



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:05 am GMT

PDB ID : 1FPY  
Title : CRYSTAL STRUCTURE OF GLUTAMINE SYNTHETASE FROM  
SALMONELLA TYPHIMURIUM WITH INHIBITOR PHOS-  
PHINOTHRICIN  
Authors : Gill, H.S.; Eisenberg, D.  
Deposited on : 2000-08-31  
Resolution : 2.89 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

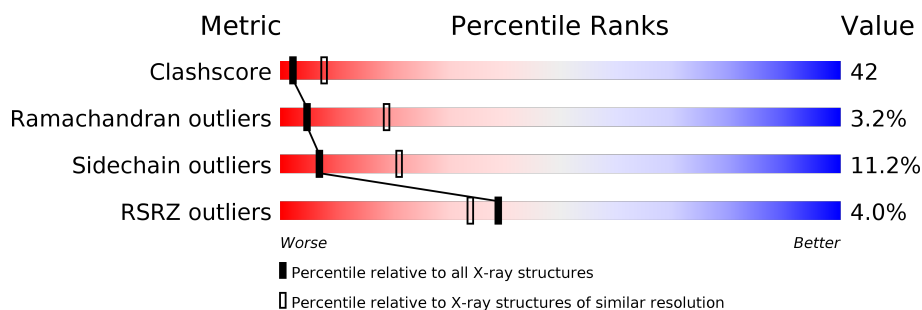
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 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))
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	468	<div> <div>6%</div> <div> <div></div> <div>50%</div> <div>41%</div> <div>8%</div> </div> </div>
1	B	468	<div> <div>4%</div> <div> <div></div> <div>52%</div> <div>40%</div> <div>8%</div> </div> </div>
1	C	468	<div> <div>4%</div> <div> <div></div> <div>50%</div> <div>41%</div> <div>8%</div> </div> </div>
1	D	468	<div> <div>4%</div> <div> <div></div> <div>51%</div> <div>40%</div> <div>8%</div> </div> </div>
1	E	468	<div> <div>4%</div> <div> <div></div> <div>50%</div> <div>41%</div> <div>8%</div> </div> </div>
1	F	468	<div> <div>5%</div> <div> <div></div> <div>52%</div> <div>40%</div> <div>8%</div> </div> </div>
1	G	468	<div> <div>4%</div> <div> <div></div> <div>51%</div> <div>41%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	H	468	
1	I	468	
1	J	468	
1	K	468	
1	L	468	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADP	C	4473	-	-	-	X
3	ADP	E	4475	-	-	-	X
3	ADP	F	4476	-	-	-	X
3	ADP	G	4477	-	-	-	X
3	ADP	H	4478	-	-	-	X
3	ADP	I	4479	-	-	-	X
3	ADP	K	4481	-	-	-	X
3	ADP	L	4482	-	-	-	X
4	PPQ	A	5900	-	-	X	-
4	PPQ	B	5901	-	-	X	-
4	PPQ	C	5902	-	-	X	-
4	PPQ	D	5903	-	-	X	-
4	PPQ	E	5904	-	-	X	-
4	PPQ	F	5905	-	-	X	-
4	PPQ	G	5906	-	-	X	-
4	PPQ	H	5907	-	-	X	-
4	PPQ	I	5908	-	-	X	-
4	PPQ	J	5909	-	-	X	-
4	PPQ	L	5911	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 47280 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 GLUTAMINE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	B	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	C	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	D	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	E	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	F	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	G	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	H	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	I	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	J	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	K	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	L	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

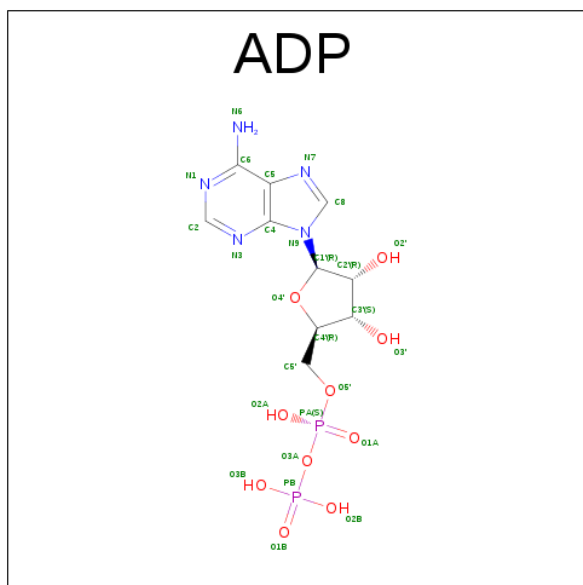
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mn	0	0
			2	2		
2	J	2	Total	Mn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Mn	0	0
			2	2		
2	K	2	Total	Mn	0	0
			2	2		
2	E	2	Total	Mn	0	0
			2	2		
2	H	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	I	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		
2	L	2	Total	Mn	0	0
			2	2		
2	F	2	Total	Mn	0	0
			2	2		

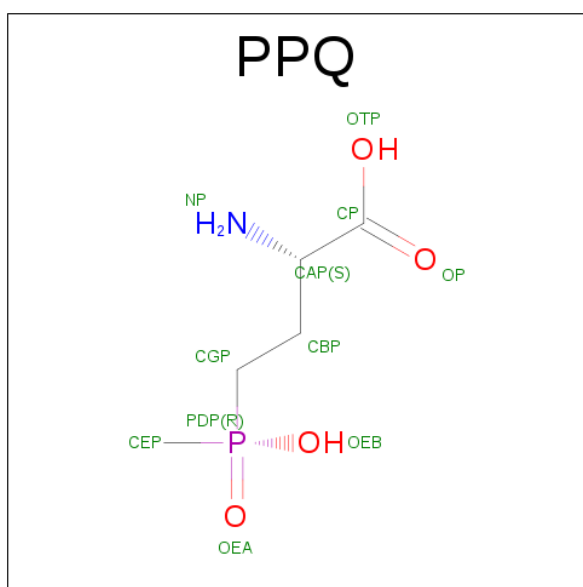
- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is PHOSPHINOTHRICIN (three-letter code: PPQ) (formula:  $C_5H_{12}NO_4P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	B	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	C	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	D	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	E	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	F	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	G	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	H	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	I	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	J	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	K	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	L	1	Total	C	N	O	P	0	0
			11	5	1	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	152	Total	O	0	0
			152	152		
5	B	155	Total	O	0	0
			155	155		
5	C	152	Total	O	0	0
			152	152		
5	D	153	Total	O	0	0
			153	153		
5	E	154	Total	O	0	0
			154	154		
5	F	152	Total	O	0	0
			152	152		
5	G	155	Total	O	0	0
			155	155		
5	H	150	Total	O	0	0
			150	150		

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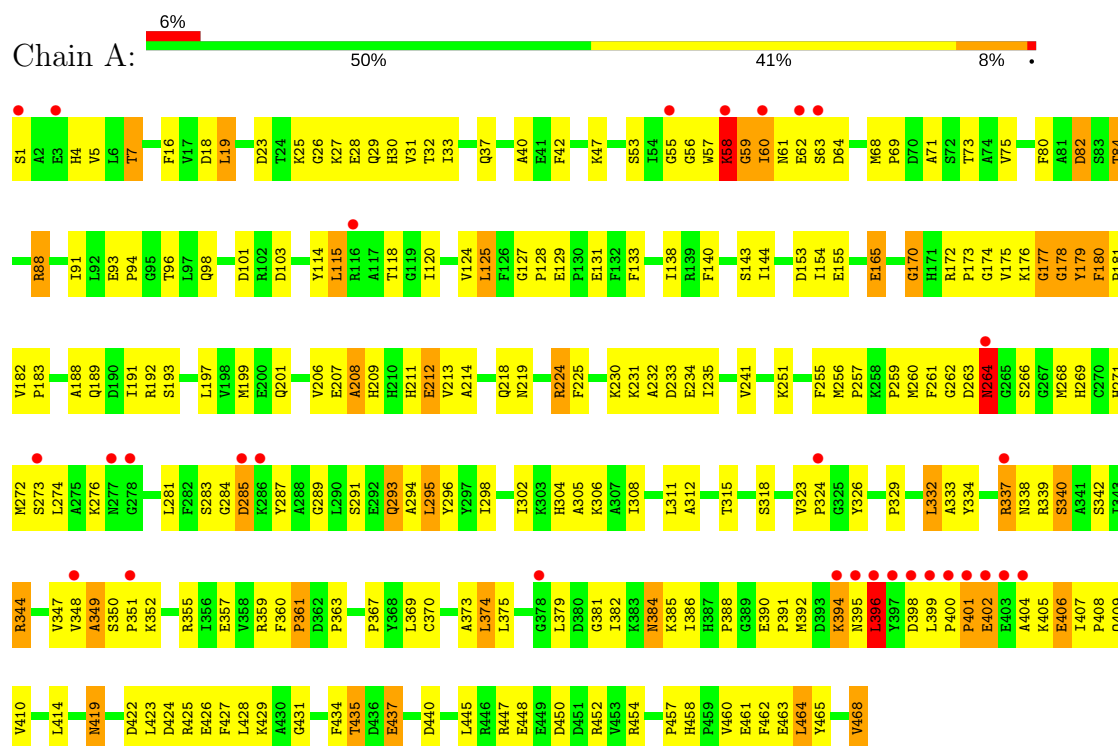
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	156	Total 156	O 156	0	0
5	J	151	Total 151	O 151	0	0
5	K	153	Total 153	O 153	0	0
5	L	153	Total 153	O 153	0	0



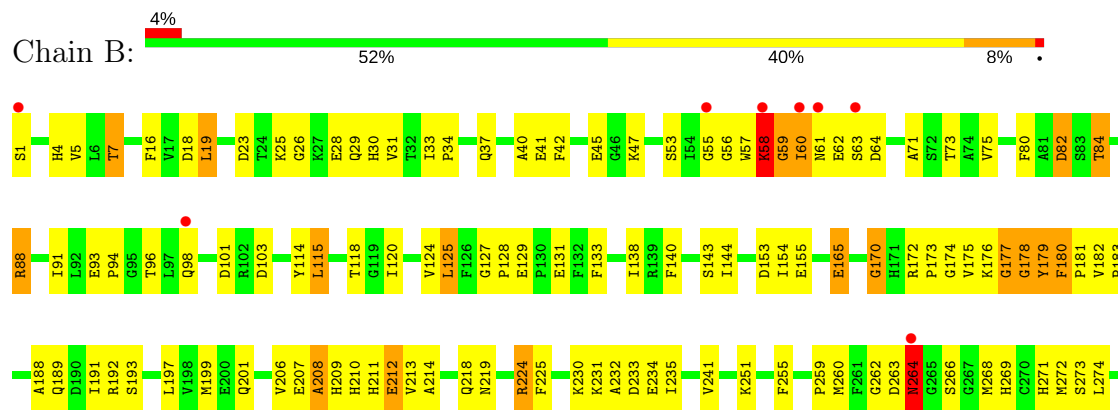
### 3 Residue-property plots

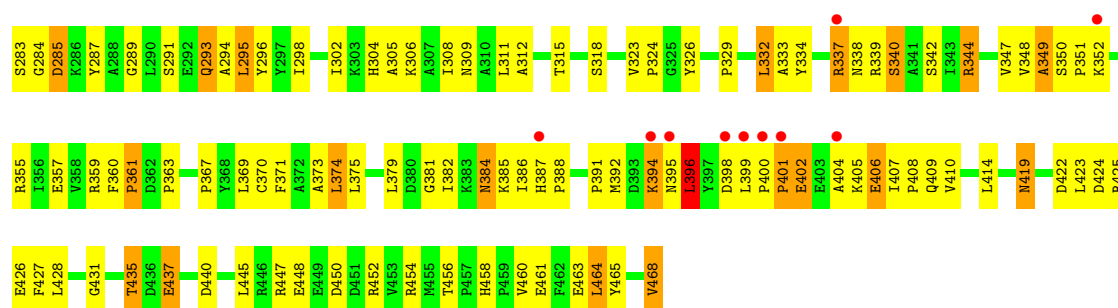
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: GLUTAMINE SYNTHETASE

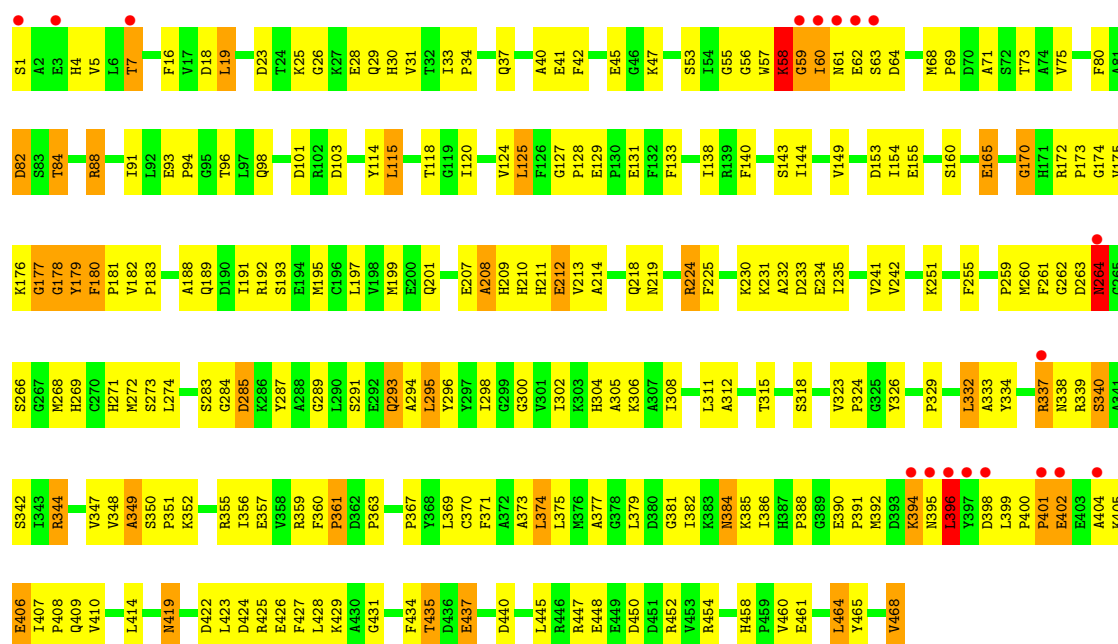


#### • Molecule 1: GLUTAMINE SYNTHETASE

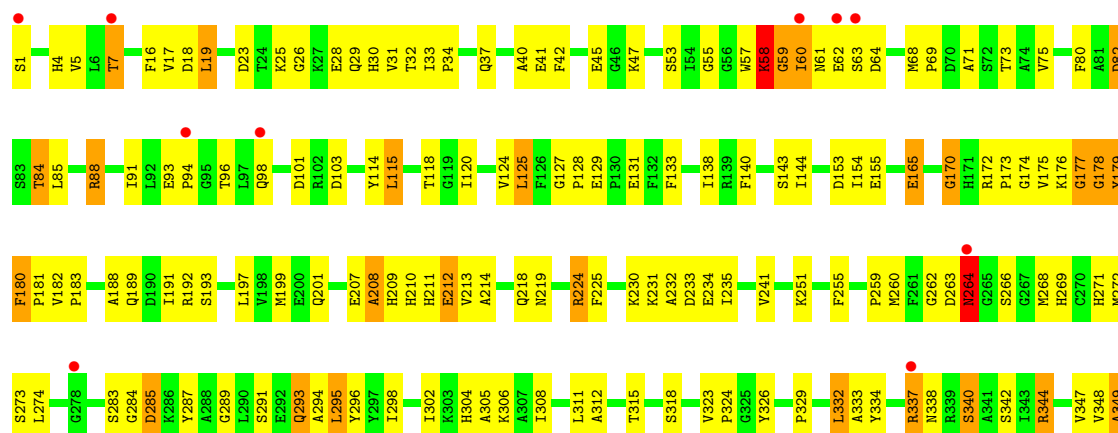


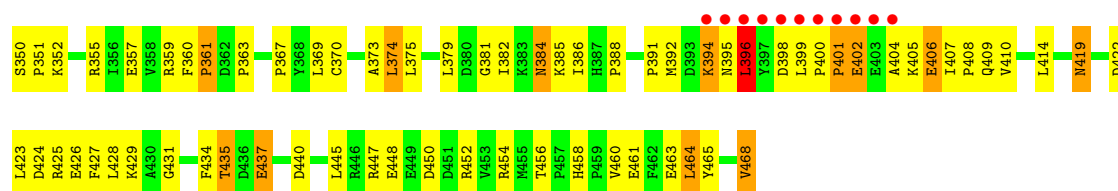


### • Molecule 1: GLUTAMINE SYNTHETASE

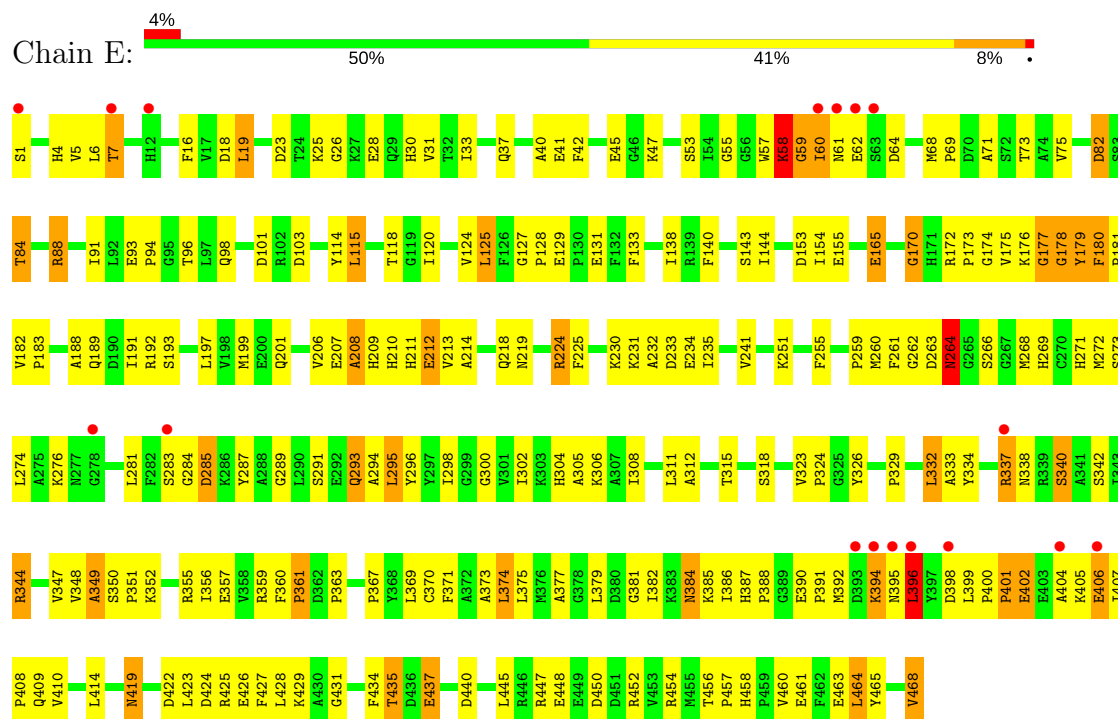


### • Molecule 1: GLUTAMINE SYNTHETASE





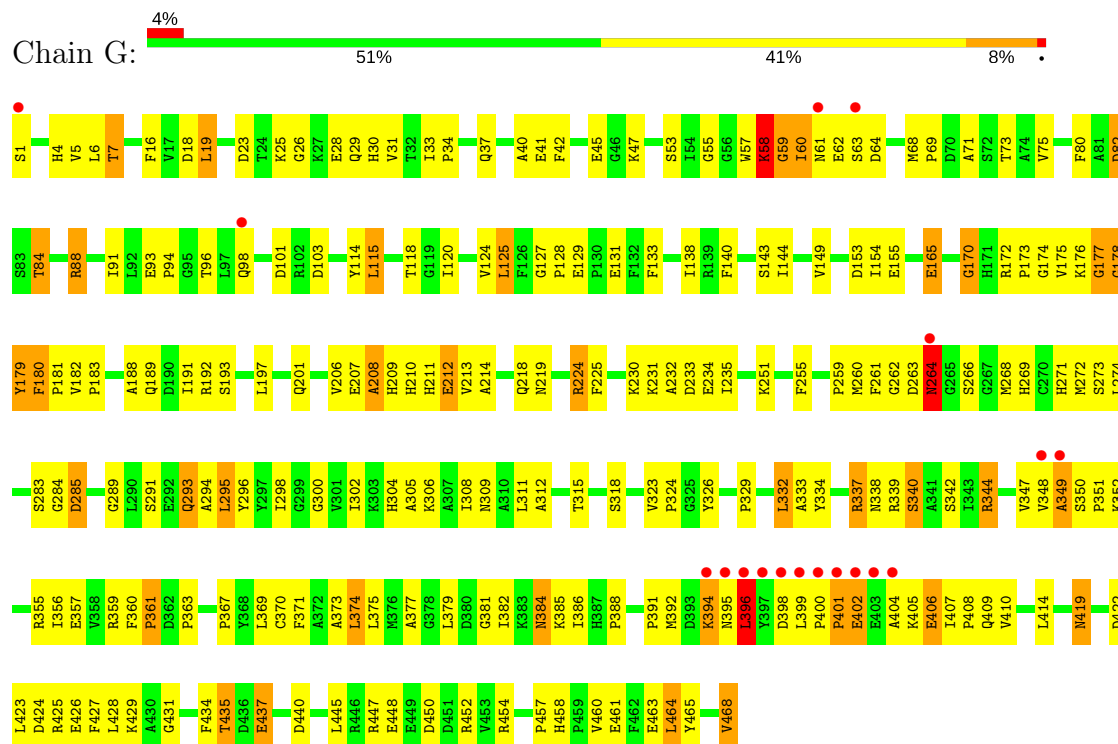
• Molecule 1: GLUTAMINE SYNTHETASE



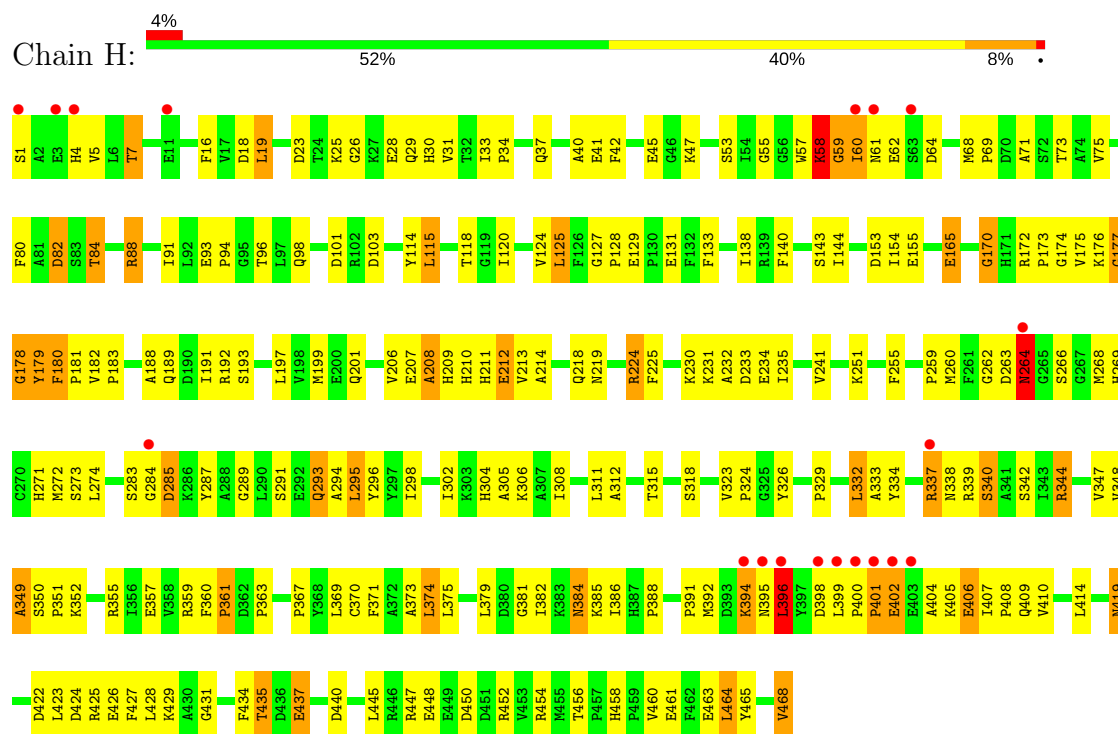
• Molecule 1: GLUTAMINE SYNTHETASE



• Molecule 1: GLUTAMINE SYNTHETASE

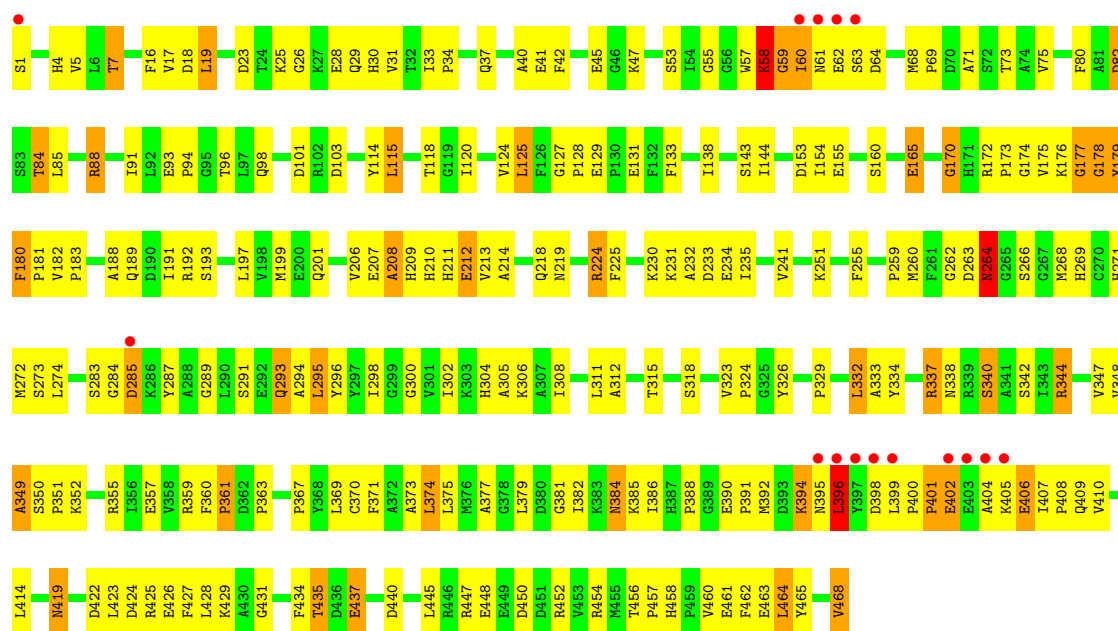


• Molecule 1: GLUTAMINE SYNTHETASE

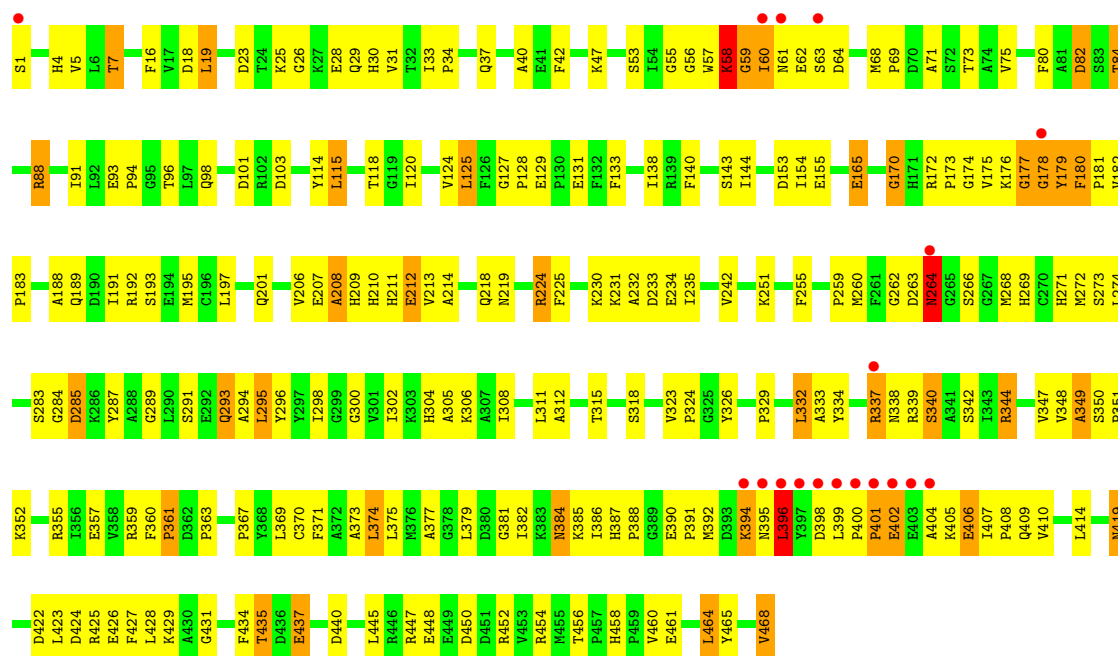


• Molecule 1: GLUTAMINE SYNTHETASE

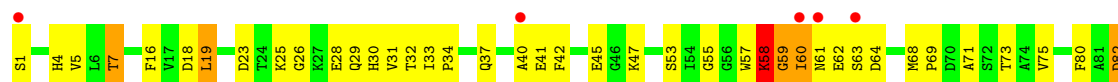


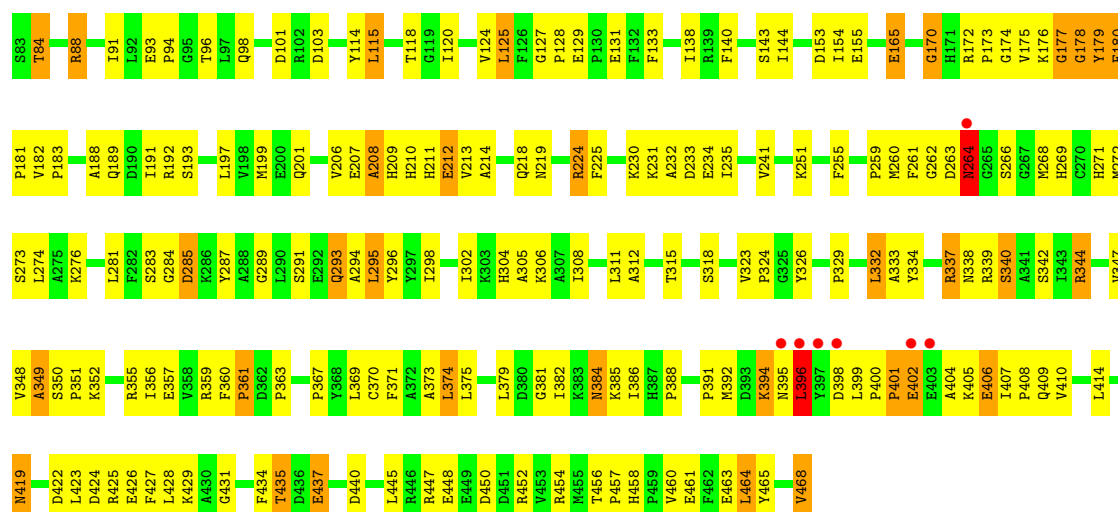


- Molecule 1: GLUTAMINE SYNTHETASE

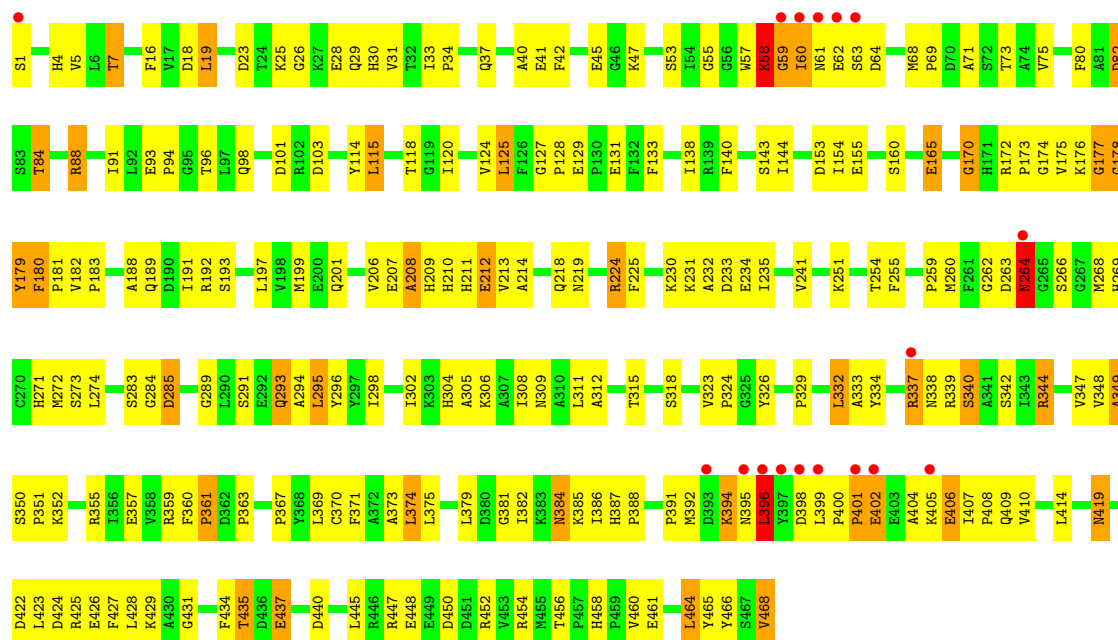


- Molecule 1: GLUTAMINE SYNTHETASE





### • Molecule 1: GLUTAMINE SYNTHETASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	230.60Å 132.50Å 195.90Å 90.00° 102.40° 90.00°	Depositor
Resolution (Å)	15.00 – 2.89 15.00 – 2.89	Depositor EDS
% Data completeness (in resolution range)	70.0 (15.00-2.89) 68.7 (15.00-2.89)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 2.91Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.248 , 0.263 0.244 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	51.1	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 69.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	47280	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: PPQ, MN, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.63	0/3850	0.90	2/5212 (0.0%)
1	B	0.63	0/3850	0.90	2/5212 (0.0%)
1	C	0.63	0/3850	0.90	2/5212 (0.0%)
1	D	0.63	0/3850	0.90	2/5212 (0.0%)
1	E	0.63	0/3850	0.90	2/5212 (0.0%)
1	F	0.63	0/3850	0.90	2/5212 (0.0%)
1	G	0.63	0/3850	0.90	2/5212 (0.0%)
1	H	0.63	0/3850	0.90	2/5212 (0.0%)
1	I	0.63	0/3850	0.90	2/5212 (0.0%)
1	J	0.63	0/3850	0.90	2/5212 (0.0%)
1	K	0.63	0/3850	0.90	2/5212 (0.0%)
1	L	0.63	0/3850	0.90	2/5212 (0.0%)
All	All	0.63	0/46200	0.90	24/62544 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
All	All	0	12

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179[A]	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	B	179[B]	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	J	179[A]	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	J	179[B]	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	C	179[A]	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	C	179[B]	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	D	179[A]	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	D	179[B]	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	A	179[A]	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	A	179[B]	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	L	179[A]	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	L	179[B]	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	K	179[A]	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	K	179[B]	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	E	179[A]	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	E	179[B]	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	F	179[A]	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	F	179[B]	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	I	179[A]	TYR	CB-CG-CD2	-5.59	117.64	121.00
1	I	179[B]	TYR	CB-CG-CD2	-5.59	117.64	121.00
1	H	179[A]	TYR	CB-CG-CD2	-5.59	117.65	121.00
1	H	179[B]	TYR	CB-CG-CD2	-5.59	117.65	121.00
1	G	179[A]	TYR	CB-CG-CD2	-5.57	117.66	121.00
1	G	179[B]	TYR	CB-CG-CD2	-5.57	117.66	121.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	ALA	Mainchain
1	B	208	ALA	Mainchain
1	C	208	ALA	Mainchain
1	D	208	ALA	Mainchain
1	E	208	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	F	208	ALA	Mainchain
1	G	208	ALA	Mainchain
1	H	208	ALA	Mainchain
1	I	208	ALA	Mainchain
1	J	208	ALA	Mainchain
1	K	208	ALA	Mainchain
1	L	208	ALA	Mainchain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3747	0	3621	330	0
1	B	3747	0	3621	325	0
1	C	3747	0	3621	330	0
1	D	3747	0	3621	320	0
1	E	3747	0	3621	322	0
1	F	3747	0	3621	325	0
1	G	3747	0	3621	328	0
1	H	3747	0	3621	324	0
1	I	3747	0	3621	334	0
1	J	3747	0	3621	333	0
1	K	3747	0	3621	328	0
1	L	3747	0	3621	323	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	27	0	10	8	0
3	B	27	0	10	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	27	0	10	8	0
3	D	27	0	10	8	0
3	E	27	0	10	8	0
3	F	27	0	10	8	0
3	G	27	0	10	8	0
3	H	27	0	10	8	0
3	I	27	0	10	8	0
3	J	27	0	10	8	0
3	K	27	0	10	8	0
3	L	27	0	10	8	0
4	A	11	0	10	7	0
4	B	11	0	10	7	0
4	C	11	0	10	6	0
4	D	11	0	10	6	0
4	E	11	0	10	6	0
4	F	11	0	10	7	0
4	G	11	0	10	6	0
4	H	11	0	10	7	0
4	I	11	0	10	6	0
4	J	11	0	10	6	0
4	K	11	0	10	5	0
4	L	11	0	10	7	0
5	A	152	0	0	89	0
5	B	155	0	0	91	0
5	C	152	0	0	93	0
5	D	153	0	0	85	0
5	E	154	0	0	91	0
5	F	152	0	0	91	0
5	G	155	0	0	91	0
5	H	150	0	0	88	0
5	I	156	0	0	92	0
5	J	151	0	0	90	0
5	K	153	0	0	85	0
5	L	153	0	0	90	0
All	All	47280	0	43692	3738	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 42.

