%) 13 11	90, 109, 135, 148	0
All	All	1291/1344 (96%)	-0.30	9 (0%) 87 82	45, 83, 117, 159	12 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	136	THR	4.6
1	C	281	ASP	3.2
1	I	137	ALA	2.9
1	D	283	GLN	2.9
2	E	410	DG	2.6
1	D	137	ALA	2.5
1	D	282	GLY	2.4
2	L	813	DT	2.1
2	E	415	DT	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	D	401	1/1	0.97	0.05	84,84,84,84	0
3	ZN	B	401	1/1	0.98	0.14	89,89,89,89	0
3	ZN	I	401	1/1	0.98	0.07	76,76,76,76	0
3	ZN	A	401	1/1	0.98	0.08	73,73,73,73	0
3	ZN	C	401	1/1	0.98	0.09	58,58,58,58	0
3	ZN	J	401	1/1	1.00	0.15	56,56,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.