All (3738) 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)
3:L:4482:ADP:C1'	3:L:4482:ADP:N9	1.70	1.54
3:C:4473:ADP:N9	3:C:4473:ADP:C1'	1.70	1.53
3:I:4479:ADP:N9	3:I:4479:ADP:C1'	1.70	1.53
3:H:4478:ADP:N9	3:H:4478:ADP:C1'	1.70	1.52
3:B:4472:ADP:C1'	3:B:4472:ADP:N9	1.70	1.52
3:J:4480:ADP:C1'	3:J:4480:ADP:N9	1.70	1.51
3:K:4481:ADP:N9	3:K:4481:ADP:C1'	1.70	1.51
3:A:4471:ADP:C1'	3:A:4471:ADP:N9	1.70	1.50
3:F:4476:ADP:N9	3:F:4476:ADP:C1'	1.70	1.50
3:G:4477:ADP:C1'	3:G:4477:ADP:N9	1.70	1.49
3:D:4474:ADP:C1'	3:D:4474:ADP:N9	1.70	1.49
3:E:4475:ADP:C1'	3:E:4475:ADP:N9	1.70	1.49
1:C:211[B]:HIS:CE1	5:C:6044:HOH:O	1.82	1.27
1:F:211[B]:HIS:CE1	5:F:5906:HOH:O	1.82	1.27
1:K:211[B]:HIS:CE1	5:K:1381:HOH:O	1.85	1.26
1:D:211[B]:HIS:O	1:D:212[B]:GLU:HG2	1.07	1.25
1:J:337:ARG:HG3	1:J:338:ASN:N	1.31	1.25
1:L:211[B]:HIS:CE1	5:L:1534:HOH:O	1.85	1.25
1:H:211[B]:HIS:CE1	5:H:5912:HOH:O	1.91	1.24
1:K:211[B]:HIS:O	1:K:212[B]:GLU:HG2	1.07	1.24
1:D:337:ARG:HG3	1:D:338:ASN:N	1.31	1.24
1:G:211[B]:HIS:O	1:G:212[B]:GLU:HG2	1.07	1.23
1:L:337:ARG:HG3	1:L:338:ASN:N	1.31	1.23
1:A:211[B]:HIS:O	1:A:212[B]:GLU:HG2	1.07	1.23
1:I:211[B]:HIS:O	1:I:212[B]:GLU:HG2	1.07	1.23
1:F:211[B]:HIS:O	1:F:212[B]:GLU:HG2	1.07	1.23
1:E:211[B]:HIS:CE1	5:E:769:HOH:O	1.87	1.22
1:C:211[B]:HIS:O	1:C:212[B]:GLU:HG2	1.07	1.22
1:G:211[B]:HIS:CE1	5:G:6054:HOH:O	1.86	1.22
1:L:211[B]:HIS:O	1:L:212[B]:GLU:HG2	1.07	1.22
1:B:211[B]:HIS:CE1	5:B:6045:HOH:O	1.92	1.22
1:H:211[B]:HIS:O	1:H:212[B]:GLU:HG2	1.07	1.21
1:E:211[B]:HIS:O	1:E:212[B]:GLU:HG2	1.07	1.21
1:A:337:ARG:HG3	1:A:338:ASN:N	1.31	1.20
1:D:211[B]:HIS:CE1	5:D:6046:HOH:O	1.90	1.20
1:B:211[B]:HIS:O	1:B:212[B]:GLU:HG2	1.07	1.20
1:J:211[B]:HIS:O	1:J:212[B]:GLU:HG2	1.07	1.20
1:G:337:ARG:HG3	1:G:338:ASN:N	1.31	1.19
1:B:337:ARG:HG3	1:B:338:ASN:N	1.32	1.19
1:K:337:ARG:HG3	1:K:338:ASN:N	1.32	1.19
1:F:337:ARG:HG3	1:F:338:ASN:N	1.31	1.19
1:I:211[B]:HIS:CE1	5:I:5913:HOH:O	1.93	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:329:PRO:HG2	1:L:359:ARG:HD2	1.24	1.19
1:F:323:VAL:HG12	5:F:6047:HOH:O	1.44	1.18
1:C:323:VAL:HG12	5:C:6037:HOH:O	1.44	1.17
1:G:323:VAL:HG12	5:G:6047:HOH:O	1.44	1.17
1:F:179[A]:TYR:OH	5:F:5911:HOH:O	1.59	1.17
1:H:337:ARG:CG	1:H:338:ASN:N	2.07	1.17
1:L:337:ARG:CG	1:L:338:ASN:N	2.07	1.17
1:I:323:VAL:HG12	5:I:6058:HOH:O	1.44	1.17
1:A:337:ARG:CG	1:A:338:ASN:N	2.07	1.16
1:H:337:ARG:HG3	1:H:338:ASN:N	1.32	1.16
1:C:337:ARG:HG3	1:C:338:ASN:N	1.31	1.16
1:J:211[B]:HIS:CE1	5:J:5914:HOH:O	1.95	1.16
1:A:211[B]:HIS:CE1	5:A:6043:HOH:O	1.95	1.16
1:J:337:ARG:CG	1:J:338:ASN:N	2.07	1.15
1:E:337:ARG:CG	1:E:338:ASN:N	2.07	1.15
1:F:329:PRO:HG2	1:F:359:ARG:HD2	1.24	1.15
1:K:323:VAL:HG12	5:K:1677:HOH:O	1.44	1.15
1:J:323:VAL:HG12	5:J:6054:HOH:O	1.44	1.15
1:F:337:ARG:CG	1:F:338:ASN:N	2.07	1.15
1:H:323:VAL:HG12	5:H:6051:HOH:O	1.44	1.15
1:L:323:VAL:HG12	5:L:1830:HOH:O	1.44	1.15
1:I:337:ARG:HG3	1:I:338:ASN:N	1.31	1.15
1:E:337:ARG:HG3	1:E:338:ASN:N	1.31	1.14
1:A:323:VAL:HG12	5:A:6037:HOH:O	1.44	1.14
1:H:211[B]:HIS:O	1:H:212[B]:GLU:CG	1.96	1.14
1:L:179[A]:TYR:OH	5:L:1632:HOH:O	1.65	1.14
1:D:323:VAL:HG12	5:D:6040:HOH:O	1.44	1.14
1:I:60:ILE:HD11	5:J:6056:HOH:O	1.47	1.14
1:C:179[A]:TYR:OH	5:C:6049:HOH:O	1.61	1.14
1:I:329:PRO:HG2	1:I:359:ARG:HD2	1.24	1.14
1:A:211[B]:HIS:O	1:A:212[B]:GLU:CG	1.96	1.14
1:D:211[B]:HIS:O	1:D:212[B]:GLU:CG	1.96	1.14
1:B:211[B]:HIS:O	1:B:212[B]:GLU:CG	1.96	1.14
1:D:360:PHE:CD2	1:D:361:PRO:HD3	1.83	1.13
1:F:211[B]:HIS:O	1:F:212[B]:GLU:CG	1.96	1.13
1:H:329:PRO:HG2	1:H:359:ARG:HD2	1.24	1.13
1:C:329:PRO:HG2	1:C:359:ARG:HD2	1.24	1.13
1:L:211[B]:HIS:O	1:L:212[B]:GLU:CG	1.96	1.13
1:H:360:PHE:CD2	1:H:361:PRO:HD3	1.83	1.13
1:K:360:PHE:CD2	1:K:361:PRO:HD3	1.83	1.13
1:A:360:PHE:CD2	1:A:361:PRO:HD3	1.83	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:VAL:HG12	5:E:759:HOH:O	1.44	1.13
1:G:211[B]:HIS:O	1:G:212[B]:GLU:CG	1.96	1.13
1:B:337:ARG:CG	1:B:338:ASN:N	2.07	1.13
1:G:360:PHE:CD2	1:G:361:PRO:HD3	1.83	1.13
1:K:211[B]:HIS:O	1:K:212[B]:GLU:CG	1.96	1.13
1:E:211[B]:HIS:O	1:E:212[B]:GLU:CG	1.96	1.12
1:J:211[B]:HIS:O	1:J:212[B]:GLU:CG	1.96	1.12
1:E:293:GLN:HB2	5:E:752:HOH:O	1.49	1.12
1:E:360:PHE:CD2	1:E:361:PRO:HD3	1.83	1.12
1:I:211[B]:HIS:O	1:I:212[B]:GLU:CG	1.96	1.12
1:L:360:PHE:CD2	1:L:361:PRO:HD3	1.83	1.12
1:C:211[B]:HIS:O	1:C:212[B]:GLU:CG	1.96	1.12
1:E:329:PRO:HG2	1:E:359:ARG:HD2	1.24	1.12
1:C:360:PHE:CD2	1:C:361:PRO:HD3	1.84	1.12
1:J:360:PHE:CD2	1:J:361:PRO:HD3	1.83	1.12
1:B:323:VAL:HG12	5:B:6038:HOH:O	1.44	1.12
1:F:360:PHE:CD2	1:F:361:PRO:HD3	1.83	1.12
1:G:293:GLN:HB2	5:G:6041:HOH:O	1.49	1.12
1:B:360:PHE:CD2	1:B:361:PRO:HD3	1.83	1.11
1:B:329:PRO:HG2	1:B:359:ARG:HD2	1.24	1.11
1:G:337:ARG:CG	1:G:338:ASN:N	2.07	1.11
1:I:360:PHE:CD2	1:I:361:PRO:HD3	1.83	1.11
1:C:293:GLN:HB2	5:C:6031:HOH:O	1.49	1.11
1:J:329:PRO:HG2	1:J:359:ARG:HD2	1.24	1.11
1:I:337:ARG:CG	1:I:338:ASN:N	2.07	1.11
1:K:179[A]:TYR:OH	5:K:1479:HOH:O	1.68	1.10
1:B:293:GLN:HB2	5:B:6032:HOH:O	1.49	1.10
1:D:337:ARG:CG	1:D:338:ASN:N	2.07	1.10
1:I:293:GLN:HB2	5:I:6052:HOH:O	1.49	1.10
1:J:293:GLN:HB2	5:J:6048:HOH:O	1.49	1.10
1:L:1:SER:HB2	1:L:4:HIS:HB3	1.34	1.10
1:D:329:PRO:HG2	1:D:359:ARG:HD2	1.24	1.10
1:H:293:GLN:HB2	5:H:6045:HOH:O	1.49	1.10
1:L:293:GLN:HB2	5:L:1823:HOH:O	1.50	1.10
1:K:1:SER:HB2	1:K:4:HIS:HB3	1.34	1.10
1:A:1:SER:HB2	1:A:4:HIS:HB3	1.34	1.09
1:G:60:ILE:HD11	5:H:6053:HOH:O	1.49	1.09
1:J:1:SER:HB2	1:J:4:HIS:HB3	1.34	1.09
1:K:293:GLN:HB2	5:K:1670:HOH:O	1.49	1.09
1:A:329:PRO:HG2	1:A:359:ARG:HD2	1.24	1.09
1:B:1:SER:HB2	1:B:4:HIS:HB3	1.34	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ARG:CD	1:B:61:ASN:HB3	1.81	1.08
1:C:337:ARG:CG	1:C:338:ASN:N	2.07	1.08
1:I:61:ASN:HB3	1:J:337:ARG:CD	1.83	1.08
1:K:329:PRO:HG2	1:K:359:ARG:HD2	1.24	1.08
1:F:293:GLN:HB2	5:F:6041:HOH:O	1.49	1.08
1:G:329:PRO:HG2	1:G:359:ARG:HD2	1.24	1.08
1:K:337:ARG:CG	1:K:338:ASN:N	2.07	1.08
1:A:293:GLN:HB2	5:A:6031:HOH:O	1.49	1.08
1:C:224:ARG:HH21	1:C:224:ARG:HG2	1.19	1.08
1:D:293:GLN:HB2	5:D:6034:HOH:O	1.49	1.08
1:J:224:ARG:HG2	1:J:224:ARG:HH21	1.19	1.08
1:D:179[A]:TYR:OH	5:D:6052:HOH:O	1.70	1.08
1:D:224:ARG:HG2	1:D:224:ARG:HH21	1.19	1.07
1:E:211[B]:HIS:C	1:E:212[B]:GLU:HG2	1.75	1.07
1:G:211[B]:HIS:C	1:G:212[B]:GLU:HG2	1.75	1.07
1:F:211[B]:HIS:C	1:F:212[B]:GLU:HG2	1.75	1.07
1:G:337:ARG:CD	1:L:61:ASN:HB3	1.84	1.07
1:F:1:SER:HB2	1:F:4:HIS:HB3	1.34	1.07
1:L:224:ARG:HH21	1:L:224:ARG:HG2	1.19	1.07
1:A:211[B]:HIS:C	1:A:212[B]:GLU:HG2	1.75	1.07
1:D:1:SER:HB2	1:D:4:HIS:HB3	1.34	1.07
1:J:211[B]:HIS:CD2	1:J:211[B]:HIS:N	2.22	1.06
1:B:211[B]:HIS:N	1:B:211[B]:HIS:CD2	2.22	1.06
1:E:1:SER:HB2	1:E:4:HIS:HB3	1.34	1.06
1:I:224:ARG:HG2	1:I:224:ARG:HH21	1.19	1.06
1:D:211[B]:HIS:C	1:D:212[B]:GLU:HG2	1.75	1.06
1:K:211[B]:HIS:C	1:K:212[B]:GLU:HG2	1.75	1.06
1:J:211[B]:HIS:C	1:J:212[B]:GLU:HG2	1.75	1.06
1:B:211[B]:HIS:C	1:B:212[B]:GLU:HG2	1.75	1.06
1:I:179[A]:TYR:OH	5:I:5921:HOH:O	1.74	1.06
1:A:224:ARG:HH21	1:A:224:ARG:HG2	1.19	1.06
1:I:211[B]:HIS:C	1:I:212[B]:GLU:HG2	1.75	1.06
1:H:211[B]:HIS:C	1:H:212[B]:GLU:HG2	1.75	1.05
1:G:179[A]:TYR:OH	5:G:6061:HOH:O	1.74	1.05
1:L:211[B]:HIS:C	1:L:212[B]:GLU:HG2	1.75	1.05
1:H:1:SER:HB2	1:H:4:HIS:HB3	1.34	1.05
1:D:211[B]:HIS:N	1:D:211[B]:HIS:CD2	2.22	1.05
1:G:211[B]:HIS:N	1:G:211[B]:HIS:CD2	2.22	1.05
1:A:211[B]:HIS:CD2	1:A:211[B]:HIS:N	2.22	1.05
1:H:176[B]:LYS:O	1:H:178[B]:GLY:N	1.90	1.05
1:E:179[A]:TYR:OH	5:E:867:HOH:O	1.73	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176[B]:LYS:O	1:F:178[B]:GLY:N	1.90	1.05
1:G:176[B]:LYS:O	1:G:178[B]:GLY:N	1.90	1.05
1:G:224:ARG:HG2	1:G:224:ARG:HH21	1.19	1.04
1:C:176[B]:LYS:O	1:C:178[B]:GLY:N	1.90	1.04
1:E:176[B]:LYS:O	1:E:178[B]:GLY:N	1.90	1.04
1:H:179[A]:TYR:OH	5:H:5917:HOH:O	1.73	1.04
1:K:176[B]:LYS:O	1:K:178[B]:GLY:N	1.90	1.04
1:G:1:SER:HB2	1:G:4:HIS:HB3	1.34	1.04
1:A:176[B]:LYS:O	1:A:178[B]:GLY:N	1.90	1.04
1:C:1:SER:HB2	1:C:4:HIS:HB3	1.34	1.04
1:I:176[B]:LYS:O	1:I:178[B]:GLY:N	1.90	1.04
1:B:176[B]:LYS:O	1:B:178[B]:GLY:N	1.90	1.04
1:I:1:SER:HB2	1:I:4:HIS:HB3	1.34	1.04
5:C:6039:HOH:O	1:D:60:ILE:HD11	1.58	1.03
1:C:211[B]:HIS:N	1:C:211[B]:HIS:CD2	2.22	1.03
1:D:179[B]:TYR:CD1	1:D:212[B]:GLU:HA	1.93	1.03
1:L:179[B]:TYR:CD1	1:L:212[B]:GLU:HA	1.93	1.03
1:C:211[B]:HIS:C	1:C:212[B]:GLU:HG2	1.75	1.03
1:E:179[B]:TYR:CD1	1:E:212[B]:GLU:HA	1.93	1.03
1:G:61:ASN:HB3	1:H:337:ARG:CD	1.89	1.03
1:H:179[B]:TYR:CD1	1:H:212[B]:GLU:HA	1.93	1.03
1:D:176[B]:LYS:O	1:D:178[B]:GLY:N	1.90	1.03
1:J:179[B]:TYR:CD1	1:J:212[B]:GLU:HA	1.93	1.03
1:K:211[B]:HIS:N	1:K:211[B]:HIS:CD2	2.22	1.03
1:F:224:ARG:HH21	1:F:224:ARG:HG2	1.19	1.03
1:G:179[B]:TYR:CD1	1:G:212[B]:GLU:HA	1.93	1.03
1:C:179[B]:TYR:CD1	1:C:212[B]:GLU:HA	1.93	1.03
1:J:176[B]:LYS:O	1:J:178[B]:GLY:N	1.90	1.03
1:J:329:PRO:CG	1:J:359:ARG:HD2	1.89	1.02
1:F:179[B]:TYR:CD1	1:F:212[B]:GLU:HA	1.93	1.02
1:H:224:ARG:HH21	1:H:224:ARG:HG2	1.19	1.02
1:B:179[A]:TYR:OH	5:B:6052:HOH:O	1.76	1.02
1:E:211[B]:HIS:N	1:E:211[B]:HIS:CD2	2.22	1.02
1:F:211[B]:HIS:CD2	1:F:211[B]:HIS:N	2.22	1.02
1:H:329:PRO:CG	1:H:359:ARG:HD2	1.90	1.02
1:L:329:PRO:CG	1:L:359:ARG:HD2	1.89	1.02
1:A:329:PRO:CG	1:A:359:ARG:HD2	1.90	1.02
1:C:329:PRO:CG	1:C:359:ARG:HD2	1.89	1.02
1:D:329:PRO:CG	1:D:359:ARG:HD2	1.90	1.02
1:B:179[B]:TYR:CD1	1:B:212[B]:GLU:HA	1.93	1.02
1:L:176[B]:LYS:O	1:L:178[B]:GLY:N	1.90	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:224:ARG:HH21	1:K:224:ARG:HG2	1.19	1.02
1:L:211[B]:HIS:N	1:L:211[B]:HIS:CD2	2.22	1.02
1:A:179[B]:TYR:CD1	1:A:212[B]:GLU:HA	1.93	1.02
1:F:329:PRO:CG	1:F:359:ARG:HD2	1.90	1.02
1:H:211[B]:HIS:N	1:H:211[B]:HIS:CD2	2.22	1.02
1:I:179[B]:TYR:CD1	1:I:212[B]:GLU:HA	1.93	1.02
1:E:224:ARG:HH21	1:E:224:ARG:HG2	1.19	1.01
1:K:329:PRO:CG	1:K:359:ARG:HD2	1.90	1.01
1:B:329:PRO:CG	1:B:359:ARG:HD2	1.90	1.01
1:K:179[B]:TYR:CD1	1:K:212[B]:GLU:HA	1.93	1.01
1:B:224:ARG:HG2	1:B:224:ARG:HH21	1.18	1.01
1:L:285:ASP:HA	5:L:1816:HOH:O	1.60	1.01
1:A:60:ILE:HD11	5:F:6049:HOH:O	1.60	1.01
1:I:211[B]:HIS:N	1:I:211[B]:HIS:CD2	2.22	1.00
1:I:329:PRO:CG	1:I:359:ARG:HD2	1.90	1.00
1:J:285:ASP:HA	5:J:6041:HOH:O	1.60	1.00
1:E:329:PRO:CG	1:E:359:ARG:HD2	1.89	1.00
1:I:285:ASP:HA	5:I:6045:HOH:O	1.60	1.00
1:G:329:PRO:CG	1:G:359:ARG:HD2	1.90	1.00
1:A:179[A]:TYR:OH	5:A:6048:HOH:O	1.78	1.00
1:A:285:ASP:HA	5:A:6024:HOH:O	1.60	1.00
1:H:285:ASP:HA	5:H:6038:HOH:O	1.61	0.99
1:B:285:ASP:HA	5:B:6025:HOH:O	1.60	0.99
1:C:285:ASP:HA	5:C:6024:HOH:O	1.60	0.99
1:G:285:ASP:HA	5:G:6034:HOH:O	1.60	0.99
1:I:61:ASN:HB3	1:J:337:ARG:HD2	1.43	0.99
1:D:285:ASP:HA	5:D:6027:HOH:O	1.60	0.98
1:L:337:ARG:CG	1:L:338:ASN:H	1.73	0.98
1:J:179[A]:TYR:OH	5:J:5919:HOH:O	1.79	0.98
1:E:285:ASP:HA	5:E:745:HOH:O	1.60	0.98
1:K:285:ASP:HA	5:K:1663:HOH:O	1.60	0.98
1:F:285:ASP:HA	5:F:6034:HOH:O	1.60	0.98
1:J:337:ARG:HG3	1:J:338:ASN:H	0.87	0.97
5:B:6040:HOH:O	1:C:60:ILE:HD11	1.62	0.97
1:F:337:ARG:CG	1:F:338:ASN:H	1.73	0.97
1:B:211[B]:HIS:C	1:B:212[B]:GLU:CG	2.33	0.97
1:J:60:ILE:HD11	5:K:1679:HOH:O	1.65	0.97
1:C:406:GLU:HA	5:C:5984:HOH:O	1.66	0.96
1:L:337:ARG:HG3	1:L:338:ASN:H	0.87	0.96
1:D:192[A]:ARG:HD3	1:D:219:ASN:HD22	1.31	0.96
1:H:399:LEU:H	1:H:400:PRO:HD2	1.30	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:406:GLU:HA	5:L:1771:HOH:O	1.66	0.96
1:D:211[B]:HIS:C	1:D:212[B]:GLU:CG	2.33	0.96
1:L:192[A]:ARG:HD3	1:L:219:ASN:HD22	1.31	0.96
1:A:192[A]:ARG:HD3	1:A:219:ASN:HD22	1.31	0.96
1:A:406:GLU:HA	5:A:5984:HOH:O	1.66	0.96
1:F:406:GLU:HA	5:F:5994:HOH:O	1.66	0.96
1:F:399:LEU:H	1:F:400:PRO:HD2	1.30	0.95
1:B:406:GLU:HA	5:B:5985:HOH:O	1.66	0.95
1:G:337:ARG:HG3	1:G:338:ASN:H	0.87	0.95
1:J:406:GLU:HA	5:J:6001:HOH:O	1.66	0.95
1:B:337:ARG:CD	1:C:61:ASN:HB3	1.96	0.95
1:I:192[A]:ARG:HD3	1:I:219:ASN:HD22	1.31	0.95
5:G:6049:HOH:O	1:L:60:ILE:HD11	1.65	0.95
1:E:337:ARG:CG	1:E:338:ASN:H	1.73	0.95
1:E:337:ARG:CD	1:F:61:ASN:HB3	1.97	0.95
1:J:192[A]:ARG:HD3	1:J:219:ASN:HD22	1.31	0.95
1:C:409:GLN:HB3	5:C:6026:HOH:O	1.67	0.95
1:J:399:LEU:H	1:J:400:PRO:HD2	1.30	0.95
1:L:409:GLN:HB3	5:L:1818:HOH:O	1.67	0.95
1:F:192[A]:ARG:HD3	1:F:219:ASN:HD22	1.31	0.94
1:H:406:GLU:HA	5:H:5998:HOH:O	1.66	0.94
1:I:337:ARG:HG3	1:I:338:ASN:H	0.87	0.94
1:K:406:GLU:HA	5:K:1618:HOH:O	1.66	0.94
1:K:399:LEU:H	1:K:400:PRO:HD2	1.30	0.94
1:A:337:ARG:CG	1:A:338:ASN:H	1.73	0.94
1:A:409:GLN:HB3	5:A:6026:HOH:O	1.67	0.94
1:J:211[B]:HIS:C	1:J:212[B]:GLU:CG	2.33	0.94
1:J:409:GLN:HB3	5:J:6043:HOH:O	1.67	0.94
1:F:211[B]:HIS:C	1:F:212[B]:GLU:CG	2.33	0.94
1:E:399:LEU:H	1:E:400:PRO:HD2	1.30	0.94
1:B:192[A]:ARG:HD3	1:B:219:ASN:HD22	1.31	0.94
1:H:409:GLN:HB3	5:H:6040:HOH:O	1.67	0.94
1:I:406:GLU:HA	5:I:6005:HOH:O	1.66	0.94
1:C:399:LEU:H	1:C:400:PRO:HD2	1.30	0.94
1:G:399:LEU:H	1:G:400:PRO:HD2	1.30	0.94
1:A:399:LEU:H	1:A:400:PRO:HD2	1.30	0.94
1:D:406:GLU:HA	5:D:5987:HOH:O	1.66	0.94
1:E:406:GLU:HA	5:E:700:HOH:O	1.66	0.94
1:A:211[B]:HIS:C	1:A:212[B]:GLU:CG	2.33	0.94
1:D:399:LEU:H	1:D:400:PRO:HD2	1.30	0.94
1:G:192[A]:ARG:HD3	1:G:219:ASN:HD22	1.31	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:61:ASN:HB3	1:I:337:ARG:CD	1.98	0.94
1:J:337:ARG:CG	1:J:338:ASN:H	1.73	0.94
1:B:399:LEU:H	1:B:400:PRO:HD2	1.30	0.93
1:H:192[A]:ARG:HD3	1:H:219:ASN:HD22	1.31	0.93
1:J:61:ASN:HB3	1:K:337:ARG:CD	1.98	0.93
1:A:337:ARG:HD2	1:B:61:ASN:HB3	1.50	0.93
1:D:409:GLN:HB3	5:D:6029:HOH:O	1.67	0.93
1:I:399:LEU:H	1:I:400:PRO:HD2	1.30	0.93
1:H:337:ARG:HG3	1:H:338:ASN:H	0.87	0.93
1:L:399:LEU:H	1:L:400:PRO:HD2	1.30	0.93
1:G:406:GLU:HA	5:G:5994:HOH:O	1.66	0.93
1:D:337:ARG:CD	1:E:61:ASN:HB3	1.99	0.93
1:K:192[A]:ARG:HD3	1:K:219:ASN:HD22	1.31	0.93
1:C:192[A]:ARG:HD3	1:C:219:ASN:HD22	1.31	0.93
1:G:61:ASN:HB3	1:H:337:ARG:HD2	1.47	0.93
1:I:409:GLN:HB3	5:I:6047:HOH:O	1.67	0.93
5:A:6039:HOH:O	1:B:60:ILE:HD11	1.68	0.92
1:L:211[B]:HIS:C	1:L:212[B]:GLU:CG	2.33	0.92
1:E:192[A]:ARG:HD3	1:E:219:ASN:HD22	1.31	0.92
1:F:409:GLN:HB3	5:F:6036:HOH:O	1.67	0.92
1:H:211[B]:HIS:C	1:H:212[B]:GLU:CG	2.33	0.92
1:K:409:GLN:HB3	5:K:1665:HOH:O	1.67	0.92
1:C:211[B]:HIS:C	1:C:212[B]:GLU:CG	2.33	0.92
1:H:211[B]:HIS:CD2	1:H:211[B]:HIS:H	1.87	0.92
1:K:337:ARG:CG	1:K:338:ASN:H	1.73	0.92
1:D:426:GLU:HB2	5:D:5963:HOH:O	1.70	0.92
1:E:409:GLN:HB3	5:E:747:HOH:O	1.67	0.92
1:H:426:GLU:HB2	5:H:5974:HOH:O	1.70	0.92
1:I:337:ARG:CG	1:I:338:ASN:H	1.73	0.92
1:B:409:GLN:HB3	5:B:6027:HOH:O	1.67	0.92
1:F:337:ARG:HG3	1:F:338:ASN:H	0.87	0.92
1:D:337:ARG:HG3	1:D:338:ASN:H	0.87	0.91
1:A:426:GLU:HB2	5:A:5960:HOH:O	1.70	0.91
1:K:211[B]:HIS:H	1:K:211[B]:HIS:CD2	1.87	0.91
1:E:211[B]:HIS:C	1:E:212[B]:GLU:CG	2.33	0.91
1:D:179[B]:TYR:CE2	1:D:211[B]:HIS:HB2	2.06	0.91
1:E:337:ARG:NH1	1:F:61:ASN:CB	2.33	0.91
1:J:426:GLU:HB2	5:J:5977:HOH:O	1.70	0.91
1:K:179[B]:TYR:CE2	1:K:211[B]:HIS:HB2	2.06	0.91
1:F:211[B]:HIS:CD2	1:F:211[B]:HIS:H	1.87	0.91
1:A:179[B]:TYR:CE2	1:A:211[B]:HIS:HB2	2.06	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:337:ARG:HH11	1:F:61:ASN:CB	1.83	0.91
1:G:179[B]:TYR:CE2	1:G:211[B]:HIS:HB2	2.06	0.91
1:G:409:GLN:HB3	5:G:6036:HOH:O	1.67	0.91
1:I:179[B]:TYR:CE2	1:I:211[B]:HIS:HB2	2.06	0.91
1:C:179[B]:TYR:CE2	1:C:211[B]:HIS:HB2	2.06	0.90
1:C:211[B]:HIS:H	1:C:211[B]:HIS:CD2	1.87	0.90
1:I:426:GLU:HB2	5:I:5981:HOH:O	1.70	0.90
1:J:179[B]:TYR:CE2	1:J:211[B]:HIS:HB2	2.06	0.90
1:K:211[B]:HIS:C	1:K:212[B]:GLU:CG	2.33	0.90
1:A:337:ARG:HG3	1:A:338:ASN:H	0.87	0.90
1:B:337:ARG:HG3	1:B:338:ASN:H	0.87	0.90
1:C:426:GLU:HB2	5:C:5960:HOH:O	1.70	0.90
1:B:337:ARG:HD2	1:C:61:ASN:HB3	1.53	0.90
1:H:323:VAL:HA	5:H:6051:HOH:O	1.72	0.90
1:L:179[B]:TYR:CE2	1:L:211[B]:HIS:HB2	2.06	0.90
1:B:179[B]:TYR:CE2	1:B:211[B]:HIS:HB2	2.06	0.90
1:B:426:GLU:HB2	5:B:5961:HOH:O	1.70	0.90
1:G:337:ARG:HD2	1:L:61:ASN:HB3	1.50	0.90
1:H:179[B]:TYR:CE2	1:H:211[B]:HIS:HB2	2.06	0.90
1:E:337:ARG:NH1	1:F:61:ASN:HB2	1.87	0.90
1:A:323:VAL:HA	5:A:6037:HOH:O	1.72	0.90
1:D:211[B]:HIS:H	1:D:211[B]:HIS:CD2	1.87	0.90
1:E:426:GLU:HB2	5:E:675:HOH:O	1.70	0.90
1:K:426:GLU:HB2	5:K:1593:HOH:O	1.70	0.90
1:B:337:ARG:CG	1:B:338:ASN:H	1.73	0.90
1:C:302:ILE:HD13	5:C:5998:HOH:O	1.72	0.90
1:E:211[B]:HIS:H	1:E:211[B]:HIS:CD2	1.87	0.90
1:L:426:GLU:HB2	5:L:1746:HOH:O	1.70	0.90
1:E:179[B]:TYR:CE2	1:E:211[B]:HIS:HB2	2.06	0.90
1:F:179[B]:TYR:CE2	1:F:211[B]:HIS:HB2	2.06	0.90
1:K:61:ASN:HB3	1:L:337:ARG:CD	2.02	0.89
1:A:302:ILE:HD13	5:A:5998:HOH:O	1.72	0.89
1:H:302:ILE:HD13	5:H:6012:HOH:O	1.72	0.89
1:D:302:ILE:HD13	5:D:6001:HOH:O	1.72	0.89
1:A:61:ASN:HB3	1:F:337:ARG:CD	2.03	0.89
1:G:426:GLU:HB2	5:G:5970:HOH:O	1.70	0.89
1:C:337:ARG:CD	1:D:61:ASN:HB3	2.01	0.89
1:E:302:ILE:HD13	5:E:717:HOH:O	1.73	0.89
1:I:302:ILE:HD13	5:I:6019:HOH:O	1.72	0.89
1:F:302:ILE:HD13	5:F:6008:HOH:O	1.72	0.89
1:D:323:VAL:HA	5:D:6040:HOH:O	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:211[B]:HIS:C	1:I:212[B]:GLU:CG	2.33	0.89
1:G:211[B]:HIS:H	1:G:211[B]:HIS:CD2	1.87	0.89
1:K:323:VAL:HA	5:K:1677:HOH:O	1.72	0.89
1:F:323:VAL:HA	5:F:6047:HOH:O	1.72	0.89
1:J:302:ILE:HD13	5:J:6015:HOH:O	1.72	0.89
1:L:302:ILE:HD13	5:L:1788:HOH:O	1.72	0.89
3:A:4471:ADP:H3'	5:A:5976:HOH:O	1.73	0.89
3:E:4475:ADP:H3'	5:E:691:HOH:O	1.73	0.89
1:C:337:ARG:CG	1:C:338:ASN:H	1.73	0.88
3:K:4481:ADP:H3'	5:K:1609:HOH:O	1.73	0.88
1:B:211[B]:HIS:H	1:B:211[B]:HIS:CD2	1.87	0.88
1:B:323:VAL:HA	5:B:6038:HOH:O	1.72	0.88
3:H:4478:ADP:H3'	5:H:5990:HOH:O	1.73	0.88
1:C:177[B]:GLY:O	1:C:178[B]:GLY:C	2.12	0.88
1:K:177[B]:GLY:O	1:K:178[B]:GLY:O	1.92	0.88
1:I:177[B]:GLY:O	1:I:178[B]:GLY:O	1.92	0.88
1:K:60:ILE:HD11	5:L:1832:HOH:O	1.73	0.88
1:L:177[B]:GLY:O	1:L:178[B]:GLY:C	2.12	0.88
1:F:426:GLU:HB2	5:F:5970:HOH:O	1.70	0.88
1:G:177[B]:GLY:O	1:G:178[B]:GLY:O	1.92	0.88
1:J:323:VAL:HA	5:J:6054:HOH:O	1.72	0.88
1:C:177[B]:GLY:O	1:C:178[B]:GLY:O	1.92	0.88
1:C:323:VAL:HA	5:C:6037:HOH:O	1.72	0.88
1:J:211[B]:HIS:CD2	1:J:211[B]:HIS:H	1.87	0.88
1:A:211[B]:HIS:CD2	1:A:211[B]:HIS:H	1.87	0.88
1:D:177[B]:GLY:O	1:D:178[B]:GLY:O	1.92	0.88
1:H:340:SER:OG	1:H:396:LEU:HA	1.74	0.88
1:I:323:VAL:HA	5:I:6058:HOH:O	1.72	0.88
1:A:177[B]:GLY:O	1:A:178[B]:GLY:O	1.92	0.88
1:B:177[B]:GLY:O	1:B:178[B]:GLY:O	1.92	0.88
1:I:340:SER:OG	1:I:396:LEU:HA	1.74	0.88
1:C:337:ARG:HG3	1:C:338:ASN:H	0.87	0.87
1:E:177[B]:GLY:O	1:E:178[B]:GLY:C	2.12	0.87
1:E:177[B]:GLY:O	1:E:178[B]:GLY:O	1.92	0.87
1:D:180[B]:PHE:CD1	1:E:31:VAL:HB	2.09	0.87
3:L:4482:ADP:H3'	5:L:1762:HOH:O	1.73	0.87
1:B:337:ARG:HH11	1:C:61:ASN:CB	1.86	0.87
1:K:302:ILE:HD13	5:K:1635:HOH:O	1.72	0.87
1:L:323:VAL:HA	5:L:1830:HOH:O	1.72	0.87
1:F:177[B]:GLY:O	1:F:178[B]:GLY:O	1.92	0.87
1:I:177[B]:GLY:O	1:I:178[B]:GLY:C	2.12	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:ILE:HD13	5:B:5999:HOH:O	1.72	0.87
1:G:302:ILE:HD13	5:G:6008:HOH:O	1.72	0.87
1:G:323:VAL:HA	5:G:6047:HOH:O	1.72	0.87
1:B:177[B]:GLY:O	1:B:178[B]:GLY:C	2.12	0.87
1:B:340:SER:OG	1:B:396:LEU:HA	1.74	0.87
1:E:340:SER:OG	1:E:396:LEU:HA	1.74	0.87
5:D:6042:HOH:O	1:E:60:ILE:HD11	1.75	0.87
3:J:4480:ADP:H3'	5:J:5993:HOH:O	1.73	0.87
1:K:177[B]:GLY:O	1:K:178[B]:GLY:C	2.12	0.87
1:L:211[B]:HIS:H	1:L:211[B]:HIS:CD2	1.87	0.87
3:F:4476:ADP:H3'	5:F:5986:HOH:O	1.73	0.87
3:C:4473:ADP:H3'	5:C:5976:HOH:O	1.73	0.87
1:E:323:VAL:HA	5:E:759:HOH:O	1.72	0.87
3:I:4479:ADP:H3'	5:I:5997:HOH:O	1.73	0.87
1:H:177[B]:GLY:O	1:H:178[B]:GLY:C	2.12	0.87
1:H:337:ARG:CG	1:H:338:ASN:H	1.73	0.87
1:L:177[B]:GLY:O	1:L:178[B]:GLY:O	1.92	0.87
1:A:177[B]:GLY:O	1:A:178[B]:GLY:C	2.12	0.87
1:D:340:SER:OG	1:D:396:LEU:HA	1.74	0.87
1:D:177[B]:GLY:O	1:D:178[B]:GLY:C	2.12	0.86
3:D:4474:ADP:H3'	5:D:5979:HOH:O	1.73	0.86
1:F:177[B]:GLY:O	1:F:178[B]:GLY:C	2.12	0.86
3:G:4477:ADP:H3'	5:G:5986:HOH:O	1.73	0.86
1:L:340:SER:OG	1:L:396:LEU:HA	1.74	0.86
1:D:337:ARG:NH1	1:E:61:ASN:HB2	1.90	0.86
3:B:4472:ADP:H3'	5:B:5977:HOH:O	1.73	0.86
1:C:340:SER:OG	1:C:396:LEU:HA	1.74	0.86
1:J:177[B]:GLY:O	1:J:178[B]:GLY:O	1.92	0.86
1:D:337:ARG:NH1	1:E:61:ASN:CB	2.38	0.86
1:K:340:SER:OG	1:K:396:LEU:HA	1.74	0.86
1:B:337:ARG:NH1	1:C:61:ASN:HB2	1.88	0.86
1:H:177[B]:GLY:O	1:H:178[B]:GLY:O	1.92	0.86
1:A:340:SER:OG	1:A:396:LEU:HA	1.74	0.86
1:G:340:SER:OG	1:G:396:LEU:HA	1.74	0.86
1:I:211[B]:HIS:H	1:I:211[B]:HIS:CD2	1.87	0.86
1:D:435:THR:HG23	5:D:5960:HOH:O	1.76	0.86
1:E:180[B]:PHE:CD1	1:F:31:VAL:HB	2.10	0.86
1:J:340:SER:OG	1:J:396:LEU:HA	1.74	0.86
1:A:344:ARG:HD2	5:A:5974:HOH:O	1.76	0.86
1:K:344:ARG:HD2	5:K:1607:HOH:O	1.76	0.86
1:G:211[B]:HIS:C	1:G:212[B]:GLU:CG	2.33	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:THR:HG23	5:A:5957:HOH:O	1.76	0.85
1:D:337:ARG:HH11	1:E:61:ASN:CB	1.87	0.85
5:E:761:HOH:O	1:F:60:ILE:HD11	1.74	0.85
1:J:435:THR:HG23	5:J:5974:HOH:O	1.76	0.85
1:L:435:THR:HG23	5:L:1742:HOH:O	1.76	0.85
1:E:344:ARG:HD2	5:E:689:HOH:O	1.76	0.85
1:D:337:ARG:CG	1:D:338:ASN:H	1.73	0.85
1:H:435:THR:HG23	5:H:5971:HOH:O	1.76	0.85
1:B:435:THR:HG23	5:B:5958:HOH:O	1.76	0.85
1:F:340:SER:OG	1:F:396:LEU:HA	1.74	0.85
1:F:344:ARG:HD2	5:F:5984:HOH:O	1.76	0.85
1:G:344:ARG:HD2	5:G:5984:HOH:O	1.76	0.85
1:L:344:ARG:HD2	5:L:1760:HOH:O	1.76	0.85
1:I:435:THR:HG23	5:I:5978:HOH:O	1.76	0.85
1:J:344:ARG:HD2	5:J:5991:HOH:O	1.76	0.84
1:B:344:ARG:HD2	5:B:5975:HOH:O	1.76	0.84
1:E:435:THR:HG23	5:E:671:HOH:O	1.76	0.84
1:H:61:ASN:CB	1:I:337:ARG:NH1	2.40	0.84
1:I:344:ARG:HD2	5:I:5995:HOH:O	1.76	0.84
1:G:165:GLU:HB2	5:G:5971:HOH:O	1.78	0.84
1:J:177[B]:GLY:O	1:J:178[B]:GLY:C	2.12	0.84
1:K:165:GLU:HB2	5:K:1594:HOH:O	1.78	0.84
1:K:435:THR:HG23	5:K:1589:HOH:O	1.76	0.84
1:E:165:GLU:HB2	5:E:676:HOH:O	1.78	0.84
1:B:337:ARG:NH1	1:C:61:ASN:CB	2.41	0.84
1:G:177[B]:GLY:O	1:G:178[B]:GLY:C	2.12	0.84
1:J:61:ASN:HB3	1:K:337:ARG:HD2	1.57	0.84
1:A:165:GLU:HB2	5:A:5961:HOH:O	1.78	0.83
1:D:344:ARG:HD2	5:D:5977:HOH:O	1.76	0.83
1:I:165:GLU:HB2	5:I:5982:HOH:O	1.78	0.83
1:C:344:ARG:HD2	5:C:5974:HOH:O	1.76	0.83
1:C:435:THR:HG23	5:C:5957:HOH:O	1.76	0.83
1:C:458:HIS:HD2	1:C:460:VAL:H	1.26	0.83
1:C:165:GLU:HB2	5:C:5961:HOH:O	1.78	0.83
1:E:337:ARG:HD2	1:F:61:ASN:HB3	1.58	0.83
1:E:337:ARG:HG3	1:E:338:ASN:H	0.87	0.83
1:F:435:THR:HG23	5:F:5967:HOH:O	1.76	0.83
1:K:458:HIS:HD2	1:K:460:VAL:H	1.26	0.83
1:B:165:GLU:HB2	5:B:5962:HOH:O	1.78	0.83
1:J:458:HIS:HD2	1:J:460:VAL:H	1.26	0.83
1:G:337:ARG:NH1	1:L:61:ASN:HB2	1.94	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:HIS:HD2	1:B:460:VAL:H	1.26	0.83
1:G:435:THR:HG23	5:G:5967:HOH:O	1.76	0.83
1:A:458:HIS:HD2	1:A:460:VAL:H	1.26	0.83
1:J:61:ASN:CB	1:K:337:ARG:HH11	1.92	0.82
1:E:458:HIS:HD2	1:E:460:VAL:H	1.26	0.82
1:J:165:GLU:HB2	5:J:5978:HOH:O	1.78	0.82
1:H:165:GLU:HB2	5:H:5975:HOH:O	1.78	0.82
1:H:60:ILE:HD11	5:I:6060:HOH:O	1.79	0.82
1:D:337:ARG:HD2	1:E:61:ASN:HB3	1.61	0.82
1:H:344:ARG:HD2	5:H:5988:HOH:O	1.76	0.82
1:L:165:GLU:HB2	5:L:1747:HOH:O	1.78	0.82
1:G:458:HIS:HD2	1:G:460:VAL:H	1.26	0.82
1:I:458:HIS:HD2	1:I:460:VAL:H	1.26	0.82
1:B:180[B]:PHE:CE1	1:C:31:VAL:HB	2.13	0.82
1:A:337:ARG:HD3	1:B:61:ASN:HB3	1.60	0.82
1:D:165:GLU:HB2	5:D:5964:HOH:O	1.78	0.82
1:E:180[B]:PHE:CE1	1:F:31:VAL:HB	2.14	0.81
1:L:458:HIS:HD2	1:L:460:VAL:H	1.26	0.81
1:A:337:ARG:NH1	1:B:61:ASN:HB2	1.96	0.81
1:J:61:ASN:HB2	1:K:337:ARG:NH1	1.95	0.81
1:F:165:GLU:HB2	5:F:5971:HOH:O	1.78	0.81
1:B:40:ALA:CB	5:B:5982:HOH:O	2.29	0.81
1:G:337:ARG:HH11	1:L:61:ASN:CB	1.92	0.81
3:D:4474:ADP:H1'	3:D:4474:ADP:N9	1.96	0.81
1:G:337:ARG:NH1	1:L:61:ASN:CB	2.44	0.81
1:L:40:ALA:CB	5:L:1768:HOH:O	2.29	0.81
3:A:4471:ADP:H1'	3:A:4471:ADP:N9	1.96	0.80
1:G:337:ARG:CG	1:G:338:ASN:H	1.73	0.80
1:K:40:ALA:CB	5:K:1615:HOH:O	2.29	0.80
1:A:337:ARG:HH11	1:B:61:ASN:CB	1.95	0.80
1:A:40:ALA:CB	5:A:5981:HOH:O	2.29	0.80
3:B:4472:ADP:H1'	3:B:4472:ADP:N9	1.96	0.80
1:C:337:ARG:HD2	1:D:61:ASN:HB3	1.62	0.80
1:C:40:ALA:CB	5:C:5981:HOH:O	2.29	0.80
1:E:170:GLY:HA2	1:E:172:ARG:HH22	1.47	0.80
1:I:170:GLY:HA2	1:I:172:ARG:HH22	1.47	0.80
1:I:61:ASN:HB3	1:J:337:ARG:HD3	1.62	0.80
1:K:170:GLY:HA2	1:K:172:ARG:HH22	1.47	0.80
1:L:347:VAL:HB	5:L:1792:HOH:O	1.82	0.80
1:B:347:VAL:HB	5:B:6003:HOH:O	1.82	0.80
3:E:4475:ADP:N9	3:E:4475:ADP:H1'	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ARG:NH1	1:B:61:ASN:CB	2.45	0.80
1:D:458:HIS:HD2	1:D:460:VAL:H	1.26	0.80
1:J:31:VAL:HB	1:K:180[B]:PHE:CD1	2.17	0.80
1:B:170:GLY:HA2	1:B:172:ARG:HH22	1.46	0.80
1:H:170:GLY:HA2	1:H:172:ARG:HH22	1.47	0.80
1:J:347:VAL:HB	5:J:6019:HOH:O	1.82	0.80
1:L:170:GLY:HA2	1:L:172:ARG:HH22	1.47	0.80
1:A:347:VAL:HB	5:A:6002:HOH:O	1.82	0.79
3:I:4479:ADP:N9	3:I:4479:ADP:H1'	1.96	0.79
1:J:170:GLY:HA2	1:J:172:ARG:HH22	1.47	0.79
1:G:40:ALA:CB	5:G:5991:HOH:O	2.29	0.79
1:H:40:ALA:HB3	5:H:5995:HOH:O	1.83	0.79
1:H:61:ASN:CB	1:I:337:ARG:HH11	1.93	0.79
1:A:170:GLY:HA2	1:A:172:ARG:HH22	1.47	0.79
1:B:40:ALA:HB3	5:B:5982:HOH:O	1.83	0.79
1:D:40:ALA:HB3	5:D:5984:HOH:O	1.83	0.79
1:E:40:ALA:HB3	5:E:697:HOH:O	1.83	0.79
1:H:347:VAL:HB	5:H:6016:HOH:O	1.82	0.79
1:I:40:ALA:CB	5:I:6002:HOH:O	2.29	0.79
1:K:347:VAL:HB	5:K:1639:HOH:O	1.82	0.79
1:H:458:HIS:HD2	1:H:460:VAL:H	1.26	0.79
1:J:40:ALA:CB	5:J:5998:HOH:O	2.29	0.79
1:J:40:ALA:HB3	5:J:5998:HOH:O	1.83	0.79
1:D:347:VAL:HB	5:D:6005:HOH:O	1.82	0.79
1:F:458:HIS:HD2	1:F:460:VAL:H	1.26	0.79
1:I:347:VAL:HB	5:I:6023:HOH:O	1.82	0.79
1:J:31:VAL:HB	1:K:180[B]:PHE:CE1	2.17	0.79
1:B:180[B]:PHE:CD1	1:C:31:VAL:HB	2.16	0.79
1:F:176[B]:LYS:HB3	5:F:5912:HOH:O	1.83	0.79
1:F:40:ALA:CB	5:F:5991:HOH:O	2.29	0.79
3:L:4482:ADP:N9	3:L:4482:ADP:H1'	1.96	0.79
1:A:40:ALA:HB3	5:A:5981:HOH:O	1.83	0.79
1:I:40:ALA:HB3	5:I:6002:HOH:O	1.83	0.79
1:D:170:GLY:HA2	1:D:172:ARG:HH22	1.47	0.79
1:D:40:ALA:CB	5:D:5984:HOH:O	2.29	0.79
1:E:40:ALA:CB	5:E:697:HOH:O	2.29	0.79
1:F:170:GLY:HA2	1:F:172:ARG:HH22	1.47	0.79
1:F:347:VAL:HB	5:F:6012:HOH:O	1.82	0.79
1:K:337:ARG:HG3	1:K:338:ASN:H	0.87	0.79
1:C:176[B]:LYS:HB3	5:C:6050:HOH:O	1.82	0.78
1:E:447:ARG:HD3	5:E:698:HOH:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:447:ARG:HD3	5:I:6003:HOH:O	1.83	0.78
1:G:170:GLY:HA2	1:G:172:ARG:HH22	1.47	0.78
1:H:40:ALA:CB	5:H:5995:HOH:O	2.29	0.78
1:L:447:ARG:HD3	5:L:1769:HOH:O	1.84	0.78
1:K:40:ALA:HB3	5:K:1615:HOH:O	1.83	0.78
1:J:447:ARG:HD3	5:J:5999:HOH:O	1.83	0.78
3:K:4481:ADP:N9	3:K:4481:ADP:H1'	1.96	0.78
1:C:347:VAL:HB	5:C:6002:HOH:O	1.82	0.78
1:F:447:ARG:HD3	5:F:5992:HOH:O	1.83	0.78
1:G:40:ALA:HB3	5:G:5991:HOH:O	1.83	0.78
1:I:61:ASN:HB2	1:J:337:ARG:NH1	1.98	0.78
1:C:170:GLY:HA2	1:C:172:ARG:HH22	1.47	0.78
1:L:75:VAL:HG23	5:L:1701:HOH:O	1.84	0.78
1:B:75:VAL:HG23	5:B:5917:HOH:O	1.84	0.78
1:J:61:ASN:CB	1:K:337:ARG:NH1	2.47	0.78
1:C:75:VAL:HG23	5:C:5917:HOH:O	1.84	0.78
1:J:75:VAL:HG23	5:J:5934:HOH:O	1.84	0.78
1:A:75:VAL:HG23	5:A:5916:HOH:O	1.84	0.78
1:C:40:ALA:HB3	5:C:5981:HOH:O	1.83	0.78
1:E:347:VAL:HB	5:E:721:HOH:O	1.82	0.78
1:K:224:ARG:NH2	1:K:224:ARG:HG2	1.97	0.77
1:C:170:GLY:HA2	1:C:172:ARG:NH2	2.00	0.77
1:H:170:GLY:HA2	1:H:172:ARG:NH2	1.99	0.77
1:H:447:ARG:HD3	5:H:5996:HOH:O	1.83	0.77
1:H:75:VAL:HG23	5:H:5932:HOH:O	1.84	0.77
1:L:40:ALA:HB3	5:L:1768:HOH:O	1.83	0.77
1:G:447:ARG:HD3	5:G:5992:HOH:O	1.84	0.77
1:J:170:GLY:HA2	1:J:172:ARG:NH2	1.99	0.77
1:G:337:ARG:HD3	1:L:61:ASN:HB3	1.65	0.77
1:B:170:GLY:HA2	1:B:172:ARG:NH2	2.00	0.77
1:F:75:VAL:HG23	5:F:5927:HOH:O	1.84	0.77
1:K:75:VAL:HG23	5:K:1548:HOH:O	1.84	0.77
1:A:61:ASN:HB3	1:F:337:ARG:HD2	1.66	0.77
1:D:180[B]:PHE:CE1	1:E:31:VAL:HB	2.20	0.77
1:H:176[B]:LYS:C	1:H:178[B]:GLY:H	1.88	0.77
1:D:170:GLY:HA2	1:D:172:ARG:NH2	2.00	0.77
1:G:170:GLY:HA2	1:G:172:ARG:NH2	2.00	0.77
1:G:61:ASN:HB2	1:H:337:ARG:NH1	1.99	0.77
3:H:4478:ADP:N9	3:H:4478:ADP:H1'	1.96	0.77
1:H:61:ASN:HB2	1:I:337:ARG:NH1	1.97	0.77
1:A:447:ARG:HD3	5:A:5982:HOH:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:GLY:HA2	1:F:172:ARG:NH2	2.00	0.77
1:B:447:ARG:HD3	5:B:5983:HOH:O	1.83	0.77
1:E:75:VAL:HG23	5:E:630:HOH:O	1.84	0.77
1:J:251:LYS:HE3	5:J:5940:HOH:O	1.85	0.77
1:L:170:GLY:HA2	1:L:172:ARG:NH2	1.99	0.77
1:B:251:LYS:HE3	5:B:5923:HOH:O	1.85	0.77
1:D:75:VAL:HG23	5:D:5919:HOH:O	1.84	0.77
1:E:170:GLY:HA2	1:E:172:ARG:NH2	2.00	0.77
1:C:447:ARG:HD3	5:C:5982:HOH:O	1.83	0.77
1:F:251:LYS:HE3	5:F:5933:HOH:O	1.85	0.77
1:G:31:VAL:HB	1:H:180[B]:PHE:CD1	2.20	0.77
1:L:191:ILE:HG13	5:L:1743:HOH:O	1.85	0.77
1:A:176[B]:LYS:C	1:A:178[B]:GLY:H	1.88	0.76
1:C:1:SER:HB2	1:C:4:HIS:CB	2.15	0.76
1:G:180[B]:PHE:CD1	1:L:31:VAL:HB	2.20	0.76
1:I:170:GLY:HA2	1:I:172:ARG:NH2	2.00	0.76
1:K:191:ILE:HG13	5:K:1590:HOH:O	1.85	0.76
1:F:191:ILE:HG13	5:F:5968:HOH:O	1.85	0.76
1:F:251:LYS:CE	5:F:5933:HOH:O	2.34	0.76
1:G:251:LYS:HE3	5:G:5932:HOH:O	1.85	0.76
1:G:347:VAL:HB	5:G:6012:HOH:O	1.82	0.76
1:H:251:LYS:HE3	5:H:5938:HOH:O	1.85	0.76
1:B:176[B]:LYS:C	1:B:178[B]:GLY:H	1.88	0.76
1:D:447:ARG:HD3	5:D:5985:HOH:O	1.83	0.76
1:E:337:ARG:HH11	1:F:61:ASN:HB3	1.48	0.76
1:K:170:GLY:HA2	1:K:172:ARG:NH2	2.00	0.76
1:C:251:LYS:HE3	5:C:5923:HOH:O	1.85	0.76
1:G:191:ILE:HG13	5:G:5968:HOH:O	1.85	0.76
1:J:191:ILE:HG13	5:J:5975:HOH:O	1.85	0.76
1:K:251:LYS:CE	5:K:1554:HOH:O	2.34	0.76
1:K:447:ARG:HD3	5:K:1616:HOH:O	1.84	0.76
1:B:191:ILE:HG13	5:B:5959:HOH:O	1.85	0.76
1:E:251:LYS:HE3	5:E:636:HOH:O	1.85	0.76
1:E:349:ALA:HB3	5:E:648:HOH:O	1.86	0.76
1:G:251:LYS:CE	5:G:5932:HOH:O	2.34	0.76
1:I:176[B]:LYS:C	1:I:178[B]:GLY:H	1.88	0.76
1:I:251:LYS:HE3	5:I:5943:HOH:O	1.85	0.76
1:K:349:ALA:HB3	5:K:1566:HOH:O	1.86	0.76
1:F:40:ALA:HB3	5:F:5991:HOH:O	1.83	0.76
1:H:251:LYS:CE	5:H:5938:HOH:O	2.34	0.76
1:D:191:ILE:HG13	5:D:5961:HOH:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:75:VAL:HG23	5:I:5937:HOH:O	1.84	0.76
1:B:251:LYS:CE	5:B:5923:HOH:O	2.34	0.76
1:E:1:SER:CB	1:E:4:HIS:HB3	2.16	0.76
1:G:75:VAL:HG23	5:G:5926:HOH:O	1.84	0.76
1:J:176[B]:LYS:C	1:J:178[B]:GLY:H	1.88	0.76
1:L:251:LYS:HE3	5:L:1707:HOH:O	1.85	0.76
1:C:311:LEU:HD13	1:C:369:LEU:HB3	1.68	0.76
1:G:176[B]:LYS:C	1:G:178[B]:GLY:H	1.88	0.76
1:A:191:ILE:HG13	5:A:5958:HOH:O	1.85	0.75
1:D:251:LYS:HE3	5:D:5925:HOH:O	1.85	0.75
1:G:61:ASN:HB3	1:H:337:ARG:HD3	1.67	0.75
1:I:31:VAL:HB	1:J:180[B]:PHE:CE1	2.21	0.75
1:K:251:LYS:HE3	5:K:1554:HOH:O	1.85	0.75
1:L:176[B]:LYS:C	1:L:178[B]:GLY:H	1.88	0.75
1:C:191:ILE:HG13	5:C:5958:HOH:O	1.85	0.75
5:G:6052:HOH:O	1:H:176[B]:LYS:HB3	1.85	0.75
1:H:349:ALA:HB3	5:H:5949:HOH:O	1.86	0.75
1:I:191:ILE:HG13	5:I:5979:HOH:O	1.85	0.75
1:I:61:ASN:CB	1:J:337:ARG:HH11	1.99	0.75
1:K:1:SER:HB2	1:K:4:HIS:CB	2.15	0.75
1:E:179[A]:TYR:O	1:E:181[A]:PRO:CD	2.35	0.75
1:G:1:SER:HB2	1:G:4:HIS:CB	2.15	0.75
3:G:4477:ADP:N9	3:G:4477:ADP:H1'	1.96	0.75
1:H:179[A]:TYR:O	1:H:181[A]:PRO:CD	2.34	0.75
1:I:251:LYS:CE	5:I:5943:HOH:O	2.34	0.75
1:L:251:LYS:CE	5:L:1707:HOH:O	2.34	0.75
1:C:179[A]:TYR:O	1:C:181[A]:PRO:CD	2.35	0.75
1:E:191:ILE:HG13	5:E:672:HOH:O	1.85	0.75
1:E:251:LYS:CE	5:E:636:HOH:O	2.34	0.75
1:G:211[B]:HIS:NE2	5:G:6054:HOH:O	2.07	0.75
1:G:349:ALA:HB3	5:G:5944:HOH:O	1.86	0.75
1:K:1:SER:CB	1:K:4:HIS:HB3	2.15	0.75
1:L:179[A]:TYR:O	1:L:181[A]:PRO:CD	2.35	0.75
1:L:211[B]:HIS:NE2	5:L:1534:HOH:O	2.05	0.75
1:G:180[B]:PHE:CE1	1:L:31:VAL:HB	2.22	0.75
1:A:251:LYS:HE3	5:A:5922:HOH:O	1.85	0.75
1:A:349:ALA:HB3	5:A:5934:HOH:O	1.86	0.75
1:D:176[B]:LYS:C	1:D:178[B]:GLY:H	1.88	0.75
1:A:170:GLY:HA2	1:A:172:ARG:NH2	2.00	0.75
1:B:224:ARG:NH2	1:B:224:ARG:HG2	1.97	0.75
1:F:176[B]:LYS:C	1:F:178[B]:GLY:H	1.88	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179[A]:TYR:O	1:F:181[A]:PRO:CD	2.35	0.75
1:K:61:ASN:HB3	1:L:337:ARG:HD2	1.68	0.75
1:C:176[B]:LYS:C	1:C:178[B]:GLY:H	1.88	0.75
1:F:189:GLN:NE2	1:F:209[A]:HIS:HE1	1.85	0.75
1:G:189:GLN:NE2	1:G:209[A]:HIS:HE1	1.85	0.75
1:G:311:LEU:HD13	1:G:369:LEU:HB3	1.69	0.75
1:H:311:LEU:HD13	1:H:369:LEU:HB3	1.69	0.75
1:K:179[A]:TYR:O	1:K:181[A]:PRO:CD	2.35	0.75
1:L:311:LEU:HD13	1:L:369:LEU:HB3	1.69	0.75
1:A:1:SER:HB2	1:A:4:HIS:CB	2.15	0.75
1:A:400:PRO:O	1:A:402:GLU:N	2.20	0.75
1:B:179[A]:TYR:O	1:B:181[A]:PRO:CD	2.34	0.75
1:B:189:GLN:NE2	1:B:209[A]:HIS:HE1	1.85	0.75
1:E:311:LEU:HD13	1:E:369:LEU:HB3	1.69	0.75
1:G:31:VAL:HB	1:H:180[B]:PHE:CE1	2.21	0.75
1:I:311:LEU:HD13	1:I:369:LEU:HB3	1.68	0.75
1:H:61:ASN:HB3	1:I:337:ARG:HD2	1.66	0.75
1:A:311:LEU:HD13	1:A:369:LEU:HB3	1.68	0.75
1:C:1:SER:CB	1:C:4:HIS:HB3	2.16	0.75
1:E:176[B]:LYS:C	1:E:178[B]:GLY:H	1.88	0.75
1:G:179[A]:TYR:O	1:G:181[A]:PRO:CD	2.34	0.75
1:J:179[A]:TYR:O	1:J:181[A]:PRO:CD	2.35	0.75
1:J:311:LEU:HD13	1:J:369:LEU:HB3	1.68	0.75
1:L:400:PRO:O	1:L:402:GLU:N	2.20	0.75
1:A:179[A]:TYR:O	1:A:181[A]:PRO:CD	2.35	0.74
1:D:349:ALA:HB3	5:D:5937:HOH:O	1.86	0.74
1:H:191:ILE:HG13	5:H:5972:HOH:O	1.85	0.74
1:J:189:GLN:NE2	1:J:209[A]:HIS:HE1	1.85	0.74
3:J:4480:ADP:H1'	3:J:4480:ADP:N9	1.96	0.74
1:B:349:ALA:HB3	5:B:5935:HOH:O	1.86	0.74
1:B:176[B]:LYS:HB3	5:C:6042:HOH:O	1.86	0.74
1:C:251:LYS:CE	5:C:5923:HOH:O	2.34	0.74
1:C:180[B]:PHE:CD1	1:D:31:VAL:HB	2.22	0.74
1:D:311:LEU:HD13	1:D:369:LEU:HB3	1.69	0.74
1:A:31:VAL:HB	1:F:180[B]:PHE:CD1	2.22	0.74
1:L:349:ALA:HB3	5:L:1719:HOH:O	1.86	0.74
1:D:337:ARG:HH11	1:E:61:ASN:HB3	1.52	0.74
1:H:224:ARG:NH2	1:H:224:ARG:HG2	1.97	0.74
1:K:189:GLN:NE2	1:K:209[A]:HIS:HE1	1.85	0.74
1:K:61:ASN:CB	1:L:337:ARG:NH1	2.51	0.74
1:A:251:LYS:CE	5:A:5922:HOH:O	2.34	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:PRO:O	1:C:402:GLU:N	2.20	0.74
1:D:251:LYS:CE	5:D:5925:HOH:O	2.34	0.74
1:E:189:GLN:NE2	1:E:209[A]:HIS:HE1	1.85	0.74
1:F:349:ALA:HB3	5:F:5944:HOH:O	1.86	0.74
1:F:1:SER:CB	1:F:4:HIS:HB3	2.15	0.74
1:I:179[A]:TYR:O	1:I:181[A]:PRO:CD	2.35	0.74
1:J:1:SER:HB2	1:J:4:HIS:CB	2.15	0.74
5:J:6059:HOH:O	1:K:176[B]:LYS:HB3	1.86	0.74
1:D:179[A]:TYR:O	1:D:181[A]:PRO:CD	2.34	0.74
1:I:189:GLN:NE2	1:I:209[A]:HIS:HE1	1.85	0.74
1:I:1:SER:CB	1:I:4:HIS:HB3	2.16	0.74
1:L:189:GLN:NE2	1:L:209[A]:HIS:HE1	1.85	0.74
1:B:1:SER:HB2	1:B:4:HIS:CB	2.15	0.74
1:J:251:LYS:CE	5:J:5940:HOH:O	2.34	0.74
1:K:176[B]:LYS:C	1:K:178[B]:GLY:H	1.88	0.74
1:B:211[B]:HIS:NE2	5:B:6045:HOH:O	2.08	0.74
1:G:61:ASN:CB	1:H:337:ARG:HH11	2.00	0.74
1:H:1:SER:CB	1:H:4:HIS:HB3	2.16	0.74
1:J:349:ALA:HB3	5:J:5951:HOH:O	1.86	0.74
1:G:407:ILE:HB	1:G:408:PRO:HD2	1.70	0.74
1:I:399:LEU:H	1:I:400:PRO:CD	2.01	0.74
1:F:407:ILE:HB	1:F:408:PRO:HD2	1.70	0.74
1:D:1:SER:HB2	1:D:4:HIS:CB	2.15	0.73
1:I:400:PRO:O	1:I:402:GLU:N	2.20	0.73
1:C:189:GLN:NE2	1:C:209[A]:HIS:HE1	1.85	0.73
1:D:189:GLN:NE2	1:D:209[A]:HIS:HE1	1.85	0.73
1:F:400:PRO:O	1:F:402:GLU:N	2.20	0.73
1:G:399:LEU:H	1:G:400:PRO:CD	2.01	0.73
1:L:399:LEU:H	1:L:400:PRO:CD	2.01	0.73
1:L:407:ILE:HB	1:L:408:PRO:HD2	1.70	0.73
1:E:400:PRO:O	1:E:402:GLU:N	2.20	0.73
1:C:349:ALA:HB3	5:C:5934:HOH:O	1.86	0.73
1:D:224:ARG:HH21	1:D:224:ARG:CG	2.01	0.73
1:E:407:ILE:HB	1:E:408:PRO:HD2	1.70	0.73
1:K:311:LEU:HD13	1:K:369:LEU:HB3	1.68	0.73
1:A:189:GLN:NE2	1:A:209[A]:HIS:HE1	1.85	0.73
1:B:311:LEU:HD13	1:B:369:LEU:HB3	1.68	0.73
1:E:1:SER:HB2	1:E:4:HIS:CB	2.15	0.73
1:J:400:PRO:O	1:J:402:GLU:N	2.20	0.73
1:K:61:ASN:CB	1:L:337:ARG:HH11	2.01	0.73
1:E:176[B]:LYS:HB3	5:F:6052:HOH:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:349:ALA:HB3	5:I:5955:HOH:O	1.86	0.73
1:A:1:SER:CB	1:A:4:HIS:HB3	2.15	0.73
1:C:57:TRP:O	1:C:58:LYS:O	2.07	0.73
1:D:399:LEU:H	1:D:400:PRO:CD	2.01	0.73
1:E:57:TRP:O	1:E:58:LYS:O	2.07	0.73
1:F:311:LEU:HD13	1:F:369:LEU:HB3	1.68	0.73
1:J:1:SER:CB	1:J:4:HIS:HB3	2.15	0.73
1:B:407:ILE:HB	1:B:408:PRO:HD2	1.70	0.73
1:C:269:HIS:HE1	4:C:5902:PPQ:CEP	2.02	0.73
1:F:269:HIS:HE1	4:F:5905:PPQ:CEP	2.02	0.73
1:H:189:GLN:NE2	1:H:209[A]:HIS:HE1	1.85	0.73
1:H:179[B]:TYR:CE1	1:H:212[B]:GLU:CA	2.72	0.73
1:I:407:ILE:HB	1:I:408:PRO:HD2	1.70	0.73
1:D:407:ILE:HB	1:D:408:PRO:HD2	1.70	0.73
1:K:179[B]:TYR:CE1	1:K:212[B]:GLU:CA	2.72	0.73
1:L:1:SER:HB2	1:L:4:HIS:CB	2.15	0.73
1:B:269:HIS:HE1	4:B:5901:PPQ:CEP	2.02	0.72
1:C:399:LEU:H	1:C:400:PRO:CD	2.01	0.72
1:G:57:TRP:O	1:G:58:LYS:O	2.07	0.72
5:I:6063:HOH:O	1:J:176[B]:LYS:HB3	1.88	0.72
1:J:57:TRP:O	1:J:58:LYS:O	2.07	0.72
1:K:57:TRP:O	1:K:58:LYS:O	2.07	0.72
1:B:57:TRP:O	1:B:58:LYS:O	2.07	0.72
1:F:179[B]:TYR:CE1	1:F:212[B]:GLU:CA	2.72	0.72
1:I:57:TRP:O	1:I:58:LYS:O	2.07	0.72
1:K:269:HIS:HE1	4:K:5910:PPQ:CEP	2.02	0.72
1:A:399:LEU:H	1:A:400:PRO:CD	2.01	0.72
1:A:407:ILE:HB	1:A:408:PRO:HD2	1.70	0.72
1:G:179[B]:TYR:CE1	1:G:212[B]:GLU:CA	2.72	0.72
1:I:269:HIS:HE1	4:I:5908:PPQ:CEP	2.02	0.72
1:J:179[B]:TYR:CE1	1:J:212[B]:GLU:CA	2.72	0.72
1:L:1:SER:CB	1:L:4:HIS:HB3	2.15	0.72
1:A:179[B]:TYR:CE1	1:A:212[B]:GLU:CA	2.72	0.72
1:B:400:PRO:O	1:B:402:GLU:N	2.20	0.72
1:C:179[B]:TYR:CE1	1:C:212[B]:GLU:CA	2.72	0.72
1:D:269:HIS:HE1	4:D:5903:PPQ:CEP	2.02	0.72
1:E:179[B]:TYR:CE1	1:E:212[B]:GLU:CA	2.72	0.72
1:E:269:HIS:HE1	4:E:5904:PPQ:CEP	2.02	0.72
1:G:269:HIS:HE1	4:G:5906:PPQ:CEP	2.02	0.72
1:I:179[B]:TYR:CE1	1:I:212[B]:GLU:CA	2.72	0.72
1:J:269:HIS:HE1	4:J:5909:PPQ:CEP	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:407:ILE:HB	1:K:408:PRO:HD2	1.70	0.72
1:D:179[B]:TYR:CE1	1:D:212[B]:GLU:CA	2.72	0.72
1:E:224:ARG:HG2	1:E:224:ARG:NH2	1.97	0.72
1:G:400:PRO:O	1:G:402:GLU:N	2.20	0.72
1:I:31:VAL:HB	1:J:180[B]:PHE:CD1	2.25	0.72
1:L:57:TRP:O	1:L:58:LYS:O	2.07	0.72
1:B:224:ARG:CG	1:B:224:ARG:HH21	2.01	0.72
1:G:1:SER:CB	1:G:4:HIS:HB3	2.15	0.72
1:K:400:PRO:O	1:K:402:GLU:N	2.20	0.72
1:A:269:HIS:HE1	4:A:5900:PPQ:CEP	2.02	0.72
1:B:337:ARG:HG3	1:B:338:ASN:CA	2.20	0.72
1:F:337:ARG:HG3	1:F:338:ASN:CA	2.20	0.72
1:J:399:LEU:H	1:J:400:PRO:CD	2.01	0.72
1:G:224:ARG:HH21	1:G:224:ARG:CG	2.01	0.72
1:J:407:ILE:HB	1:J:408:PRO:HD2	1.70	0.72
1:L:179[B]:TYR:CE1	1:L:212[B]:GLU:CA	2.72	0.72
1:B:179[B]:TYR:CE1	1:B:212[B]:GLU:CA	2.72	0.72
1:C:224:ARG:HH21	1:C:224:ARG:CG	2.01	0.72
1:K:399:LEU:H	1:K:400:PRO:CD	2.01	0.72
1:B:399:LEU:H	1:B:400:PRO:CD	2.01	0.71
1:C:407:ILE:HB	1:C:408:PRO:HD2	1.70	0.71
3:C:4473:ADP:H1'	3:C:4473:ADP:N9	1.96	0.71
1:H:400:PRO:O	1:H:402:GLU:N	2.20	0.71
1:H:57:TRP:O	1:H:58:LYS:O	2.07	0.71
1:L:176[B]:LYS:HB3	5:L:1682:HOH:O	1.90	0.71
1:A:180[B]:PHE:CD1	1:B:31:VAL:HB	2.25	0.71
1:F:57:TRP:O	1:F:58:LYS:O	2.07	0.71
1:G:384:ASN:HD22	1:G:384:ASN:N	1.88	0.71
1:H:407:ILE:HB	1:H:408:PRO:HD2	1.70	0.71
1:D:400:PRO:O	1:D:402:GLU:N	2.20	0.71
1:E:399:LEU:H	1:E:400:PRO:CD	2.01	0.71
1:K:61:ASN:HB2	1:L:337:ARG:NH1	2.05	0.71
1:D:57:TRP:O	1:D:58:LYS:O	2.07	0.71
1:G:337:ARG:HG3	1:G:338:ASN:CA	2.20	0.71
1:H:224:ARG:HH21	1:H:224:ARG:CG	2.01	0.71
1:E:384:ASN:N	1:E:384:ASN:HD22	1.88	0.71
1:L:269:HIS:HE1	4:L:5911:PPQ:CEP	2.02	0.71
1:A:57:TRP:O	1:A:58:LYS:O	2.07	0.71
1:F:399:LEU:H	1:F:400:PRO:CD	2.01	0.71
1:H:31:VAL:HB	1:I:180[B]:PHE:CD1	2.25	0.71
1:J:337:ARG:HG3	1:J:338:ASN:CA	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1:SER:HB2	1:F:4:HIS:CB	2.15	0.71
1:K:31:VAL:HB	1:L:180[B]:PHE:CD1	2.25	0.71
1:A:179[A]:TYR:O	1:A:181[A]:PRO:HD3	1.91	0.71
1:C:384:ASN:HD22	1:C:384:ASN:N	1.88	0.71
1:H:269:HIS:HE1	4:H:5907:PPQ:CEP	2.02	0.71
1:I:179[A]:TYR:O	1:I:181[A]:PRO:HD3	1.91	0.70
1:H:384:ASN:HD22	1:H:384:ASN:N	1.88	0.70
1:I:381:GLY:HA2	1:I:386:ILE:HG13	1.74	0.70
1:A:384:ASN:N	1:A:384:ASN:HD22	1.88	0.70
1:J:211[B]:HIS:NE2	5:J:5914:HOH:O	2.10	0.70
1:K:179[A]:TYR:O	1:K:181[A]:PRO:HD3	1.91	0.70
1:E:337:ARG:HG3	1:E:338:ASN:CA	2.20	0.70
1:H:399:LEU:H	1:H:400:PRO:CD	2.01	0.70
1:I:401:PRO:HA	1:I:404:ALA:HA	1.74	0.70
1:J:384:ASN:N	1:J:384:ASN:HD22	1.89	0.70
1:C:337:ARG:HG3	1:C:338:ASN:CA	2.20	0.70
1:D:176[B]:LYS:HB3	5:E:764:HOH:O	1.90	0.70
1:I:1:SER:HB2	1:I:4:HIS:CB	2.15	0.70
1:K:401:PRO:HA	1:K:404:ALA:HA	1.74	0.70
1:C:381:GLY:HA2	1:C:386:ILE:HG13	1.74	0.70
1:E:179[A]:TYR:O	1:E:181[A]:PRO:HD3	1.92	0.70
1:I:179[B]:TYR:CE1	1:I:212[B]:GLU:HA	2.27	0.70
1:I:384:ASN:HD22	1:I:384:ASN:N	1.88	0.70
1:L:179[A]:TYR:O	1:L:181[A]:PRO:HD3	1.92	0.70
1:B:1:SER:CB	1:B:4:HIS:HB3	2.15	0.70
1:D:401:PRO:HA	1:D:404:ALA:HA	1.74	0.70
1:J:179[A]:TYR:O	1:J:181[A]:PRO:HD3	1.91	0.70
1:B:401:PRO:HA	1:B:404:ALA:HA	1.74	0.70
1:D:381:GLY:HA2	1:D:386:ILE:HG13	1.74	0.70
1:E:224:ARG:CG	1:E:224:ARG:HH21	2.01	0.70
1:F:381:GLY:HA2	1:F:386:ILE:HG13	1.74	0.70
1:F:384:ASN:N	1:F:384:ASN:HD22	1.88	0.70
1:G:381:GLY:HA2	1:G:386:ILE:HG13	1.74	0.70
1:A:401:PRO:HA	1:A:404:ALA:HA	1.74	0.69
1:E:381:GLY:HA2	1:E:386:ILE:HG13	1.74	0.69
1:H:1:SER:HB2	1:H:4:HIS:CB	2.15	0.69
1:B:337:ARG:HH11	1:C:61:ASN:HB3	1.56	0.69
1:C:179[B]:TYR:CE1	1:C:212[B]:GLU:HA	2.27	0.69
1:F:179[B]:TYR:CE1	1:F:212[B]:GLU:HA	2.27	0.69
3:F:4476:ADP:N9	3:F:4476:ADP:H1'	1.96	0.69
1:B:179[A]:TYR:O	1:B:181[A]:PRO:HD3	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ASN:N	1:B:384:ASN:HD22	1.88	0.69
1:C:179[A]:TYR:O	1:C:181[A]:PRO:HD3	1.91	0.69
1:D:426:GLU:HG2	5:D:5936:HOH:O	1.93	0.69
1:F:179[A]:TYR:O	1:F:181[A]:PRO:HD3	1.91	0.69
1:H:179[A]:TYR:O	1:H:181[A]:PRO:HD3	1.91	0.69
1:K:384:ASN:HD22	1:K:384:ASN:N	1.88	0.69
1:L:224:ARG:HG2	1:L:224:ARG:NH2	1.97	0.69
1:D:1:SER:CB	1:D:4:HIS:HB3	2.16	0.69
1:A:381:GLY:HA2	1:A:386:ILE:HG13	1.74	0.69
1:A:426:GLU:HG2	5:A:5933:HOH:O	1.93	0.69
1:C:211[B]:HIS:NE2	5:C:6044:HOH:O	2.05	0.69
1:C:401:PRO:HA	1:C:404:ALA:HA	1.74	0.69
1:D:179[B]:TYR:CE1	1:D:212[B]:GLU:HA	2.27	0.69
1:F:224:ARG:HH21	1:F:224:ARG:CG	2.01	0.69
1:G:179[B]:TYR:CE1	1:G:212[B]:GLU:HA	2.27	0.69
1:H:381:GLY:HA2	1:H:386:ILE:HG13	1.74	0.69
1:J:401:PRO:HA	1:J:404:ALA:HA	1.74	0.69
1:B:381:GLY:HA2	1:B:386:ILE:HG13	1.74	0.69
1:D:384:ASN:HD22	1:D:384:ASN:N	1.88	0.69
1:B:179[B]:TYR:CE1	1:B:212[B]:GLU:HA	2.27	0.69
1:D:179[A]:TYR:O	1:D:181[A]:PRO:HD3	1.91	0.69
1:H:61:ASN:HB3	1:I:337:ARG:HH11	1.55	0.69
1:G:176[B]:LYS:HB3	5:L:1835:HOH:O	1.92	0.69
1:G:179[A]:TYR:O	1:G:181[A]:PRO:HD3	1.91	0.69
1:J:231:LYS:HE2	5:J:5926:HOH:O	1.93	0.69
1:K:426:GLU:HG2	5:K:1565:HOH:O	1.93	0.69
1:G:211[A]:HIS:CD2	1:G:212[A]:GLU:H	2.11	0.69
1:G:231:LYS:HE2	5:G:5917:HOH:O	1.93	0.69
1:I:211[A]:HIS:CD2	1:I:212[A]:GLU:H	2.11	0.69
1:B:426:GLU:HG2	5:B:5934:HOH:O	1.93	0.69
1:F:231:LYS:HE2	5:F:5919:HOH:O	1.93	0.69
1:F:269:HIS:HE1	4:F:5905:PPQ:HEP3	1.58	0.69
1:H:401:PRO:HA	1:H:404:ALA:HA	1.74	0.69
1:I:224:ARG:CG	1:I:224:ARG:HH21	2.01	0.69
1:A:211[A]:HIS:CD2	1:A:212[A]:GLU:H	2.11	0.69
1:A:180[B]:PHE:CE1	1:B:31:VAL:HB	2.28	0.69
1:F:426:GLU:HG2	5:F:5943:HOH:O	1.92	0.69
1:G:269:HIS:HE1	4:G:5906:PPQ:HEP3	1.58	0.69
1:H:426:GLU:HG2	5:H:5948:HOH:O	1.92	0.69
1:L:381:GLY:HA2	1:L:386:ILE:HG13	1.74	0.69
1:A:337:ARG:HG3	1:A:338:ASN:CA	2.20	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:427:PHE:HB2	5:J:6046:HOH:O	1.93	0.68
1:L:179[B]:TYR:CE1	1:L:212[B]:GLU:HA	2.27	0.68
1:L:211[A]:HIS:CD2	1:L:212[A]:GLU:H	2.11	0.68
1:E:179[B]:TYR:CE1	1:E:212[B]:GLU:HA	2.27	0.68
1:K:179[B]:TYR:CE1	1:K:212[B]:GLU:HA	2.27	0.68
1:B:231:LYS:HE2	5:B:5908:HOH:O	1.93	0.68
1:H:427:PHE:HB2	5:H:6043:HOH:O	1.94	0.68
1:J:179[B]:TYR:CE1	1:J:212[B]:GLU:HA	2.27	0.68
1:K:329:PRO:HG3	5:K:1655:HOH:O	1.94	0.68
1:K:381:GLY:HA2	1:K:386:ILE:HG13	1.74	0.68
1:A:427:PHE:HB2	5:A:6029:HOH:O	1.94	0.68
1:C:180[B]:PHE:CE1	1:D:31:VAL:HB	2.29	0.68
1:D:427:PHE:HB2	5:D:6032:HOH:O	1.94	0.68
1:E:329:PRO:HG3	5:E:737:HOH:O	1.94	0.68
1:G:224:ARG:HG2	1:G:224:ARG:NH2	1.97	0.68
1:G:426:GLU:HG2	5:G:5943:HOH:O	1.93	0.68
1:I:269:HIS:HE1	4:I:5908:PPQ:HEP3	1.58	0.68
1:A:179[B]:TYR:CE1	1:A:212[B]:GLU:HA	2.27	0.68
1:A:269:HIS:HE1	4:A:5900:PPQ:HEP3	1.58	0.68
1:B:329:PRO:HG3	5:B:6017:HOH:O	1.94	0.68
1:C:114:TYR:CD2	1:C:431:GLY:HA3	2.29	0.68
1:C:337:ARG:NH1	1:D:61:ASN:HB2	2.09	0.68
1:H:337:ARG:HG3	1:H:338:ASN:CA	2.20	0.68
1:L:427:PHE:HB2	5:L:1821:HOH:O	1.94	0.68
1:A:224:ARG:HH21	1:A:224:ARG:CG	2.01	0.68
1:C:427:PHE:HB2	5:C:6029:HOH:O	1.94	0.68
1:E:211[A]:HIS:CD2	1:E:212[A]:GLU:H	2.11	0.68
1:E:426:GLU:HG2	5:E:647:HOH:O	1.92	0.68
1:J:114:TYR:CD2	1:J:431:GLY:HA3	2.29	0.68
1:J:224:ARG:CG	1:J:224:ARG:HH21	2.01	0.68
1:J:381:GLY:HA2	1:J:386:ILE:HG13	1.74	0.68
1:J:426:GLU:HG2	5:J:5950:HOH:O	1.93	0.68
1:K:269:HIS:HE1	4:K:5910:PPQ:HEP3	1.58	0.68
1:B:269:HIS:HE1	4:B:5901:PPQ:HEP3	1.58	0.68
1:E:114:TYR:CD2	1:E:431:GLY:HA3	2.29	0.68
1:F:401:PRO:HA	1:F:404:ALA:HA	1.74	0.68
1:G:114:TYR:CD2	1:G:431:GLY:HA3	2.29	0.68
1:H:179[B]:TYR:CE1	1:H:212[B]:GLU:HA	2.27	0.68
1:H:31:VAL:HB	1:I:180[B]:PHE:CE1	2.28	0.68
1:J:211[A]:HIS:CD2	1:J:212[A]:GLU:H	2.11	0.68
1:I:61:ASN:CB	1:J:337:ARG:NH1	2.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:211[A]:HIS:CD2	1:K:212[A]:GLU:H	2.11	0.68
1:L:337:ARG:HG3	1:L:338:ASN:CA	2.20	0.68
1:L:401:PRO:HA	1:L:404:ALA:HA	1.74	0.68
1:D:231:LYS:HE2	5:D:5910:HOH:O	1.93	0.68
1:D:269:HIS:HE1	4:D:5903:PPQ:HEP3	1.58	0.68
1:D:337:ARG:HG3	1:D:338:ASN:CA	2.20	0.68
1:H:211[A]:HIS:CD2	1:H:212[A]:GLU:H	2.11	0.68
1:I:231:LYS:HE2	5:I:5928:HOH:O	1.93	0.68
1:I:337:ARG:HG3	1:I:338:ASN:CA	2.20	0.68
1:K:114:TYR:CD2	1:K:431:GLY:HA3	2.29	0.68
1:A:231:LYS:HE2	5:A:5907:HOH:O	1.93	0.68
1:A:114:TYR:CD2	1:A:431:GLY:HA3	2.29	0.68
1:G:401:PRO:HA	1:G:404:ALA:HA	1.74	0.68
1:I:224:ARG:HG2	1:I:224:ARG:NH2	1.97	0.68
1:K:323:VAL:CG1	5:K:1677:HOH:O	2.20	0.68
1:K:337:ARG:HG3	1:K:338:ASN:CA	2.20	0.68
1:K:427:PHE:HB2	5:K:1668:HOH:O	1.93	0.68
1:E:231:LYS:HE2	5:E:621:HOH:O	1.93	0.68
1:F:427:PHE:HB2	5:F:6039:HOH:O	1.94	0.68
1:I:114:TYR:CD2	1:I:431:GLY:HA3	2.29	0.68
1:L:360:PHE:CE2	1:L:361:PRO:HD3	2.29	0.68
1:B:427:PHE:HB2	5:B:6030:HOH:O	1.94	0.67
1:D:211[A]:HIS:CD2	1:D:212[A]:GLU:H	2.11	0.67
1:F:211[A]:HIS:CD2	1:F:212[A]:GLU:H	2.11	0.67
1:G:212[A]:GLU:HG3	1:G:218:GLN:NE2	2.10	0.67
1:C:211[A]:HIS:CD2	1:C:212[A]:GLU:H	2.11	0.67
1:F:114:TYR:CD2	1:F:431:GLY:HA3	2.29	0.67
1:I:360:PHE:CE2	1:I:361:PRO:HD3	2.29	0.67
1:J:360:PHE:CE2	1:J:361:PRO:HD3	2.29	0.67
1:L:114:TYR:CD2	1:L:431:GLY:HA3	2.29	0.67
1:L:269:HIS:HE1	4:L:5911:PPQ:HEP3	1.58	0.67
1:A:329:PRO:HG3	5:A:6016:HOH:O	1.94	0.67
1:B:114:TYR:CD2	1:B:431:GLY:HA3	2.29	0.67
1:C:231:LYS:HE2	5:C:5909:HOH:O	1.93	0.67
1:C:426:GLU:HG2	5:C:5933:HOH:O	1.93	0.67
1:D:212[A]:GLU:HG3	1:D:218:GLN:NE2	2.10	0.67
1:C:337:ARG:HH11	1:D:61:ASN:CB	2.08	0.67
1:I:61:ASN:CB	1:J:337:ARG:CD	2.67	0.67
1:K:224:ARG:HH21	1:K:224:ARG:CG	2.01	0.67
1:F:211[B]:HIS:NE2	5:F:5906:HOH:O	2.08	0.67
1:G:329:PRO:HG3	5:G:6026:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:212[A]:GLU:HG3	1:H:218:GLN:NE2	2.10	0.67
1:L:384:ASN:N	1:L:384:ASN:HD22	1.88	0.67
1:A:212[A]:GLU:HG3	1:A:218:GLN:NE2	2.10	0.67
1:A:224:ARG:NH2	1:A:224:ARG:HG2	1.97	0.67
1:C:337:ARG:HD3	1:D:61:ASN:HB3	1.75	0.67
1:E:401:PRO:HA	1:E:404:ALA:HA	1.74	0.67
1:F:329:PRO:HG3	5:F:6026:HOH:O	1.94	0.67
1:F:360:PHE:CE2	1:F:361:PRO:HD3	2.29	0.67
1:H:329:PRO:HG3	5:H:6030:HOH:O	1.94	0.67
1:I:426:GLU:HG2	5:I:5954:HOH:O	1.92	0.67
1:J:212[A]:GLU:HG3	1:J:218:GLN:NE2	2.10	0.67
1:K:212[A]:GLU:HG3	1:K:218:GLN:NE2	2.10	0.67
1:K:231:LYS:HE2	5:K:1539:HOH:O	1.93	0.67
1:L:224:ARG:HH21	1:L:224:ARG:CG	2.01	0.67
1:L:231:LYS:HE2	5:L:1692:HOH:O	1.93	0.67
1:G:360:PHE:CE2	1:G:361:PRO:HD3	2.29	0.67
1:H:114:TYR:CD2	1:H:431:GLY:HA3	2.29	0.67
1:H:269:HIS:HE1	4:H:5907:PPQ:HEP3	1.58	0.67
1:I:212[A]:GLU:HG3	1:I:218:GLN:NE2	2.10	0.67
1:B:211[A]:HIS:CD2	1:B:212[A]:GLU:H	2.11	0.67
1:B:360:PHE:CE2	1:B:361:PRO:HD3	2.29	0.67
1:C:269:HIS:HE1	4:C:5902:PPQ:HEP3	1.58	0.67
1:D:114:TYR:CD2	1:D:431:GLY:HA3	2.29	0.67
1:E:360:PHE:CE2	1:E:361:PRO:HD3	2.29	0.67
1:E:399:LEU:N	1:E:400:PRO:HD2	2.09	0.67
1:H:176[B]:LYS:C	1:H:178[B]:GLY:N	2.47	0.67
1:I:427:PHE:HB2	5:I:6050:HOH:O	1.94	0.67
1:L:426:GLU:HG2	5:L:1718:HOH:O	1.93	0.67
1:E:212[A]:GLU:HG3	1:E:218:GLN:NE2	2.10	0.67
1:B:179[A]:TYR:C	1:B:181[A]:PRO:HD2	2.16	0.67
1:B:212[A]:GLU:HG3	1:B:218:GLN:NE2	2.10	0.67
1:G:61:ASN:CB	1:H:337:ARG:NH1	2.58	0.67
1:H:211[B]:HIS:NE2	5:H:5912:HOH:O	2.11	0.67
1:E:269:HIS:HE1	4:E:5904:PPQ:HEP3	1.58	0.67
1:C:212[A]:GLU:HG3	1:C:218:GLN:NE2	2.10	0.66
1:E:315:THR:O	1:E:318:SER:HB2	1.96	0.66
1:E:427:PHE:HB2	5:E:750:HOH:O	1.94	0.66
1:H:179[A]:TYR:C	1:H:181[A]:PRO:HD2	2.16	0.66
1:I:329:PRO:HG3	5:I:6037:HOH:O	1.94	0.66
1:J:179[A]:TYR:C	1:J:181[A]:PRO:HD2	2.16	0.66
1:K:179[A]:TYR:C	1:K:181[A]:PRO:HD2	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ASP:HB3	5:A:5943:HOH:O	1.96	0.66
1:B:323:VAL:CG1	5:B:6038:HOH:O	2.20	0.66
1:C:82:ASP:HB3	5:C:5943:HOH:O	1.96	0.66
1:D:179[A]:TYR:C	1:D:181[A]:PRO:HD2	2.16	0.66
1:D:360:PHE:CE2	1:D:361:PRO:HD3	2.29	0.66
1:G:179[A]:TYR:C	1:G:181[A]:PRO:HD2	2.16	0.66
1:H:360:PHE:CE2	1:H:361:PRO:HD3	2.29	0.66
1:I:385:LYS:HE2	5:I:5992:HOH:O	1.95	0.66
1:K:315:THR:O	1:K:318:SER:HB2	1.96	0.66
1:E:179[A]:TYR:C	1:E:181[A]:PRO:HD2	2.16	0.66
1:G:385:LYS:HE2	5:G:5981:HOH:O	1.95	0.66
1:J:329:PRO:HG3	5:J:6033:HOH:O	1.94	0.66
1:C:179[A]:TYR:C	1:C:181[A]:PRO:HD2	2.16	0.66
1:C:329:PRO:HG3	5:C:6016:HOH:O	1.94	0.66
1:C:360:PHE:CE2	1:C:361:PRO:HD3	2.29	0.66
1:D:329:PRO:HG3	5:D:6019:HOH:O	1.94	0.66
1:F:298:ILE:O	1:F:302:ILE:HG13	1.96	0.66
1:A:179[A]:TYR:C	1:A:181[A]:PRO:HD2	2.16	0.66
1:A:298:ILE:O	1:A:302:ILE:HG13	1.96	0.66
1:B:315:THR:O	1:B:318:SER:HB2	1.96	0.66
1:B:55:GLY:HA3	5:B:5947:HOH:O	1.96	0.66
1:K:360:PHE:CE2	1:K:361:PRO:HD3	2.29	0.66
1:L:329:PRO:HG3	5:L:1808:HOH:O	1.94	0.66
1:L:82:ASP:HB3	5:L:1728:HOH:O	1.96	0.66
1:A:179[B]:TYR:CD1	1:A:212[B]:GLU:CA	2.77	0.66
1:C:385:LYS:HE2	5:C:5971:HOH:O	1.95	0.66
1:A:61:ASN:HB3	1:F:337:ARG:HD3	1.76	0.66
1:F:385:LYS:HE2	5:F:5981:HOH:O	1.95	0.66
1:H:231:LYS:HE2	5:H:5924:HOH:O	1.93	0.66
1:H:315:THR:O	1:H:318:SER:HB2	1.95	0.66
1:I:315:THR:O	1:I:318:SER:HB2	1.96	0.66
1:K:211[B]:HIS:NE2	5:K:1381:HOH:O	2.04	0.66
1:K:298:ILE:O	1:K:302:ILE:HG13	1.96	0.66
1:C:298:ILE:O	1:C:302:ILE:HG13	1.96	0.66
1:D:25:LYS:HD3	5:D:5949:HOH:O	1.96	0.66
1:I:399:LEU:N	1:I:400:PRO:HD2	2.09	0.66
1:K:31:VAL:HB	1:L:180[B]:PHE:CE1	2.31	0.66
1:L:212[A]:GLU:HG3	1:L:218:GLN:NE2	2.10	0.66
1:A:360:PHE:CE2	1:A:361:PRO:HD3	2.29	0.66
1:B:82:ASP:HB3	5:B:5944:HOH:O	1.96	0.66
1:F:212[A]:GLU:HG3	1:F:218:GLN:NE2	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:269:HIS:HE1	4:J:5909:PPQ:HEP3	1.58	0.66
1:K:385:LYS:HE2	5:K:1604:HOH:O	1.95	0.66
1:L:315:THR:O	1:L:318:SER:HB2	1.96	0.66
1:L:385:LYS:HE2	5:L:1757:HOH:O	1.95	0.66
1:G:427:PHE:HB2	5:G:6039:HOH:O	1.94	0.66
1:I:298:ILE:O	1:I:302:ILE:HG13	1.96	0.66
1:L:179[A]:TYR:C	1:L:181[A]:PRO:HD2	2.16	0.66
1:L:298:ILE:O	1:L:302:ILE:HG13	1.96	0.66
1:B:176[B]:LYS:C	1:B:178[B]:GLY:N	2.47	0.66
1:F:179[A]:TYR:C	1:F:181[A]:PRO:HD2	2.16	0.66
1:A:61:ASN:HB2	1:F:337:ARG:NH1	2.11	0.66
1:G:315:THR:O	1:G:318:SER:HB2	1.96	0.66
1:I:25:LYS:HD3	5:I:5967:HOH:O	1.96	0.66
1:J:82:ASP:HB3	5:J:5960:HOH:O	1.95	0.66
1:L:176[B]:LYS:C	1:L:178[B]:GLY:N	2.47	0.66
1:L:334:TYR:CD1	5:L:1764:HOH:O	2.49	0.66
1:A:334:TYR:CD1	5:A:5978:HOH:O	2.49	0.65
1:E:298:ILE:O	1:E:302:ILE:HG13	1.96	0.65
1:G:334:TYR:CD1	5:G:5988:HOH:O	2.49	0.65
1:K:308:ILE:HG21	1:K:374:LEU:HD13	1.78	0.65
1:K:82:ASP:HB3	5:K:1575:HOH:O	1.96	0.65
1:A:315:THR:O	1:A:318:SER:HB2	1.96	0.65
1:B:206:VAL:O	1:C:34:PRO:HG2	1.97	0.65
1:D:298:ILE:O	1:D:302:ILE:HG13	1.96	0.65
1:F:315:THR:O	1:F:318:SER:HB2	1.96	0.65
1:H:55:GLY:HA3	5:H:5961:HOH:O	1.96	0.65
1:I:211[B]:HIS:NE2	5:I:5913:HOH:O	2.09	0.65
1:I:308:ILE:HG21	1:I:374:LEU:HD13	1.78	0.65
1:J:385:LYS:HE2	5:J:5988:HOH:O	1.96	0.65
1:C:25:LYS:HD3	5:C:5946:HOH:O	1.96	0.65
1:C:315:THR:O	1:C:318:SER:HB2	1.96	0.65
1:E:25:LYS:CD	5:E:660:HOH:O	2.45	0.65
1:E:385:LYS:HE2	5:E:686:HOH:O	1.95	0.65
1:F:82:ASP:HB3	5:F:5953:HOH:O	1.96	0.65
1:J:25:LYS:HD3	5:J:5963:HOH:O	1.96	0.65
1:J:315:THR:O	1:J:318:SER:HB2	1.95	0.65
1:J:55:GLY:HA3	5:J:5963:HOH:O	1.96	0.65
1:A:458:HIS:CD2	1:A:460:VAL:H	2.14	0.65
1:B:25:LYS:HD3	5:B:5947:HOH:O	1.96	0.65
1:B:385:LYS:HE2	5:B:5972:HOH:O	1.95	0.65
1:D:315:THR:O	1:D:318:SER:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:298:ILE:O	1:G:302:ILE:HG13	1.96	0.65
1:I:334:TYR:CD1	5:I:5999:HOH:O	2.49	0.65
1:I:82:ASP:HB3	5:I:5964:HOH:O	1.96	0.65
1:K:55:GLY:HA3	5:K:1578:HOH:O	1.96	0.65
1:B:308:ILE:HG21	1:B:374:LEU:HD13	1.78	0.65
1:C:25:LYS:CD	5:C:5946:HOH:O	2.45	0.65
1:C:308:ILE:HG21	1:C:374:LEU:HD13	1.78	0.65
1:E:179[B]:TYR:CD1	1:E:212[B]:GLU:CA	2.77	0.65
1:F:334:TYR:CD1	5:F:5988:HOH:O	2.49	0.65
1:H:82:ASP:HB3	5:H:5958:HOH:O	1.96	0.65
1:H:61:ASN:HB3	1:I:337:ARG:HD3	1.78	0.65
1:I:458:HIS:CD2	1:I:460:VAL:H	2.14	0.65
1:A:323:VAL:CG1	5:A:6037:HOH:O	2.20	0.65
1:C:334:TYR:CD1	5:C:5978:HOH:O	2.49	0.65
1:F:25:LYS:HD3	5:F:5956:HOH:O	1.96	0.65
1:I:179[A]:TYR:C	1:I:181[A]:PRO:HD2	2.16	0.65
1:J:298:ILE:O	1:J:302:ILE:HG13	1.96	0.65
1:K:61:ASN:HB3	1:L:337:ARG:HD3	1.78	0.65
1:F:201:GLN:HA	5:F:6013:HOH:O	1.97	0.65
1:F:224:ARG:NH2	1:F:224:ARG:HG2	1.97	0.65
1:A:61:ASN:CB	1:F:337:ARG:HH11	2.10	0.65
1:H:298:ILE:O	1:H:302:ILE:HG13	1.96	0.65
1:J:61:ASN:HB3	1:K:337:ARG:HH11	1.61	0.65
1:C:201:GLN:HA	5:C:6003:HOH:O	1.97	0.65
1:G:201:GLN:HA	5:G:6013:HOH:O	1.97	0.65
1:B:298:ILE:O	1:B:302:ILE:HG13	1.96	0.65
1:D:59:GLY:C	1:D:61:ASN:H	2.01	0.65
1:E:82:ASP:HB3	5:E:657:HOH:O	1.96	0.65
1:H:385:LYS:HE2	5:H:5985:HOH:O	1.95	0.65
1:I:201:GLN:HA	5:I:6024:HOH:O	1.97	0.65
1:J:334:TYR:CD1	5:J:5995:HOH:O	2.49	0.65
1:L:25:LYS:HD3	5:L:1731:HOH:O	1.96	0.65
1:B:334:TYR:CD1	5:B:5979:HOH:O	2.49	0.65
1:D:25:LYS:CD	5:D:5949:HOH:O	2.45	0.65
1:D:399:LEU:N	1:D:400:PRO:HD2	2.09	0.65
1:E:55:GLY:HA3	5:E:660:HOH:O	1.96	0.65
1:F:179[B]:TYR:CD1	1:F:212[B]:GLU:CA	2.77	0.65
1:I:323:VAL:CG1	5:I:6058:HOH:O	2.20	0.65
1:L:179[B]:TYR:CD1	1:L:212[B]:GLU:CA	2.77	0.65
1:A:211[B]:HIS:NE2	5:A:6043:HOH:O	2.15	0.64
1:C:59:GLY:C	1:C:61:ASN:H	2.01	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:LYS:CD	5:F:5956:HOH:O	2.45	0.64
1:F:308:ILE:HG21	1:F:374:LEU:HD13	1.78	0.64
1:F:399:LEU:N	1:F:400:PRO:HD2	2.09	0.64
1:G:82:ASP:HB3	5:G:5953:HOH:O	1.95	0.64
1:H:308:ILE:HG21	1:H:374:LEU:HD13	1.78	0.64
1:I:176[B]:LYS:C	1:I:178[B]:GLY:N	2.47	0.64
1:K:25:LYS:CD	5:K:1578:HOH:O	2.45	0.64
1:A:55:GLY:HA3	5:A:5946:HOH:O	1.96	0.64
1:C:55:GLY:HA3	5:C:5946:HOH:O	1.96	0.64
1:F:55:GLY:HA3	5:F:5956:HOH:O	1.96	0.64
1:G:25:LYS:HD3	5:G:5956:HOH:O	1.96	0.64
1:H:399:LEU:N	1:H:400:PRO:HD2	2.09	0.64
1:I:55:GLY:HA3	5:I:5967:HOH:O	1.96	0.64
1:J:25:LYS:CD	5:J:5963:HOH:O	2.45	0.64
1:L:201:GLN:HA	5:L:1793:HOH:O	1.97	0.64
1:A:31:VAL:HB	1:F:180[B]:PHE:CE1	2.31	0.64
1:E:201:GLN:HA	5:E:722:HOH:O	1.97	0.64
1:E:334:TYR:CD1	5:E:693:HOH:O	2.49	0.64
1:H:25:LYS:HD3	5:H:5961:HOH:O	1.96	0.64
1:J:308:ILE:HG21	1:J:374:LEU:HD13	1.78	0.64
1:L:25:LYS:CD	5:L:1731:HOH:O	2.45	0.64
1:A:25:LYS:HD3	5:A:5946:HOH:O	1.96	0.64
1:A:308:ILE:HG21	1:A:374:LEU:HD13	1.78	0.64
1:D:201:GLN:HA	5:D:6006:HOH:O	1.97	0.64
1:E:308:ILE:HG21	1:E:374:LEU:HD13	1.78	0.64
1:G:323:VAL:CG1	5:G:6047:HOH:O	2.20	0.64
1:K:25:LYS:HD3	5:K:1578:HOH:O	1.96	0.64
1:B:399:LEU:N	1:B:400:PRO:HD2	2.09	0.64
1:B:59:GLY:C	1:B:61:ASN:H	2.01	0.64
1:D:55:GLY:HA3	5:D:5949:HOH:O	1.96	0.64
1:D:82:ASP:HB3	5:D:5946:HOH:O	1.96	0.64
5:H:6056:HOH:O	1:I:176[B]:LYS:HB3	1.96	0.64
1:I:25:LYS:CD	5:I:5967:HOH:O	2.45	0.64
1:L:458:HIS:CD2	1:L:460:VAL:H	2.14	0.64
1:A:385:LYS:HE2	5:A:5971:HOH:O	1.95	0.64
1:D:385:LYS:HE2	5:D:5974:HOH:O	1.95	0.64
1:B:25:LYS:CD	5:B:5947:HOH:O	2.45	0.64
1:F:176[B]:LYS:C	1:F:178[B]:GLY:N	2.47	0.64
1:G:25:LYS:CD	5:G:5956:HOH:O	2.45	0.64
1:H:334:TYR:CD1	5:H:5992:HOH:O	2.49	0.64
1:J:59:GLY:C	1:J:61:ASN:H	2.01	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLN:HA	5:A:6003:HOH:O	1.97	0.64
1:D:308:ILE:HG21	1:D:374:LEU:HD13	1.78	0.64
1:G:59:GLY:C	1:G:61:ASN:H	2.01	0.64
1:L:308:ILE:HG21	1:L:374:LEU:HD13	1.78	0.64
1:A:59:GLY:C	1:A:61:ASN:H	2.01	0.64
1:A:82:ASP:O	1:A:84:THR:HG22	1.98	0.64
1:I:82:ASP:O	1:I:84:THR:HG22	1.98	0.64
1:K:155:GLU:OE1	1:K:211[A]:HIS:HE1	1.81	0.64
1:L:59:GLY:C	1:L:61:ASN:H	2.01	0.64
1:L:82:ASP:O	1:L:84:THR:HG22	1.98	0.64
1:B:201:GLN:HA	5:B:6004:HOH:O	1.97	0.64
1:F:174[B]:GLY:O	1:F:177[B]:GLY:N	2.31	0.64
1:F:59:GLY:C	1:F:61:ASN:H	2.01	0.64
1:H:155:GLU:OE1	1:H:211[A]:HIS:HE1	1.82	0.64
1:H:25:LYS:CD	5:H:5961:HOH:O	2.45	0.64
1:I:61:ASN:CB	1:J:337:ARG:HD3	2.27	0.64
1:J:201:GLN:HA	5:J:6020:HOH:O	1.97	0.64
1:K:458:HIS:CD2	1:K:460:VAL:H	2.14	0.64
1:G:308:ILE:HG21	1:G:374:LEU:HD13	1.78	0.63
1:G:55:GLY:HA3	5:G:5956:HOH:O	1.96	0.63
1:K:176[B]:LYS:C	1:K:178[B]:GLY:N	2.47	0.63
1:L:55:GLY:HA3	5:L:1731:HOH:O	1.96	0.63
1:D:165:GLU:CB	5:D:5964:HOH:O	2.43	0.63
1:D:334:TYR:CD1	5:D:5981:HOH:O	2.49	0.63
1:G:174[B]:GLY:O	1:G:177[B]:GLY:N	2.31	0.63
1:G:179[B]:TYR:CD1	1:G:212[B]:GLU:CA	2.77	0.63
5:I:5969:HOH:O	1:J:182:VAL:HG23	1.97	0.63
1:K:334:TYR:CD1	5:K:1611:HOH:O	2.49	0.63
1:C:174[B]:GLY:O	1:C:177[B]:GLY:N	2.31	0.63
1:C:82:ASP:O	1:C:84:THR:HG22	1.98	0.63
1:D:82:ASP:O	1:D:84:THR:HG22	1.98	0.63
1:E:155:GLU:OE1	1:E:211[A]:HIS:HE1	1.81	0.63
1:E:82:ASP:O	1:E:84:THR:HG22	1.98	0.63
1:G:155:GLU:OE1	1:G:211[A]:HIS:HE1	1.81	0.63
1:J:224:ARG:HG2	1:J:224:ARG:NH2	1.97	0.63
1:K:174[B]:GLY:O	1:K:177[B]:GLY:N	2.31	0.63
1:D:458:HIS:CD2	1:D:460:VAL:H	2.14	0.63
1:I:59:GLY:C	1:I:61:ASN:H	2.01	0.63
1:J:360:PHE:CG	1:J:361:PRO:HD3	2.34	0.63
1:A:155:GLU:OE1	1:A:211[A]:HIS:HE1	1.81	0.63
1:J:155:GLU:OE1	1:J:211[A]:HIS:HE1	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:59:GLY:C	1:K:61:ASN:H	2.01	0.63
1:A:25:LYS:CD	5:A:5946:HOH:O	2.45	0.63
1:H:201:GLN:HA	5:H:6017:HOH:O	1.97	0.63
1:I:155:GLU:OE1	1:I:211[A]:HIS:HE1	1.81	0.63
1:L:155:GLU:OE1	1:L:211[A]:HIS:HE1	1.81	0.63
1:B:165:GLU:CB	5:B:5962:HOH:O	2.43	0.62
1:B:155:GLU:OE1	1:B:211[A]:HIS:HE1	1.81	0.62
1:E:360:PHE:CG	1:E:361:PRO:HD3	2.34	0.62
1:F:155:GLU:OE1	1:F:211[A]:HIS:HE1	1.81	0.62
1:I:174[B]:GLY:O	1:I:177[B]:GLY:N	2.31	0.62
1:A:176[B]:LYS:HB3	5:B:6043:HOH:O	1.99	0.62
1:C:155:GLU:OE1	1:C:211[A]:HIS:HE1	1.81	0.62
1:E:25:LYS:HD3	5:E:660:HOH:O	1.96	0.62
1:G:61:ASN:CB	1:H:337:ARG:CD	2.73	0.62
1:G:82:ASP:O	1:G:84:THR:HG22	1.98	0.62
1:K:201:GLN:HA	5:K:1640:HOH:O	1.97	0.62
1:F:82:ASP:O	1:F:84:THR:HG22	1.98	0.62
1:J:174[B]:GLY:O	1:J:177[B]:GLY:N	2.32	0.62
1:J:82:ASP:O	1:J:84:THR:HG22	1.98	0.62
1:K:269:HIS:CE1	4:K:5910:PPQ:HEP3	2.35	0.62
1:A:452:ARG:HA	5:A:6015:HOH:O	2.00	0.62
1:B:174[B]:GLY:O	1:B:177[B]:GLY:N	2.31	0.62
1:B:269:HIS:CE1	4:B:5901:PPQ:HEP3	2.35	0.62
1:D:155:GLU:OE1	1:D:211[A]:HIS:HE1	1.82	0.62
1:D:269:HIS:CE1	4:D:5903:PPQ:HEP3	2.35	0.62
1:F:269:HIS:CE1	4:F:5905:PPQ:HEP3	2.35	0.62
1:G:360:PHE:CG	1:G:361:PRO:HD3	2.34	0.62
1:H:399:LEU:N	1:H:400:PRO:CD	2.62	0.62
1:I:269:HIS:CE1	4:I:5908:PPQ:HEP3	2.35	0.62
1:D:179[B]:TYR:CD1	1:D:212[B]:GLU:CA	2.77	0.62
1:E:59:GLY:C	1:E:61:ASN:H	2.01	0.62
1:H:82:ASP:O	1:H:84:THR:HG22	1.98	0.62
1:J:452:ARG:HA	5:J:6032:HOH:O	2.00	0.62
1:K:82:ASP:O	1:K:84:THR:HG22	1.98	0.62
1:B:82:ASP:O	1:B:84:THR:HG22	1.98	0.62
1:C:165:GLU:CB	5:C:5961:HOH:O	2.43	0.62
1:F:128:PRO:HD2	5:F:5919:HOH:O	2.00	0.62
1:H:360:PHE:CG	1:H:361:PRO:HD3	2.34	0.62
1:K:61:ASN:HB3	1:L:337:ARG:HH11	1.65	0.62
1:L:452:ARG:HA	5:L:1807:HOH:O	2.00	0.62
1:B:128:PRO:HD2	5:B:5908:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:PHE:CG	1:C:361:PRO:HD3	2.34	0.62
1:C:452:ARG:HA	5:C:6015:HOH:O	2.00	0.62
1:H:174[B]:GLY:O	1:H:177[B]:GLY:N	2.31	0.62
1:I:329:PRO:CG	1:I:359:ARG:CD	2.75	0.62
1:K:437:GLU:HA	5:K:1656:HOH:O	2.00	0.62
1:E:174[B]:GLY:O	1:E:177[B]:GLY:N	2.31	0.62
1:H:59:GLY:C	1:H:61:ASN:H	2.01	0.62
1:I:128:PRO:HD2	5:I:5928:HOH:O	2.00	0.62
1:I:437:GLU:HA	5:I:6038:HOH:O	2.00	0.62
1:A:174[B]:GLY:O	1:A:177[B]:GLY:N	2.31	0.62
1:A:437:GLU:HA	5:A:6017:HOH:O	2.00	0.62
1:C:128:PRO:HD2	5:C:5909:HOH:O	2.00	0.62
1:C:437:GLU:HA	5:C:6017:HOH:O	2.00	0.62
1:G:452:ARG:HA	5:G:6025:HOH:O	2.00	0.62
1:I:452:ARG:HA	5:I:6036:HOH:O	2.00	0.62
1:D:211[B]:HIS:HD2	1:D:211[B]:HIS:N	1.96	0.61
1:J:61:ASN:HB3	1:K:337:ARG:HD3	1.80	0.61
1:B:452:ARG:HA	5:B:6016:HOH:O	2.00	0.61
1:D:437:GLU:HA	5:D:6020:HOH:O	2.00	0.61
1:F:452:ARG:HA	5:F:6025:HOH:O	2.00	0.61
1:J:269:HIS:CE1	4:J:5909:PPQ:HEP3	2.35	0.61
1:L:399:LEU:N	1:L:400:PRO:HD2	2.09	0.61
1:D:174[B]:GLY:O	1:D:177[B]:GLY:N	2.31	0.61
1:D:224:ARG:HG2	1:D:224:ARG:NH2	1.97	0.61
1:E:128:PRO:HD2	5:E:621:HOH:O	2.00	0.61
1:J:437:GLU:HA	5:J:6034:HOH:O	2.00	0.61
1:L:269:HIS:CE1	4:L:5911:PPQ:HEP3	2.35	0.61
1:B:437:GLU:HA	5:B:6018:HOH:O	2.00	0.61
1:C:337:ARG:NH1	1:D:61:ASN:CB	2.63	0.61
1:L:350:SER:HB2	1:L:351:PRO:HD2	1.83	0.61
1:C:350:SER:HB2	1:C:351:PRO:HD2	1.83	0.61
1:E:269:HIS:CE1	4:E:5904:PPQ:HEP3	2.35	0.61
1:E:437:GLU:HA	5:E:738:HOH:O	2.00	0.61
1:G:128:PRO:HD2	5:G:5917:HOH:O	2.00	0.61
1:G:269:HIS:CE1	4:G:5906:PPQ:HEP3	2.35	0.61
1:E:452:ARG:HA	5:E:736:HOH:O	2.00	0.61
1:G:437:GLU:HA	5:G:6027:HOH:O	2.00	0.61
1:J:128:PRO:HD2	5:J:5926:HOH:O	2.00	0.61
1:K:165:GLU:CB	5:K:1594:HOH:O	2.43	0.61
1:B:182:VAL:HG23	5:C:5948:HOH:O	2.00	0.61
1:D:360:PHE:CG	1:D:361:PRO:HD3	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:437:GLU:HA	5:F:6027:HOH:O	2.00	0.61
1:F:458:HIS:CD2	1:F:460:VAL:H	2.14	0.61
1:G:458:HIS:CD2	1:G:460:VAL:H	2.14	0.61
1:I:360:PHE:CG	1:I:361:PRO:HD3	2.34	0.61
1:J:165:GLU:CB	5:J:5978:HOH:O	2.43	0.61
1:K:42:PHE:HA	5:K:1622:HOH:O	2.01	0.61
1:L:165:GLU:CB	5:L:1747:HOH:O	2.43	0.61
1:A:128:PRO:HD2	5:A:5907:HOH:O	2.00	0.61
1:A:61:ASN:CB	1:F:337:ARG:NH1	2.64	0.61
1:H:269:HIS:CE1	4:H:5907:PPQ:HEP3	2.35	0.61
1:K:360:PHE:CG	1:K:361:PRO:HD3	2.34	0.61
1:L:174[B]:GLY:O	1:L:177[B]:GLY:N	2.31	0.61
1:L:329:PRO:CG	1:L:359:ARG:CD	2.75	0.61
1:L:360:PHE:CG	1:L:361:PRO:HD3	2.34	0.61
1:A:269:HIS:CE1	4:A:5900:PPQ:HEP3	2.35	0.61
1:C:269:HIS:CE1	4:C:5902:PPQ:HEP3	2.35	0.61
1:E:42:PHE:HA	5:E:704:HOH:O	2.01	0.61
1:E:458:HIS:CD2	1:E:460:VAL:H	2.14	0.61
1:H:350:SER:HB2	1:H:351:PRO:HD2	1.83	0.61
1:K:128:PRO:HD2	5:K:1539:HOH:O	2.00	0.61
1:A:360:PHE:CG	1:A:361:PRO:HD3	2.34	0.61
1:J:192[A]:ARG:HD3	1:J:219:ASN:ND2	2.11	0.61
1:I:63:SER:N	1:J:339:ARG:HH12	1.98	0.61
1:J:350:SER:HB2	1:J:351:PRO:HD2	1.83	0.61
1:K:179[B]:TYR:CD1	1:K:212[B]:GLU:CA	2.77	0.61
1:F:350:SER:HB2	1:F:351:PRO:HD2	1.83	0.60
1:F:360:PHE:CG	1:F:361:PRO:HD3	2.34	0.60
1:I:399:LEU:N	1:I:400:PRO:CD	2.62	0.60
1:J:323:VAL:CG1	5:J:6054:HOH:O	2.20	0.60
1:K:452:ARG:HA	5:K:1654:HOH:O	2.00	0.60
1:L:128:PRO:HD2	5:L:1692:HOH:O	2.00	0.60
1:L:192[A]:ARG:HD3	1:L:219:ASN:ND2	2.11	0.60
1:L:399:LEU:N	1:L:400:PRO:CD	2.62	0.60
1:L:437:GLU:HA	5:L:1809:HOH:O	2.00	0.60
1:A:350:SER:HB2	1:A:351:PRO:HD2	1.83	0.60
3:C:4473:ADP:C8	3:C:4473:ADP:C1'	2.81	0.60
3:D:4474:ADP:C8	3:D:4474:ADP:C1'	2.81	0.60
1:E:350:SER:HB2	1:E:351:PRO:HD2	1.83	0.60
1:I:29[A]:GLN:HB3	1:J:180[A]:PHE:HB3	1.83	0.60
1:B:42:PHE:HA	5:B:5989:HOH:O	2.01	0.60
1:C:211[B]:HIS:HD2	1:C:211[B]:HIS:N	1.96	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:458:HIS:CD2	1:H:460:VAL:H	2.14	0.60
1:A:192[A]:ARG:HD3	1:A:219:ASN:ND2	2.11	0.60
1:D:128:PRO:HD2	5:D:5910:HOH:O	2.00	0.60
1:J:285:ASP:CA	5:J:6041:HOH:O	2.35	0.60
1:K:350:SER:HB2	1:K:351:PRO:HD2	1.83	0.60
1:A:337:ARG:HD3	1:B:61:ASN:CB	2.30	0.60
1:E:337:ARG:HD3	1:F:61:ASN:HB3	1.82	0.60
1:H:179[B]:TYR:CD1	1:H:212[B]:GLU:CA	2.77	0.60
1:L:323:VAL:CG1	5:L:1830:HOH:O	2.20	0.60
1:A:42:PHE:HA	5:A:5988:HOH:O	2.01	0.60
1:B:350:SER:HB2	1:B:351:PRO:HD2	1.83	0.60
1:E:329:PRO:CG	1:E:359:ARG:CD	2.75	0.60
1:H:437:GLU:HA	5:H:6031:HOH:O	2.00	0.60
1:D:350:SER:HB2	1:D:351:PRO:HD2	1.83	0.60
1:G:63:SER:N	1:H:339:ARG:HH12	1.99	0.60
1:H:452:ARG:HA	5:H:6029:HOH:O	2.00	0.60
1:J:329:PRO:CG	1:J:359:ARG:CD	2.75	0.60
1:J:458:HIS:CD2	1:J:460:VAL:H	2.14	0.60
1:A:465:TYR:O	1:A:468:VAL:HB	2.02	0.60
1:B:458:HIS:CD2	1:B:460:VAL:H	2.14	0.60
1:D:465:TYR:O	1:D:468:VAL:HB	2.02	0.60
1:E:211[B]:HIS:N	1:E:211[B]:HIS:HD2	1.96	0.60
1:F:42:PHE:HA	5:F:5998:HOH:O	2.01	0.60
1:I:465:TYR:O	1:I:468:VAL:HB	2.02	0.60
1:J:465:TYR:O	1:J:468:VAL:HB	2.02	0.60
1:K:26:GLY:HA3	5:K:1592:HOH:O	2.02	0.60
1:G:337:ARG:HH11	1:L:61:ASN:HB3	1.65	0.60
1:F:465:TYR:O	1:F:468:VAL:HB	2.02	0.60
1:H:42:PHE:HA	5:H:6002:HOH:O	2.01	0.60
1:I:350:SER:HB2	1:I:351:PRO:HD2	1.83	0.60
1:E:26:GLY:HA3	5:E:674:HOH:O	2.02	0.60
1:E:465:TYR:O	1:E:468:VAL:HB	2.02	0.60
1:H:128:PRO:HD2	5:H:5924:HOH:O	2.00	0.60
1:K:465:TYR:O	1:K:468:VAL:HB	2.02	0.60
1:A:26:GLY:HA3	5:A:5959:HOH:O	2.02	0.59
1:D:42:PHE:HA	5:D:5991:HOH:O	2.01	0.59
1:G:42:PHE:HA	5:G:5998:HOH:O	2.01	0.59
1:J:42:PHE:HA	5:J:6005:HOH:O	2.01	0.59
1:K:251:LYS:HE2	5:K:1554:HOH:O	2.01	0.59
1:C:465:TYR:O	1:C:468:VAL:HB	2.02	0.59
1:D:452:ARG:HA	5:D:6018:HOH:O	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:28:GLU:HB2	5:H:5945:HOH:O	2.03	0.59
1:L:26:GLY:HA3	5:L:1745:HOH:O	2.02	0.59
1:A:30[A]:HIS:CE1	1:F:183:PRO:HD3	2.37	0.59
1:B:465:TYR:O	1:B:468:VAL:HB	2.02	0.59
1:G:350:SER:HB2	1:G:351:PRO:HD2	1.83	0.59
3:J:4480:ADP:C3'	5:J:5993:HOH:O	2.43	0.59
1:A:28:GLU:HB2	5:A:5930:HOH:O	2.03	0.59
1:D:183:PRO:HB2	5:E:684:HOH:O	2.01	0.59
1:H:192[A]:ARG:HD3	1:H:219:ASN:ND2	2.11	0.59
1:J:34:PRO:HG2	1:K:206:VAL:O	2.02	0.59
1:B:329:PRO:CG	1:B:359:ARG:CD	2.75	0.59
1:D:329:PRO:CG	1:D:359:ARG:CD	2.75	0.59
3:J:4480:ADP:C1'	3:J:4480:ADP:C8	2.81	0.59
3:K:4481:ADP:C8	3:K:4481:ADP:C1'	2.81	0.59
1:C:339:ARG:HH12	1:D:63:SER:N	2.00	0.59
1:F:26:GLY:HA3	5:F:5969:HOH:O	2.02	0.59
1:G:26:GLY:HA3	5:G:5969:HOH:O	2.02	0.59
3:G:4477:ADP:C3'	5:G:5986:HOH:O	2.43	0.59
1:I:26:GLY:HA3	5:I:5980:HOH:O	2.02	0.59
1:L:42:PHE:HA	5:L:1775:HOH:O	2.01	0.59
1:B:211[B]:HIS:N	1:B:211[B]:HIS:HD2	1.96	0.59
1:L:28:GLU:HB2	5:L:1715:HOH:O	2.03	0.59
1:C:192[A]:ARG:HD3	1:C:219:ASN:ND2	2.11	0.59
1:G:212[A]:GLU:HG3	1:G:218:GLN:HE21	1.68	0.59
1:G:465:TYR:O	1:G:468:VAL:HB	2.02	0.59
1:D:212[A]:GLU:HG3	1:D:218:GLN:HE21	1.68	0.59
1:D:28:GLU:HB2	5:D:5933:HOH:O	2.03	0.59
1:D:323:VAL:CG1	5:D:6040:HOH:O	2.20	0.59
1:H:131:GLU:OE2	4:H:5907:PPQ:NP	2.36	0.59
1:K:28:GLU:HB2	5:K:1562:HOH:O	2.03	0.59
1:L:465:TYR:O	1:L:468:VAL:HB	2.02	0.59
1:A:419:ASN:O	1:A:422:ASP:HB3	2.03	0.59
1:C:419:ASN:O	1:C:422:ASP:HB3	2.03	0.59
1:A:176[B]:LYS:C	1:A:178[B]:GLY:N	2.47	0.58
1:F:212[A]:GLU:HG3	1:F:218:GLN:HE21	1.68	0.58
1:H:329:PRO:CG	1:H:359:ARG:CD	2.75	0.58
1:I:165:GLU:CB	5:I:5982:HOH:O	2.43	0.58
1:K:131:GLU:OE2	4:K:5910:PPQ:NP	2.36	0.58
1:A:182:VAL:HG23	5:B:5949:HOH:O	2.01	0.58
1:D:131:GLU:OE2	4:D:5903:PPQ:NP	2.36	0.58
1:E:419:ASN:O	1:E:422:ASP:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:GLU:OE2	4:E:5904:PPQ:NP	2.36	0.58
1:F:285:ASP:CA	5:F:6034:HOH:O	2.35	0.58
1:A:63:SER:N	1:F:339:ARG:HH12	2.01	0.58
1:I:212[A]:GLU:HG3	1:I:218:GLN:HE21	1.68	0.58
1:I:42:PHE:HA	5:I:6009:HOH:O	2.01	0.58
1:J:399:LEU:N	1:J:400:PRO:HD2	2.09	0.58
1:K:285:ASP:CA	5:K:1663:HOH:O	2.35	0.58
1:G:337:ARG:HD3	1:L:61:ASN:CB	2.33	0.58
1:A:285:ASP:CA	5:A:6024:HOH:O	2.35	0.58
3:B:4472:ADP:C1'	3:B:4472:ADP:C8	2.81	0.58
1:C:178[A]:GLY:O	1:C:212[A]:GLU:C	2.42	0.58
1:C:26:GLY:HA3	5:C:5959:HOH:O	2.02	0.58
1:B:337:ARG:HD3	1:C:61:ASN:HB3	1.81	0.58
1:E:28:GLU:HB2	5:E:644:HOH:O	2.03	0.58
1:G:28:GLU:HB2	5:G:5940:HOH:O	2.03	0.58
1:G:131:GLU:OE2	4:G:5906:PPQ:NP	2.36	0.58
1:H:165:GLU:CB	5:H:5975:HOH:O	2.43	0.58
1:I:419:ASN:O	1:I:422:ASP:HB3	2.03	0.58
1:A:337:ARG:CD	1:B:61:ASN:CB	2.70	0.58
1:B:360:PHE:CG	1:B:361:PRO:HD3	2.34	0.58
1:C:212[A]:GLU:HG3	1:C:218:GLN:HE21	1.68	0.58
1:C:399:LEU:N	1:C:400:PRO:HD2	2.09	0.58
1:F:28:GLU:HB2	5:F:5940:HOH:O	2.03	0.58
1:H:211[B]:HIS:N	1:H:211[B]:HIS:HD2	1.96	0.58
1:H:26:GLY:HA3	5:H:5973:HOH:O	2.02	0.58
1:H:465:TYR:O	1:H:468:VAL:HB	2.02	0.58
1:J:251:LYS:HE2	5:J:5940:HOH:O	2.00	0.58
1:K:211[B]:HIS:N	1:K:211[B]:HIS:HD2	1.96	0.58
1:L:419:ASN:O	1:L:422:ASP:HB3	2.03	0.58
1:J:178[A]:GLY:O	1:J:212[A]:GLU:C	2.42	0.58
1:K:178[A]:GLY:O	1:K:212[A]:GLU:C	2.42	0.58
1:K:212[A]:GLU:HG3	1:K:218:GLN:HE21	1.68	0.58
1:B:131:GLU:OE2	4:B:5901:PPQ:NP	2.36	0.58
1:C:131:GLU:OE2	4:C:5902:PPQ:NP	2.36	0.58
1:D:26:GLY:HA3	5:D:5962:HOH:O	2.02	0.58
1:F:329:PRO:CG	1:F:359:ARG:CD	2.75	0.58
1:G:419:ASN:O	1:G:422:ASP:HB3	2.03	0.58
1:J:131:GLU:OE2	4:J:5909:PPQ:NP	2.36	0.58
1:K:419:ASN:O	1:K:422:ASP:HB3	2.03	0.58
1:L:212[A]:GLU:HG3	1:L:218:GLN:HE21	1.68	0.58
1:A:131:GLU:OE2	4:A:5900:PPQ:NP	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178[A]:GLY:O	1:B:212[A]:GLU:C	2.42	0.58
1:B:189:GLN:HG3	1:C:80:PHE:CZ	2.39	0.58
1:B:192[A]:ARG:HD3	1:B:219:ASN:ND2	2.11	0.58
1:C:28:GLU:HB2	5:C:5930:HOH:O	2.03	0.58
1:C:360:PHE:CD2	1:C:361:PRO:CD	2.75	0.58
1:C:42:PHE:HA	5:C:5988:HOH:O	2.01	0.58
1:E:211[B]:HIS:NE2	5:E:769:HOH:O	2.10	0.58
1:G:285:ASP:CA	5:G:6034:HOH:O	2.35	0.58
1:H:419:ASN:O	1:H:422:ASP:HB3	2.03	0.58
1:I:131:GLU:OE2	4:I:5908:PPQ:NP	2.36	0.58
1:I:211[B]:HIS:HD2	1:I:211[B]:HIS:N	1.96	0.58
1:J:114:TYR:HD2	1:J:431:GLY:HA3	1.69	0.58
1:J:419:ASN:O	1:J:422:ASP:HB3	2.03	0.58
1:K:192[A]:ARG:HD3	1:K:219:ASN:ND2	2.11	0.58
1:A:178[A]:GLY:O	1:A:212[A]:GLU:C	2.42	0.58
1:B:26:GLY:HA3	5:B:5960:HOH:O	2.02	0.58
1:C:224:ARG:NH2	1:C:224:ARG:HG2	1.97	0.58
1:E:183:PRO:HB2	5:F:5979:HOH:O	2.03	0.58
1:E:192[A]:ARG:HD3	1:E:219:ASN:ND2	2.11	0.58
1:F:399:LEU:N	1:F:400:PRO:CD	2.63	0.58
1:G:360:PHE:CD2	1:G:361:PRO:CD	2.75	0.58
1:H:178[A]:GLY:O	1:H:212[A]:GLU:C	2.42	0.58
1:J:28:GLU:HB2	5:J:5947:HOH:O	2.03	0.58
1:L:114:TYR:HD2	1:L:431:GLY:HA3	1.69	0.58
1:A:212[A]:GLU:HG3	1:A:218:GLN:HE21	1.68	0.58
3:A:4471:ADP:C8	3:A:4471:ADP:C1'	2.81	0.58
1:D:178[A]:GLY:O	1:D:212[A]:GLU:C	2.42	0.58
1:D:211[B]:HIS:NE2	5:D:6046:HOH:O	2.20	0.58
1:F:131:GLU:OE2	4:F:5905:PPQ:NP	2.36	0.58
1:H:34:PRO:HG2	1:I:206:VAL:O	2.03	0.58
1:L:131:GLU:OE2	4:L:5911:PPQ:NP	2.36	0.58
1:L:211[B]:HIS:HD2	1:L:211[B]:HIS:N	1.96	0.58
1:B:419:ASN:O	1:B:422:ASP:HB3	2.03	0.58
1:D:192[A]:ARG:HD3	1:D:219:ASN:ND2	2.11	0.58
3:D:4474:ADP:C3'	5:D:5979:HOH:O	2.43	0.58
3:E:4475:ADP:C1'	3:E:4475:ADP:C8	2.81	0.58
1:G:211[B]:HIS:HD2	1:G:211[B]:HIS:N	1.96	0.58
1:G:399:LEU:N	1:G:400:PRO:HD2	2.09	0.58
3:G:4477:ADP:C1'	3:G:4477:ADP:C8	2.81	0.58
1:I:28:GLU:HB2	5:I:5951:HOH:O	2.03	0.58
1:D:114:TYR:HD2	1:D:431:GLY:HA3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:4479:ADP:C3'	5:I:5997:HOH:O	2.42	0.57
1:J:26:GLY:HA3	5:J:5976:HOH:O	2.02	0.57
1:B:251:LYS:HE2	5:B:5923:HOH:O	2.00	0.57
1:E:178[A]:GLY:O	1:E:212[A]:GLU:C	2.42	0.57
1:F:458:HIS:HD2	1:F:460:VAL:N	2.01	0.57
1:G:399:LEU:N	1:G:400:PRO:CD	2.63	0.57
1:B:360:PHE:CD2	1:B:361:PRO:CD	2.75	0.57
1:G:178[A]:GLY:O	1:G:212[A]:GLU:C	2.42	0.57
1:I:178[A]:GLY:O	1:I:212[A]:GLU:C	2.42	0.57
1:I:179[B]:TYR:CD1	1:I:212[B]:GLU:CA	2.77	0.57
1:E:347:VAL:HA	5:E:670:HOH:O	2.04	0.57
1:K:291:SER:O	1:K:295:LEU:HD12	2.05	0.57
1:B:28:GLU:HB2	5:B:5931:HOH:O	2.03	0.57
1:B:291:SER:O	1:B:295:LEU:HD12	2.05	0.57
5:B:5946:HOH:O	1:C:84:THR:HG21	2.05	0.57
1:F:178[A]:GLY:O	1:F:212[A]:GLU:C	2.42	0.57
1:I:114:TYR:HD2	1:I:431:GLY:HA3	1.69	0.57
1:J:179[B]:TYR:CD1	1:J:212[B]:GLU:CA	2.77	0.57
1:J:212[A]:GLU:HG3	1:J:218:GLN:HE21	1.68	0.57
1:K:29[A]:GLN:HB3	1:L:180[A]:PHE:HB3	1.87	0.57
1:B:312:ALA:HB2	1:B:370:CYS:SG	2.45	0.57
1:F:347:VAL:HA	5:F:5966:HOH:O	2.04	0.57
1:G:291:SER:O	1:G:295:LEU:HD12	2.05	0.57
3:I:4479:ADP:C8	3:I:4479:ADP:C1'	2.81	0.57
1:C:312:ALA:HB2	1:C:370:CYS:SG	2.45	0.57
1:D:311:LEU:HD12	1:D:373:ALA:HB2	1.87	0.57
1:E:323:VAL:CG1	5:E:759:HOH:O	2.20	0.57
1:F:201:GLN:CA	5:F:6013:HOH:O	2.53	0.57
1:G:165:GLU:CB	5:G:5971:HOH:O	2.43	0.57
1:H:285:ASP:CA	5:H:6038:HOH:O	2.35	0.57
1:K:312:ALA:HB2	1:K:370:CYS:SG	2.45	0.57
1:L:178[A]:GLY:O	1:L:212[A]:GLU:C	2.42	0.57
3:L:4482:ADP:C3'	5:L:1762:HOH:O	2.43	0.57
1:A:311:LEU:HD12	1:A:373:ALA:HB2	1.87	0.57
1:A:312:ALA:HB2	1:A:370:CYS:SG	2.45	0.57
1:B:212[A]:GLU:HG3	1:B:218:GLN:HE21	1.68	0.57
1:D:419:ASN:O	1:D:422:ASP:HB3	2.03	0.57
1:G:312:ALA:HB2	1:G:370:CYS:SG	2.45	0.57
1:H:291:SER:O	1:H:295:LEU:HD12	2.05	0.57
1:H:311:LEU:HD12	1:H:373:ALA:HB2	1.87	0.57
1:H:458:HIS:HD2	1:H:460:VAL:N	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ARG:HH11	1:B:61:ASN:HB3	1.68	0.57
1:B:285:ASP:CA	5:B:6025:HOH:O	2.35	0.57
1:C:180[A]:PHE:HB3	1:D:29[A]:GLN:HB3	1.86	0.57
1:D:312:ALA:HB2	1:D:370:CYS:SG	2.45	0.57
1:E:291:SER:O	1:E:295:LEU:HD12	2.05	0.57
1:F:291:SER:O	1:F:295:LEU:HD12	2.05	0.57
1:F:419:ASN:O	1:F:422:ASP:HB3	2.03	0.57
1:G:114:TYR:HD2	1:G:431:GLY:HA3	1.69	0.57
1:G:347:VAL:HA	5:G:5966:HOH:O	2.04	0.57
1:H:312:ALA:HB2	1:H:370:CYS:SG	2.45	0.57
1:I:291:SER:O	1:I:295:LEU:HD12	2.05	0.57
1:L:311:LEU:HD12	1:L:373:ALA:HB2	1.87	0.57
1:L:360:PHE:CD2	1:L:361:PRO:CD	2.75	0.57
1:A:114:TYR:HD2	1:A:431:GLY:HA3	1.69	0.57
1:E:165:GLU:CB	5:E:676:HOH:O	2.43	0.57
1:G:61:ASN:CB	1:H:337:ARG:HD3	2.33	0.57
5:G:5958:HOH:O	1:H:182:VAL:HG23	2.04	0.57
1:H:347:VAL:HA	5:H:5970:HOH:O	2.04	0.57
1:I:311:LEU:HD12	1:I:373:ALA:HB2	1.87	0.57
1:I:312:ALA:HB2	1:I:370:CYS:SG	2.45	0.57
1:J:84:THR:HG21	5:K:1577:HOH:O	2.05	0.57
1:L:264[B]:ASN:HA	1:L:326:TYR:HB3	1.87	0.57
1:A:347:VAL:HA	5:A:5956:HOH:O	2.04	0.56
3:A:4471:ADP:C3'	5:A:5976:HOH:O	2.43	0.56
1:B:1:SER:C	1:B:71:ALA:HB1	2.25	0.56
1:C:291:SER:O	1:C:295:LEU:HD12	2.05	0.56
1:F:1:SER:C	1:F:71:ALA:HB1	2.26	0.56
1:J:230:LYS:O	1:J:233:ASP:HB2	2.05	0.56
1:K:347:VAL:HA	5:K:1588:HOH:O	2.04	0.56
1:K:114:TYR:HD2	1:K:431:GLY:HA3	1.69	0.56
1:K:1:SER:C	1:K:71:ALA:HB1	2.25	0.56
1:B:399:LEU:N	1:B:400:PRO:CD	2.62	0.56
1:B:180[A]:PHE:HB3	1:C:29[A]:GLN:HB3	1.88	0.56
1:F:264[B]:ASN:HA	1:F:326:TYR:HB3	1.87	0.56
1:F:57:TRP:C	1:F:58:LYS:O	2.42	0.56
1:H:264[B]:ASN:HA	1:H:326:TYR:HB3	1.87	0.56
1:I:360:PHE:CD2	1:I:361:PRO:CD	2.75	0.56
1:J:291:SER:O	1:J:295:LEU:HD12	2.05	0.56
1:K:311:LEU:HD12	1:K:373:ALA:HB2	1.87	0.56
1:C:251:LYS:HE2	5:C:5923:HOH:O	2.01	0.56
1:C:264[B]:ASN:HA	1:C:326:TYR:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:LYS:O	1:E:233:ASP:HB2	2.05	0.56
1:E:311:LEU:HD12	1:E:373:ALA:HB2	1.87	0.56
1:E:360:PHE:CD2	1:E:361:PRO:CD	2.75	0.56
1:G:1:SER:C	1:G:71:ALA:HB1	2.26	0.56
1:H:1:SER:C	1:H:71:ALA:HB1	2.26	0.56
1:H:57:TRP:C	1:H:58:LYS:O	2.42	0.56
1:H:61:ASN:HB3	1:I:337:ARG:NH1	2.14	0.56
1:K:57:TRP:C	1:K:58:LYS:O	2.42	0.56
1:L:230:LYS:O	1:L:233:ASP:HB2	2.05	0.56
1:L:312:ALA:HB2	1:L:370:CYS:SG	2.45	0.56
1:B:230:LYS:O	1:B:233:ASP:HB2	2.05	0.56
1:C:230:LYS:O	1:C:233:ASP:HB2	2.05	0.56
1:C:347:VAL:HA	5:C:5956:HOH:O	2.04	0.56
1:C:114:TYR:HD2	1:C:431:GLY:HA3	1.69	0.56
1:G:189:GLN:NE2	1:G:209[A]:HIS:CE1	2.72	0.56
1:H:212[A]:GLU:HG3	1:H:218:GLN:HE21	1.68	0.56
1:H:230:LYS:O	1:H:233:ASP:HB2	2.05	0.56
1:J:264[B]:ASN:HA	1:J:326:TYR:HB3	1.87	0.56
1:J:80:PHE:CZ	1:K:189:GLN:HG3	2.40	0.56
1:A:165:GLU:CB	5:A:5961:HOH:O	2.43	0.56
1:A:1:SER:C	1:A:71:ALA:HB1	2.26	0.56
1:B:311:LEU:HD12	1:B:373:ALA:HB2	1.87	0.56
1:C:1:SER:C	1:C:71:ALA:HB1	2.26	0.56
1:E:212[A]:GLU:HG3	1:E:218:GLN:HE21	1.68	0.56
1:E:312:ALA:HB2	1:E:370:CYS:SG	2.45	0.56
3:E:4475:ADP:C3'	5:E:691:HOH:O	2.43	0.56
1:I:347:VAL:HA	5:I:5977:HOH:O	2.04	0.56
1:I:61:ASN:O	1:J:337:ARG:O	2.23	0.56
1:C:458:HIS:CD2	1:C:460:VAL:H	2.14	0.56
1:D:347:VAL:HA	5:D:5959:HOH:O	2.04	0.56
1:E:1:SER:C	1:E:71:ALA:HB1	2.26	0.56
1:F:311:LEU:HD12	1:F:373:ALA:HB2	1.87	0.56
1:G:192[A]:ARG:HD3	1:G:219:ASN:ND2	2.11	0.56
3:H:4478:ADP:C8	3:H:4478:ADP:C1'	2.81	0.56
1:J:347:VAL:HA	5:J:5973:HOH:O	2.04	0.56
1:J:360:PHE:CD2	1:J:361:PRO:CD	2.75	0.56
1:J:399:LEU:N	1:J:400:PRO:CD	2.63	0.56
1:K:264[B]:ASN:HA	1:K:326:TYR:HB3	1.87	0.56
1:B:264[B]:ASN:HA	1:B:326:TYR:HB3	1.87	0.56
1:B:57:TRP:C	1:B:58:LYS:O	2.42	0.56
1:C:329:PRO:CG	1:C:359:ARG:CD	2.75	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:201:GLN:CA	5:G:6013:HOH:O	2.53	0.56
1:I:1:SER:C	1:I:71:ALA:HB1	2.25	0.56
1:J:29[A]:GLN:HB3	1:K:180[A]:PHE:HB3	1.87	0.56
1:L:347:VAL:HA	5:L:1741:HOH:O	2.04	0.56
1:F:114:TYR:HD2	1:F:431:GLY:HA3	1.69	0.56
1:F:312:ALA:HB2	1:F:370:CYS:SG	2.45	0.56
1:G:29[A]:GLN:HB3	1:H:180[A]:PHE:HB3	1.88	0.56
1:G:60:ILE:CD1	5:H:6053:HOH:O	2.27	0.56
1:I:182:VAL:HG23	5:I:5916:HOH:O	2.05	0.56
1:J:1:SER:C	1:J:71:ALA:HB1	2.26	0.56
1:J:312:ALA:HB2	1:J:370:CYS:SG	2.45	0.56
1:L:291:SER:O	1:L:295:LEU:HD12	2.05	0.56
3:L:4482:ADP:C1'	3:L:4482:ADP:C8	2.81	0.56
1:A:291:SER:O	1:A:295:LEU:HD12	2.05	0.56
1:C:311:LEU:HD12	1:C:373:ALA:HB2	1.87	0.56
1:E:285:ASP:CA	5:E:745:HOH:O	2.35	0.56
1:E:458:HIS:HB3	1:E:461:GLU:HG3	1.88	0.56
1:E:57:TRP:C	1:E:58:LYS:O	2.42	0.56
1:F:230:LYS:O	1:F:233:ASP:HB2	2.05	0.56
1:G:57:TRP:C	1:G:58:LYS:O	2.42	0.56
1:H:179[A]:TYR:O	1:H:181[A]:PRO:HD2	2.05	0.56
1:H:201:GLN:CA	5:H:6017:HOH:O	2.53	0.56
1:C:269:HIS:CD2	1:C:359:ARG:HG3	2.41	0.56
3:F:4476:ADP:C1'	3:F:4476:ADP:C8	2.81	0.56
1:H:251:LYS:HE2	5:H:5938:HOH:O	2.00	0.56
1:I:179[A]:TYR:C	1:I:181[A]:PRO:CD	2.75	0.56
1:K:201:GLN:CA	5:K:1640:HOH:O	2.53	0.56
1:L:179[A]:TYR:O	1:L:181[A]:PRO:HD2	2.05	0.56
1:L:211[B]:HIS:O	1:L:212[B]:GLU:CB	2.54	0.56
1:B:347:VAL:HA	5:B:5957:HOH:O	2.04	0.56
1:D:269:HIS:CD2	1:D:359:ARG:HG3	2.41	0.56
1:F:192[A]:ARG:HD3	1:F:219:ASN:ND2	2.11	0.56
1:G:311:LEU:HD12	1:G:373:ALA:HB2	1.87	0.56
3:H:4478:ADP:C3'	5:H:5990:HOH:O	2.43	0.56
1:H:29[A]:GLN:HB3	1:I:180[A]:PHE:HB3	1.88	0.56
1:I:251:LYS:HE2	5:I:5943:HOH:O	2.01	0.56
1:I:458:HIS:HB3	1:I:461:GLU:HG3	1.88	0.56
1:J:269:HIS:CD2	1:J:359:ARG:HG3	2.41	0.56
1:K:179[A]:TYR:O	1:K:181[A]:PRO:HD2	2.05	0.56
5:J:5965:HOH:O	1:K:182:VAL:HG23	2.06	0.56
1:K:399:LEU:N	1:K:400:PRO:HD2	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:HIS:HB3	1:A:461:GLU:HG3	1.88	0.55
1:C:201:GLN:CA	5:C:6003:HOH:O	2.53	0.55
1:C:91:ILE:HB	1:C:103:ASP:HB2	1.88	0.55
1:I:230:LYS:O	1:I:233:ASP:HB2	2.05	0.55
1:I:264[B]:ASN:HA	1:I:326:TYR:HB3	1.87	0.55
1:I:269:HIS:CD2	1:I:359:ARG:HG3	2.41	0.55
1:I:57:TRP:C	1:I:58:LYS:O	2.42	0.55
1:L:1:SER:C	1:L:71:ALA:HB1	2.26	0.55
1:A:230:LYS:O	1:A:233:ASP:HB2	2.05	0.55
1:C:57:TRP:C	1:C:58:LYS:O	2.42	0.55
1:D:251:LYS:HE2	5:D:5925:HOH:O	2.01	0.55
1:D:458:HIS:HB3	1:D:461:GLU:HG3	1.88	0.55
1:E:91:ILE:HB	1:E:103:ASP:HB2	1.89	0.55
1:D:337:ARG:HD3	1:E:61:ASN:HB3	1.82	0.55
1:G:179[A]:TYR:C	1:G:181[A]:PRO:CD	2.75	0.55
1:G:269:HIS:CD2	1:G:359:ARG:HG3	2.41	0.55
1:G:334:TYR:HD1	5:G:5988:HOH:O	1.88	0.55
1:G:458:HIS:HD2	1:G:460:VAL:N	2.01	0.55
1:G:61:ASN:O	1:H:337:ARG:O	2.24	0.55
1:H:360:PHE:CD2	1:H:361:PRO:CD	2.75	0.55
1:I:192[A]:ARG:HD3	1:I:219:ASN:ND2	2.11	0.55
1:J:458:HIS:HB3	1:J:461:GLU:HG3	1.88	0.55
1:L:458:HIS:HB3	1:L:461:GLU:HG3	1.88	0.55
1:A:264[B]:ASN:HA	1:A:326:TYR:HB3	1.87	0.55
1:B:179[A]:TYR:C	1:B:181[A]:PRO:CD	2.75	0.55
1:E:251:LYS:HE2	5:E:636:HOH:O	2.01	0.55
1:G:91:ILE:HB	1:G:103:ASP:HB2	1.88	0.55
1:G:337:ARG:CD	1:L:61:ASN:CB	2.72	0.55
1:K:230:LYS:O	1:K:233:ASP:HB2	2.05	0.55
1:C:183:PRO:HD3	1:D:30[A]:HIS:CE1	2.41	0.55
1:D:1:SER:C	1:D:71:ALA:HB1	2.26	0.55
1:E:179[A]:TYR:O	1:E:181[A]:PRO:HD2	2.05	0.55
1:H:80:PHE:CZ	1:I:189:GLN:HG3	2.42	0.55
1:I:189:GLN:NE2	1:I:209[A]:HIS:CE1	2.72	0.55
1:I:201:GLN:CA	5:I:6024:HOH:O	2.53	0.55
1:J:189:GLN:NE2	1:J:209[A]:HIS:CE1	2.72	0.55
1:J:458:HIS:HD2	1:J:460:VAL:N	2.01	0.55
1:K:360:PHE:CD2	1:K:361:PRO:CD	2.75	0.55
1:A:179[A]:TYR:O	1:A:181[A]:PRO:HD2	2.05	0.55
1:E:264[B]:ASN:HA	1:E:326:TYR:HB3	1.87	0.55
1:A:29[A]:GLN:HB3	1:F:180[A]:PHE:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:91:ILE:HB	1:J:103:ASP:HB2	1.88	0.55
1:J:179[A]:TYR:C	1:J:181[A]:PRO:CD	2.75	0.55
1:K:458:HIS:HD2	1:K:460:VAL:N	2.01	0.55
1:B:179[A]:TYR:O	1:B:181[A]:PRO:HD2	2.05	0.55
1:D:291:SER:O	1:D:295:LEU:HD12	2.05	0.55
1:D:264[B]:ASN:HA	1:D:326:TYR:HB3	1.87	0.55
1:F:323:VAL:CG1	5:F:6047:HOH:O	2.20	0.55
1:E:189:GLN:HG3	1:F:80:PHE:CZ	2.41	0.55
1:H:179[A]:TYR:C	1:H:181[A]:PRO:CD	2.75	0.55
1:H:323:VAL:CG1	5:H:6051:HOH:O	2.20	0.55
1:B:458:HIS:HD2	1:B:460:VAL:N	2.01	0.55
1:F:269:HIS:CD2	1:F:359:ARG:HG3	2.41	0.55
1:G:230:LYS:O	1:G:233:ASP:HB2	2.05	0.55
1:I:179[A]:TYR:O	1:I:181[A]:PRO:HD2	2.05	0.55
1:J:201:GLN:CA	5:J:6020:HOH:O	2.53	0.55
1:J:211[B]:HIS:HD2	1:J:211[B]:HIS:N	1.96	0.55
1:L:91:ILE:HB	1:L:103:ASP:HB2	1.88	0.55
1:A:334:TYR:HD1	5:A:5978:HOH:O	1.88	0.55
1:B:458:HIS:HB3	1:B:461:GLU:HG3	1.88	0.55
1:E:269:HIS:CD2	1:E:359:ARG:HG3	2.41	0.55
1:H:91:ILE:HB	1:H:103:ASP:HB2	1.88	0.55
1:H:269:HIS:CD2	1:H:359:ARG:HG3	2.41	0.55
1:K:334:TYR:HD1	5:K:1611:HOH:O	1.88	0.55
1:K:399:LEU:N	1:K:400:PRO:CD	2.62	0.55
1:F:179[A]:TYR:C	1:F:181[A]:PRO:CD	2.75	0.55
1:G:264[B]:ASN:HA	1:G:326:TYR:HB3	1.87	0.55
1:I:34:PRO:HG2	1:J:206:VAL:O	2.06	0.55
1:K:269:HIS:CD2	1:K:359:ARG:HG3	2.41	0.55
1:L:201:GLN:CA	5:L:1793:HOH:O	2.53	0.55
1:A:201:GLN:CA	5:A:6003:HOH:O	2.53	0.55
1:A:454:ARG:NH2	1:A:454:ARG:HB3	2.22	0.55
1:B:454:ARG:NH2	1:B:454:ARG:HB3	2.22	0.55
1:C:176[B]:LYS:C	1:C:178[B]:GLY:N	2.47	0.55
3:C:4473:ADP:C3'	5:C:5976:HOH:O	2.43	0.55
1:E:458:HIS:HD2	1:E:460:VAL:N	2.01	0.55
1:I:91:ILE:HB	1:I:103:ASP:HB2	1.89	0.55
1:L:269:HIS:CD2	1:L:359:ARG:HG3	2.41	0.55
1:C:454:ARG:NH2	1:C:454:ARG:HB3	2.22	0.54
1:D:201:GLN:CA	5:D:6006:HOH:O	2.53	0.54
1:D:230:LYS:O	1:D:233:ASP:HB2	2.05	0.54
1:D:360:PHE:CD2	1:D:361:PRO:CD	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:GLN:CA	5:E:722:HOH:O	2.53	0.54
1:F:165:GLU:CB	5:F:5971:HOH:O	2.43	0.54
1:G:189:GLN:HG3	1:L:80:PHE:CZ	2.42	0.54
1:K:211[B]:HIS:O	1:K:212[B]:GLU:CB	2.54	0.54
1:K:458:HIS:HB3	1:K:461:GLU:HG3	1.88	0.54
1:A:269:HIS:CD2	1:A:359:ARG:HG3	2.41	0.54
1:B:269:HIS:CD2	1:B:359:ARG:HG3	2.41	0.54
1:C:179[A]:TYR:C	1:C:181[A]:PRO:CD	2.75	0.54
1:D:91:ILE:HB	1:D:103:ASP:HB2	1.89	0.54
1:E:337:ARG:NH1	1:F:61:ASN:HB3	2.12	0.54
1:H:458:HIS:HB3	1:H:461:GLU:HG3	1.88	0.54
1:K:329:PRO:CG	1:K:359:ARG:CD	2.75	0.54
1:K:91:ILE:HB	1:K:103:ASP:HB2	1.89	0.54
1:D:179[A]:TYR:C	1:D:181[A]:PRO:CD	2.75	0.54
1:G:179[A]:TYR:O	1:G:181[A]:PRO:HD2	2.05	0.54
1:G:458:HIS:HB3	1:G:461:GLU:HG3	1.88	0.54
1:L:57:TRP:C	1:L:58:LYS:O	2.42	0.54
1:A:179[A]:TYR:C	1:A:181[A]:PRO:CD	2.75	0.54
1:A:189:GLN:NE2	1:A:209[A]:HIS:CE1	2.72	0.54
1:A:57:TRP:C	1:A:58:LYS:O	2.42	0.54
1:A:91:ILE:HB	1:A:103:ASP:HB2	1.89	0.54
1:C:458:HIS:HB3	1:C:461:GLU:HG3	1.88	0.54
1:F:334:TYR:HD1	5:F:5988:HOH:O	1.89	0.54
1:E:206:VAL:O	1:F:34:PRO:HG2	2.08	0.54
1:F:458:HIS:HB3	1:F:461:GLU:HG3	1.88	0.54
1:G:183:PRO:HB2	5:L:1755:HOH:O	2.06	0.54
1:H:114:TYR:HD2	1:H:431:GLY:HA3	1.69	0.54
1:I:129:GLU:HA	5:I:5925:HOH:O	2.08	0.54
1:J:311:LEU:HD12	1:J:373:ALA:HB2	1.87	0.54
1:D:454:ARG:HB3	1:D:454:ARG:NH2	2.22	0.54
1:D:57:TRP:O	1:D:58:LYS:C	2.46	0.54
1:D:57:TRP:C	1:D:58:LYS:O	2.42	0.54
1:E:454:ARG:NH2	1:E:454:ARG:HB3	2.22	0.54
1:F:189:GLN:NE2	1:F:209[A]:HIS:CE1	2.72	0.54
1:F:211[A]:HIS:CD2	1:F:212[A]:GLU:N	2.76	0.54
1:F:454:ARG:NH2	1:F:454:ARG:HB3	2.22	0.54
1:G:182:VAL:HG23	5:L:1733:HOH:O	2.07	0.54
1:K:179[A]:TYR:C	1:K:181[A]:PRO:CD	2.75	0.54
1:L:129:GLU:HA	5:L:1689:HOH:O	2.08	0.54
1:L:454:ARG:NH2	1:L:454:ARG:HB3	2.22	0.54
1:B:91:ILE:HB	1:B:103:ASP:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:454:ARG:HB3	1:G:454:ARG:NH2	2.23	0.54
1:H:454:ARG:HB3	1:H:454:ARG:NH2	2.22	0.54
1:H:84:THR:HG21	5:I:5966:HOH:O	2.08	0.54
1:I:59:GLY:O	1:I:61:ASN:N	2.41	0.54
1:J:454:ARG:HB3	1:J:454:ARG:NH2	2.22	0.54
1:C:399:LEU:N	1:C:400:PRO:CD	2.62	0.54
1:D:211[B]:HIS:O	1:D:212[B]:GLU:CB	2.54	0.54
1:D:211[A]:HIS:CD2	1:D:212[A]:GLU:N	2.76	0.54
1:F:57:TRP:O	1:F:58:LYS:C	2.46	0.54
1:G:211[A]:HIS:CD2	1:G:212[A]:GLU:N	2.76	0.54
1:I:57:TRP:O	1:I:58:LYS:C	2.46	0.54
1:L:57:TRP:O	1:L:58:LYS:C	2.46	0.54
1:A:211[A]:HIS:CD2	1:A:212[A]:GLU:N	2.76	0.54
1:A:251:LYS:HE2	5:A:5922:HOH:O	2.00	0.54
1:B:57:TRP:O	1:B:58:LYS:C	2.46	0.54
1:C:211[A]:HIS:CD2	1:C:212[A]:GLU:N	2.76	0.54
1:D:179[A]:TYR:O	1:D:181[A]:PRO:HD2	2.05	0.54
1:D:268:MET:HB2	1:D:363:PRO:HD3	1.90	0.54
1:E:334:TYR:CE2	1:E:391:PRO:HG3	2.43	0.54
1:F:211[B]:HIS:O	1:F:212[B]:GLU:CB	2.54	0.54
1:G:251:LYS:HE2	5:G:5932:HOH:O	2.01	0.54
1:I:268:MET:HB2	1:I:363:PRO:HD3	1.90	0.54
1:I:454:ARG:NH2	1:I:454:ARG:HB3	2.22	0.54
1:J:57:TRP:C	1:J:58:LYS:O	2.42	0.54
1:K:211[A]:HIS:CD2	1:K:212[A]:GLU:N	2.76	0.54
1:A:57:TRP:O	1:A:58:LYS:C	2.46	0.54
1:D:59:GLY:O	1:D:61:ASN:N	2.41	0.54
1:F:59:GLY:O	1:F:61:ASN:N	2.41	0.54
1:D:189:GLN:HE22	1:D:209[A]:HIS:CE1	2.26	0.54
1:F:268:MET:HB2	1:F:363:PRO:HD3	1.90	0.54
1:G:180[A]:PHE:HB3	1:L:29[A]:GLN:HB3	1.89	0.54
1:K:189:GLN:NE2	1:K:209[A]:HIS:CE1	2.72	0.54
1:L:268:MET:HB2	1:L:363:PRO:HD3	1.90	0.54
1:E:334:TYR:HD1	5:E:693:HOH:O	1.88	0.53
1:D:337:ARG:NH1	1:E:61:ASN:HB3	2.16	0.53
1:G:332:LEU:HD22	1:G:409:GLN:C	2.29	0.53
1:J:308:ILE:HG21	1:J:374:LEU:CD1	2.39	0.53
1:K:454:ARG:HB3	1:K:454:ARG:NH2	2.22	0.53
1:L:334:TYR:HD1	5:L:1764:HOH:O	1.88	0.53
1:B:308:ILE:HG21	1:B:374:LEU:CD1	2.39	0.53
1:B:332:LEU:HD22	1:B:409:GLN:C	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4472:ADP:C3'	5:B:5977:HOH:O	2.43	0.53
1:C:332:LEU:HD22	1:C:409:GLN:C	2.29	0.53
1:E:176[B]:LYS:C	1:E:178[B]:GLY:N	2.47	0.53
1:F:91:ILE:HB	1:F:103:ASP:HB2	1.89	0.53
1:G:308:ILE:HG21	1:G:374:LEU:CD1	2.39	0.53
1:G:57:TRP:O	1:G:58:LYS:C	2.46	0.53
1:A:118:THR:OG1	1:A:120:ILE:HG13	2.09	0.53
1:B:268:MET:HB2	1:B:363:PRO:HD3	1.90	0.53
1:C:189:GLN:NE2	1:C:209[A]:HIS:CE1	2.72	0.53
1:E:189:GLN:NE2	1:E:209[A]:HIS:CE1	2.72	0.53
1:F:129:GLU:HA	5:F:5916:HOH:O	2.08	0.53
1:F:334:TYR:CE2	1:F:391:PRO:HG3	2.43	0.53
1:F:332:LEU:HD22	1:F:409:GLN:C	2.29	0.53
1:G:129:GLU:HA	5:G:5914:HOH:O	2.08	0.53
5:G:5979:HOH:O	1:H:183:PRO:HB2	2.07	0.53
1:J:332:LEU:HD22	1:J:409:GLN:C	2.29	0.53
1:J:334:TYR:CE2	1:J:391:PRO:HG3	2.43	0.53
1:J:57:TRP:O	1:J:58:LYS:C	2.46	0.53
1:K:129:GLU:HA	5:K:1536:HOH:O	2.08	0.53
1:K:334:TYR:CE2	1:K:391:PRO:HG3	2.43	0.53
1:L:332:LEU:HD22	1:L:409:GLN:C	2.29	0.53
1:B:129:GLU:HA	5:B:5905:HOH:O	2.08	0.53
1:B:334:TYR:CE2	1:B:391:PRO:HG3	2.43	0.53
1:C:118:THR:OG1	1:C:120:ILE:HG13	2.09	0.53
1:E:189:GLN:HE22	1:E:209[A]:HIS:CE1	2.26	0.53
1:G:268:MET:HB2	1:G:363:PRO:HD3	1.90	0.53
1:J:118:THR:OG1	1:J:120:ILE:HG13	2.09	0.53
1:L:179[A]:TYR:C	1:L:181[A]:PRO:CD	2.75	0.53
1:A:334:TYR:CE2	1:A:391:PRO:HG3	2.43	0.53
1:A:399:LEU:N	1:A:400:PRO:CD	2.62	0.53
1:A:60:ILE:CD1	5:F:6049:HOH:O	2.35	0.53
1:B:189:GLN:HE22	1:B:209[A]:HIS:CE1	2.26	0.53
1:B:211[A]:HIS:CD2	1:B:212[A]:GLU:N	2.76	0.53
1:D:308:ILE:HG21	1:D:374:LEU:CD1	2.38	0.53
1:E:114:TYR:HD2	1:E:431:GLY:HA3	1.69	0.53
1:G:334:TYR:CE2	1:G:391:PRO:HG3	2.43	0.53
1:H:189:GLN:HE22	1:H:209[A]:HIS:CE1	2.26	0.53
1:H:211[A]:HIS:CD2	1:H:212[A]:GLU:N	2.76	0.53
1:H:334:TYR:CE2	1:H:391:PRO:HG3	2.43	0.53
1:J:268:MET:HB2	1:J:363:PRO:HD3	1.90	0.53
1:K:189:GLN:HE22	1:K:209[A]:HIS:CE1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:118:THR:OG1	1:L:120:ILE:HG13	2.09	0.53
1:B:337:ARG:CD	1:B:338:ASN:N	2.72	0.53
1:C:308:ILE:HG21	1:C:374:LEU:CD1	2.38	0.53
1:F:251:LYS:HE2	5:F:5933:HOH:O	2.01	0.53
5:E:659:HOH:O	1:F:84:THR:HG21	2.08	0.53
1:H:308:ILE:HG21	1:H:374:LEU:CD1	2.39	0.53
1:H:57:TRP:O	1:H:58:LYS:C	2.46	0.53
1:I:332:LEU:HD22	1:I:409:GLN:C	2.29	0.53
1:K:57:TRP:O	1:K:58:LYS:C	2.46	0.53
1:L:189:GLN:HE22	1:L:209[A]:HIS:CE1	2.26	0.53
1:A:19:LEU:O	1:A:30[A]:HIS:HA	2.09	0.53
1:A:337:ARG:CD	1:A:338:ASN:N	2.72	0.53
1:C:255:PHE:O	1:C:363:PRO:HB2	2.09	0.53
1:C:57:TRP:O	1:C:58:LYS:C	2.46	0.53
1:D:334:TYR:CE2	1:D:391:PRO:HG3	2.43	0.53
1:D:399:LEU:HB3	1:D:400:PRO:HD3	1.91	0.53
1:D:458:HIS:HD2	1:D:460:VAL:N	2.01	0.53
1:H:255:PHE:O	1:H:363:PRO:HB2	2.09	0.53
1:I:211[A]:HIS:CD2	1:I:212[A]:GLU:N	2.76	0.53
1:J:19:LEU:O	1:J:30[A]:HIS:HA	2.09	0.53
1:K:189:GLN:HE22	1:K:209[A]:HIS:HE1	1.57	0.53
1:L:47:LYS:HD3	5:L:1827:HOH:O	2.09	0.53
1:A:399:LEU:HB3	1:A:400:PRO:HD3	1.91	0.53
1:B:19:LEU:O	1:B:30[A]:HIS:HA	2.09	0.53
1:E:129:GLU:HA	5:E:618:HOH:O	2.08	0.53
1:E:57:TRP:O	1:E:58:LYS:C	2.46	0.53
1:F:118:THR:OG1	1:F:120:ILE:HG13	2.09	0.53
1:F:337:ARG:CD	1:F:338:ASN:N	2.72	0.53
1:F:255:PHE:O	1:F:363:PRO:HB2	2.09	0.53
1:I:308:ILE:HG21	1:I:374:LEU:CD1	2.38	0.53
1:K:118:THR:OG1	1:K:120:ILE:HG13	2.09	0.53
1:K:255:PHE:O	1:K:363:PRO:HB2	2.09	0.53
1:K:30[A]:HIS:CE1	1:L:183:PRO:HD3	2.44	0.53
1:A:308:ILE:HG21	1:A:374:LEU:CD1	2.39	0.53
1:A:47:LYS:HD3	5:A:6035:HOH:O	2.09	0.53
1:B:114:TYR:HD2	1:B:431:GLY:HA3	1.69	0.53
1:B:255:PHE:O	1:B:363:PRO:HB2	2.09	0.53
1:C:285:ASP:CA	5:C:6024:HOH:O	2.35	0.53
1:C:334:TYR:CE2	1:C:391:PRO:HG3	2.43	0.53
1:E:179[A]:TYR:C	1:E:181[A]:PRO:CD	2.75	0.53
1:E:211[A]:HIS:CD2	1:E:212[A]:GLU:N	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:332:LEU:HD22	1:E:409:GLN:C	2.29	0.53
1:H:47:LYS:HD3	5:H:6049:HOH:O	2.09	0.53
1:I:189:GLN:HE22	1:I:209[A]:HIS:CE1	2.26	0.53
1:J:211[A]:HIS:CD2	1:J:212[A]:GLU:N	2.76	0.53
1:L:19:LEU:O	1:L:30[A]:HIS:HA	2.09	0.53
1:A:268:MET:HB2	1:A:363:PRO:HD3	1.90	0.53
1:B:201:GLN:CA	5:B:6004:HOH:O	2.53	0.53
1:D:19:LEU:O	1:D:30[A]:HIS:HA	2.09	0.53
1:E:118:THR:OG1	1:E:120:ILE:HG13	2.09	0.53
1:G:189:GLN:HE22	1:G:209[A]:HIS:CE1	2.26	0.53
1:G:329:PRO:CG	1:G:359:ARG:CD	2.75	0.53
1:G:255:PHE:O	1:G:363:PRO:HB2	2.09	0.53
1:K:399:LEU:HB3	1:K:400:PRO:HD3	1.91	0.53
1:K:59:GLY:O	1:K:61:ASN:N	2.41	0.53
1:C:268:MET:HB2	1:C:363:PRO:HD3	1.90	0.52
1:D:332:LEU:HD22	1:D:409:GLN:C	2.29	0.52
1:E:255:PHE:O	1:E:363:PRO:HB2	2.09	0.52
1:E:19:LEU:O	1:E:30[A]:HIS:HA	2.09	0.52
1:F:308:ILE:HG21	1:F:374:LEU:CD1	2.39	0.52
1:H:19:LEU:O	1:H:30[A]:HIS:HA	2.09	0.52
1:H:399:LEU:HB3	1:H:400:PRO:HD3	1.91	0.52
1:I:118:THR:OG1	1:I:120:ILE:HG13	2.09	0.52
1:I:334:TYR:CE2	1:I:391:PRO:HG3	2.43	0.52
1:J:255:PHE:O	1:J:363:PRO:HB2	2.09	0.52
1:L:334:TYR:CE2	1:L:391:PRO:HG3	2.43	0.52
1:C:129:GLU:HA	5:C:5906:HOH:O	2.08	0.52
1:D:129:GLU:HA	5:D:5907:HOH:O	2.08	0.52
1:D:189:GLN:HE22	1:D:209[A]:HIS:HE1	1.57	0.52
1:D:47:LYS:HD3	5:D:6038:HOH:O	2.09	0.52
1:E:47:LYS:HD3	5:E:756:HOH:O	2.09	0.52
1:G:329:PRO:CD	1:G:359:ARG:CD	2.87	0.52
1:I:255:PHE:O	1:I:363:PRO:HB2	2.09	0.52
1:L:285:ASP:CA	5:L:1816:HOH:O	2.35	0.52
1:B:47:LYS:HD3	5:B:6036:HOH:O	2.09	0.52
1:C:179[A]:TYR:O	1:C:181[A]:PRO:HD2	2.05	0.52
1:C:329:PRO:CD	1:C:359:ARG:CD	2.87	0.52
1:C:458:HIS:HD2	1:C:460:VAL:N	2.01	0.52
1:D:118:THR:OG1	1:D:120:ILE:HG13	2.09	0.52
1:E:308:ILE:HG21	1:E:374:LEU:CD1	2.39	0.52
1:G:19:LEU:O	1:G:30[A]:HIS:HA	2.09	0.52
1:H:118:THR:OG1	1:H:120:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:332:LEU:HD22	1:H:409:GLN:C	2.29	0.52
1:I:295:LEU:HB3	1:I:388:PRO:HG3	1.91	0.52
1:I:334:TYR:HD1	5:I:5999:HOH:O	1.88	0.52
1:K:329:PRO:CD	1:K:359:ARG:CD	2.87	0.52
1:K:332:LEU:HD22	1:K:409:GLN:C	2.29	0.52
1:L:255:PHE:O	1:L:363:PRO:HB2	2.09	0.52
1:A:189:GLN:HE22	1:A:209[A]:HIS:CE1	2.26	0.52
1:A:332:LEU:HD22	1:A:409:GLN:C	2.29	0.52
1:A:458:HIS:HD2	1:A:460:VAL:N	2.01	0.52
1:C:189:GLN:HE22	1:C:209[A]:HIS:CE1	2.26	0.52
1:D:255:PHE:O	1:D:363:PRO:HB2	2.09	0.52
1:E:268:MET:HB2	1:E:363:PRO:HD3	1.90	0.52
1:E:295:LEU:HB3	1:E:388:PRO:HG3	1.92	0.52
1:H:268:MET:HB2	1:H:363:PRO:HD3	1.90	0.52
1:D:189:GLN:NE2	1:D:209[A]:HIS:CE1	2.72	0.52
1:E:337:ARG:CD	1:E:338:ASN:N	2.72	0.52
1:E:329:PRO:CD	1:E:359:ARG:CD	2.87	0.52
1:F:19:LEU:O	1:F:30[A]:HIS:HA	2.09	0.52
1:F:329:PRO:CD	1:F:359:ARG:CD	2.87	0.52
1:F:47:LYS:HD3	5:F:6045:HOH:O	2.09	0.52
1:H:295:LEU:HB3	1:H:388:PRO:HG3	1.91	0.52
1:H:334:TYR:HD1	5:H:5992:HOH:O	1.88	0.52
1:J:129:GLU:HA	5:J:5923:HOH:O	2.08	0.52
1:J:329:PRO:CD	1:J:359:ARG:CD	2.87	0.52
1:L:211[A]:HIS:CD2	1:L:212[A]:GLU:N	2.76	0.52
1:A:129:GLU:HA	5:A:5904:HOH:O	2.08	0.52
1:A:329:PRO:CD	1:A:359:ARG:CD	2.87	0.52
1:B:189:GLN:NE2	1:B:209[A]:HIS:CE1	2.72	0.52
1:B:295:LEU:HB3	1:B:388:PRO:HG3	1.91	0.52
1:B:329:PRO:CD	1:B:359:ARG:CD	2.87	0.52
1:C:47:LYS:HD3	5:C:6035:HOH:O	2.09	0.52
1:F:189:GLN:HE22	1:F:209[A]:HIS:CE1	2.26	0.52
1:F:437:GLU:CA	5:F:6027:HOH:O	2.58	0.52
1:G:59:GLY:O	1:G:61:ASN:N	2.41	0.52
1:H:129:GLU:HA	5:H:5921:HOH:O	2.08	0.52
1:J:47:LYS:HD3	5:J:6052:HOH:O	2.09	0.52
1:K:308:ILE:HG21	1:K:374:LEU:CD1	2.39	0.52
1:L:295:LEU:HB3	1:L:388:PRO:HG3	1.92	0.52
1:L:399:LEU:HB3	1:L:400:PRO:HD3	1.91	0.52
1:A:59:GLY:O	1:A:61:ASN:N	2.41	0.52
1:D:295:LEU:HB3	1:D:388:PRO:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:THR:OG1	1:G:120:ILE:HG13	2.09	0.52
1:H:211[B]:HIS:O	1:H:212[B]:GLU:CB	2.54	0.52
1:I:437:GLU:CA	5:I:6038:HOH:O	2.58	0.52
1:J:179[A]:TYR:O	1:J:181[A]:PRO:HD2	2.05	0.52
1:J:334:TYR:HD1	5:J:5995:HOH:O	1.88	0.52
1:K:80:PHE:CZ	1:L:189:GLN:HG3	2.45	0.52
5:G:5955:HOH:O	1:L:84:THR:HG21	2.09	0.52
1:D:28:GLU:CB	5:D:5933:HOH:O	2.58	0.52
1:D:329:PRO:CD	1:D:359:ARG:CD	2.87	0.52
1:G:47:LYS:HD3	5:G:6045:HOH:O	2.09	0.52
1:I:60:ILE:CD1	5:J:6056:HOH:O	2.25	0.52
1:K:19:LEU:O	1:K:30[A]:HIS:HA	2.09	0.52
1:B:118:THR:OG1	1:B:120:ILE:HG13	2.09	0.52
1:C:295:LEU:HB3	1:C:388:PRO:HG3	1.91	0.52
1:H:189:GLN:NE2	1:H:209[A]:HIS:CE1	2.72	0.52
1:H:329:PRO:CD	1:H:359:ARG:CD	2.87	0.52
1:I:285:ASP:CA	5:I:6045:HOH:O	2.35	0.52
1:I:399:LEU:HB3	1:I:400:PRO:HD3	1.91	0.52
1:A:329:PRO:CG	1:A:359:ARG:CD	2.75	0.52
1:A:235:ILE:HG21	1:A:367:PRO:HG3	1.92	0.52
1:A:457:PRO:HD3	1:G:261[A]:PHE:HB2	1.92	0.52
1:C:334:TYR:HD1	5:C:5978:HOH:O	1.89	0.52
1:D:235:ILE:HG21	1:D:367:PRO:HG3	1.92	0.52
1:E:399:LEU:HB3	1:E:400:PRO:HD3	1.91	0.52
1:F:360:PHE:CD2	1:F:361:PRO:CD	2.75	0.52
1:G:295:LEU:HB3	1:G:388:PRO:HG3	1.92	0.52
1:G:47:LYS:HA	5:G:6045:HOH:O	2.10	0.52
1:H:337:ARG:CD	1:H:338:ASN:N	2.72	0.52
1:L:308:ILE:HG21	1:L:374:LEU:CD1	2.39	0.52
1:A:414:LEU:HD23	1:A:450:ASP:HB2	1.93	0.51
1:E:33:ILE:HG23	1:E:37:GLN:HB2	1.92	0.51
1:I:19:LEU:O	1:I:30[A]:HIS:HA	2.09	0.51
1:I:329:PRO:CD	1:I:359:ARG:CD	2.87	0.51
1:I:337:ARG:CD	1:I:338:ASN:N	2.72	0.51
1:A:255:PHE:O	1:A:363:PRO:HB2	2.09	0.51
1:B:33:ILE:HG23	1:B:37:GLN:HB2	1.92	0.51
1:E:47:LYS:HA	5:E:756:HOH:O	2.10	0.51
1:F:414:LEU:HD23	1:F:450:ASP:HB2	1.92	0.51
1:G:399:LEU:HB3	1:G:400:PRO:HD3	1.91	0.51
1:G:437:GLU:CA	5:G:6027:HOH:O	2.58	0.51
1:H:59:GLY:O	1:H:61:ASN:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:414:LEU:HD23	1:I:450:ASP:HB2	1.93	0.51
1:J:189:GLN:HE22	1:J:209[A]:HIS:HE1	1.57	0.51
1:K:33:ILE:HG23	1:K:37:GLN:HB2	1.92	0.51
1:K:47:LYS:HA	5:K:1674:HOH:O	2.10	0.51
1:A:360:PHE:CD2	1:A:361:PRO:CD	2.75	0.51
1:B:211[B]:HIS:O	1:B:212[B]:GLU:CB	2.54	0.51
1:D:334:TYR:HD1	5:D:5981:HOH:O	1.88	0.51
1:J:189:GLN:HE22	1:J:209[A]:HIS:CE1	2.26	0.51
1:L:329:PRO:CD	1:L:359:ARG:CD	2.87	0.51
1:L:235:ILE:HG21	1:L:367:PRO:HG3	1.92	0.51
1:L:414:LEU:HD23	1:L:450:ASP:HB2	1.93	0.51
1:A:211[B]:HIS:N	1:A:211[B]:HIS:HD2	1.96	0.51
1:A:437:GLU:CA	5:A:6017:HOH:O	2.58	0.51
1:E:399:LEU:N	1:E:400:PRO:CD	2.62	0.51
1:G:33:ILE:HG23	1:G:37:GLN:HB2	1.92	0.51
1:J:414:LEU:HD23	1:J:450:ASP:HB2	1.93	0.51
1:K:295:LEU:HB3	1:K:388:PRO:HG3	1.92	0.51
1:K:115:LEU:HD23	1:K:379:LEU:HD21	1.93	0.51
1:K:47:LYS:HD3	5:K:1674:HOH:O	2.09	0.51
1:A:28:GLU:CB	5:A:5930:HOH:O	2.58	0.51
1:A:115:LEU:HD23	1:A:379:LEU:HD21	1.93	0.51
1:A:4:HIS:O	1:A:7:THR:HG23	2.11	0.51
1:C:179[B]:TYR:CE1	1:C:212[B]:GLU:N	2.79	0.51
1:D:414:LEU:HD23	1:D:450:ASP:HB2	1.93	0.51
1:E:4:HIS:O	1:E:7:THR:HG23	2.11	0.51
1:F:115:LEU:HD23	1:F:379:LEU:HD21	1.93	0.51
1:F:47:LYS:HA	5:F:6045:HOH:O	2.10	0.51
1:G:206:VAL:O	1:L:34:PRO:HG2	2.11	0.51
1:G:414:LEU:HD23	1:G:450:ASP:HB2	1.93	0.51
1:H:179[B]:TYR:CE1	1:H:212[B]:GLU:N	2.79	0.51
1:I:33:ILE:HG23	1:I:37:GLN:HB2	1.92	0.51
1:J:179[B]:TYR:CE1	1:J:212[B]:GLU:N	2.79	0.51
1:K:268:MET:HB2	1:K:363:PRO:HD3	1.90	0.51
1:A:180[A]:PHE:HB3	1:B:29[A]:GLN:HB3	1.92	0.51
1:A:179[B]:TYR:CE1	1:A:212[B]:GLU:N	2.79	0.51
1:A:295:LEU:HB3	1:A:388:PRO:HG3	1.91	0.51
1:B:399:LEU:HB3	1:B:400:PRO:HD3	1.91	0.51
1:B:59:GLY:O	1:B:61:ASN:N	2.41	0.51
1:C:323:VAL:CG1	5:C:6037:HOH:O	2.20	0.51
1:E:179[B]:TYR:CE1	1:E:212[B]:GLU:N	2.79	0.51
1:F:179[B]:TYR:CE1	1:F:212[B]:GLU:N	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:399:LEU:HB3	1:F:400:PRO:HD3	1.91	0.51
1:H:235:ILE:HG21	1:H:367:PRO:HG3	1.92	0.51
1:J:337:ARG:CD	1:J:338:ASN:N	2.72	0.51
1:K:188:ALA:HA	5:K:1590:HOH:O	2.11	0.51
1:K:414:LEU:HD23	1:K:450:ASP:HB2	1.93	0.51
1:L:4:HIS:O	1:L:7:THR:HG23	2.11	0.51
1:B:179[B]:TYR:CE1	1:B:212[B]:GLU:N	2.79	0.51
1:C:19:LEU:O	1:C:30[A]:HIS:HA	2.09	0.51
1:D:183:PRO:HD3	1:E:30[A]:HIS:CE1	2.46	0.51
1:D:115:LEU:HD23	1:D:379:LEU:HD21	1.93	0.51
1:D:384:ASN:N	1:D:384:ASN:ND2	2.59	0.51
1:H:394:LYS:HD3	1:H:395:ASN:H	1.76	0.51
1:J:115:LEU:HD23	1:J:379:LEU:HD21	1.93	0.51
1:L:251:LYS:HE2	5:L:1707:HOH:O	2.01	0.51
1:L:28:GLU:CB	5:L:1715:HOH:O	2.58	0.51
1:B:25:LYS:HD2	5:B:5947:HOH:O	2.10	0.51
1:C:115:LEU:HD23	1:C:379:LEU:HD21	1.93	0.51
1:C:394:LYS:HD3	1:C:395:ASN:H	1.76	0.51
1:D:4:HIS:O	1:D:7:THR:HG23	2.11	0.51
1:E:394:LYS:HD3	1:E:395:ASN:H	1.76	0.51
1:E:437:GLU:CA	5:E:738:HOH:O	2.58	0.51
1:F:28:GLU:CB	5:F:5940:HOH:O	2.58	0.51
1:G:115:LEU:HD23	1:G:379:LEU:HD21	1.93	0.51
1:I:179[B]:TYR:CE1	1:I:212[B]:GLU:N	2.79	0.51
1:I:115:LEU:HD23	1:I:379:LEU:HD21	1.93	0.51
1:I:445:LEU:O	1:I:448:GLU:HG2	2.11	0.51
1:J:445:LEU:O	1:J:448:GLU:HG2	2.11	0.51
1:L:189:GLN:NE2	1:L:209[A]:HIS:CE1	2.72	0.51
1:L:179[B]:TYR:CE1	1:L:212[B]:GLU:N	2.79	0.51
1:L:47:LYS:HA	5:L:1827:HOH:O	2.10	0.51
1:A:189:GLN:HE22	1:A:209[A]:HIS:HE1	1.57	0.51
1:C:264[B]:ASN:CA	1:C:326:TYR:HB3	2.41	0.51
1:C:399:LEU:HB3	1:C:400:PRO:HD3	1.91	0.51
1:D:399:LEU:N	1:D:400:PRO:CD	2.62	0.51
1:D:47:LYS:HA	5:D:6038:HOH:O	2.10	0.51
1:G:179[B]:TYR:CE1	1:G:212[B]:GLU:N	2.79	0.51
1:H:445:LEU:O	1:H:448:GLU:HG2	2.11	0.51
1:I:189:GLN:HE22	1:I:209[A]:HIS:HE1	1.57	0.51
1:J:211[B]:HIS:O	1:J:212[B]:GLU:CB	2.54	0.51
1:J:28:GLU:CB	5:J:5947:HOH:O	2.58	0.51
1:J:4:HIS:O	1:J:7:THR:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:264[B]:ASN:CA	1:K:326:TYR:HB3	2.41	0.51
1:L:384:ASN:N	1:L:384:ASN:ND2	2.59	0.51
1:A:33:ILE:HG23	1:A:37:GLN:HB2	1.92	0.51
1:A:394:LYS:HD3	1:A:395:ASN:H	1.76	0.51
1:B:179[B]:TYR:CD1	1:B:212[B]:GLU:CA	2.77	0.51
1:B:183:PRO:HB2	5:C:5969:HOH:O	2.10	0.51
1:B:264[B]:ASN:CA	1:B:326:TYR:HB3	2.41	0.51
1:B:47:LYS:HA	5:B:6036:HOH:O	2.10	0.51
1:D:264[B]:ASN:CA	1:D:326:TYR:HB3	2.41	0.51
1:D:33:ILE:HG23	1:D:37:GLN:HB2	1.92	0.51
1:D:445:LEU:O	1:D:448:GLU:HG2	2.11	0.51
1:D:73:THR:HG21	1:D:88:ARG:HB3	1.93	0.51
1:G:188:ALA:HA	5:G:5968:HOH:O	2.11	0.51
1:H:188:ALA:HA	5:H:5972:HOH:O	2.11	0.51
1:I:235:ILE:HG21	1:I:367:PRO:HG3	1.92	0.51
1:J:399:LEU:HB3	1:J:400:PRO:HD3	1.91	0.51
5:J:5986:HOH:O	1:K:183:PRO:HB2	2.11	0.51
1:L:445:LEU:O	1:L:448:GLU:HG2	2.11	0.51
1:A:47:LYS:HA	5:A:6035:HOH:O	2.10	0.50
1:B:384:ASN:ND2	1:B:384:ASN:N	2.59	0.50
1:C:33:ILE:HG23	1:C:37:GLN:HB2	1.92	0.50
5:C:6039:HOH:O	1:D:60:ILE:CD1	2.33	0.50
1:F:33:ILE:HG23	1:F:37:GLN:HB2	1.93	0.50
1:G:445:LEU:O	1:G:448:GLU:HG2	2.11	0.50
1:H:33:ILE:HG23	1:H:37:GLN:HB2	1.92	0.50
1:I:211[B]:HIS:O	1:I:212[B]:GLU:CB	2.54	0.50
1:I:264[B]:ASN:CA	1:I:326:TYR:HB3	2.41	0.50
1:I:4:HIS:O	1:I:7:THR:HG23	2.11	0.50
1:I:59:GLY:O	1:J:339:ARG:NH1	2.42	0.50
1:K:394:LYS:HD3	1:K:395:ASN:H	1.76	0.50
1:A:445:LEU:O	1:A:448:GLU:HG2	2.11	0.50
1:C:445:LEU:O	1:C:448:GLU:HG2	2.11	0.50
1:D:188:ALA:HA	5:D:5961:HOH:O	2.11	0.50
1:E:125:LEU:O	1:E:272:MET:HA	2.12	0.50
1:F:445:LEU:O	1:F:448:GLU:HG2	2.11	0.50
3:F:4476:ADP:C3'	5:F:5986:HOH:O	2.43	0.50
1:G:264[B]:ASN:CA	1:G:326:TYR:HB3	2.41	0.50
1:H:334:TYR:CZ	1:H:391:PRO:HG3	2.47	0.50
1:H:460:VAL:HG12	1:H:464:LEU:HD22	1.93	0.50
1:K:179[B]:TYR:CE1	1:K:212[B]:GLU:N	2.79	0.50
1:K:460:VAL:HG12	1:K:464:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:337:ARG:CD	1:L:338:ASN:N	2.72	0.50
1:A:264[B]:ASN:CA	1:A:326:TYR:HB3	2.41	0.50
1:B:337:ARG:CD	1:C:61:ASN:CB	2.81	0.50
1:C:337:ARG:CD	1:C:338:ASN:N	2.72	0.50
1:D:179[B]:TYR:CE1	1:D:212[B]:GLU:N	2.79	0.50
1:D:337:ARG:CD	1:D:338:ASN:N	2.72	0.50
1:D:460:VAL:HG12	1:D:464:LEU:HD22	1.94	0.50
1:F:394:LYS:HD3	1:F:395:ASN:H	1.76	0.50
1:H:73:THR:HG21	1:H:88:ARG:HB3	1.93	0.50
1:I:80:PHE:CZ	1:J:189:GLN:HG3	2.46	0.50
1:J:47:LYS:HA	5:J:6052:HOH:O	2.10	0.50
1:K:235:ILE:HG21	1:K:367:PRO:HG3	1.92	0.50
1:K:334:TYR:CZ	1:K:391:PRO:HG3	2.47	0.50
1:B:188:ALA:HA	5:B:5959:HOH:O	2.11	0.50
1:D:125:LEU:O	1:D:272:MET:HA	2.12	0.50
1:F:460:VAL:HG12	1:F:464:LEU:HD22	1.94	0.50
1:H:125:LEU:O	1:H:272:MET:HA	2.12	0.50
5:I:5990:HOH:O	1:J:183:PRO:HB2	2.11	0.50
1:J:264[B]:ASN:CA	1:J:326:TYR:HB3	2.41	0.50
1:J:125:LEU:O	1:J:272:MET:HA	2.12	0.50
1:J:33:ILE:HG23	1:J:37:GLN:HB2	1.92	0.50
1:J:59:GLY:C	1:J:61:ASN:N	2.65	0.50
1:L:188:ALA:HA	5:L:1743:HOH:O	2.11	0.50
1:A:25:LYS:HD2	5:A:5946:HOH:O	2.10	0.50
1:C:125:LEU:O	1:C:272:MET:HA	2.12	0.50
1:C:28:GLU:CB	5:C:5930:HOH:O	2.58	0.50
1:E:445:LEU:O	1:E:448:GLU:HG2	2.11	0.50
1:G:176[B]:LYS:C	1:G:178[B]:GLY:N	2.47	0.50
1:G:394:LYS:HD3	1:G:395:ASN:H	1.76	0.50
1:H:25:LYS:HD2	5:H:5961:HOH:O	2.10	0.50
1:H:264[B]:ASN:CA	1:H:326:TYR:HB3	2.41	0.50
1:H:4:HIS:O	1:H:7:THR:HG23	2.11	0.50
1:I:394:LYS:HD3	1:I:395:ASN:H	1.76	0.50
1:I:460:VAL:HG12	1:I:464:LEU:HD22	1.94	0.50
1:J:25:LYS:HD2	5:J:5963:HOH:O	2.11	0.50
1:J:235:ILE:HG21	1:J:367:PRO:HG3	1.92	0.50
1:K:28:GLU:CB	5:K:1562:HOH:O	2.58	0.50
1:K:337:ARG:CD	1:K:338:ASN:N	2.72	0.50
1:L:334:TYR:CZ	1:L:391:PRO:HG3	2.46	0.50
1:L:33:ILE:HG23	1:L:37:GLN:HB2	1.92	0.50
1:A:334:TYR:CZ	1:A:391:PRO:HG3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:TYR:CZ	1:B:391:PRO:HG3	2.47	0.50
1:D:272:MET:O	1:D:355:ARG:HB2	2.12	0.50
1:E:235:ILE:HG21	1:E:367:PRO:HG3	1.92	0.50
1:F:179[A]:TYR:O	1:F:181[A]:PRO:HD2	2.05	0.50
1:F:235:ILE:HG21	1:F:367:PRO:HG3	1.92	0.50
1:F:59:GLY:C	1:F:61:ASN:N	2.65	0.50
1:G:28:GLU:CB	5:G:5940:HOH:O	2.58	0.50
1:G:337:ARG:CD	1:G:338:ASN:N	2.72	0.50
1:G:235:ILE:HG21	1:G:367:PRO:HG3	1.92	0.50
1:G:4:HIS:O	1:G:7:THR:HG23	2.11	0.50
1:I:73:THR:HG21	1:I:88:ARG:HB3	1.93	0.50
1:L:25:LYS:HD2	5:L:1731:HOH:O	2.10	0.50
1:A:188:ALA:HA	5:A:5958:HOH:O	2.11	0.50
1:A:460:VAL:HG12	1:A:464:LEU:HD22	1.94	0.50
1:C:235:ILE:HG21	1:C:367:PRO:HG3	1.92	0.50
1:C:4:HIS:O	1:C:7:THR:HG23	2.11	0.50
1:C:60:ILE:O	1:C:60:ILE:HG23	2.12	0.50
1:D:59:GLY:C	1:D:61:ASN:N	2.65	0.50
1:E:183:PRO:CB	5:F:5979:HOH:O	2.59	0.50
1:F:295:LEU:HB3	1:F:388:PRO:HG3	1.91	0.50
1:F:334:TYR:CZ	1:F:391:PRO:HG3	2.47	0.50
1:H:272:MET:O	1:H:355:ARG:HB2	2.12	0.50
1:H:47:LYS:HA	5:H:6049:HOH:O	2.10	0.50
1:H:59:GLY:C	1:H:61:ASN:N	2.65	0.50
1:I:334:TYR:CZ	1:I:391:PRO:HG3	2.46	0.50
1:I:47:LYS:HD3	5:I:6056:HOH:O	2.09	0.50
1:J:295:LEU:HB3	1:J:388:PRO:HG3	1.91	0.50
1:J:384:ASN:ND2	1:J:384:ASN:N	2.59	0.50
1:K:272:MET:O	1:K:355:ARG:HB2	2.12	0.50
1:A:25:LYS:NZ	5:A:5919:HOH:O	2.45	0.50
1:B:414:LEU:HD23	1:B:450:ASP:HB2	1.93	0.50
1:C:334:TYR:CZ	1:C:391:PRO:HG3	2.47	0.50
1:C:414:LEU:HD23	1:C:450:ASP:HB2	1.93	0.50
1:E:384:ASN:N	1:E:384:ASN:ND2	2.59	0.50
1:F:4:HIS:O	1:F:7:THR:HG23	2.11	0.50
1:I:384:ASN:N	1:I:384:ASN:ND2	2.59	0.50
1:I:458:HIS:HD2	1:I:460:VAL:N	2.01	0.50
1:I:47:LYS:HA	5:I:6056:HOH:O	2.10	0.50
1:J:394:LYS:HD3	1:J:395:ASN:H	1.76	0.50
1:J:63:SER:N	1:K:339:ARG:HH12	2.09	0.50
1:K:445:LEU:O	1:K:448:GLU:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:4:HIS:O	1:K:7:THR:HG23	2.11	0.50
1:L:115:LEU:HD23	1:L:379:LEU:HD21	1.93	0.50
1:L:460:VAL:HG12	1:L:464:LEU:HD22	1.93	0.50
1:L:59:GLY:C	1:L:61:ASN:N	2.65	0.50
1:B:125:LEU:O	1:B:272:MET:HA	2.12	0.50
1:C:59:GLY:C	1:C:61:ASN:N	2.65	0.50
1:E:460:VAL:HG12	1:E:464:LEU:HD22	1.94	0.50
1:E:59:GLY:O	1:E:61:ASN:N	2.41	0.50
1:F:211[B]:HIS:N	1:F:211[B]:HIS:HD2	1.96	0.50
1:F:272:MET:O	1:F:355:ARG:HB2	2.12	0.50
1:G:59:GLY:C	1:G:61:ASN:N	2.65	0.50
1:I:125:LEU:O	1:I:272:MET:HA	2.12	0.50
1:J:188:ALA:HA	5:J:5975:HOH:O	2.11	0.50
1:K:125:LEU:O	1:K:272:MET:HA	2.12	0.50
1:L:264[B]:ASN:CA	1:L:326:TYR:HB3	2.41	0.50
1:L:59:GLY:O	1:L:61:ASN:N	2.41	0.50
1:B:235:ILE:HG21	1:B:367:PRO:HG3	1.92	0.49
1:D:394:LYS:HD3	1:D:395:ASN:H	1.76	0.49
1:D:437:GLU:CA	5:D:6020:HOH:O	2.58	0.49
1:E:414:LEU:HD23	1:E:450:ASP:HB2	1.93	0.49
1:F:188:ALA:HA	5:F:5968:HOH:O	2.11	0.49
1:G:272:MET:O	1:G:355:ARG:HB2	2.12	0.49
1:G:334:TYR:CZ	1:G:391:PRO:HG3	2.47	0.49
1:G:73:THR:HG21	1:G:88:ARG:HB3	1.93	0.49
1:H:179[B]:TYR:CD2	1:H:211[B]:HIS:HB2	2.47	0.49
1:I:60:ILE:HG23	1:I:60:ILE:O	2.12	0.49
1:L:125:LEU:O	1:L:272:MET:HA	2.12	0.49
1:B:394:LYS:HD3	1:B:395:ASN:H	1.76	0.49
1:C:47:LYS:HA	5:C:6035:HOH:O	2.10	0.49
1:E:115:LEU:HD23	1:E:379:LEU:HD21	1.93	0.49
1:E:73:THR:HG21	1:E:88:ARG:HB3	1.93	0.49
1:H:115:LEU:HD23	1:H:379:LEU:HD21	1.93	0.49
1:I:188:ALA:HA	5:I:5979:HOH:O	2.11	0.49
1:K:59:GLY:C	1:K:61:ASN:N	2.65	0.49
1:L:394:LYS:HD3	1:L:395:ASN:H	1.76	0.49
1:A:384:ASN:ND2	1:A:384:ASN:N	2.59	0.49
1:B:175[B]:VAL:O	1:B:175[B]:VAL:HG12	2.13	0.49
1:B:272:MET:O	1:B:355:ARG:HB2	2.12	0.49
1:B:445:LEU:O	1:B:448:GLU:HG2	2.11	0.49
1:B:460:VAL:HG12	1:B:464:LEU:HD22	1.93	0.49
1:C:124:VAL:HA	1:C:274:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:VAL:CG2	5:D:5919:HOH:O	2.53	0.49
1:E:188:ALA:HA	5:E:672:HOH:O	2.11	0.49
1:E:334:TYR:CZ	1:E:391:PRO:HG3	2.47	0.49
1:E:59:GLY:C	1:E:61:ASN:N	2.65	0.49
1:F:125:LEU:O	1:F:272:MET:HA	2.12	0.49
1:F:73:THR:HG21	1:F:88:ARG:HB3	1.93	0.49
1:H:414:LEU:HD23	1:H:450:ASP:HB2	1.93	0.49
1:I:272:MET:O	1:I:355:ARG:HB2	2.12	0.49
1:J:178[A]:GLY:O	1:J:212[A]:GLU:O	2.31	0.49
1:J:25:LYS:NZ	5:J:5937:HOH:O	2.45	0.49
1:J:460:VAL:HG12	1:J:464:LEU:HD22	1.94	0.49
1:K:175[B]:VAL:HG12	1:K:175[B]:VAL:O	2.13	0.49
3:K:4481:ADP:C3'	5:K:1609:HOH:O	2.42	0.49
1:L:178[A]:GLY:O	1:L:212[A]:GLU:O	2.31	0.49
1:L:179[B]:TYR:CD2	1:L:211[B]:HIS:HB2	2.47	0.49
1:A:59:GLY:C	1:A:61:ASN:N	2.65	0.49
1:B:115:LEU:HD23	1:B:379:LEU:HD21	1.93	0.49
1:B:73:THR:HG21	1:B:88:ARG:HB3	1.93	0.49
1:C:384:ASN:ND2	1:C:384:ASN:N	2.59	0.49
1:D:178[A]:GLY:O	1:D:212[A]:GLU:O	2.31	0.49
1:E:25:LYS:HD2	5:E:660:HOH:O	2.10	0.49
1:G:125:LEU:O	1:G:272:MET:HA	2.12	0.49
1:H:175[B]:VAL:O	1:H:175[B]:VAL:HG12	2.13	0.49
1:J:334:TYR:CZ	1:J:391:PRO:HG3	2.47	0.49
1:K:73:THR:HG21	1:K:88:ARG:HB3	1.93	0.49
1:L:458:HIS:HD2	1:L:460:VAL:N	2.01	0.49
1:L:60:ILE:O	1:L:60:ILE:HG23	2.12	0.49
1:B:259:PRO:HG2	1:B:260[A]:MET:H	1.78	0.49
1:B:4:HIS:O	1:B:7:THR:HG23	2.11	0.49
1:C:188:ALA:HA	5:C:5958:HOH:O	2.11	0.49
1:C:178[A]:GLY:O	1:C:212[A]:GLU:O	2.31	0.49
1:D:179[B]:TYR:CD2	1:D:211[B]:HIS:HB2	2.47	0.49
1:E:28:GLU:CB	5:E:644:HOH:O	2.58	0.49
1:E:272:MET:O	1:E:355:ARG:HB2	2.12	0.49
1:F:178[A]:GLY:O	1:F:212[A]:GLU:O	2.31	0.49
1:F:264[B]:ASN:CA	1:F:326:TYR:HB3	2.41	0.49
1:G:178[A]:GLY:O	1:G:212[A]:GLU:O	2.31	0.49
1:G:60:ILE:HG23	1:G:60:ILE:O	2.12	0.49
1:H:60:ILE:HG23	1:H:60:ILE:O	2.12	0.49
1:J:73:THR:HG21	1:J:88:ARG:HB3	1.93	0.49
1:B:178[A]:GLY:O	1:B:212[A]:GLU:O	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179[B]:TYR:CD2	1:C:211[B]:HIS:HB2	2.47	0.49
1:C:259:PRO:HG2	1:C:260[A]:MET:H	1.77	0.49
1:C:73:THR:HG21	1:C:88:ARG:HB3	1.93	0.49
1:E:182:VAL:HG23	5:F:5958:HOH:O	2.11	0.49
1:A:463:GLU:HA	1:G:140:PHE:CE1	2.47	0.49
1:I:124:VAL:HA	1:I:274:LEU:HD23	1.95	0.49
1:J:59:GLY:O	1:J:61:ASN:N	2.41	0.49
1:J:33:ILE:CD1	1:K:208:ALA:HB2	2.42	0.49
1:K:60:ILE:O	1:K:60:ILE:HG23	2.12	0.49
1:L:73:THR:HG21	1:L:88:ARG:HB3	1.93	0.49
1:B:348:VAL:HG22	5:B:5935:HOH:O	2.13	0.49
1:D:334:TYR:CZ	1:D:391:PRO:HG3	2.47	0.49
1:E:175[B]:VAL:HG12	1:E:175[B]:VAL:O	2.13	0.49
1:E:264[B]:ASN:CA	1:E:326:TYR:HB3	2.41	0.49
1:E:60:ILE:HG23	1:E:60:ILE:O	2.12	0.49
1:F:179[B]:TYR:CD2	1:F:211[B]:HIS:HB2	2.47	0.49
1:F:60:ILE:HG23	1:F:60:ILE:O	2.12	0.49
1:G:25:LYS:NZ	5:G:5929:HOH:O	2.45	0.49
1:G:329:PRO:CD	1:G:359:ARG:HD2	2.42	0.49
1:K:124:VAL:HA	1:K:274:LEU:HD23	1.95	0.49
1:L:75:VAL:CG2	5:L:1701:HOH:O	2.53	0.49
1:A:178[A]:GLY:O	1:A:212[A]:GLU:O	2.31	0.49
1:A:183:PRO:HB2	5:B:5970:HOH:O	2.12	0.49
1:B:28:GLU:CB	5:B:5931:HOH:O	2.58	0.49
1:C:460:VAL:HG12	1:C:464:LEU:HD22	1.94	0.49
1:D:175[B]:VAL:O	1:D:175[B]:VAL:HG12	2.12	0.49
1:D:348:VAL:HG22	5:D:5937:HOH:O	2.13	0.49
1:H:437:GLU:CA	5:H:6031:HOH:O	2.58	0.49
1:I:178[A]:GLY:O	1:I:212[A]:GLU:O	2.31	0.49
1:J:179[B]:TYR:CD2	1:J:211[B]:HIS:HB2	2.47	0.49
1:K:437:GLU:CA	5:K:1656:HOH:O	2.58	0.49
1:A:272:MET:O	1:A:355:ARG:HB2	2.12	0.49
1:A:73:THR:HG21	1:A:88:ARG:HB3	1.93	0.49
1:C:25:LYS:HD2	5:C:5946:HOH:O	2.10	0.49
1:E:178[A]:GLY:O	1:E:212[A]:GLU:O	2.31	0.49
1:E:75:VAL:CG2	5:E:630:HOH:O	2.53	0.49
1:I:179[B]:TYR:CD2	1:I:211[B]:HIS:HB2	2.47	0.49
1:J:259:PRO:HG2	1:J:260[A]:MET:H	1.78	0.49
1:K:25:LYS:NZ	5:K:1551:HOH:O	2.45	0.49
1:L:25:LYS:NZ	5:L:1704:HOH:O	2.45	0.49
1:A:124:VAL:HA	1:A:274:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ILE:HG23	1:A:60:ILE:O	2.12	0.49
1:D:25:LYS:HD2	5:D:5949:HOH:O	2.11	0.49
1:E:259:PRO:HG2	1:E:260[A]:MET:H	1.78	0.49
1:A:32:THR:OG1	1:F:189:GLN:NE2	2.46	0.49
1:H:25:LYS:NZ	5:H:5935:HOH:O	2.45	0.49
1:I:174[B]:GLY:O	1:I:177[B]:GLY:HA2	2.13	0.49
1:K:348:VAL:HG22	5:K:1566:HOH:O	2.13	0.49
1:A:179[B]:TYR:CD2	1:A:211[B]:HIS:HB2	2.47	0.48
1:B:174[B]:GLY:O	1:B:177[B]:GLY:HA2	2.13	0.48
1:C:25:LYS:NZ	5:C:5920:HOH:O	2.45	0.48
1:D:174[B]:GLY:O	1:D:177[B]:GLY:HA2	2.13	0.48
1:D:25:LYS:NZ	5:D:5922:HOH:O	2.45	0.48
1:F:259:PRO:HG2	1:F:260[A]:MET:H	1.78	0.48
1:F:25:LYS:NZ	5:F:5930:HOH:O	2.45	0.48
1:F:329:PRO:CD	1:F:359:ARG:HD2	2.42	0.48
1:G:460:VAL:HG12	1:G:464:LEU:HD22	1.94	0.48
1:H:231:LYS:CE	5:H:5924:HOH:O	2.59	0.48
1:I:348:VAL:HG22	5:I:5955:HOH:O	2.13	0.48
1:J:60:ILE:HG23	1:J:60:ILE:O	2.12	0.48
1:J:61:ASN:CB	1:K:337:ARG:CD	2.84	0.48
5:K:1580:HOH:O	1:L:182:VAL:HG23	2.13	0.48
1:A:175[B]:VAL:HG12	1:A:175[B]:VAL:O	2.13	0.48
1:C:59:GLY:O	1:C:61:ASN:N	2.41	0.48
1:F:348:VAL:HG22	5:F:5944:HOH:O	2.13	0.48
1:H:259:PRO:HG2	1:H:260[A]:MET:H	1.77	0.48
1:K:174[B]:GLY:O	1:K:177[B]:GLY:HA2	2.13	0.48
1:L:437:GLU:CA	5:L:1809:HOH:O	2.58	0.48
1:A:125:LEU:O	1:A:272:MET:HA	2.12	0.48
1:B:25:LYS:NZ	5:B:5920:HOH:O	2.45	0.48
1:B:124:VAL:HA	1:B:274:LEU:HD23	1.95	0.48
1:C:337:ARG:HH11	1:D:61:ASN:HB3	1.78	0.48
1:F:124:VAL:HA	1:F:274:LEU:HD23	1.95	0.48
1:G:175[B]:VAL:O	1:G:175[B]:VAL:HG12	2.13	0.48
1:G:124:VAL:HA	1:G:274:LEU:HD23	1.95	0.48
1:H:178[A]:GLY:O	1:H:212[A]:GLU:O	2.31	0.48
1:H:348:VAL:HG22	5:H:5949:HOH:O	2.13	0.48
1:I:25:LYS:HD2	5:I:5967:HOH:O	2.10	0.48
1:J:272:MET:O	1:J:355:ARG:HB2	2.12	0.48
1:L:174[B]:GLY:O	1:L:177[B]:GLY:HA2	2.13	0.48
1:L:230:LYS:HG2	5:L:1749:HOH:O	2.14	0.48
1:B:334:TYR:HD1	5:B:5979:HOH:O	1.88	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ILE:HG13	5:C:5977:HOH:O	2.14	0.48
1:A:61:ASN:HB3	1:F:337:ARG:HH11	1.79	0.48
1:G:25:LYS:HD2	5:G:5956:HOH:O	2.10	0.48
1:I:25:LYS:NZ	5:I:5940:HOH:O	2.45	0.48
1:J:329:PRO:HG2	1:J:359:ARG:CD	2.18	0.48
1:K:259:PRO:HG2	1:K:260[A]:MET:H	1.78	0.48
1:L:348:VAL:HG22	5:L:1719:HOH:O	2.13	0.48
1:B:59:GLY:C	1:B:61:ASN:N	2.65	0.48
1:D:124:VAL:HA	1:D:274:LEU:HD23	1.95	0.48
1:E:360:PHE:CG	1:E:361:PRO:CD	2.97	0.48
3:E:4475:ADP:H5'1	5:E:691:HOH:O	2.14	0.48
1:G:384:ASN:ND2	1:G:384:ASN:N	2.59	0.48
1:H:154:ILE:HG13	5:H:5991:HOH:O	2.13	0.48
1:H:28:GLU:CB	5:H:5945:HOH:O	2.58	0.48
1:I:259:PRO:HG2	1:I:260[A]:MET:H	1.78	0.48
1:I:59:GLY:C	1:I:61:ASN:N	2.65	0.48
1:I:60:ILE:O	1:J:339:ARG:HB2	2.14	0.48
1:J:410:VAL:HG22	5:J:6043:HOH:O	2.14	0.48
1:K:178[A]:GLY:O	1:K:212[A]:GLU:O	2.31	0.48
1:L:175[B]:VAL:O	1:L:175[B]:VAL:HG12	2.13	0.48
1:L:259:PRO:HG2	1:L:260[A]:MET:H	1.78	0.48
1:L:272:MET:O	1:L:355:ARG:HB2	2.12	0.48
1:A:399:LEU:N	1:A:400:PRO:HD2	2.09	0.48
1:B:179[B]:TYR:CD2	1:B:211[B]:HIS:HB2	2.47	0.48
1:B:437:GLU:CA	5:B:6018:HOH:O	2.58	0.48
1:D:60:ILE:O	1:D:60:ILE:HG23	2.12	0.48
1:E:211[B]:HIS:O	1:E:212[B]:GLU:CB	2.54	0.48
1:F:174[B]:GLY:O	1:F:177[B]:GLY:HA2	2.13	0.48
1:F:410:VAL:HG22	5:F:6036:HOH:O	2.14	0.48
1:G:329:PRO:HG2	1:G:359:ARG:CD	2.18	0.48
1:A:174[B]:GLY:O	1:A:177[B]:GLY:HA2	2.13	0.48
1:A:259:PRO:HG2	1:A:260[A]:MET:H	1.78	0.48
1:A:329:PRO:CD	1:A:359:ARG:HD2	2.42	0.48
1:C:175[B]:VAL:O	1:C:175[B]:VAL:HG12	2.13	0.48
1:C:230:LYS:HG2	5:C:5963:HOH:O	2.14	0.48
1:C:272:MET:O	1:C:355:ARG:HB2	2.12	0.48
1:D:285:ASP:CA	5:D:6027:HOH:O	2.35	0.48
1:F:175[B]:VAL:HG12	1:F:175[B]:VAL:O	2.12	0.48
1:G:211[B]:HIS:O	1:G:212[B]:GLU:CB	2.54	0.48
1:J:175[B]:VAL:HG12	1:J:175[B]:VAL:O	2.13	0.48
1:J:124:VAL:HA	1:J:274:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176[B]:LYS:C	1:D:178[B]:GLY:N	2.47	0.48
1:E:179[B]:TYR:CD2	1:E:211[B]:HIS:HB2	2.47	0.48
1:E:348:VAL:HG22	5:E:648:HOH:O	2.13	0.48
1:H:75:VAL:CG2	5:H:5932:HOH:O	2.53	0.48
1:C:183:PRO:HB2	5:D:5972:HOH:O	2.14	0.48
1:D:259:PRO:HG2	1:D:260[A]:MET:H	1.78	0.48
1:D:329:PRO:CD	1:D:359:ARG:HD2	2.42	0.48
1:E:230:LYS:HG2	5:E:678:HOH:O	2.14	0.48
1:E:25:LYS:NZ	5:E:633:HOH:O	2.45	0.48
1:E:124:VAL:HA	1:E:274:LEU:HD23	1.95	0.48
1:G:179[B]:TYR:CD2	1:G:211[B]:HIS:HB2	2.47	0.48
1:H:269:HIS:CE1	4:H:5907:PPQ:CEP	2.92	0.48
1:L:410:VAL:HG22	5:L:1818:HOH:O	2.14	0.48
1:A:206:VAL:O	1:B:34:PRO:HG2	2.13	0.48
1:B:410:VAL:HG22	5:B:6027:HOH:O	2.14	0.48
1:C:304:HIS:O	1:C:308:ILE:HG13	2.14	0.48
1:D:456:THR:O	1:J:458:HIS:HE1	1.97	0.48
1:E:180[A]:PHE:HB3	1:F:29[A]:GLN:HB3	1.96	0.48
1:G:174[B]:GLY:O	1:G:177[B]:GLY:HA2	2.13	0.48
1:H:174[B]:GLY:O	1:H:177[B]:GLY:HA2	2.13	0.48
1:H:124:VAL:HA	1:H:274:LEU:HD23	1.95	0.48
1:H:304:HIS:O	1:H:308:ILE:HG13	2.14	0.48
1:H:463:GLU:OE1	5:H:5909:HOH:O	2.20	0.48
1:J:154:ILE:HG13	5:J:5994:HOH:O	2.14	0.48
1:K:25:LYS:HD2	5:K:1578:HOH:O	2.11	0.48
1:K:360:PHE:CG	1:K:361:PRO:CD	2.97	0.48
1:L:128:PRO:CD	5:L:1692:HOH:O	2.61	0.48
1:L:360:PHE:CG	1:L:361:PRO:CD	2.97	0.48
1:A:304:HIS:O	1:A:308:ILE:HG13	2.14	0.47
1:A:348:VAL:HG22	5:A:5934:HOH:O	2.13	0.47
1:B:60:ILE:O	1:B:60:ILE:HG23	2.12	0.47
1:D:304:HIS:O	1:D:308:ILE:HG13	2.14	0.47
1:D:329:PRO:HB2	1:D:342:SER:HA	1.96	0.47
1:G:189:GLN:HE22	1:G:209[A]:HIS:HE1	1.57	0.47
1:G:230:LYS:HG2	5:G:5973:HOH:O	2.14	0.47
3:G:4477:ADP:H5'1	5:G:5986:HOH:O	2.14	0.47
3:H:4478:ADP:H5'1	5:H:5990:HOH:O	2.14	0.47
1:I:154:ILE:HG13	5:I:5998:HOH:O	2.14	0.47
1:I:269:HIS:CE1	4:I:5908:PPQ:CEP	2.92	0.47
1:I:68:MET:HA	1:I:69:PRO:HD2	1.78	0.47
1:L:124:VAL:HA	1:L:274:LEU:HD23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LYS:HG2	5:A:5963:HOH:O	2.14	0.47
1:C:360:PHE:CG	1:C:361:PRO:CD	2.97	0.47
1:E:154:ILE:HG13	5:E:692:HOH:O	2.14	0.47
1:F:304:HIS:O	1:F:308:ILE:HG13	2.14	0.47
1:F:329:PRO:HB2	1:F:342:SER:HA	1.97	0.47
1:F:68:MET:HA	1:F:69:PRO:HD2	1.78	0.47
1:G:259:PRO:HG2	1:G:260[A]:MET:H	1.78	0.47
1:H:230:LYS:HG2	5:H:5977:HOH:O	2.14	0.47
1:H:360:PHE:CG	1:H:361:PRO:CD	2.97	0.47
1:I:175[B]:VAL:HG12	1:I:175[B]:VAL:O	2.12	0.47
1:I:224:ARG:CG	1:I:224:ARG:NH2	2.69	0.47
1:J:437:GLU:CA	5:J:6034:HOH:O	2.58	0.47
1:K:34:PRO:HG2	1:L:206:VAL:O	2.14	0.47
1:B:154:ILE:HG13	5:B:5978:HOH:O	2.14	0.47
1:C:261[A]:PHE:HB2	1:I:457:PRO:HD3	1.97	0.47
1:D:154:ILE:HG13	5:D:5980:HOH:O	2.14	0.47
1:D:410:VAL:HG22	5:D:6029:HOH:O	2.14	0.47
1:E:174[B]:GLY:O	1:E:177[B]:GLY:HA2	2.13	0.47
1:F:230:LYS:HG2	5:F:5973:HOH:O	2.14	0.47
1:G:154:ILE:HG13	5:G:5987:HOH:O	2.14	0.47
1:G:329:PRO:HB2	1:G:342:SER:HA	1.96	0.47
1:H:410:VAL:HG22	5:H:6040:HOH:O	2.14	0.47
1:J:174[B]:GLY:O	1:J:177[B]:GLY:HA2	2.13	0.47
1:K:230:LYS:HG2	5:K:1596:HOH:O	2.14	0.47
1:L:154:ILE:HG13	5:L:1763:HOH:O	2.14	0.47
1:A:360:PHE:CG	1:A:361:PRO:CD	2.97	0.47
1:B:329:PRO:HB2	1:B:342:SER:HA	1.96	0.47
3:B:4472:ADP:H5'1	5:B:5977:HOH:O	2.14	0.47
1:C:174[B]:GLY:O	1:C:177[B]:GLY:HA2	2.13	0.47
1:D:128:PRO:CD	5:D:5910:HOH:O	2.61	0.47
1:I:231:LYS:CE	5:I:5928:HOH:O	2.59	0.47
1:K:179[B]:TYR:CD2	1:K:211[B]:HIS:HB2	2.47	0.47
1:A:128:PRO:CD	5:A:5907:HOH:O	2.61	0.47
1:A:154:ILE:HG13	5:A:5977:HOH:O	2.14	0.47
1:C:140:PHE:CE1	1:I:463:GLU:HA	2.49	0.47
1:C:232:ALA:HB1	1:C:367:PRO:HB2	1.97	0.47
1:D:68:MET:HA	1:D:69:PRO:HD2	1.78	0.47
1:I:329:PRO:HB2	1:I:342:SER:HA	1.96	0.47
1:I:329:PRO:CD	1:I:359:ARG:HD2	2.42	0.47
1:J:329:PRO:CD	1:J:359:ARG:HD2	2.42	0.47
1:K:304:HIS:O	1:K:308:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:84:THR:HG21	5:L:1730:HOH:O	2.12	0.47
1:A:296:TYR:HB3	1:A:382:ILE:HA	1.97	0.47
1:B:174[B]:GLY:O	1:B:177[B]:GLY:CA	2.63	0.47
1:C:165:GLU:N	5:C:5961:HOH:O	2.46	0.47
1:C:207:GLU:O	1:C:208:ALA:HB2	2.15	0.47
1:E:329:PRO:HB2	1:E:342:SER:HA	1.96	0.47
1:F:154:ILE:HG13	5:F:5987:HOH:O	2.14	0.47
1:G:165:GLU:N	5:G:5971:HOH:O	2.46	0.47
1:H:207:GLU:O	1:H:208:ALA:HB2	2.15	0.47
1:H:329:PRO:CD	1:H:359:ARG:HD2	2.42	0.47
1:K:231:LYS:CE	5:K:1539:HOH:O	2.59	0.47
1:K:447:ARG:HD2	5:K:1647:HOH:O	2.15	0.47
1:L:304:HIS:O	1:L:308:ILE:HG13	2.14	0.47
1:A:230:LYS:O	1:A:234:GLU:HG3	2.15	0.47
1:A:339:ARG:NH1	1:B:59:GLY:O	2.44	0.47
1:C:174[B]:GLY:O	1:C:177[B]:GLY:CA	2.63	0.47
1:C:348:VAL:HG22	5:C:5934:HOH:O	2.13	0.47
1:D:360:PHE:CG	1:D:361:PRO:CD	2.97	0.47
1:D:296:TYR:HB3	1:D:382:ILE:HA	1.97	0.47
1:E:68:MET:HA	1:E:69:PRO:HD2	1.78	0.47
1:G:1:SER:N	1:G:71:ALA:CB	2.78	0.47
1:H:296:TYR:HB3	1:H:382:ILE:HA	1.97	0.47
1:G:60:ILE:O	1:H:339:ARG:HB2	2.15	0.47
1:I:360:PHE:CG	1:I:361:PRO:CD	2.97	0.47
1:J:304:HIS:O	1:J:308:ILE:HG13	2.14	0.47
1:J:348:VAL:HG22	5:J:5951:HOH:O	2.13	0.47
1:J:360:PHE:CG	1:J:361:PRO:CD	2.97	0.47
3:J:4480:ADP:H5'1	5:J:5993:HOH:O	2.14	0.47
3:K:4481:ADP:H5'1	5:K:1609:HOH:O	2.14	0.47
1:L:174[B]:GLY:O	1:L:177[B]:GLY:CA	2.63	0.47
1:A:401:PRO:HA	1:A:404:ALA:CA	2.44	0.47
1:B:230:LYS:HG2	5:B:5964:HOH:O	2.14	0.47
1:D:332:LEU:O	5:D:6001:HOH:O	2.20	0.47
1:E:232:ALA:HB1	1:E:367:PRO:HB2	1.97	0.47
1:F:128:PRO:CD	5:F:5919:HOH:O	2.61	0.47
1:F:174[B]:GLY:O	1:F:177[B]:GLY:CA	2.63	0.47
1:F:1:SER:N	1:F:71:ALA:CB	2.78	0.47
1:G:447:ARG:HD2	5:G:6019:HOH:O	2.15	0.47
1:G:1:SER:O	1:G:5:VAL:HG23	2.15	0.47
1:G:34:PRO:HG2	1:H:206:VAL:O	2.15	0.47
1:H:230:LYS:O	1:H:234:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:174[B]:GLY:O	1:I:177[B]:GLY:CA	2.63	0.47
1:I:28:GLU:CB	5:I:5951:HOH:O	2.58	0.47
1:I:410:VAL:HG22	5:I:6047:HOH:O	2.14	0.47
1:J:174[B]:GLY:O	1:J:177[B]:GLY:CA	2.63	0.47
1:J:75:VAL:CG2	5:J:5934:HOH:O	2.53	0.47
1:K:296:TYR:HB3	1:K:382:ILE:HA	1.97	0.47
1:K:332:LEU:O	5:K:1635:HOH:O	2.20	0.47
1:L:165:GLU:N	5:L:1747:HOH:O	2.46	0.47
1:A:332:LEU:O	5:A:5998:HOH:O	2.20	0.47
1:D:230:LYS:O	1:D:234:GLU:HG3	2.15	0.47
1:F:207:GLU:O	1:F:208:ALA:HB2	2.15	0.47
1:H:1:SER:O	1:H:5:VAL:HG23	2.15	0.47
1:I:207:GLU:O	1:I:208:ALA:HB2	2.15	0.47
1:J:230:LYS:HG2	5:J:5980:HOH:O	2.14	0.47
1:J:329:PRO:HB2	1:J:342:SER:HA	1.96	0.47
1:L:232:ALA:HB1	1:L:367:PRO:HB2	1.97	0.47
1:A:232:ALA:HB1	1:A:367:PRO:HB2	1.97	0.47
1:A:261[A]:PHE:HB2	1:G:457:PRO:HD3	1.96	0.47
1:B:165:GLU:N	5:B:5962:HOH:O	2.46	0.47
1:C:1:SER:N	1:C:71:ALA:CB	2.78	0.47
1:C:273:SER:OG	3:C:4473:ADP:N6	2.48	0.47
1:B:208:ALA:HB2	1:C:33:ILE:CD1	2.44	0.47
3:C:4473:ADP:H5'1	5:C:5976:HOH:O	2.14	0.47
1:G:174[B]:GLY:O	1:G:177[B]:GLY:CA	2.63	0.47
1:G:232:ALA:HB1	1:G:367:PRO:HB2	1.97	0.47
1:H:329:PRO:HB2	1:H:342:SER:HA	1.97	0.47
1:I:230:LYS:HG2	5:I:5984:HOH:O	2.14	0.47
1:I:230:LYS:O	1:I:234:GLU:HG3	2.15	0.47
1:J:273:SER:OG	3:J:4480:ADP:N6	2.48	0.47
1:K:1:SER:O	1:K:5:VAL:HG23	2.15	0.47
1:L:207:GLU:O	1:L:208:ALA:HB2	2.15	0.47
1:A:211[B]:HIS:O	1:A:212[B]:GLU:CB	2.54	0.47
1:A:410:VAL:HG22	5:A:6026:HOH:O	2.14	0.47
1:A:447:ARG:HD2	5:A:6009:HOH:O	2.15	0.47
1:B:360:PHE:CG	1:B:361:PRO:CD	2.97	0.47
1:B:296:TYR:HB3	1:B:382:ILE:HA	1.97	0.47
1:B:273:SER:OG	3:B:4472:ADP:N6	2.48	0.47
1:B:447:ARG:HD2	5:B:6010:HOH:O	2.15	0.47
1:A:337:ARG:CZ	1:B:61:ASN:HB2	2.44	0.47
1:C:1:SER:O	1:C:5:VAL:HG23	2.15	0.47
1:C:329:PRO:CD	1:C:359:ARG:HD2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:PHE:CE2	1:D:218:GLN:HB2	2.50	0.47
1:D:273:SER:OG	3:D:4474:ADP:N6	2.48	0.47
1:E:1:SER:O	1:E:5:VAL:HG23	2.15	0.47
1:F:1:SER:O	1:F:5:VAL:HG23	2.15	0.47
1:G:133:PHE:CE2	1:G:218:GLN:HB2	2.50	0.47
1:G:304:HIS:O	1:G:308:ILE:HG13	2.14	0.47
1:G:348:VAL:HG22	5:G:5944:HOH:O	2.13	0.47
1:G:410:VAL:HG22	5:G:6036:HOH:O	2.14	0.47
1:I:232:ALA:HB1	1:I:367:PRO:HB2	1.97	0.47
1:I:329:PRO:HG2	1:I:359:ARG:CD	2.18	0.47
1:K:1:SER:N	1:K:71:ALA:CB	2.78	0.47
1:K:61:ASN:HB3	1:L:337:ARG:NH1	2.27	0.47
1:L:1:SER:O	1:L:5:VAL:HG23	2.15	0.47
1:A:224:ARG:NH2	1:A:224:ARG:CG	2.69	0.46
1:A:1:SER:N	1:A:71:ALA:CB	2.78	0.46
1:B:133:PHE:CE2	1:B:218:GLN:HB2	2.50	0.46
1:B:339:ARG:HH12	1:C:63:SER:N	2.13	0.46
1:B:1:SER:N	1:B:71:ALA:CB	2.78	0.46
1:D:174[B]:GLY:O	1:D:177[B]:GLY:CA	2.63	0.46
3:D:4474:ADP:H5'1	5:D:5979:HOH:O	2.14	0.46
1:E:296:TYR:HB3	1:E:382:ILE:HA	1.97	0.46
1:E:304:HIS:O	1:E:308:ILE:HG13	2.14	0.46
1:E:329:PRO:HG2	1:E:359:ARG:CD	2.18	0.46
1:E:273:SER:OG	3:E:4475:ADP:N6	2.48	0.46
1:G:75:VAL:CG2	5:G:5926:HOH:O	2.53	0.46
1:H:232:ALA:HB1	1:H:367:PRO:HB2	1.97	0.46
1:I:128:PRO:CD	5:I:5928:HOH:O	2.61	0.46
1:J:232:ALA:HB1	1:J:367:PRO:HB2	1.97	0.46
1:J:1:SER:N	1:J:71:ALA:CB	2.78	0.46
1:K:329:PRO:HG2	1:K:359:ARG:CD	2.18	0.46
1:K:232:ALA:HB1	1:K:367:PRO:HB2	1.97	0.46
1:L:230:LYS:O	1:L:234:GLU:HG3	2.15	0.46
1:L:273:SER:OG	3:L:4482:ADP:N6	2.48	0.46
1:L:329:PRO:HB2	1:L:342:SER:HA	1.97	0.46
3:A:4471:ADP:H5'1	5:A:5976:HOH:O	2.14	0.46
1:B:207:GLU:O	1:B:208:ALA:HB2	2.15	0.46
1:B:458:HIS:HE1	1:H:456:THR:O	1.98	0.46
1:C:75:VAL:CG2	5:C:5917:HOH:O	2.53	0.46
5:A:5969:HOH:O	1:F:183:PRO:HB2	2.14	0.46
1:G:207:GLU:O	1:G:208:ALA:HB2	2.15	0.46
1:G:360:PHE:CG	1:G:361:PRO:CD	2.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:4479:ADP:H5'1	5:I:5997:HOH:O	2.14	0.46
1:K:329:PRO:HB2	1:K:342:SER:HA	1.96	0.46
1:B:304:HIS:O	1:B:308:ILE:HG13	2.14	0.46
1:B:1:SER:O	1:B:5:VAL:HG23	2.15	0.46
1:C:133:PHE:CE2	1:C:218:GLN:HB2	2.50	0.46
1:D:230:LYS:HG2	5:D:5966:HOH:O	2.14	0.46
1:D:294:ALA:O	1:D:298:ILE:HG13	2.16	0.46
1:D:447:ARG:HD2	5:D:6012:HOH:O	2.15	0.46
1:D:1:SER:N	1:D:71:ALA:CB	2.78	0.46
1:E:174[B]:GLY:O	1:E:177[B]:GLY:CA	2.63	0.46
1:F:230:LYS:O	1:F:234:GLU:HG3	2.15	0.46
1:H:133:PHE:CE2	1:H:218:GLN:HB2	2.50	0.46
1:K:273:SER:OG	3:K:4481:ADP:N6	2.48	0.46
1:L:1:SER:N	1:L:71:ALA:CB	2.78	0.46
1:C:329:PRO:HB2	1:C:342:SER:HA	1.96	0.46
1:E:1:SER:N	1:E:71:ALA:CB	2.78	0.46
1:E:230:LYS:O	1:E:234:GLU:HG3	2.15	0.46
1:F:332:LEU:O	5:F:6008:HOH:O	2.20	0.46
1:G:273:SER:OG	3:G:4477:ADP:N6	2.48	0.46
1:H:447:ARG:HD2	5:H:6023:HOH:O	2.15	0.46
1:I:133:PHE:CE2	1:I:218:GLN:HB2	2.50	0.46
1:I:1:SER:N	1:I:71:ALA:CB	2.78	0.46
1:I:447:ARG:HD2	5:I:6030:HOH:O	2.15	0.46
1:J:1:SER:O	1:J:5:VAL:HG23	2.15	0.46
1:K:133:PHE:CE2	1:K:218:GLN:HB2	2.50	0.46
1:K:174[B]:GLY:O	1:K:177[B]:GLY:CA	2.63	0.46
1:K:207:GLU:O	1:K:208:ALA:HB2	2.15	0.46
1:L:401:PRO:HA	1:L:404:ALA:CA	2.44	0.46
1:C:447:ARG:HD2	5:C:6009:HOH:O	2.15	0.46
1:E:207:GLU:O	1:E:208:ALA:HB2	2.15	0.46
1:E:333:ALA:HB1	1:E:392:MET:HG2	1.97	0.46
1:E:410:VAL:HG22	5:E:747:HOH:O	2.14	0.46
1:F:18:ASP:OD2	1:F:30[A]:HIS:HD2	1.99	0.46
1:F:273:SER:OG	3:F:4476:ADP:N6	2.48	0.46
1:G:18:ASP:OD2	1:G:30[A]:HIS:HD2	1.99	0.46
1:H:273:SER:OG	3:H:4478:ADP:N6	2.48	0.46
1:I:332:LEU:O	5:I:6019:HOH:O	2.20	0.46
1:I:333:ALA:HB1	1:I:392:MET:HG2	1.97	0.46
1:I:84:THR:HG21	5:J:5962:HOH:O	2.16	0.46
1:J:207:GLU:O	1:J:208:ALA:HB2	2.15	0.46
1:I:33:ILE:CD1	1:J:208:ALA:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:401:PRO:HA	1:K:404:ALA:CA	2.44	0.46
3:L:4482:ADP:H5'1	5:L:1762:HOH:O	2.14	0.46
1:A:133:PHE:CE2	1:A:218:GLN:HB2	2.50	0.46
1:A:174[B]:GLY:O	1:A:177[B]:GLY:CA	2.63	0.46
1:B:232:ALA:HB1	1:B:367:PRO:HB2	1.97	0.46
1:C:410:VAL:HG22	5:C:6026:HOH:O	2.14	0.46
1:D:182:VAL:HG23	5:E:662:HOH:O	2.16	0.46
1:D:183:PRO:CB	5:E:684:HOH:O	2.62	0.46
1:E:390:GLU:HA	1:E:391:PRO:HD3	1.84	0.46
1:F:447:ARG:HD2	5:F:6019:HOH:O	2.15	0.46
1:I:304:HIS:O	1:I:308:ILE:HG13	2.14	0.46
1:K:410:VAL:HG22	5:K:1665:HOH:O	2.14	0.46
1:L:296:TYR:HB3	1:L:382:ILE:HA	1.97	0.46
1:L:447:ARG:HD2	5:L:1800:HOH:O	2.15	0.46
1:A:333:ALA:HB1	1:A:392:MET:HG2	1.97	0.46
1:A:269:HIS:CE1	4:A:5900:PPQ:CEP	2.92	0.46
1:C:437:GLU:CA	5:C:6017:HOH:O	2.58	0.46
1:D:232:ALA:HB1	1:D:367:PRO:HB2	1.97	0.46
1:D:1:SER:O	1:D:5:VAL:HG23	2.15	0.46
1:E:306:LYS:HE2	5:E:751:HOH:O	2.16	0.46
1:F:133:PHE:CE2	1:F:218:GLN:HB2	2.51	0.46
3:F:4476:ADP:H5'1	5:F:5986:HOH:O	2.14	0.46
1:J:18:ASP:OD2	1:J:30[A]:HIS:HD2	1.99	0.46
1:J:133:PHE:CE2	1:J:218:GLN:HB2	2.50	0.46
1:J:230:LYS:O	1:J:234:GLU:HG3	2.15	0.46
1:I:63:SER:N	1:J:339:ARG:NH1	2.62	0.46
1:J:447:ARG:HD2	5:J:6026:HOH:O	2.15	0.46
1:L:332:LEU:O	5:L:1788:HOH:O	2.20	0.46
1:A:207:GLU:O	1:A:208:ALA:HB2	2.15	0.46
1:B:294:ALA:O	1:B:298:ILE:HG13	2.16	0.46
1:B:332:LEU:O	5:B:5999:HOH:O	2.20	0.46
1:B:333:ALA:HB1	1:B:392:MET:HG2	1.97	0.46
1:D:207:GLU:O	1:D:208:ALA:HB2	2.15	0.46
1:D:333:ALA:HB1	1:D:392:MET:HG2	1.97	0.46
1:D:395:ASN:HB2	1:D:399:LEU:HD12	1.98	0.46
1:E:447:ARG:HD2	5:E:729:HOH:O	2.15	0.46
1:I:296:TYR:HB3	1:I:382:ILE:HA	1.97	0.46
1:I:401:PRO:HA	1:I:404:ALA:CA	2.44	0.46
1:I:1:SER:O	1:I:5:VAL:HG23	2.15	0.46
1:A:273:SER:OG	3:A:4471:ADP:N6	2.48	0.46
1:C:18:ASP:OD2	1:C:30[A]:HIS:HD2	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:ASP:OD2	1:D:30[A]:HIS:HD2	1.99	0.46
1:G:230:LYS:O	1:G:234:GLU:HG3	2.15	0.46
1:B:140:PHE:CE1	1:H:463:GLU:HA	2.51	0.46
1:I:294:ALA:O	1:I:298:ILE:HG13	2.16	0.46
1:I:273:SER:OG	3:I:4479:ADP:N6	2.48	0.46
1:K:154:ILE:HG13	5:K:1610:HOH:O	2.14	0.46
1:K:18:ASP:OD2	1:K:30[A]:HIS:HD2	1.99	0.46
1:A:294:ALA:O	1:A:298:ILE:HG13	2.16	0.46
1:B:344:ARG:HB3	1:B:344:ARG:HE	1.59	0.46
1:C:333:ALA:HB1	1:C:392:MET:HG2	1.97	0.46
1:C:68:MET:HA	1:C:69:PRO:HD2	1.78	0.46
1:C:189:GLN:NE2	1:D:32:THR:OG1	2.48	0.46
1:E:210[A]:HIS:ND1	1:E:211[A]:HIS:O	2.47	0.46
1:F:395:ASN:HB2	1:F:399:LEU:HD12	1.98	0.46
1:G:235:ILE:HA	1:G:235:ILE:HD13	1.80	0.46
1:H:172:ARG:HA	1:H:173[A]:PRO:HD3	1.80	0.46
1:H:174[B]:GLY:O	1:H:177[B]:GLY:CA	2.63	0.46
1:H:1:SER:N	1:H:71:ALA:CB	2.78	0.46
1:I:61:ASN:HB3	1:J:337:ARG:HH11	1.79	0.46
1:G:337:ARG:CZ	1:L:61:ASN:HB2	2.45	0.46
1:A:18:ASP:OD2	1:A:30[A]:HIS:HD2	1.99	0.45
1:A:1:SER:O	1:A:5:VAL:HG23	2.15	0.45
1:B:306:LYS:HE2	5:B:6031:HOH:O	2.16	0.45
1:C:180[A]:PHE:O	1:D:29[A]:GLN:HA	2.16	0.45
1:D:231:LYS:CE	5:D:5910:HOH:O	2.59	0.45
1:E:165:GLU:N	5:E:676:HOH:O	2.46	0.45
1:E:133:PHE:CE2	1:E:218:GLN:HB2	2.50	0.45
1:G:125:LEU:HA	1:G:125:LEU:HD12	1.79	0.45
1:G:339:ARG:HH12	1:L:63:SER:N	2.14	0.45
1:H:294:ALA:O	1:H:298:ILE:HG13	2.16	0.45
1:J:165:GLU:N	5:J:5978:HOH:O	2.46	0.45
1:J:332:LEU:O	5:J:6015:HOH:O	2.20	0.45
1:J:333:ALA:HB1	1:J:392:MET:HG2	1.97	0.45
1:K:230:LYS:O	1:K:234:GLU:HG3	2.15	0.45
1:L:133:PHE:CE2	1:L:218:GLN:HB2	2.51	0.45
1:L:333:ALA:HB1	1:L:392:MET:HG2	1.97	0.45
1:C:230:LYS:O	1:C:234:GLU:HG3	2.15	0.45
1:E:294:ALA:O	1:E:298:ILE:HG13	2.16	0.45
1:F:232:ALA:HB1	1:F:367:PRO:HB2	1.97	0.45
1:G:80:PHE:CZ	1:H:189:GLN:HG3	2.51	0.45
1:I:165:GLU:N	5:I:5982:HOH:O	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:210[A]:HIS:ND1	1:K:211[A]:HIS:O	2.47	0.45
1:L:18:ASP:OD2	1:L:30[A]:HIS:HD2	1.99	0.45
1:L:294:ALA:O	1:L:298:ILE:HG13	2.16	0.45
1:A:329:PRO:HB2	1:A:342:SER:HA	1.96	0.45
1:A:47:LYS:CD	5:A:6035:HOH:O	2.65	0.45
1:B:230:LYS:O	1:B:234:GLU:HG3	2.15	0.45
1:C:296:TYR:HB3	1:C:382:ILE:HA	1.97	0.45
1:D:47:LYS:CD	5:D:6038:HOH:O	2.65	0.45
1:E:269:HIS:CE1	4:E:5904:PPQ:CEP	2.92	0.45
1:F:296:TYR:HB3	1:F:382:ILE:HA	1.97	0.45
1:G:155:GLU:OE1	1:G:211[A]:HIS:CE1	2.68	0.45
1:H:333:ALA:HB1	1:H:392:MET:HG2	1.97	0.45
1:H:401:PRO:HA	1:H:404:ALA:CA	2.44	0.45
1:J:128:PRO:CD	5:J:5926:HOH:O	2.61	0.45
1:J:294:ALA:O	1:J:298:ILE:HG13	2.16	0.45
1:J:296:TYR:HB3	1:J:382:ILE:HA	1.97	0.45
1:J:47:LYS:CD	5:J:6052:HOH:O	2.65	0.45
1:K:128:PRO:CD	5:K:1539:HOH:O	2.61	0.45
1:K:294:ALA:O	1:K:298:ILE:HG13	2.16	0.45
1:C:182:VAL:HG23	5:D:5951:HOH:O	2.16	0.45
1:E:18:ASP:OD2	1:E:30[A]:HIS:HD2	1.99	0.45
1:G:172:ARG:HA	1:G:173[A]:PRO:HD3	1.80	0.45
1:G:296:TYR:HB3	1:G:382:ILE:HA	1.97	0.45
1:H:18:ASP:OD2	1:H:30[A]:HIS:HD2	1.99	0.45
1:A:165:GLU:N	5:A:5961:HOH:O	2.46	0.45
1:A:329:PRO:HD2	1:A:359:ARG:HG2	1.99	0.45
1:D:165:GLU:N	5:D:5964:HOH:O	2.46	0.45
1:F:153:ASP:OD1	1:F:251:LYS:NZ	2.50	0.45
1:F:333:ALA:HB1	1:F:392:MET:HG2	1.97	0.45
1:F:344:ARG:HE	1:F:344:ARG:HB3	1.59	0.45
1:G:153:ASP:OD1	1:G:251:LYS:NZ	2.50	0.45
1:G:333:ALA:HB1	1:G:392:MET:HG2	1.97	0.45
1:H:306:LYS:HE2	5:H:6044:HOH:O	2.16	0.45
1:I:395:ASN:HB2	1:I:399:LEU:HD12	1.98	0.45
1:K:333:ALA:HB1	1:K:392:MET:HG2	1.97	0.45
1:L:395:ASN:HB2	1:L:399:LEU:HD12	1.98	0.45
1:B:153:ASP:OD1	1:B:251:LYS:NZ	2.50	0.45
1:B:284:GLY:HA3	1:B:291:SER:HA	1.99	0.45
1:B:395:ASN:HB2	1:B:399:LEU:HD12	1.98	0.45
1:C:128:PRO:CD	5:C:5909:HOH:O	2.61	0.45
1:E:172:ARG:HA	1:E:173[A]:PRO:HD3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:395:ASN:HB2	1:H:399:LEU:HD12	1.98	0.45
1:A:189:GLN:HG3	1:B:80:PHE:CZ	2.51	0.45
1:C:306:LYS:HE2	5:C:6030:HOH:O	2.16	0.45
1:F:294:ALA:O	1:F:298:ILE:HG13	2.16	0.45
1:G:183:PRO:CB	5:L:1755:HOH:O	2.62	0.45
1:G:294:ALA:O	1:G:298:ILE:HG13	2.16	0.45
1:G:306:LYS:HE2	5:G:6040:HOH:O	2.16	0.45
1:H:329:PRO:HD2	1:H:359:ARG:HG2	1.99	0.45
1:I:306:LYS:HE2	5:I:6051:HOH:O	2.16	0.45
1:J:306:LYS:HE2	5:J:6047:HOH:O	2.16	0.45
1:K:165:GLU:N	5:K:1594:HOH:O	2.46	0.45
1:K:306:LYS:HE2	5:K:1669:HOH:O	2.16	0.45
1:L:329:PRO:HD2	1:L:359:ARG:HG2	1.99	0.45
1:A:153:ASP:OD1	1:A:251:LYS:NZ	2.50	0.45
1:A:4:HIS:CE1	5:A:5986:HOH:O	2.70	0.45
1:D:329:PRO:HD2	1:D:359:ARG:HG2	1.99	0.45
1:E:128:PRO:CD	5:E:621:HOH:O	2.61	0.45
1:G:332:LEU:O	5:G:6008:HOH:O	2.20	0.45
1:G:63:SER:N	1:H:339:ARG:NH1	2.62	0.45
1:I:40:ALA:HB2	5:I:6002:HOH:O	2.10	0.45
1:K:29[A]:GLN:HA	1:L:180[A]:PHE:O	2.17	0.45
1:B:183:PRO:CB	5:C:5969:HOH:O	2.65	0.45
1:B:18:ASP:OD2	1:B:30[A]:HIS:HD2	1.99	0.45
1:D:447:ARG:HG3	1:D:447:ARG:HH21	1.82	0.45
1:C:189:GLN:HG3	1:D:80:PHE:CZ	2.51	0.45
1:F:210[A]:HIS:ND1	1:F:211[A]:HIS:O	2.47	0.45
1:F:306:LYS:HE2	5:F:6040:HOH:O	2.16	0.45
1:F:401:PRO:HA	1:F:404:ALA:CA	2.44	0.45
1:H:284:GLY:HA3	1:H:291:SER:HA	1.99	0.45
1:I:18:ASP:OD2	1:I:30[A]:HIS:HD2	1.99	0.45
1:I:210[B]:HIS:C	1:I:211[B]:HIS:CD2	2.90	0.45
1:I:4:HIS:CE1	5:I:6007:HOH:O	2.70	0.45
1:J:401:PRO:CA	1:J:404:ALA:HA	2.46	0.45
1:K:193:SER:O	1:K:197:LEU:HG	2.17	0.45
1:K:395:ASN:HB2	1:K:399:LEU:HD12	1.98	0.45
1:A:395:ASN:HB2	1:A:399:LEU:HD12	1.98	0.45
1:B:269:HIS:HE1	4:B:5901:PPQ:HEP2	1.82	0.45
1:C:294:ALA:O	1:C:298:ILE:HG13	2.16	0.45
1:D:359:ARG:HD3	1:D:359:ARG:HH11	1.65	0.45
1:D:458:HIS:HE1	1:J:456:THR:O	2.00	0.45
1:E:47:LYS:CD	5:E:756:HOH:O	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:153:ASP:OD1	1:H:251:LYS:NZ	2.50	0.45
1:H:193:SER:O	1:H:197:LEU:HG	2.17	0.45
1:K:447:ARG:HG3	1:K:447:ARG:HH21	1.83	0.45
1:L:306:LYS:HE2	5:L:1822:HOH:O	2.16	0.45
1:C:149:VAL:HG21	1:I:462:PHE:CE1	2.52	0.44
1:C:268:MET:N	1:C:363:PRO:HD3	2.33	0.44
1:D:284:GLY:HA3	1:D:291:SER:HA	1.99	0.44
1:E:447:ARG:HG3	1:E:447:ARG:HH21	1.82	0.44
1:F:155:GLU:OE1	1:F:211[A]:HIS:CE1	2.68	0.44
1:F:25:LYS:HD2	5:F:5956:HOH:O	2.10	0.44
1:G:447:ARG:HH21	1:G:447:ARG:HG3	1.82	0.44
1:G:47:LYS:CD	5:G:6045:HOH:O	2.65	0.44
1:H:210[A]:HIS:ND1	1:H:211[A]:HIS:O	2.47	0.44
1:J:395:ASN:HB2	1:J:399:LEU:HD12	1.98	0.44
1:J:401:PRO:HA	1:J:404:ALA:CA	2.44	0.44
1:L:387:HIS:HA	1:L:388:PRO:HD2	1.85	0.44
1:A:447:ARG:HG3	1:A:447:ARG:HH21	1.82	0.44
1:A:462:PHE:CE1	1:G:149:VAL:HG21	2.52	0.44
1:B:115:LEU:CD2	1:B:379:LEU:HD21	2.48	0.44
1:B:193:SER:O	1:B:197:LEU:HG	2.17	0.44
1:B:401:PRO:HA	1:B:404:ALA:CA	2.44	0.44
1:C:153:ASP:OD1	1:C:251:LYS:NZ	2.50	0.44
1:B:337:ARG:HD3	1:C:61:ASN:CB	2.46	0.44
1:C:339:ARG:HB2	1:D:60:ILE:O	2.18	0.44
1:E:115:LEU:CD2	1:E:379:LEU:HD21	2.48	0.44
1:I:268:MET:N	1:I:363:PRO:HD3	2.33	0.44
1:K:153:ASP:OD1	1:K:251:LYS:NZ	2.50	0.44
1:L:210[A]:HIS:ND1	1:L:211[A]:HIS:O	2.47	0.44
1:A:231:LYS:CE	5:A:5907:HOH:O	2.59	0.44
1:B:401:PRO:CA	1:B:404:ALA:HA	2.47	0.44
1:D:153:ASP:OD1	1:D:251:LYS:NZ	2.50	0.44
1:D:289:GLY:HA2	5:D:6027:HOH:O	2.18	0.44
1:D:401:PRO:HA	1:D:404:ALA:CA	2.44	0.44
1:E:289:GLY:HA2	5:E:745:HOH:O	2.18	0.44
1:A:60:ILE:O	1:F:339:ARG:HB2	2.17	0.44
1:F:360:PHE:CG	1:F:361:PRO:CD	2.97	0.44
1:F:75:VAL:CG2	5:F:5927:HOH:O	2.53	0.44
1:H:268:MET:N	1:H:363:PRO:HD3	2.33	0.44
1:H:401:PRO:CA	1:H:404:ALA:HA	2.47	0.44
1:I:329:PRO:HD2	1:I:359:ARG:HG2	1.99	0.44
1:I:447:ARG:HH21	1:I:447:ARG:HG3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:447:ARG:HG3	1:J:447:ARG:HH21	1.82	0.44
1:J:4:HIS:CE1	5:J:6003:HOH:O	2.70	0.44
1:K:329:PRO:HD2	1:K:359:ARG:HG2	1.99	0.44
1:K:68:MET:HA	1:K:69:PRO:HD2	1.78	0.44
1:B:268:MET:N	1:B:363:PRO:HD3	2.33	0.44
1:B:447:ARG:HG3	1:B:447:ARG:HH21	1.82	0.44
1:C:210[A]:HIS:ND1	1:C:211[A]:HIS:O	2.47	0.44
1:C:324:PRO:N	5:C:6020:HOH:O	2.51	0.44
1:C:332:LEU:O	5:C:5998:HOH:O	2.20	0.44
1:C:395:ASN:HB2	1:C:399:LEU:HD12	1.98	0.44
1:E:153:ASP:OD1	1:E:251:LYS:NZ	2.50	0.44
1:F:268:MET:N	1:F:363:PRO:HD3	2.33	0.44
1:H:324:PRO:N	5:H:6034:HOH:O	2.51	0.44
1:H:447:ARG:HH21	1:H:447:ARG:HG3	1.82	0.44
1:H:4:HIS:CE1	5:H:6000:HOH:O	2.70	0.44
1:J:284:GLY:HA3	1:J:291:SER:HA	1.99	0.44
1:K:63:SER:N	1:L:339:ARG:HH12	2.15	0.44
1:C:329:PRO:HD2	1:C:359:ARG:HG2	1.99	0.44
1:D:4:HIS:CE1	5:D:5989:HOH:O	2.70	0.44
1:E:193:SER:O	1:E:197:LEU:HG	2.18	0.44
1:F:193:SER:O	1:F:197:LEU:HG	2.17	0.44
1:F:284:GLY:HA3	1:F:291:SER:HA	1.99	0.44
1:G:289:GLY:HA2	5:G:6034:HOH:O	2.18	0.44
1:I:153:ASP:OD1	1:I:251:LYS:NZ	2.50	0.44
1:J:153:ASP:OD1	1:J:251:LYS:NZ	2.50	0.44
1:A:306:LYS:HE2	5:A:6030:HOH:O	2.16	0.44
1:A:268:MET:N	1:A:363:PRO:HD3	2.33	0.44
1:C:337:ARG:O	1:D:61:ASN:O	2.35	0.44
1:D:115:LEU:CD2	1:D:379:LEU:HD21	2.48	0.44
1:D:193:SER:O	1:D:197:LEU:HG	2.17	0.44
1:D:306:LYS:HE2	5:D:6033:HOH:O	2.16	0.44
1:G:193:SER:O	1:G:197:LEU:HG	2.17	0.44
1:H:289:GLY:HA2	5:H:6038:HOH:O	2.18	0.44
1:J:231:LYS:CE	5:J:5926:HOH:O	2.59	0.44
1:K:284:GLY:HA3	1:K:291:SER:HA	1.99	0.44
1:K:359:ARG:HH11	1:K:359:ARG:HD3	1.65	0.44
1:K:47:LYS:CD	5:K:1674:HOH:O	2.65	0.44
1:L:324:PRO:N	5:L:1812:HOH:O	2.51	0.44
1:L:447:ARG:HH21	1:L:447:ARG:HG3	1.82	0.44
1:A:68:MET:HA	1:A:69:PRO:HD2	1.78	0.44
1:C:269:HIS:HE1	4:C:5902:PPQ:HEP2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:MET:N	1:D:363:PRO:HD3	2.33	0.44
1:E:401:PRO:HA	1:E:404:ALA:CA	2.44	0.44
1:F:352:LYS:HE2	1:F:352:LYS:HA	2.00	0.44
1:F:329:PRO:HD2	1:F:359:ARG:HG2	1.99	0.44
1:F:4:HIS:CE1	5:F:5996:HOH:O	2.70	0.44
1:G:210[A]:HIS:ND1	1:G:211[A]:HIS:O	2.47	0.44
1:G:268:MET:N	1:G:363:PRO:HD3	2.33	0.44
1:G:68:MET:HA	1:G:69:PRO:HD2	1.78	0.44
1:I:193:SER:O	1:I:197:LEU:HG	2.17	0.44
1:J:115:LEU:CD2	1:J:379:LEU:HD21	2.48	0.44
1:K:178[A]:GLY:O	1:K:211[A]:HIS:HD2	2.01	0.44
1:L:284:GLY:HA3	1:L:291:SER:HA	1.99	0.44
1:L:268:MET:N	1:L:363:PRO:HD3	2.33	0.44
1:A:40:ALA:HB2	5:A:5981:HOH:O	2.10	0.44
1:B:231:LYS:CE	5:B:5908:HOH:O	2.59	0.44
1:E:324:PRO:N	5:E:741:HOH:O	2.51	0.44
1:G:208:ALA:HB2	1:L:33:ILE:CD1	2.48	0.44
1:K:344:ARG:HB3	1:K:344:ARG:HE	1.59	0.44
1:K:4:HIS:CE1	5:K:1620:HOH:O	2.70	0.44
1:L:153:ASP:OD1	1:L:251:LYS:NZ	2.50	0.44
1:C:4:HIS:CE1	5:C:5986:HOH:O	2.70	0.44
1:E:284:GLY:HA3	1:E:291:SER:HA	1.99	0.44
1:F:128:PRO:HA	1:F:269:HIS:O	2.18	0.44
1:A:61:ASN:CB	1:F:337:ARG:HD3	2.46	0.44
1:G:230:LYS:CG	5:G:5973:HOH:O	2.66	0.44
1:G:324:PRO:N	5:G:6030:HOH:O	2.51	0.44
1:G:269:HIS:CE1	4:G:5906:PPQ:CEP	2.92	0.44
1:H:115:LEU:CD2	1:H:379:LEU:HD21	2.48	0.44
1:H:230:LYS:CG	5:H:5977:HOH:O	2.66	0.44
1:H:323:VAL:O	5:H:5936:HOH:O	2.21	0.44
1:J:324:PRO:N	5:J:6037:HOH:O	2.51	0.44
1:K:289:GLY:HA2	5:K:1663:HOH:O	2.18	0.44
1:K:115:LEU:CD2	1:K:379:LEU:HD21	2.48	0.44
1:K:401:PRO:CA	1:K:404:ALA:HA	2.47	0.44
1:L:128:PRO:HA	1:L:269:HIS:O	2.18	0.44
1:L:231:LYS:CE	5:L:1692:HOH:O	2.59	0.44
1:L:4:HIS:CE1	5:L:1773:HOH:O	2.70	0.44
1:L:269:HIS:CE1	4:L:5911:PPQ:CEP	2.92	0.44
1:A:193:SER:O	1:A:197:LEU:HG	2.17	0.43
1:B:329:PRO:HD2	1:B:359:ARG:HG2	1.99	0.43
1:B:4:HIS:CE1	5:B:5987:HOH:O	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:SER:O	1:C:197:LEU:HG	2.18	0.43
1:C:211[B]:HIS:O	1:C:212[B]:GLU:CB	2.54	0.43
1:C:230:LYS:CG	5:C:5963:HOH:O	2.66	0.43
1:D:178[A]:GLY:O	1:D:211[A]:HIS:HD2	2.01	0.43
1:D:235:ILE:HD13	1:D:235:ILE:HA	1.80	0.43
1:F:230:LYS:CG	5:F:5973:HOH:O	2.66	0.43
1:G:401:PRO:HA	1:G:404:ALA:CA	2.44	0.43
1:J:268:MET:N	1:J:363:PRO:HD3	2.33	0.43
1:K:16:PHE:HB2	1:K:84:THR:HB	2.00	0.43
1:K:268:MET:N	1:K:363:PRO:HD3	2.33	0.43
1:J:61:ASN:CB	1:K:337:ARG:HD3	2.47	0.43
1:L:193:SER:O	1:L:197:LEU:HG	2.18	0.43
1:L:210[B]:HIS:C	1:L:211[B]:HIS:CD2	2.89	0.43
1:L:289:GLY:HA2	5:L:1816:HOH:O	2.18	0.43
1:A:374:LEU:HD12	1:A:374:LEU:HA	1.91	0.43
1:B:128:PRO:CD	5:B:5908:HOH:O	2.61	0.43
1:C:128:PRO:HA	1:C:269:HIS:O	2.18	0.43
1:C:178[A]:GLY:O	1:C:211[A]:HIS:HD2	2.01	0.43
1:D:323:VAL:O	5:D:5923:HOH:O	2.21	0.43
1:E:231:LYS:CE	5:E:621:HOH:O	2.59	0.43
1:E:323:VAL:O	5:E:634:HOH:O	2.21	0.43
1:E:4:HIS:CE1	5:E:702:HOH:O	2.70	0.43
1:G:16:PHE:HB2	1:G:84:THR:HB	2.00	0.43
1:G:395:ASN:HB2	1:G:399:LEU:HD12	1.98	0.43
1:G:4:HIS:CE1	5:G:5996:HOH:O	2.70	0.43
1:H:30[A]:HIS:CE1	1:I:183:PRO:HD3	2.54	0.43
1:H:68:MET:HA	1:H:69:PRO:HD2	1.78	0.43
1:I:128:PRO:HA	1:I:269:HIS:O	2.18	0.43
1:I:47:LYS:CD	5:I:6056:HOH:O	2.65	0.43
1:L:172:ARG:HA	1:L:173[A]:PRO:HD3	1.80	0.43
1:L:323:VAL:O	5:L:1705:HOH:O	2.21	0.43
1:A:16:PHE:HB2	1:A:84:THR:HB	2.00	0.43
1:B:323:VAL:O	5:B:5921:HOH:O	2.21	0.43
1:C:339:ARG:NH1	1:D:63:SER:N	2.65	0.43
1:D:155:GLU:OE1	1:D:211[A]:HIS:CE1	2.68	0.43
1:D:423:LEU:C	1:D:425:ARG:H	2.22	0.43
1:E:128:PRO:HA	1:E:269:HIS:O	2.18	0.43
1:E:395:ASN:HB2	1:E:399:LEU:HD12	1.98	0.43
1:E:463:GLU:HA	1:K:140:PHE:CE1	2.53	0.43
1:F:178[A]:GLY:O	1:F:211[A]:HIS:HD2	2.01	0.43
1:F:324:PRO:N	5:F:6030:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:LYS:CD	5:F:6045:HOH:O	2.65	0.43
1:G:183:PRO:HD3	1:L:30[A]:HIS:CE1	2.52	0.43
1:H:33:ILE:HA	1:H:34:PRO:HD3	1.90	0.43
1:I:284:GLY:HA3	1:I:291:SER:HA	1.99	0.43
1:I:115:LEU:CD2	1:I:379:LEU:HD21	2.48	0.43
1:K:323:VAL:O	5:K:1552:HOH:O	2.21	0.43
1:K:127:GLY:HA3	3:K:4481:ADP:H1'	2.00	0.43
1:L:178[A]:GLY:O	1:L:211[A]:HIS:HD2	2.01	0.43
1:L:352:LYS:HA	1:L:352:LYS:HE2	2.00	0.43
1:A:390:GLU:HA	1:A:391:PRO:HD3	1.84	0.43
1:A:423:LEU:C	1:A:425:ARG:H	2.22	0.43
1:B:456:THR:O	1:H:458:HIS:HE1	2.00	0.43
1:B:56:GLY:N	5:B:5994:HOH:O	2.40	0.43
1:C:284:GLY:HA3	1:C:291:SER:HA	1.99	0.43
1:C:115:LEU:CD2	1:C:379:LEU:HD21	2.48	0.43
1:D:344:ARG:HB3	1:D:344:ARG:HE	1.58	0.43
1:F:447:ARG:HG3	1:F:447:ARG:HH21	1.82	0.43
1:G:178[A]:GLY:O	1:G:211[A]:HIS:HD2	2.01	0.43
1:G:329:PRO:HD2	1:G:359:ARG:HG2	1.99	0.43
1:I:289:GLY:HA2	5:I:6045:HOH:O	2.18	0.43
1:J:193:SER:O	1:J:197:LEU:HG	2.17	0.43
1:J:29[A]:GLN:HA	1:K:180[A]:PHE:O	2.18	0.43
1:L:115:LEU:CD2	1:L:379:LEU:HD21	2.48	0.43
1:L:68:MET:HA	1:L:69:PRO:HD2	1.78	0.43
1:A:289:GLY:HA2	5:A:6024:HOH:O	2.18	0.43
1:B:127:GLY:HA3	3:B:4472:ADP:H1'	2.00	0.43
1:B:128:PRO:HA	1:B:269:HIS:O	2.18	0.43
1:B:180[A]:PHE:O	1:C:29[A]:GLN:HA	2.19	0.43
1:D:128:PRO:HA	1:D:269:HIS:O	2.18	0.43
1:D:33:ILE:HA	1:D:34:PRO:HD3	1.90	0.43
1:E:230:LYS:CG	5:E:678:HOH:O	2.66	0.43
1:E:401:PRO:CA	1:E:404:ALA:HA	2.47	0.43
1:F:423:LEU:C	1:F:425:ARG:H	2.22	0.43
1:G:284:GLY:HA3	1:G:291:SER:HA	1.99	0.43
1:G:30[A]:HIS:CE1	1:H:183:PRO:HD3	2.54	0.43
1:H:178[A]:GLY:O	1:H:211[A]:HIS:HD2	2.01	0.43
1:H:269:HIS:HE1	4:H:5907:PPQ:HEP2	1.82	0.43
1:I:16:PHE:HB2	1:I:84:THR:HB	2.00	0.43
1:I:178[A]:GLY:O	1:I:211[A]:HIS:HD2	2.01	0.43
1:I:75:VAL:CG2	5:I:5937:HOH:O	2.53	0.43
1:J:178[A]:GLY:O	1:J:211[A]:HIS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:329:PRO:HD2	1:J:359:ARG:HG2	1.99	0.43
1:K:125:LEU:HA	1:K:125:LEU:HD12	1.79	0.43
1:K:32:THR:OG1	1:L:189:GLN:NE2	2.50	0.43
1:A:230:LYS:CG	5:A:5963:HOH:O	2.66	0.43
1:A:284:GLY:HA3	1:A:291:SER:HA	1.99	0.43
1:A:324:PRO:N	5:A:6020:HOH:O	2.51	0.43
1:B:289:GLY:HA2	5:B:6025:HOH:O	2.18	0.43
1:B:16:PHE:HB2	1:B:84:THR:HB	2.00	0.43
1:C:230:LYS:HE2	1:C:230:LYS:HB2	1.85	0.43
1:C:231:LYS:CE	5:C:5909:HOH:O	2.59	0.43
1:C:33:ILE:HA	1:C:34:PRO:HD3	1.90	0.43
1:C:271:HIS:CD2	1:C:357:GLU:HB2	2.54	0.43
1:D:16:PHE:HB2	1:D:84:THR:HB	2.00	0.43
1:E:1:SER:N	1:E:71:ALA:HB3	2.34	0.43
1:E:302:ILE:CD1	5:E:717:HOH:O	2.49	0.43
1:F:165:GLU:N	5:F:5971:HOH:O	2.46	0.43
1:F:16:PHE:HB2	1:F:84:THR:HB	2.00	0.43
1:F:269:HIS:CE1	4:F:5905:PPQ:CEP	2.91	0.43
1:F:82:ASP:O	1:F:84:THR:CG2	2.67	0.43
1:G:144:ILE:HG22	5:G:5922:HOH:O	2.19	0.43
1:G:271:HIS:CD2	1:G:357:GLU:HB2	2.54	0.43
1:G:115:LEU:CD2	1:G:379:LEU:HD21	2.48	0.43
1:G:40:ALA:HB2	5:G:5991:HOH:O	2.10	0.43
1:G:423:LEU:C	1:G:425:ARG:H	2.22	0.43
1:A:140:PHE:CE1	1:G:463:GLU:HA	2.54	0.43
1:J:230:LYS:CG	5:J:5980:HOH:O	2.66	0.43
1:J:30[A]:HIS:CE1	1:K:183:PRO:HD3	2.53	0.43
1:E:261[A]:PHE:HB2	1:K:457:PRO:HD3	2.01	0.43
1:E:140:PHE:CE1	1:K:463:GLU:HA	2.54	0.43
1:A:339:ARG:HH12	1:B:63:SER:N	2.16	0.43
1:C:359:ARG:HH12	4:C:5902:PPQ:HEP2	1.84	0.43
1:D:352:LYS:HE2	1:D:352:LYS:HA	2.00	0.43
1:E:192[A]:ARG:HH21	1:E:219:ASN:ND2	2.17	0.43
1:E:268:MET:N	1:E:363:PRO:HD3	2.33	0.43
1:E:337:ARG:CD	1:F:61:ASN:CB	2.84	0.43
1:E:16:PHE:HB2	1:E:84:THR:HB	2.00	0.43
1:F:144:ILE:HG22	5:F:5923:HOH:O	2.19	0.43
1:A:29[A]:GLN:HA	1:F:180[A]:PHE:O	2.18	0.43
1:F:359:ARG:HH12	4:F:5905:PPQ:HEP2	1.84	0.43
1:H:128:PRO:HA	1:H:269:HIS:O	2.18	0.43
1:H:423:LEU:C	1:H:425:ARG:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:HIS:HE1	1:I:456:THR:O	2.02	0.43
1:J:210[A]:HIS:ND1	1:J:211[A]:HIS:O	2.47	0.43
1:J:390:GLU:HA	1:J:391:PRO:HD3	1.84	0.43
1:K:271:HIS:CD2	1:K:357:GLU:HB2	2.54	0.43
1:L:423:LEU:C	1:L:425:ARG:H	2.22	0.43
1:A:155:GLU:OE1	1:A:211[A]:HIS:CE1	2.68	0.43
5:A:5945:HOH:O	1:B:84:THR:HG21	2.18	0.43
1:C:144:ILE:HG22	5:C:5913:HOH:O	2.19	0.43
1:C:16:PHE:HB2	1:C:84:THR:HB	2.00	0.43
1:F:115:LEU:CD2	1:F:379:LEU:HD21	2.48	0.43
1:H:1:SER:N	1:H:71:ALA:HB3	2.34	0.43
1:H:201:GLN:N	5:H:6017:HOH:O	2.52	0.43
1:H:305:ALA:CB	1:H:332:LEU:HD21	2.49	0.43
1:I:230:LYS:CG	5:I:5984:HOH:O	2.66	0.43
1:I:323:VAL:O	5:I:5941:HOH:O	2.21	0.43
1:D:463:GLU:HA	1:J:140:PHE:CE1	2.54	0.43
1:K:324:PRO:N	5:K:1659:HOH:O	2.51	0.43
1:K:423:LEU:C	1:K:425:ARG:H	2.22	0.43
1:A:192[A]:ARG:HH21	1:A:219:ASN:ND2	2.17	0.43
1:A:115:LEU:CD2	1:A:379:LEU:HD21	2.48	0.43
1:B:178[A]:GLY:O	1:B:211[A]:HIS:HD2	2.01	0.43
1:B:1:SER:N	1:B:71:ALA:HB3	2.34	0.43
1:B:210[B]:HIS:C	1:B:211[B]:HIS:CD2	2.90	0.43
1:B:305:ALA:CB	1:B:332:LEU:HD21	2.49	0.43
1:C:201:GLN:N	5:C:6003:HOH:O	2.52	0.43
1:C:305:ALA:CB	1:C:332:LEU:HD21	2.49	0.43
1:C:401:PRO:CA	1:C:404:ALA:HA	2.47	0.43
1:C:447:ARG:HH21	1:C:447:ARG:HG3	1.82	0.43
1:D:192[A]:ARG:HH21	1:D:219:ASN:ND2	2.17	0.43
1:E:127:GLY:HA3	3:E:4475:ADP:H1'	2.00	0.43
1:E:329:PRO:HD2	1:E:359:ARG:HG2	1.99	0.43
1:A:140:PHE:CE1	1:F:160:SER:HB2	2.54	0.43
1:F:401:PRO:CA	1:F:404:ALA:HA	2.46	0.43
1:G:192[A]:ARG:HH21	1:G:219:ASN:ND2	2.17	0.43
1:I:172:ARG:HA	1:I:173[A]:PRO:HD3	1.80	0.43
1:I:305:ALA:CB	1:I:332:LEU:HD21	2.49	0.43
1:I:423:LEU:C	1:I:425:ARG:H	2.22	0.43
1:J:128:PRO:HA	1:J:269:HIS:O	2.18	0.43
1:J:423:LEU:C	1:J:425:ARG:H	2.22	0.43
5:J:5986:HOH:O	1:K:183:PRO:CB	2.66	0.43
1:K:201:GLN:N	5:K:1640:HOH:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:305:ALA:CB	1:K:332:LEU:HD21	2.49	0.43
1:L:201:GLN:N	5:L:1793:HOH:O	2.52	0.43
1:A:271:HIS:CD2	1:A:357:GLU:HB2	2.54	0.43
1:B:352:LYS:HA	1:B:352:LYS:HE2	2.00	0.43
1:C:352:LYS:HA	1:C:352:LYS:HE2	2.00	0.43
1:C:40:ALA:HB2	5:C:5981:HOH:O	2.10	0.43
1:D:305:ALA:CB	1:D:332:LEU:HD21	2.49	0.43
1:E:332:LEU:O	5:E:717:HOH:O	2.20	0.43
1:F:127:GLY:HA3	3:F:4476:ADP:H1'	2.00	0.43
1:F:192[A]:ARG:HH21	1:F:219:ASN:ND2	2.17	0.43
1:F:289:GLY:HA2	5:F:6034:HOH:O	2.18	0.43
1:E:337:ARG:CZ	1:F:61:ASN:HB2	2.46	0.43
1:G:128:PRO:HA	1:G:269:HIS:O	2.18	0.43
1:G:210[B]:HIS:C	1:G:211[B]:HIS:CD2	2.89	0.43
1:H:324:PRO:HA	5:H:6034:HOH:O	2.19	0.43
1:I:144:ILE:HG22	5:I:5933:HOH:O	2.19	0.43
1:I:452:ARG:HG2	5:I:6036:HOH:O	2.19	0.43
1:J:289:GLY:HA2	5:J:6041:HOH:O	2.18	0.43
1:J:31:VAL:HG23	1:K:210[A]:HIS:HB3	2.00	0.43
1:I:61:ASN:CA	1:J:337:ARG:HD3	2.48	0.43
1:K:197:LEU:O	1:K:201:GLN:HG3	2.19	0.43
1:K:192[A]:ARG:HH21	1:K:219:ASN:ND2	2.17	0.43
1:K:352:LYS:HA	1:K:352:LYS:HE2	2.00	0.43
1:B:309:ASN:HA	1:B:309:ASN:HD22	1.71	0.42
1:D:175[B]:VAL:O	1:D:176[B]:LYS:HB2	2.20	0.42
1:D:324:PRO:N	5:D:6023:HOH:O	2.51	0.42
1:D:359:ARG:HH12	4:D:5903:PPQ:HEP2	1.84	0.42
1:D:127:GLY:HA3	3:D:4474:ADP:H1'	2.00	0.42
1:E:305:ALA:CB	1:E:332:LEU:HD21	2.49	0.42
1:F:210[B]:HIS:C	1:F:211[B]:HIS:CD2	2.89	0.42
1:G:93:GLU:OE2	1:G:94:PRO:HD2	2.20	0.42
5:G:5979:HOH:O	1:H:183:PRO:CB	2.66	0.42
1:I:192[A]:ARG:HH21	1:I:219:ASN:ND2	2.17	0.42
1:I:324:PRO:N	5:I:6041:HOH:O	2.51	0.42
1:I:359:ARG:HH12	4:I:5908:PPQ:HEP2	1.84	0.42
1:I:29[A]:GLN:HA	1:J:180[A]:PHE:O	2.19	0.42
1:K:1:SER:N	1:K:71:ALA:HB3	2.34	0.42
1:L:16:PHE:HB2	1:L:84:THR:HB	2.00	0.42
1:L:127:GLY:HA3	3:L:4482:ADP:H1'	2.00	0.42
1:L:452:ARG:HG2	5:L:1807:HOH:O	2.19	0.42
1:A:128:PRO:HA	1:A:269:HIS:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178[A]:GLY:O	1:A:211[A]:HIS:HD2	2.01	0.42
1:B:271:HIS:CD2	1:B:357:GLU:HB2	2.54	0.42
1:B:47:LYS:CD	5:B:6036:HOH:O	2.65	0.42
1:C:289:GLY:HA2	5:C:6024:HOH:O	2.18	0.42
1:E:125:LEU:HA	1:E:125:LEU:HD12	1.79	0.42
1:E:178[A]:GLY:O	1:E:211[A]:HIS:HD2	2.01	0.42
1:E:93:GLU:OE2	1:E:94:PRO:HD2	2.19	0.42
1:F:197:LEU:O	1:F:201:GLN:HG3	2.19	0.42
1:H:210[B]:HIS:C	1:H:211[B]:HIS:CD2	2.89	0.42
1:H:47:LYS:CD	5:H:6049:HOH:O	2.65	0.42
1:J:144:ILE:HG22	5:J:5930:HOH:O	2.19	0.42
1:J:197:LEU:O	1:J:201:GLN:HG3	2.20	0.42
1:J:323:VAL:O	5:J:5938:HOH:O	2.21	0.42
1:J:387:HIS:HA	1:J:388:PRO:HD2	1.85	0.42
1:L:230:LYS:CG	5:L:1749:HOH:O	2.66	0.42
1:B:359:ARG:HH12	4:B:5901:PPQ:HEP2	1.84	0.42
1:C:160:SER:HB2	1:D:140:PHE:CE1	2.54	0.42
1:D:269:HIS:HE1	4:D:5903:PPQ:HEP2	1.82	0.42
1:E:183:PRO:HD3	1:F:30[A]:HIS:CE1	2.54	0.42
1:E:337:ARG:HD3	1:F:61:ASN:CB	2.49	0.42
1:F:374:LEU:HA	1:F:374:LEU:HD12	1.91	0.42
1:F:458:HIS:HE1	1:L:456:THR:O	2.02	0.42
1:G:175[B]:VAL:O	1:G:176[B]:LYS:HB2	2.20	0.42
1:G:352:LYS:HE2	1:G:352:LYS:HA	2.00	0.42
1:G:127:GLY:HA3	3:G:4477:ADP:H1'	2.00	0.42
1:H:352:LYS:HA	1:H:352:LYS:HE2	2.00	0.42
1:H:271:HIS:CD2	1:H:357:GLU:HB2	2.54	0.42
1:I:175[B]:VAL:O	1:I:176[B]:LYS:HB2	2.20	0.42
1:I:201:GLN:N	5:I:6024:HOH:O	2.52	0.42
1:I:271:HIS:CD2	1:I:357:GLU:HB2	2.54	0.42
1:J:305:ALA:CB	1:J:332:LEU:HD21	2.49	0.42
1:L:192[A]:ARG:HH21	1:L:219:ASN:ND2	2.17	0.42
1:A:197:LEU:O	1:A:201:GLN:HG3	2.20	0.42
1:A:324:PRO:HA	5:A:6020:HOH:O	2.19	0.42
1:A:82:ASP:O	1:A:84:THR:CG2	2.67	0.42
1:B:144:ILE:HG22	5:B:5913:HOH:O	2.19	0.42
1:B:423:LEU:C	1:B:425:ARG:H	2.22	0.42
1:D:230:LYS:CG	5:D:5966:HOH:O	2.66	0.42
1:D:324:PRO:HA	5:D:6023:HOH:O	2.19	0.42
1:D:271:HIS:CD2	1:D:357:GLU:HB2	2.54	0.42
1:E:271:HIS:CD2	1:E:357:GLU:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:271:HIS:CD2	1:F:357:GLU:HB2	2.54	0.42
1:G:197:LEU:O	1:G:201:GLN:HG3	2.19	0.42
1:G:309:ASN:HA	1:G:309:ASN:HD22	1.71	0.42
1:G:1:SER:N	1:G:71:ALA:HB3	2.34	0.42
1:H:127:GLY:HA3	3:H:4478:ADP:H1'	2.00	0.42
1:J:210[B]:HIS:C	1:J:211[B]:HIS:CD2	2.89	0.42
1:K:128:PRO:HA	1:K:269:HIS:O	2.18	0.42
1:L:47:LYS:CD	5:L:1827:HOH:O	2.65	0.42
1:A:172:ARG:HA	1:A:173[A]:PRO:HD3	1.80	0.42
1:A:175[B]:VAL:O	1:A:176[B]:LYS:HB2	2.20	0.42
1:A:183:PRO:HD3	1:B:30[A]:HIS:CE1	2.54	0.42
1:A:269:HIS:HE1	4:A:5900:PPQ:HEP2	1.82	0.42
1:A:305:ALA:CB	1:A:332:LEU:HD21	2.49	0.42
1:A:127:GLY:HA3	3:A:4471:ADP:H1'	2.00	0.42
1:A:452:ARG:HG2	5:A:6015:HOH:O	2.19	0.42
1:A:1:SER:N	1:A:71:ALA:HB3	2.34	0.42
1:A:93:GLU:OE2	1:A:94:PRO:HD2	2.19	0.42
1:B:324:PRO:N	5:B:6021:HOH:O	2.51	0.42
1:C:155:GLU:OE1	1:C:211[A]:HIS:CE1	2.68	0.42
1:C:192[A]:ARG:HH21	1:C:219:ASN:ND2	2.17	0.42
1:C:323:VAL:O	5:C:5921:HOH:O	2.21	0.42
1:D:374:LEU:HA	1:D:374:LEU:HD12	1.91	0.42
1:E:175[B]:VAL:O	1:E:176[B]:LYS:HB2	2.20	0.42
1:E:201:GLN:N	5:E:722:HOH:O	2.52	0.42
1:E:324:PRO:CA	5:E:741:HOH:O	2.68	0.42
1:E:329:PRO:CD	1:E:359:ARG:HD2	2.42	0.42
1:E:359:ARG:HH12	4:E:5904:PPQ:HEP2	1.84	0.42
1:G:401:PRO:CA	1:G:404:ALA:HA	2.47	0.42
1:H:324:PRO:CA	5:H:6034:HOH:O	2.68	0.42
1:H:359:ARG:HH12	4:H:5907:PPQ:HEP2	1.84	0.42
1:I:352:LYS:HE2	1:I:352:LYS:HA	2.00	0.42
1:I:93:GLU:OE2	1:I:94:PRO:HD2	2.19	0.42
1:J:155:GLU:OE1	1:J:211[A]:HIS:CE1	2.68	0.42
1:J:271:HIS:CD2	1:J:357:GLU:HB2	2.54	0.42
1:J:359:ARG:HH12	4:J:5909:PPQ:HEP2	1.84	0.42
1:K:93:GLU:OE2	1:K:94:PRO:HD2	2.19	0.42
1:L:144:ILE:HG22	5:L:1697:HOH:O	2.19	0.42
1:C:127:GLY:HA3	3:C:4473:ADP:H1'	2.00	0.42
1:C:1:SER:N	1:C:71:ALA:HB3	2.34	0.42
1:C:93:GLU:OE2	1:C:94:PRO:HD2	2.19	0.42
1:D:172:ARG:HA	1:D:173[A]:PRO:HD3	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:SER:N	1:D:71:ALA:HB3	2.34	0.42
1:E:197:LEU:O	1:E:201:GLN:HG3	2.20	0.42
1:E:332:LEU:HD12	1:E:332:LEU:HA	1.90	0.42
1:E:352:LYS:HA	1:E:352:LYS:HE2	2.00	0.42
1:F:201:GLN:N	5:F:6013:HOH:O	2.52	0.42
1:F:231:LYS:CE	5:F:5919:HOH:O	2.59	0.42
1:G:324:PRO:CA	5:G:6030:HOH:O	2.68	0.42
1:H:192[A]:ARG:HH21	1:H:219:ASN:ND2	2.17	0.42
1:I:127:GLY:HA3	3:I:4479:ADP:HI'	2.00	0.42
1:I:1:SER:N	1:I:71:ALA:HB3	2.34	0.42
1:J:33:ILE:HA	1:J:34:PRO:HD3	1.90	0.42
1:J:352:LYS:HE2	1:J:352:LYS:HA	2.00	0.42
1:L:271:HIS:CD2	1:L:357:GLU:HB2	2.54	0.42
1:L:93:GLU:OE2	1:L:94:PRO:HD2	2.19	0.42
1:A:352:LYS:HE2	1:A:352:LYS:HA	2.00	0.42
1:B:197:LEU:O	1:B:201:GLN:HG3	2.20	0.42
1:C:197:LEU:O	1:C:201:GLN:HG3	2.19	0.42
1:C:235:ILE:HD13	1:C:235:ILE:HA	1.80	0.42
1:C:324:PRO:CA	5:C:6020:HOH:O	2.68	0.42
1:C:47:LYS:CD	5:C:6035:HOH:O	2.65	0.42
1:E:210[B]:HIS:C	1:E:211[B]:HIS:CD2	2.89	0.42
1:E:457:PRO:HD3	1:K:261[A]:PHE:HB2	2.01	0.42
5:A:5948:HOH:O	1:F:182:VAL:HG23	2.20	0.42
1:F:324:PRO:CA	5:F:6030:HOH:O	2.68	0.42
1:G:359:ARG:HH12	4:G:5906:PPQ:HEP2	1.84	0.42
1:H:197:LEU:O	1:H:201:GLN:HG3	2.19	0.42
1:H:332:LEU:O	5:H:6012:HOH:O	2.20	0.42
1:H:16:PHE:HB2	1:H:84:THR:HB	2.00	0.42
1:I:197:LEU:O	1:I:201:GLN:HG3	2.19	0.42
1:J:16:PHE:HB2	1:J:84:THR:HB	2.00	0.42
1:J:192[A]:ARG:HH21	1:J:219:ASN:ND2	2.17	0.42
1:J:324:PRO:HA	5:J:6037:HOH:O	2.19	0.42
1:J:127:GLY:HA3	3:J:4480:ADP:HI'	2.00	0.42
1:J:56:GLY:N	5:J:6010:HOH:O	2.40	0.42
1:J:33:ILE:HD12	1:K:208:ALA:CB	2.49	0.42
1:K:140:PHE:CE1	1:L:160:SER:HB2	2.55	0.42
1:L:359:ARG:HH12	4:L:5911:PPQ:HEP2	1.84	0.42
1:B:155:GLU:OE1	1:B:211[A]:HIS:CE1	2.68	0.42
1:B:175[B]:VAL:O	1:B:176[B]:LYS:HB2	2.20	0.42
1:B:192[A]:ARG:HH21	1:B:219:ASN:ND2	2.17	0.42
1:C:401:PRO:HA	1:C:404:ALA:CA	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210[B]:HIS:C	1:D:211[B]:HIS:CD2	2.89	0.42
1:E:155:GLU:OE1	1:E:211[A]:HIS:CE1	2.68	0.42
1:E:452:ARG:HG2	5:E:736:HOH:O	2.19	0.42
1:F:125:LEU:HD12	1:F:125:LEU:HA	1.79	0.42
1:F:456:THR:O	1:L:458:HIS:HE1	2.02	0.42
1:G:305:ALA:CB	1:G:332:LEU:HD21	2.49	0.42
1:H:175[B]:VAL:O	1:H:176[B]:LYS:HB2	2.20	0.42
1:H:447:ARG:CD	5:H:6023:HOH:O	2.68	0.42
1:J:125:LEU:HD12	1:J:125:LEU:HA	1.79	0.42
1:K:175[B]:VAL:O	1:K:176[B]:LYS:HB2	2.20	0.42
1:K:230:LYS:CG	5:K:1596:HOH:O	2.66	0.42
1:L:175[B]:VAL:O	1:L:176[B]:LYS:HB2	2.20	0.42
1:L:305:ALA:CB	1:L:332:LEU:HD21	2.49	0.42
1:A:440:ASP:HB2	5:A:6028:HOH:O	2.20	0.42
1:B:210[A]:HIS:ND1	1:B:211[A]:HIS:O	2.47	0.42
1:B:463:GLU:HA	1:H:140:PHE:CE1	2.54	0.42
1:C:324:PRO:HA	5:C:6020:HOH:O	2.19	0.42
1:D:447:ARG:CD	5:D:6012:HOH:O	2.68	0.42
1:E:144:ILE:HG22	5:E:626:HOH:O	2.19	0.42
1:E:387:HIS:HA	1:E:388:PRO:HD2	1.85	0.42
1:E:456:THR:O	1:K:458:HIS:HE1	2.03	0.42
1:F:1:SER:N	1:F:71:ALA:HB3	2.34	0.42
1:F:305:ALA:CB	1:F:332:LEU:HD21	2.49	0.42
1:F:93:GLU:OE2	1:F:94:PRO:HD2	2.20	0.42
1:G:201:GLN:N	5:G:6013:HOH:O	2.52	0.42
1:G:59:GLY:O	1:H:339:ARG:NH1	2.47	0.42
1:H:93:GLU:OE2	1:H:94:PRO:HD2	2.20	0.42
1:I:401:PRO:CA	1:I:404:ALA:HA	2.46	0.42
1:J:201:GLN:N	5:J:6020:HOH:O	2.52	0.42
1:L:1:SER:N	1:L:71:ALA:HB3	2.34	0.42
1:A:332:LEU:HA	1:A:332:LEU:HD12	1.90	0.42
1:B:125:LEU:HA	1:B:125:LEU:HD12	1.79	0.42
1:B:201:GLN:N	5:B:6004:HOH:O	2.52	0.42
1:B:208:ALA:CB	1:C:33:ILE:HD12	2.50	0.42
1:E:423:LEU:C	1:E:425:ARG:H	2.22	0.42
1:G:323:VAL:O	5:G:5930:HOH:O	2.21	0.42
1:H:144:ILE:HG22	5:H:5928:HOH:O	2.19	0.42
1:J:129:GLU:O	1:J:268:MET:HA	2.20	0.42
1:K:324:PRO:CA	5:K:1659:HOH:O	2.68	0.42
1:L:324:PRO:HA	5:L:1812:HOH:O	2.19	0.42
1:L:401:PRO:CA	1:L:404:ALA:HA	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:VAL:O	5:A:5920:HOH:O	2.21	0.41
1:C:175[B]:VAL:O	1:C:176[B]:LYS:HB2	2.20	0.41
1:C:195:MET:HE1	1:C:242:VAL:HG13	2.02	0.41
1:C:210[B]:HIS:C	1:C:211[B]:HIS:CD2	2.90	0.41
1:C:390:GLU:HA	1:C:391:PRO:HD3	1.84	0.41
1:C:452:ARG:HG2	5:C:6015:HOH:O	2.19	0.41
1:C:82:ASP:O	1:C:84:THR:CG2	2.67	0.41
1:D:214:ALA:HA	1:D:263[A]:ASP:OD2	2.21	0.41
1:D:452:ARG:HG2	5:D:6018:HOH:O	2.19	0.41
1:E:447:ARG:CD	5:E:729:HOH:O	2.68	0.41
1:F:175[B]:VAL:O	1:F:176[B]:LYS:HB2	2.20	0.41
1:A:61:ASN:O	1:F:337:ARG:O	2.38	0.41
1:F:452:ARG:HG2	5:F:6025:HOH:O	2.19	0.41
1:H:129:GLU:O	1:H:268:MET:HA	2.20	0.41
1:H:165:GLU:N	5:H:5975:HOH:O	2.46	0.41
1:H:29[A]:GLN:HA	1:I:180[A]:PHE:O	2.20	0.41
1:I:324:PRO:CA	5:I:6041:HOH:O	2.68	0.41
1:I:390:GLU:HA	1:I:391:PRO:HD3	1.84	0.41
1:J:172:ARG:HA	1:J:173[A]:PRO:HD3	1.80	0.41
1:J:440:ASP:HB2	5:J:6045:HOH:O	2.20	0.41
1:K:210[B]:HIS:C	1:K:211[B]:HIS:CD2	2.89	0.41
1:L:197:LEU:O	1:L:201:GLN:HG3	2.20	0.41
1:L:440:ASP:HB2	5:L:1820:HOH:O	2.20	0.41
1:A:201:GLN:N	5:A:6003:HOH:O	2.52	0.41
1:A:401:PRO:CA	1:A:404:ALA:HA	2.46	0.41
1:A:56:GLY:N	5:A:5993:HOH:O	2.40	0.41
1:C:179[B]:TYR:CD1	1:C:212[B]:GLU:CA	2.77	0.41
1:C:423:LEU:C	1:C:425:ARG:H	2.22	0.41
1:D:138:ILE:O	1:D:138:ILE:HG23	2.20	0.41
1:F:129:GLU:O	1:F:268:MET:HA	2.20	0.41
1:F:324:PRO:HA	5:F:6030:HOH:O	2.19	0.41
1:G:128:PRO:CD	5:G:5917:HOH:O	2.61	0.41
1:G:129:GLU:O	1:G:268:MET:HA	2.20	0.41
1:G:461:GLU:O	1:G:465:TYR:N	2.50	0.41
1:H:138:ILE:O	1:H:138:ILE:HG23	2.21	0.41
1:H:140:PHE:CE1	1:I:160:SER:HB2	2.55	0.41
1:H:283:SER:O	1:H:291:SER:HB3	2.21	0.41
1:I:447:ARG:CD	5:I:6030:HOH:O	2.68	0.41
1:I:461:GLU:O	1:I:465:TYR:N	2.50	0.41
1:I:82:ASP:O	1:I:84:THR:CG2	2.67	0.41
1:J:176[B]:LYS:C	1:J:178[B]:GLY:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:440:ASP:HB2	5:K:1667:HOH:O	2.20	0.41
1:L:82:ASP:O	1:L:84:THR:CG2	2.67	0.41
1:A:144:ILE:HG22	5:A:5912:HOH:O	2.19	0.41
1:A:80:PHE:CZ	1:F:189:GLN:HG3	2.55	0.41
1:B:359:ARG:HD3	1:B:359:ARG:HH11	1.65	0.41
1:B:269:HIS:CE1	4:B:5901:PPQ:CEP	2.92	0.41
1:C:129:GLU:O	1:C:268:MET:HA	2.20	0.41
1:C:125:LEU:HG	1:C:225:PHE:CD2	2.56	0.41
1:E:129:GLU:O	1:E:268:MET:HA	2.20	0.41
1:E:283:SER:O	1:E:291:SER:HB3	2.20	0.41
1:E:440:ASP:HB2	5:E:749:HOH:O	2.20	0.41
1:F:254:THR:HB	1:L:466:TYR:CE1	2.54	0.41
1:F:384:ASN:ND2	1:F:384:ASN:N	2.59	0.41
1:F:440:ASP:HB2	5:F:6038:HOH:O	2.20	0.41
1:G:452:ARG:HG2	5:G:6025:HOH:O	2.19	0.41
1:J:1:SER:N	1:J:71:ALA:HB3	2.34	0.41
1:J:93:GLU:OE2	1:J:94:PRO:HD2	2.19	0.41
1:K:359:ARG:HH12	4:K:5910:PPQ:HEP2	1.84	0.41
1:L:125:LEU:HG	1:L:225:PHE:CD2	2.56	0.41
1:A:447:ARG:CD	5:A:6009:HOH:O	2.68	0.41
1:B:138:ILE:HG23	1:B:138:ILE:O	2.20	0.41
1:B:1:SER:OG	1:B:1:SER:O	2.39	0.41
1:B:214:ALA:HA	1:B:263[A]:ASP:OD2	2.21	0.41
1:B:302:ILE:CD1	5:B:5999:HOH:O	2.49	0.41
1:B:419:ASN:ND2	5:B:5993:HOH:O	2.42	0.41
1:C:210[A]:HIS:HB3	1:D:31:VAL:HG23	2.02	0.41
1:C:359:ARG:HH11	1:C:359:ARG:HD3	1.65	0.41
1:D:93:GLU:OE2	1:D:94:PRO:HD2	2.19	0.41
1:G:125:LEU:HG	1:G:225:PHE:CD2	2.56	0.41
1:H:125:LEU:HG	1:H:225:PHE:CD2	2.56	0.41
1:J:175[B]:VAL:O	1:J:176[B]:LYS:HB2	2.20	0.41
5:I:5990:HOH:O	1:J:183:PRO:CB	2.68	0.41
1:J:224:ARG:NH2	1:J:224:ARG:CG	2.69	0.41
1:J:283:SER:O	1:J:291:SER:HB3	2.21	0.41
1:J:324:PRO:CA	5:J:6037:HOH:O	2.68	0.41
1:J:452:ARG:HG2	5:J:6032:HOH:O	2.19	0.41
1:K:75:VAL:CG2	5:K:1548:HOH:O	2.53	0.41
1:L:129:GLU:O	1:L:268:MET:HA	2.20	0.41
1:A:125:LEU:HG	1:A:225:PHE:CD2	2.56	0.41
1:A:359:ARG:HH12	4:A:5900:PPQ:HEP2	1.84	0.41
1:B:230:LYS:CG	5:B:5964:HOH:O	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:PHE:N	1:B:371:PHE:CD2	2.89	0.41
1:B:93:GLU:OE2	1:B:94:PRO:HD2	2.19	0.41
1:C:211[B]:HIS:HE1	5:C:6044:HOH:O	1.60	0.41
1:C:429:LYS:HA	1:C:434:PHE:O	2.21	0.41
1:D:175[B]:VAL:O	1:D:176[B]:LYS:CB	2.69	0.41
1:D:197:LEU:O	1:D:201:GLN:HG3	2.20	0.41
1:D:201:GLN:N	5:D:6006:HOH:O	2.52	0.41
1:E:125:LEU:HG	1:E:225:PHE:CD2	2.56	0.41
1:F:125:LEU:HG	1:F:225:PHE:CD2	2.56	0.41
1:F:323:VAL:O	5:F:5931:HOH:O	2.21	0.41
1:F:447:ARG:CD	5:F:6019:HOH:O	2.68	0.41
1:H:214:ALA:HA	1:H:263[A]:ASP:OD2	2.21	0.41
1:I:138:ILE:HG23	1:I:138:ILE:O	2.20	0.41
1:I:324:PRO:HA	5:I:6041:HOH:O	2.19	0.41
1:K:129:GLU:O	1:K:268:MET:HA	2.20	0.41
1:K:199:MET:HG3	1:K:241:VAL:HG11	2.03	0.41
1:L:155:GLU:OE1	1:L:211[A]:HIS:CE1	2.68	0.41
1:A:283:SER:O	1:A:291:SER:HB3	2.20	0.41
1:B:129:GLU:O	1:B:268:MET:HA	2.20	0.41
1:B:324:PRO:HA	5:B:6021:HOH:O	2.19	0.41
1:C:175[B]:VAL:O	1:C:176[B]:LYS:CB	2.69	0.41
1:C:337:ARG:CD	1:D:61:ASN:CB	2.87	0.41
1:C:337:ARG:HD3	1:D:61:ASN:CB	2.45	0.41
1:D:129:GLU:O	1:D:268:MET:HA	2.20	0.41
1:E:324:PRO:HA	5:E:741:HOH:O	2.19	0.41
1:E:429:LYS:HA	1:E:434:PHE:O	2.21	0.41
1:E:82:ASP:O	1:E:84:THR:CG2	2.67	0.41
1:F:387:HIS:HA	1:F:388:PRO:HD2	1.85	0.41
1:G:324:PRO:HA	5:G:6030:HOH:O	2.19	0.41
1:G:344:ARG:HB3	1:G:344:ARG:HE	1.58	0.41
1:H:235:ILE:HD13	1:H:235:ILE:HA	1.80	0.41
1:I:129:GLU:O	1:I:268:MET:HA	2.20	0.41
1:I:199:MET:HG3	1:I:241:VAL:HG11	2.03	0.41
1:I:61:ASN:C	1:J:337:ARG:HD3	2.41	0.41
1:J:214:ALA:HA	1:J:263[A]:ASP:OD2	2.21	0.41
1:J:82:ASP:O	1:J:84:THR:CG2	2.67	0.41
1:K:138:ILE:HG23	1:K:138:ILE:O	2.20	0.41
1:K:144:ILE:HG22	5:K:1544:HOH:O	2.19	0.41
1:K:175[B]:VAL:O	1:K:176[B]:LYS:CB	2.69	0.41
1:K:461:GLU:O	1:K:465:TYR:N	2.50	0.41
1:L:138:ILE:O	1:L:138:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:214:ALA:HA	1:L:263[A]:ASP:OD2	2.21	0.41
1:L:324:PRO:CA	5:L:1812:HOH:O	2.68	0.41
1:A:138:ILE:HG23	1:A:138:ILE:O	2.20	0.41
1:A:235:ILE:HD13	1:A:235:ILE:HA	1.80	0.41
1:A:27:LYS:HA	1:A:27:LYS:HD2	1.95	0.41
1:A:324:PRO:CA	5:A:6020:HOH:O	2.68	0.41
1:A:75:VAL:CG2	5:A:5916:HOH:O	2.53	0.41
1:B:199:MET:HG3	1:B:241:VAL:HG11	2.03	0.41
1:B:452:ARG:HG2	5:B:6016:HOH:O	2.19	0.41
1:C:56:GLY:N	5:C:5993:HOH:O	2.40	0.41
1:D:324:PRO:CA	5:D:6023:HOH:O	2.68	0.41
1:D:401:PRO:CA	1:D:404:ALA:HA	2.47	0.41
1:F:302:ILE:CD1	5:F:6008:HOH:O	2.49	0.41
1:F:466:TYR:CE1	1:L:254:THR:HB	2.56	0.41
1:G:214:ALA:HA	1:G:263[A]:ASP:OD2	2.21	0.41
1:H:429:LYS:HA	1:H:434:PHE:O	2.21	0.41
1:K:287:TYR:CD1	1:K:391:PRO:HG2	2.56	0.41
1:K:33:ILE:HA	1:K:34:PRO:HD3	1.90	0.41
1:L:269:HIS:HE1	4:L:5911:PPQ:HEP2	1.82	0.41
5:G:6049:HOH:O	1:L:60:ILE:CD1	2.45	0.41
1:A:199:MET:HG3	1:A:241:VAL:HG11	2.03	0.41
1:A:429:LYS:HA	1:A:434:PHE:O	2.21	0.41
1:B:172:ARG:HA	1:B:173[A]:PRO:HD3	1.80	0.41
1:B:387:HIS:HA	1:B:388:PRO:HD2	1.85	0.41
1:C:138:ILE:O	1:C:138:ILE:HG23	2.20	0.41
1:D:179[B]:TYR:HB3	1:D:180[B]:PHE:CD2	2.56	0.41
1:D:199:MET:HG3	1:D:241:VAL:HG11	2.03	0.41
1:E:235:ILE:HD13	1:E:235:ILE:HA	1.80	0.41
1:E:199:MET:HG3	1:E:241:VAL:HG11	2.03	0.41
1:E:276:LYS:HB3	1:E:281:LEU:HD11	2.03	0.41
1:E:6:LEU:HD13	1:E:6:LEU:HA	1.93	0.41
1:F:269:HIS:HE1	4:F:5905:PPQ:HEP2	1.82	0.41
1:H:199:MET:HG3	1:H:241:VAL:HG11	2.03	0.41
1:H:287:TYR:CD1	1:H:391:PRO:HG2	2.56	0.41
1:H:82:ASP:CB	5:H:5958:HOH:O	2.64	0.41
1:I:440:ASP:HB2	5:I:6049:HOH:O	2.20	0.41
1:J:138:ILE:O	1:J:138:ILE:HG23	2.21	0.41
1:K:283:SER:O	1:K:291:SER:HB3	2.21	0.41
1:K:41:GLU:O	1:K:45:GLU:HG2	2.21	0.41
1:L:283:SER:O	1:L:291:SER:HB3	2.21	0.41
1:K:61:ASN:CB	1:L:337:ARG:HD3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:429:LYS:HA	1:L:434:PHE:O	2.21	0.41
1:A:211[A]:HIS:HD2	1:A:212[A]:GLU:O	2.04	0.41
1:A:256:MET:HA	1:A:257:PRO:HD2	1.89	0.41
1:A:264[B]:ASN:N	1:A:326:TYR:HD2	2.19	0.41
1:B:283:SER:O	1:B:291:SER:HB3	2.21	0.41
1:B:41:GLU:O	1:B:45:GLU:HG2	2.21	0.41
1:D:125:LEU:HG	1:D:225:PHE:CD2	2.56	0.41
1:E:371:PHE:CD2	1:E:371:PHE:N	2.89	0.41
1:F:138:ILE:HG23	1:F:138:ILE:O	2.21	0.41
1:G:138:ILE:O	1:G:138:ILE:HG23	2.20	0.41
1:G:175[B]:VAL:O	1:G:176[B]:LYS:CB	2.69	0.41
1:G:447:ARG:CD	5:G:5992:HOH:O	2.58	0.41
1:G:33:ILE:CD1	1:H:208:ALA:HB2	2.51	0.41
1:H:440:ASP:HB2	5:H:6042:HOH:O	2.20	0.41
1:I:211[A]:HIS:HD2	1:I:212[A]:GLU:O	2.04	0.41
1:I:125:LEU:HG	1:I:225:PHE:CD2	2.56	0.41
1:K:276:LYS:HB3	1:K:281:LEU:HD11	2.03	0.41
1:K:324:PRO:HA	5:K:1659:HOH:O	2.19	0.41
1:K:452:ARG:HG2	5:K:1654:HOH:O	2.20	0.41
1:L:211[A]:HIS:HD2	1:L:212[A]:GLU:O	2.04	0.41
1:L:199:MET:HG3	1:L:241:VAL:HG11	2.03	0.41
1:A:332:LEU:HB2	1:A:408:PRO:O	2.21	0.41
1:B:329:PRO:HG2	1:B:359:ARG:CD	2.18	0.41
1:B:447:ARG:CD	5:B:6010:HOH:O	2.68	0.41
1:C:440:ASP:HB2	5:C:6028:HOH:O	2.20	0.41
1:D:144:ILE:HG22	5:D:5915:HOH:O	2.19	0.41
1:D:332:LEU:HB2	1:D:408:PRO:O	2.21	0.41
1:D:41:GLU:O	1:D:45:GLU:HG2	2.21	0.41
1:E:1:SER:O	1:E:1:SER:OG	2.39	0.41
1:E:214:ALA:HA	1:E:263[A]:ASP:OD2	2.21	0.41
1:E:41:GLU:O	1:E:45:GLU:HG2	2.21	0.41
1:F:214:ALA:HA	1:F:263[A]:ASP:OD2	2.21	0.41
1:H:128:PRO:CD	5:H:5924:HOH:O	2.61	0.41
1:I:264[B]:ASN:N	1:I:326:TYR:HD2	2.19	0.41
1:I:371:PHE:N	1:I:371:PHE:CD2	2.89	0.41
1:I:429:LYS:HA	1:I:434:PHE:O	2.21	0.41
1:J:269:HIS:CE1	4:J:5909:PPQ:CEP	2.92	0.41
1:K:1:SER:O	1:K:1:SER:OG	2.39	0.41
1:K:214:ALA:HA	1:K:263[A]:ASP:OD2	2.21	0.41
1:K:371:PHE:CD2	1:K:371:PHE:N	2.89	0.41
1:L:179[B]:TYR:HB3	1:L:180[B]:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:1602:HOH:O	1:L:183:PRO:HB2	2.21	0.41
1:L:309:ASN:HA	1:L:309:ASN:HD22	1.71	0.41
1:L:264[B]:ASN:N	1:L:326:TYR:HD2	2.19	0.41
1:L:371:PHE:CD2	1:L:371:PHE:N	2.89	0.41
1:L:426:GLU:CB	5:L:1746:HOH:O	2.49	0.41
1:A:276:LYS:HB3	1:A:281:LEU:HD11	2.03	0.41
1:B:175[B]:VAL:O	1:B:176[B]:LYS:CB	2.69	0.41
1:B:264[B]:ASN:N	1:B:326:TYR:HD2	2.19	0.41
1:B:324:PRO:CA	5:B:6021:HOH:O	2.68	0.41
1:B:80:PHE:HE2	5:B:5970:HOH:O	2.04	0.41
1:C:287:TYR:CD1	1:C:391:PRO:HG2	2.56	0.41
1:C:271:HIS:HA	1:C:356:ILE:O	2.21	0.41
1:C:371:PHE:N	1:C:371:PHE:CD2	2.89	0.41
1:D:211[A]:HIS:HD2	1:D:212[A]:GLU:O	2.04	0.41
1:D:210[A]:HIS:ND1	1:D:211[A]:HIS:O	2.47	0.41
1:D:283:SER:O	1:D:291:SER:HB3	2.20	0.41
1:D:440:ASP:HB2	5:D:6031:HOH:O	2.20	0.41
1:E:138:ILE:O	1:E:138:ILE:HG23	2.20	0.41
1:E:359:ARG:HH11	1:E:359:ARG:HD3	1.65	0.41
1:G:271:HIS:HA	1:G:356:ILE:O	2.21	0.41
1:G:283:SER:O	1:G:291:SER:HB3	2.20	0.41
1:G:429:LYS:HA	1:G:434:PHE:O	2.21	0.41
1:G:6:LEU:HA	1:G:6:LEU:HD13	1.93	0.41
1:H:179[B]:TYR:HB3	1:H:180[B]:PHE:CD2	2.56	0.41
1:I:283:SER:O	1:I:291:SER:HB3	2.20	0.41
1:I:29[A]:GLN:HB3	1:J:180[A]:PHE:CB	2.49	0.41
1:J:1:SER:OG	1:J:1:SER:O	2.39	0.41
1:J:195:MET:HE1	1:J:242:VAL:HG13	2.03	0.41
1:J:287:TYR:CD1	1:J:391:PRO:HG2	2.56	0.41
1:J:302:ILE:CD1	5:J:6015:HOH:O	2.49	0.41
1:K:264[B]:ASN:N	1:K:326:TYR:HD2	2.19	0.41
1:F:463:GLU:HA	1:L:140:PHE:CE1	2.56	0.41
1:L:175[B]:VAL:O	1:L:176[B]:LYS:CB	2.69	0.41
1:L:447:ARG:CD	5:L:1800:HOH:O	2.68	0.41
1:A:129:GLU:O	1:A:268:MET:HA	2.20	0.40
1:B:179[B]:TYR:HB3	1:B:180[B]:PHE:CD2	2.56	0.40
1:C:199:MET:HG3	1:C:241:VAL:HG11	2.03	0.40
1:C:300:GLY:HA3	1:C:377:ALA:O	2.21	0.40
1:C:41:GLU:O	1:C:45:GLU:HG2	2.21	0.40
1:D:287:TYR:CD1	1:D:391:PRO:HG2	2.56	0.40
1:D:429:LYS:HA	1:D:434:PHE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:ARG:NH1	1:D:59:GLY:O	2.53	0.40
1:F:175[B]:VAL:O	1:F:176[B]:LYS:CB	2.69	0.40
1:G:82:ASP:CB	5:G:5953:HOH:O	2.64	0.40
1:H:155:GLU:OE1	1:H:211[A]:HIS:CE1	2.68	0.40
1:H:461:GLU:O	1:H:465:TYR:N	2.50	0.40
1:I:214:ALA:HA	1:I:263[A]:ASP:OD2	2.21	0.40
1:I:287:TYR:CD1	1:I:391:PRO:HG2	2.56	0.40
1:H:61:ASN:CB	1:I:337:ARG:HD3	2.50	0.40
1:I:41:GLU:O	1:I:45:GLU:HG2	2.21	0.40
1:J:179[B]:TYR:HB3	1:J:180[B]:PHE:CD2	2.56	0.40
1:K:125:LEU:HG	1:K:225:PHE:CD2	2.56	0.40
1:K:172:ARG:HA	1:K:173[A]:PRO:HD3	1.80	0.40
1:K:332:LEU:HB2	1:K:408:PRO:O	2.21	0.40
1:K:429:LYS:HA	1:K:434:PHE:O	2.21	0.40
1:E:458:HIS:HE1	1:K:456:THR:O	2.04	0.40
1:A:179[B]:TYR:HB3	1:A:180[B]:PHE:CD2	2.56	0.40
1:A:31:VAL:HG23	1:F:210[A]:HIS:HB3	2.03	0.40
1:A:63:SER:N	1:F:339:ARG:NH1	2.67	0.40
1:B:75:VAL:CG2	5:B:5917:HOH:O	2.53	0.40
1:C:447:ARG:CD	5:C:6009:HOH:O	2.68	0.40
1:E:447:ARG:CD	5:E:698:HOH:O	2.58	0.40
1:F:1:SER:O	1:F:1:SER:OG	2.39	0.40
1:F:332:LEU:HB2	1:F:408:PRO:O	2.21	0.40
1:G:231:LYS:CE	5:G:5917:HOH:O	2.59	0.40
1:G:371:PHE:N	1:G:371:PHE:CD2	2.89	0.40
1:H:371:PHE:N	1:H:371:PHE:CD2	2.89	0.40
1:I:82:ASP:CB	5:I:5964:HOH:O	2.64	0.40
1:J:264[B]:ASN:N	1:J:326:TYR:HD2	2.19	0.40
1:J:429:LYS:HA	1:J:434:PHE:O	2.21	0.40
1:L:230:LYS:HB2	1:L:230:LYS:HE2	1.85	0.40
1:L:332:LEU:HB2	1:L:408:PRO:O	2.21	0.40
1:A:214:ALA:HA	1:A:263[A]:ASP:OD2	2.21	0.40
1:A:302:ILE:CD1	5:A:5998:HOH:O	2.49	0.40
1:A:344:ARG:HE	1:A:344:ARG:HB3	1.59	0.40
1:B:125:LEU:HG	1:B:225:PHE:CD2	2.56	0.40
1:B:440:ASP:HB2	5:B:6029:HOH:O	2.20	0.40
1:E:300:GLY:HA3	1:E:377:ALA:O	2.21	0.40
1:E:332:LEU:HB2	1:E:408:PRO:O	2.21	0.40
1:F:179[B]:TYR:HB3	1:F:180[B]:PHE:CD2	2.56	0.40
1:F:283:SER:O	1:F:291:SER:HB3	2.20	0.40
1:F:300:GLY:HA3	1:F:377:ALA:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:287:TYR:CD1	1:F:391:PRO:HG2	2.56	0.40
1:F:41:GLU:O	1:F:45:GLU:HG2	2.21	0.40
1:G:440:ASP:HB2	5:G:6038:HOH:O	2.20	0.40
1:H:452:ARG:HG2	5:H:6029:HOH:O	2.19	0.40
1:H:41:GLU:O	1:H:45:GLU:HG2	2.21	0.40
1:H:61:ASN:HB2	1:I:337:ARG:CZ	2.51	0.40
1:I:175[B]:VAL:O	1:I:176[B]:LYS:CB	2.69	0.40
1:I:60:ILE:HG12	1:J:339:ARG:HB2	2.03	0.40
1:L:41:GLU:O	1:L:45:GLU:HG2	2.21	0.40
1:A:287:TYR:CD1	1:A:391:PRO:HG2	2.56	0.40
1:B:211[A]:HIS:HD2	1:B:212[A]:GLU:O	2.04	0.40
1:C:179[B]:TYR:HB3	1:C:180[B]:PHE:CD2	2.56	0.40
1:D:17:VAL:HA	1:D:85:LEU:O	2.22	0.40
1:F:271:HIS:HA	1:F:356:ILE:O	2.21	0.40
1:G:264[B]:ASN:N	1:G:326:TYR:HD2	2.19	0.40
1:G:29[A]:GLN:HA	1:H:180[A]:PHE:O	2.21	0.40
1:G:300:GLY:HA3	1:G:377:ALA:O	2.21	0.40
1:G:41:GLU:O	1:G:45:GLU:HG2	2.21	0.40
1:H:82:ASP:O	1:H:84:THR:CG2	2.67	0.40
1:I:210[A]:HIS:ND1	1:I:211[A]:HIS:O	2.47	0.40
1:I:300:GLY:HA3	1:I:377:ALA:O	2.21	0.40
1:I:80:PHE:HE2	5:I:5990:HOH:O	2.04	0.40
1:J:175[B]:VAL:O	1:J:176[B]:LYS:CB	2.69	0.40
1:J:125:LEU:HG	1:J:225:PHE:CD2	2.56	0.40
1:J:371:PHE:N	1:J:371:PHE:CD2	2.89	0.40
1:J:68:MET:HA	1:J:69:PRO:HD2	1.78	0.40
1:K:329:PRO:CD	1:K:359:ARG:HD2	2.42	0.40
1:B:287:TYR:CD1	1:B:391:PRO:HG2	2.56	0.40
1:C:172:ARG:HA	1:C:173[A]:PRO:HD3	1.80	0.40
1:C:214:ALA:HA	1:C:263[A]:ASP:OD2	2.21	0.40
1:C:283:SER:O	1:C:291:SER:HB3	2.21	0.40
5:C:5945:HOH:O	1:D:84:THR:HG21	2.21	0.40
1:E:271:HIS:HA	1:E:356:ILE:O	2.21	0.40
1:E:287:TYR:CD1	1:E:391:PRO:HG2	2.56	0.40
1:E:419:ASN:ND2	5:E:709:HOH:O	2.42	0.40
1:F:176[B]:LYS:CB	5:F:5912:HOH:O	2.55	0.40
1:F:27:LYS:HA	1:F:27:LYS:HD2	1.95	0.40
1:H:332:LEU:HB2	1:H:408:PRO:O	2.21	0.40
1:H:82:ASP:OD2	5:H:5937:HOH:O	2.22	0.40
1:I:155:GLU:OE1	1:I:211[A]:HIS:CE1	2.68	0.40
1:I:179[B]:TYR:HB3	1:I:180[B]:PHE:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1:SER:OG	1:I:5:VAL:HG23	2.22	0.40
1:I:17:VAL:HA	1:I:85:LEU:O	2.22	0.40
1:J:300:GLY:HA3	1:J:377:ALA:O	2.21	0.40
1:K:179[B]:TYR:HB3	1:K:180[B]:PHE:CD2	2.56	0.40
1:K:271:HIS:HA	1:K:356:ILE:O	2.22	0.40
1:K:423:LEU:O	1:K:425:ARG:N	2.53	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	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	B	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	C	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	D	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	E	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	F	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	G	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	H	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	I	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	J	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	K	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	L	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
All	All	5784/5616 (103%)	4932 (85%)	600 (10%)	252 (4%)	5	11

All (252) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	58	LYS
1	A	177[A]	GLY
1	A	177[B]	GLY
1	A	180[A]	PHE
1	A	180[B]	PHE
1	A	212[A]	GLU
1	A	212[B]	GLU
1	A	213[A]	VAL
1	A	262[A]	GLY
1	A	262[B]	GLY
1	A	396	LEU
1	B	58	LYS
1	B	177[A]	GLY
1	B	177[B]	GLY
1	B	180[A]	PHE
1	B	180[B]	PHE
1	B	212[A]	GLU
1	B	212[B]	GLU
1	B	213[A]	VAL
1	B	262[A]	GLY
1	B	262[B]	GLY
1	B	396	LEU
1	C	58	LYS
1	C	177[A]	GLY
1	C	177[B]	GLY
1	C	180[A]	PHE
1	C	180[B]	PHE
1	C	212[A]	GLU
1	C	212[B]	GLU
1	C	213[A]	VAL
1	C	262[A]	GLY
1	C	262[B]	GLY
1	C	396	LEU
1	D	58	LYS
1	D	177[A]	GLY
1	D	177[B]	GLY
1	D	180[A]	PHE
1	D	180[B]	PHE
1	D	212[A]	GLU
1	D	212[B]	GLU
1	D	213[A]	VAL
1	D	262[A]	GLY
1	D	262[B]	GLY

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Mol	Chain	Res	Type
1	D	396	LEU
1	E	58	LYS
1	E	177[A]	GLY
1	E	177[B]	GLY
1	E	180[A]	PHE
1	E	180[B]	PHE
1	E	212[A]	GLU
1	E	212[B]	GLU
1	E	213[A]	VAL
1	E	262[A]	GLY
1	E	262[B]	GLY
1	E	396	LEU
1	F	58	LYS
1	F	177[A]	GLY
1	F	177[B]	GLY
1	F	180[A]	PHE
1	F	180[B]	PHE
1	F	212[A]	GLU
1	F	212[B]	GLU
1	F	213[A]	VAL
1	F	262[A]	GLY
1	F	262[B]	GLY
1	F	396	LEU
1	G	58	LYS
1	G	177[A]	GLY
1	G	177[B]	GLY
1	G	180[A]	PHE
1	G	180[B]	PHE
1	G	212[A]	GLU
1	G	212[B]	GLU
1	G	213[A]	VAL
1	G	262[A]	GLY
1	G	262[B]	GLY
1	G	396	LEU
1	H	58	LYS
1	H	177[A]	GLY
1	H	177[B]	GLY
1	H	180[A]	PHE
1	H	180[B]	PHE
1	H	212[A]	GLU
1	H	212[B]	GLU
1	H	213[A]	VAL

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Mol	Chain	Res	Type
1	H	262[A]	GLY
1	H	262[B]	GLY
1	H	396	LEU
1	I	58	LYS
1	I	177[A]	GLY
1	I	177[B]	GLY
1	I	180[A]	PHE
1	I	180[B]	PHE
1	I	212[A]	GLU
1	I	212[B]	GLU
1	I	213[A]	VAL
1	I	262[A]	GLY
1	I	262[B]	GLY
1	I	396	LEU
1	J	58	LYS
1	J	177[A]	GLY
1	J	177[B]	GLY
1	J	180[A]	PHE
1	J	180[B]	PHE
1	J	212[A]	GLU
1	J	212[B]	GLU
1	J	213[A]	VAL
1	J	262[A]	GLY
1	J	262[B]	GLY
1	J	396	LEU
1	K	58	LYS
1	K	177[A]	GLY
1	K	177[B]	GLY
1	K	180[A]	PHE
1	K	180[B]	PHE
1	K	212[A]	GLU
1	K	212[B]	GLU
1	K	213[A]	VAL
1	K	262[A]	GLY
1	K	262[B]	GLY
1	K	396	LEU
1	L	58	LYS
1	L	177[A]	GLY
1	L	177[B]	GLY
1	L	180[A]	PHE
1	L	180[B]	PHE
1	L	212[A]	GLU

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Mol	Chain	Res	Type
1	L	212[B]	GLU
1	L	213[A]	VAL
1	L	262[A]	GLY
1	L	262[B]	GLY
1	L	396	LEU
1	A	60	ILE
1	A	178[A]	GLY
1	A	178[B]	GLY
1	A	264[A]	ASN
1	A	264[B]	ASN
1	A	349	ALA
1	B	60	ILE
1	B	178[A]	GLY
1	B	178[B]	GLY
1	B	264[A]	ASN
1	B	264[B]	ASN
1	B	349	ALA
1	C	60	ILE
1	C	178[A]	GLY
1	C	178[B]	GLY
1	C	264[A]	ASN
1	C	264[B]	ASN
1	C	349	ALA
1	D	60	ILE
1	D	178[A]	GLY
1	D	178[B]	GLY
1	D	264[A]	ASN
1	D	264[B]	ASN
1	D	349	ALA
1	E	60	ILE
1	E	178[A]	GLY
1	E	178[B]	GLY
1	E	264[A]	ASN
1	E	264[B]	ASN
1	E	349	ALA
1	F	60	ILE
1	F	178[A]	GLY
1	F	178[B]	GLY
1	F	264[A]	ASN
1	F	264[B]	ASN
1	F	349	ALA
1	G	60	ILE

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Mol	Chain	Res	Type
1	G	178[A]	GLY
1	G	178[B]	GLY
1	G	264[A]	ASN
1	G	264[B]	ASN
1	G	349	ALA
1	H	60	ILE
1	H	178[A]	GLY
1	H	178[B]	GLY
1	H	264[A]	ASN
1	H	264[B]	ASN
1	H	349	ALA
1	I	60	ILE
1	I	178[A]	GLY
1	I	178[B]	GLY
1	I	264[A]	ASN
1	I	264[B]	ASN
1	I	349	ALA
1	J	60	ILE
1	J	178[A]	GLY
1	J	178[B]	GLY
1	J	264[A]	ASN
1	J	264[B]	ASN
1	J	349	ALA
1	K	60	ILE
1	K	178[A]	GLY
1	K	178[B]	GLY
1	K	264[A]	ASN
1	K	264[B]	ASN
1	K	349	ALA
1	L	60	ILE
1	L	178[A]	GLY
1	L	178[B]	GLY
1	L	264[A]	ASN
1	L	264[B]	ASN
1	L	349	ALA
1	A	59	GLY
1	A	170	GLY
1	A	424	ASP
1	B	59	GLY
1	B	170	GLY
1	B	424	ASP
1	C	59	GLY

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Mol	Chain	Res	Type
1	C	170	GLY
1	C	424	ASP
1	D	59	GLY
1	D	170	GLY
1	D	424	ASP
1	E	59	GLY
1	E	170	GLY
1	E	424	ASP
1	F	59	GLY
1	F	170	GLY
1	F	424	ASP
1	G	59	GLY
1	G	170	GLY
1	G	424	ASP
1	H	59	GLY
1	H	170	GLY
1	H	424	ASP
1	I	59	GLY
1	I	170	GLY
1	I	424	ASP
1	J	59	GLY
1	J	170	GLY
1	J	424	ASP
1	K	59	GLY
1	K	170	GLY
1	K	424	ASP
1	L	59	GLY
1	L	170	GLY
1	L	424	ASP
1	A	401	PRO
1	B	401	PRO
1	C	401	PRO
1	D	401	PRO
1	E	401	PRO
1	F	401	PRO
1	G	401	PRO
1	H	401	PRO
1	I	401	PRO
1	J	401	PRO
1	K	401	PRO
1	L	401	PRO

### 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	395/384 (103%)	350 (89%)	45 (11%)	7	20
1	B	395/384 (103%)	350 (89%)	45 (11%)	7	20
1	C	395/384 (103%)	350 (89%)	45 (11%)	7	20
1	D	395/384 (103%)	350 (89%)	45 (11%)	7	20
1	E	395/384 (103%)	350 (89%)	45 (11%)	7	20
1	F	395/384 (103%)	350 (89%)	45 (11%)	7	20
1	G	395/384 (103%)	350 (89%)	45 (11%)	7	20
1	H	395/384 (103%)	350 (89%)	45 (11%)	7	20
1	I	395/384 (103%)	350 (89%)	45 (11%)	7	20
1	J	395/384 (103%)	350 (89%)	45 (11%)	7	20
1	K	395/384 (103%)	350 (89%)	45 (11%)	7	20
1	L	395/384 (103%)	350 (89%)	45 (11%)	7	20
All	All	4740/4608 (103%)	4200 (89%)	540 (11%)	7	20

All (540) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	19	LEU
1	A	23	ASP
1	A	53	SER
1	A	58	LYS
1	A	62	GLU
1	A	64	ASP
1	A	82	ASP
1	A	84	THR
1	A	88	ARG
1	A	96	THR
1	A	98	GLN
1	A	101	ASP
1	A	115	LEU

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Mol	Chain	Res	Type
1	A	125	LEU
1	A	143	SER
1	A	165	GLU
1	A	224	ARG
1	A	264[A]	ASN
1	A	264[B]	ASN
1	A	266[A]	SER
1	A	266[B]	SER
1	A	285	ASP
1	A	293	GLN
1	A	295	LEU
1	A	332	LEU
1	A	337	ARG
1	A	340	SER
1	A	344	ARG
1	A	361	PRO
1	A	374	LEU
1	A	375	LEU
1	A	384	ASN
1	A	394	LYS
1	A	396	LEU
1	A	398	ASP
1	A	402	GLU
1	A	405	LYS
1	A	406	GLU
1	A	419	ASN
1	A	428	LEU
1	A	435	THR
1	A	437	GLU
1	A	464	LEU
1	A	468	VAL
1	B	7	THR
1	B	19	LEU
1	B	23	ASP
1	B	53	SER
1	B	58	LYS
1	B	62	GLU
1	B	64	ASP
1	B	82	ASP
1	B	84	THR
1	B	88	ARG
1	B	96	THR

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Mol	Chain	Res	Type
1	B	98	GLN
1	B	101	ASP
1	B	115	LEU
1	B	125	LEU
1	B	143	SER
1	B	165	GLU
1	B	224	ARG
1	B	264[A]	ASN
1	B	264[B]	ASN
1	B	266[A]	SER
1	B	266[B]	SER
1	B	285	ASP
1	B	293	GLN
1	B	295	LEU
1	B	332	LEU
1	B	337	ARG
1	B	340	SER
1	B	344	ARG
1	B	361	PRO
1	B	374	LEU
1	B	375	LEU
1	B	384	ASN
1	B	394	LYS
1	B	396	LEU
1	B	398	ASP
1	B	402	GLU
1	B	405	LYS
1	B	406	GLU
1	B	419	ASN
1	B	428	LEU
1	B	435	THR
1	B	437	GLU
1	B	464	LEU
1	B	468	VAL
1	C	7	THR
1	C	19	LEU
1	C	23	ASP
1	C	53	SER
1	C	58	LYS
1	C	62	GLU
1	C	64	ASP
1	C	82	ASP

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Mol	Chain	Res	Type
1	C	84	THR
1	C	88	ARG
1	C	96	THR
1	C	98	GLN
1	C	101	ASP
1	C	115	LEU
1	C	125	LEU
1	C	143	SER
1	C	165	GLU
1	C	224	ARG
1	C	264[A]	ASN
1	C	264[B]	ASN
1	C	266[A]	SER
1	C	266[B]	SER
1	C	285	ASP
1	C	293	GLN
1	C	295	LEU
1	C	332	LEU
1	C	337	ARG
1	C	340	SER
1	C	344	ARG
1	C	361	PRO
1	C	374	LEU
1	C	375	LEU
1	C	384	ASN
1	C	394	LYS
1	C	396	LEU
1	C	398	ASP
1	C	402	GLU
1	C	405	LYS
1	C	406	GLU
1	C	419	ASN
1	C	428	LEU
1	C	435	THR
1	C	437	GLU
1	C	464	LEU
1	C	468	VAL
1	D	7	THR
1	D	19	LEU
1	D	23	ASP
1	D	53	SER
1	D	58	LYS

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Mol	Chain	Res	Type
1	D	62	GLU
1	D	64	ASP
1	D	82	ASP
1	D	84	THR
1	D	88	ARG
1	D	96	THR
1	D	98	GLN
1	D	101	ASP
1	D	115	LEU
1	D	125	LEU
1	D	143	SER
1	D	165	GLU
1	D	224	ARG
1	D	264[A]	ASN
1	D	264[B]	ASN
1	D	266[A]	SER
1	D	266[B]	SER
1	D	285	ASP
1	D	293	GLN
1	D	295	LEU
1	D	332	LEU
1	D	337	ARG
1	D	340	SER
1	D	344	ARG
1	D	361	PRO
1	D	374	LEU
1	D	375	LEU
1	D	384	ASN
1	D	394	LYS
1	D	396	LEU
1	D	398	ASP
1	D	402	GLU
1	D	405	LYS
1	D	406	GLU
1	D	419	ASN
1	D	428	LEU
1	D	435	THR
1	D	437	GLU
1	D	464	LEU
1	D	468	VAL
1	E	7	THR
1	E	19	LEU

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Mol	Chain	Res	Type
1	E	23	ASP
1	E	53	SER
1	E	58	LYS
1	E	62	GLU
1	E	64	ASP
1	E	82	ASP
1	E	84	THR
1	E	88	ARG
1	E	96	THR
1	E	98	GLN
1	E	101	ASP
1	E	115	LEU
1	E	125	LEU
1	E	143	SER
1	E	165	GLU
1	E	224	ARG
1	E	264[A]	ASN
1	E	264[B]	ASN
1	E	266[A]	SER
1	E	266[B]	SER
1	E	285	ASP
1	E	293	GLN
1	E	295	LEU
1	E	332	LEU
1	E	337	ARG
1	E	340	SER
1	E	344	ARG
1	E	361	PRO
1	E	374	LEU
1	E	375	LEU
1	E	384	ASN
1	E	394	LYS
1	E	396	LEU
1	E	398	ASP
1	E	402	GLU
1	E	405	LYS
1	E	406	GLU
1	E	419	ASN
1	E	428	LEU
1	E	435	THR
1	E	437	GLU
1	E	464	LEU

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Mol	Chain	Res	Type
1	E	468	VAL
1	F	7	THR
1	F	19	LEU
1	F	23	ASP
1	F	53	SER
1	F	58	LYS
1	F	62	GLU
1	F	64	ASP
1	F	82	ASP
1	F	84	THR
1	F	88	ARG
1	F	96	THR
1	F	98	GLN
1	F	101	ASP
1	F	115	LEU
1	F	125	LEU
1	F	143	SER
1	F	165	GLU
1	F	224	ARG
1	F	264[A]	ASN
1	F	264[B]	ASN
1	F	266[A]	SER
1	F	266[B]	SER
1	F	285	ASP
1	F	293	GLN
1	F	295	LEU
1	F	332	LEU
1	F	337	ARG
1	F	340	SER
1	F	344	ARG
1	F	361	PRO
1	F	374	LEU
1	F	375	LEU
1	F	384	ASN
1	F	394	LYS
1	F	396	LEU
1	F	398	ASP
1	F	402	GLU
1	F	405	LYS
1	F	406	GLU
1	F	419	ASN
1	F	428	LEU

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Mol	Chain	Res	Type
1	F	435	THR
1	F	437	GLU
1	F	464	LEU
1	F	468	VAL
1	G	7	THR
1	G	19	LEU
1	G	23	ASP
1	G	53	SER
1	G	58	LYS
1	G	62	GLU
1	G	64	ASP
1	G	82	ASP
1	G	84	THR
1	G	88	ARG
1	G	96	THR
1	G	98	GLN
1	G	101	ASP
1	G	115	LEU
1	G	125	LEU
1	G	143	SER
1	G	165	GLU
1	G	224	ARG
1	G	264[A]	ASN
1	G	264[B]	ASN
1	G	266[A]	SER
1	G	266[B]	SER
1	G	285	ASP
1	G	293	GLN
1	G	295	LEU
1	G	332	LEU
1	G	337	ARG
1	G	340	SER
1	G	344	ARG
1	G	361	PRO
1	G	374	LEU
1	G	375	LEU
1	G	384	ASN
1	G	394	LYS
1	G	396	LEU
1	G	398	ASP
1	G	402	GLU
1	G	405	LYS

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Mol	Chain	Res	Type
1	G	406	GLU
1	G	419	ASN
1	G	428	LEU
1	G	435	THR
1	G	437	GLU
1	G	464	LEU
1	G	468	VAL
1	H	7	THR
1	H	19	LEU
1	H	23	ASP
1	H	53	SER
1	H	58	LYS
1	H	62	GLU
1	H	64	ASP
1	H	82	ASP
1	H	84	THR
1	H	88	ARG
1	H	96	THR
1	H	98	GLN
1	H	101	ASP
1	H	115	LEU
1	H	125	LEU
1	H	143	SER
1	H	165	GLU
1	H	224	ARG
1	H	264[A]	ASN
1	H	264[B]	ASN
1	H	266[A]	SER
1	H	266[B]	SER
1	H	285	ASP
1	H	293	GLN
1	H	295	LEU
1	H	332	LEU
1	H	337	ARG
1	H	340	SER
1	H	344	ARG
1	H	361	PRO
1	H	374	LEU
1	H	375	LEU
1	H	384	ASN
1	H	394	LYS
1	H	396	LEU

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Mol	Chain	Res	Type
1	H	398	ASP
1	H	402	GLU
1	H	405	LYS
1	H	406	GLU
1	H	419	ASN
1	H	428	LEU
1	H	435	THR
1	H	437	GLU
1	H	464	LEU
1	H	468	VAL
1	I	7	THR
1	I	19	LEU
1	I	23	ASP
1	I	53	SER
1	I	58	LYS
1	I	62	GLU
1	I	64	ASP
1	I	82	ASP
1	I	84	THR
1	I	88	ARG
1	I	96	THR
1	I	98	GLN
1	I	101	ASP
1	I	115	LEU
1	I	125	LEU
1	I	143	SER
1	I	165	GLU
1	I	224	ARG
1	I	264[A]	ASN
1	I	264[B]	ASN
1	I	266[A]	SER
1	I	266[B]	SER
1	I	285	ASP
1	I	293	GLN
1	I	295	LEU
1	I	332	LEU
1	I	337	ARG
1	I	340	SER
1	I	344	ARG
1	I	361	PRO
1	I	374	LEU
1	I	375	LEU

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Mol	Chain	Res	Type
1	I	384	ASN
1	I	394	LYS
1	I	396	LEU
1	I	398	ASP
1	I	402	GLU
1	I	405	LYS
1	I	406	GLU
1	I	419	ASN
1	I	428	LEU
1	I	435	THR
1	I	437	GLU
1	I	464	LEU
1	I	468	VAL
1	J	7	THR
1	J	19	LEU
1	J	23	ASP
1	J	53	SER
1	J	58	LYS
1	J	62	GLU
1	J	64	ASP
1	J	82	ASP
1	J	84	THR
1	J	88	ARG
1	J	96	THR
1	J	98	GLN
1	J	101	ASP
1	J	115	LEU
1	J	125	LEU
1	J	143	SER
1	J	165	GLU
1	J	224	ARG
1	J	264[A]	ASN
1	J	264[B]	ASN
1	J	266[A]	SER
1	J	266[B]	SER
1	J	285	ASP
1	J	293	GLN
1	J	295	LEU
1	J	332	LEU
1	J	337	ARG
1	J	340	SER
1	J	344	ARG

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Mol	Chain	Res	Type
1	J	361	PRO
1	J	374	LEU
1	J	375	LEU
1	J	384	ASN
1	J	394	LYS
1	J	396	LEU
1	J	398	ASP
1	J	402	GLU
1	J	405	LYS
1	J	406	GLU
1	J	419	ASN
1	J	428	LEU
1	J	435	THR
1	J	437	GLU
1	J	464	LEU
1	J	468	VAL
1	K	7	THR
1	K	19	LEU
1	K	23	ASP
1	K	53	SER
1	K	58	LYS
1	K	62	GLU
1	K	64	ASP
1	K	82	ASP
1	K	84	THR
1	K	88	ARG
1	K	96	THR
1	K	98	GLN
1	K	101	ASP
1	K	115	LEU
1	K	125	LEU
1	K	143	SER
1	K	165	GLU
1	K	224	ARG
1	K	264[A]	ASN
1	K	264[B]	ASN
1	K	266[A]	SER
1	K	266[B]	SER
1	K	285	ASP
1	K	293	GLN
1	K	295	LEU
1	K	332	LEU

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Mol	Chain	Res	Type
1	K	337	ARG
1	K	340	SER
1	K	344	ARG
1	K	361	PRO
1	K	374	LEU
1	K	375	LEU
1	K	384	ASN
1	K	394	LYS
1	K	396	LEU
1	K	398	ASP
1	K	402	GLU
1	K	405	LYS
1	K	406	GLU
1	K	419	ASN
1	K	428	LEU
1	K	435	THR
1	K	437	GLU
1	K	464	LEU
1	K	468	VAL
1	L	7	THR
1	L	19	LEU
1	L	23	ASP
1	L	53	SER
1	L	58	LYS
1	L	62	GLU
1	L	64	ASP
1	L	82	ASP
1	L	84	THR
1	L	88	ARG
1	L	96	THR
1	L	98	GLN
1	L	101	ASP
1	L	115	LEU
1	L	125	LEU
1	L	143	SER
1	L	165	GLU
1	L	224	ARG
1	L	264[A]	ASN
1	L	264[B]	ASN
1	L	266[A]	SER
1	L	266[B]	SER
1	L	285	ASP

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Mol	Chain	Res	Type
1	L	293	GLN
1	L	295	LEU
1	L	332	LEU
1	L	337	ARG
1	L	340	SER
1	L	344	ARG
1	L	361	PRO
1	L	374	LEU
1	L	375	LEU
1	L	384	ASN
1	L	394	LYS
1	L	396	LEU
1	L	398	ASP
1	L	402	GLU
1	L	405	LYS
1	L	406	GLU
1	L	419	ASN
1	L	428	LEU
1	L	435	THR
1	L	437	GLU
1	L	464	LEU
1	L	468	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29[A]	GLN
1	A	30[A]	HIS
1	A	189	GLN
1	A	218	GLN
1	A	219	ASN
1	A	277	ASN
1	A	313	ASN
1	A	384	ASN
1	A	458	HIS
1	B	29[A]	GLN
1	B	30[A]	HIS
1	B	189	GLN
1	B	218	GLN
1	B	219	ASN
1	B	277	ASN
1	B	313	ASN

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Mol	Chain	Res	Type
1	B	384	ASN
1	B	458	HIS
1	C	29[A]	GLN
1	C	189	GLN
1	C	218	GLN
1	C	219	ASN
1	C	277	ASN
1	C	313	ASN
1	C	384	ASN
1	C	458	HIS
1	D	29[A]	GLN
1	D	30[A]	HIS
1	D	189	GLN
1	D	218	GLN
1	D	219	ASN
1	D	277	ASN
1	D	313	ASN
1	D	384	ASN
1	D	458	HIS
1	E	29[A]	GLN
1	E	30[A]	HIS
1	E	189	GLN
1	E	218	GLN
1	E	219	ASN
1	E	277	ASN
1	E	313	ASN
1	E	384	ASN
1	E	458	HIS
1	F	29[A]	GLN
1	F	189	GLN
1	F	218	GLN
1	F	219	ASN
1	F	277	ASN
1	F	313	ASN
1	F	384	ASN
1	F	458	HIS
1	G	29[A]	GLN
1	G	30[A]	HIS
1	G	189	GLN
1	G	218	GLN
1	G	219	ASN
1	G	277	ASN

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Mol	Chain	Res	Type
1	G	313	ASN
1	G	384	ASN
1	G	458	HIS
1	H	29[A]	GLN
1	H	189	GLN
1	H	218	GLN
1	H	219	ASN
1	H	277	ASN
1	H	313	ASN
1	H	384	ASN
1	H	458	HIS
1	I	29[A]	GLN
1	I	189	GLN
1	I	218	GLN
1	I	219	ASN
1	I	277	ASN
1	I	313	ASN
1	I	384	ASN
1	I	458	HIS
1	J	29[A]	GLN
1	J	189	GLN
1	J	218	GLN
1	J	219	ASN
1	J	277	ASN
1	J	313	ASN
1	J	384	ASN
1	J	458	HIS
1	K	29[A]	GLN
1	K	30[A]	HIS
1	K	189	GLN
1	K	218	GLN
1	K	219	ASN
1	K	277	ASN
1	K	313	ASN
1	K	384	ASN
1	K	458	HIS
1	L	29[A]	GLN
1	L	189	GLN
1	L	218	GLN
1	L	219	ASN
1	L	277	ASN
1	L	313	ASN

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Mol	Chain	Res	Type
1	L	384	ASN
1	L	458	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 48 ligands modelled in this entry, 24 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	ADP	A	4471	2	25,29,29	2.90	9 (36%)	24,45,45	3.22	9 (37%)
4	PPQ	A	5900	2	2,10,10	1.75	0	2,14,14	8.51	2 (100%)
3	ADP	B	4472	2	25,29,29	2.89	9 (36%)	24,45,45	3.21	9 (37%)
4	PPQ	B	5901	2	2,10,10	1.74	0	2,14,14	8.52	2 (100%)
3	ADP	C	4473	2	25,29,29	2.90	9 (36%)	24,45,45	3.21	9 (37%)
4	PPQ	C	5902	2	2,10,10	1.76	0	2,14,14	8.50	2 (100%)
3	ADP	D	4474	2	25,29,29	2.90	9 (36%)	24,45,45	3.21	9 (37%)
4	PPQ	D	5903	2	2,10,10	1.75	0	2,14,14	8.51	2 (100%)
3	ADP	E	4475	2	25,29,29	2.89	9 (36%)	24,45,45	3.22	9 (37%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PPQ	E	5904	2	2,10,10	1.76	0	2,14,14	8.51	2 (100%)
3	ADP	F	4476	2	25,29,29	2.89	9 (36%)	24,45,45	3.21	9 (37%)
4	PPQ	F	5905	2	2,10,10	1.73	0	2,14,14	8.51	2 (100%)
3	ADP	G	4477	2	25,29,29	2.90	9 (36%)	24,45,45	3.22	9 (37%)
4	PPQ	G	5906	2	2,10,10	1.74	0	2,14,14	8.52	2 (100%)
3	ADP	H	4478	2	25,29,29	2.90	9 (36%)	24,45,45	3.22	9 (37%)
4	PPQ	H	5907	2	2,10,10	1.77	0	2,14,14	8.52	2 (100%)
3	ADP	I	4479	2	25,29,29	2.90	9 (36%)	24,45,45	3.22	9 (37%)
4	PPQ	I	5908	2	2,10,10	1.79	0	2,14,14	8.51	2 (100%)
3	ADP	J	4480	2	25,29,29	2.90	9 (36%)	24,45,45	3.21	9 (37%)
4	PPQ	J	5909	2	2,10,10	1.76	0	2,14,14	8.51	2 (100%)
3	ADP	K	4481	2	25,29,29	2.90	9 (36%)	24,45,45	3.22	9 (37%)
4	PPQ	K	5910	2	2,10,10	1.68	0	2,14,14	8.50	2 (100%)
3	ADP	L	4482	2	25,29,29	2.91	9 (36%)	24,45,45	3.22	9 (37%)
4	PPQ	L	5911	2	2,10,10	1.73	0	2,14,14	8.51	2 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	4471	2	-	0/12/32/32	0/3/3/3
4	PPQ	A	5900	2	-	0/6/10/10	0/0/0/0
3	ADP	B	4472	2	-	0/12/32/32	0/3/3/3
4	PPQ	B	5901	2	-	0/6/10/10	0/0/0/0
3	ADP	C	4473	2	-	0/12/32/32	0/3/3/3
4	PPQ	C	5902	2	-	0/6/10/10	0/0/0/0
3	ADP	D	4474	2	-	0/12/32/32	0/3/3/3
4	PPQ	D	5903	2	-	0/6/10/10	0/0/0/0
3	ADP	E	4475	2	-	0/12/32/32	0/3/3/3
4	PPQ	E	5904	2	-	0/6/10/10	0/0/0/0
3	ADP	F	4476	2	-	0/12/32/32	0/3/3/3
4	PPQ	F	5905	2	-	0/6/10/10	0/0/0/0
3	ADP	G	4477	2	-	0/12/32/32	0/3/3/3
4	PPQ	G	5906	2	-	0/6/10/10	0/0/0/0
3	ADP	H	4478	2	-	0/12/32/32	0/3/3/3
4	PPQ	H	5907	2	-	0/6/10/10	0/0/0/0
3	ADP	I	4479	2	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PPQ	I	5908	2	-	0/6/10/10	0/0/0/0
3	ADP	J	4480	2	-	0/12/32/32	0/3/3/3
4	PPQ	J	5909	2	-	0/6/10/10	0/0/0/0
3	ADP	K	4481	2	-	0/12/32/32	0/3/3/3
4	PPQ	K	5910	2	-	0/6/10/10	0/0/0/0
3	ADP	L	4482	2	-	0/12/32/32	0/3/3/3
4	PPQ	L	5911	2	-	0/6/10/10	0/0/0/0

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	4479	ADP	C6-N6	-2.85	1.22	1.34
3	E	4475	ADP	C6-N6	-2.85	1.22	1.34
3	D	4474	ADP	C6-N6	-2.85	1.22	1.34
3	J	4480	ADP	C6-N6	-2.84	1.22	1.34
3	B	4472	ADP	C6-N6	-2.84	1.22	1.34
3	L	4482	ADP	C6-N6	-2.84	1.22	1.34
3	A	4471	ADP	C6-N6	-2.84	1.22	1.34
3	H	4478	ADP	C6-N6	-2.84	1.22	1.34
3	F	4476	ADP	C6-N6	-2.84	1.22	1.34
3	G	4477	ADP	C6-N6	-2.83	1.22	1.34
3	K	4481	ADP	C6-N6	-2.83	1.22	1.34
3	C	4473	ADP	C6-N6	-2.83	1.22	1.34
3	H	4478	ADP	C3'-C4'	-2.27	1.47	1.53
3	L	4482	ADP	C3'-C4'	-2.26	1.47	1.53
3	J	4480	ADP	C3'-C4'	-2.26	1.47	1.53
3	B	4472	ADP	C3'-C4'	-2.25	1.47	1.53
3	A	4471	ADP	C3'-C4'	-2.25	1.47	1.53
3	G	4477	ADP	C3'-C4'	-2.25	1.47	1.53
3	I	4479	ADP	C3'-C4'	-2.24	1.47	1.53
3	D	4474	ADP	C3'-C4'	-2.24	1.47	1.53
3	F	4476	ADP	C3'-C4'	-2.24	1.47	1.53
3	K	4481	ADP	C3'-C4'	-2.24	1.47	1.53
3	E	4475	ADP	C3'-C4'	-2.24	1.47	1.53
3	C	4473	ADP	C3'-C4'	-2.23	1.47	1.53
3	J	4480	ADP	C5-C4	2.05	1.45	1.40
3	E	4475	ADP	C5-C4	2.06	1.45	1.40
3	G	4477	ADP	C5-C4	2.06	1.45	1.40
3	A	4471	ADP	C5-C4	2.07	1.45	1.40
3	C	4473	ADP	C5-C4	2.07	1.45	1.40
3	L	4482	ADP	C5-C4	2.07	1.45	1.40
3	K	4481	ADP	C5-C4	2.07	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4476	ADP	C5-C4	2.07	1.45	1.40
3	H	4478	ADP	C5-C4	2.08	1.45	1.40
3	B	4472	ADP	C5-C4	2.08	1.45	1.40
3	D	4474	ADP	C5-C4	2.08	1.45	1.40
3	I	4479	ADP	C5-C4	2.10	1.45	1.40
3	F	4476	ADP	PB-O3B	3.59	1.69	1.54
3	E	4475	ADP	PB-O3B	3.60	1.69	1.54
3	G	4477	ADP	PB-O3B	3.60	1.69	1.54
3	D	4474	ADP	PB-O3B	3.60	1.69	1.54
3	A	4471	ADP	PB-O3B	3.60	1.69	1.54
3	K	4481	ADP	PB-O3B	3.61	1.69	1.54
3	B	4472	ADP	PB-O3B	3.61	1.69	1.54
3	L	4482	ADP	PB-O3B	3.61	1.69	1.54
3	C	4473	ADP	PB-O3B	3.62	1.69	1.54
3	J	4480	ADP	PB-O3B	3.62	1.69	1.54
3	I	4479	ADP	PB-O3B	3.62	1.69	1.54
3	H	4478	ADP	PB-O3B	3.62	1.69	1.54
3	G	4477	ADP	C2-N3	4.04	1.38	1.32
3	J	4480	ADP	O4'-C4'	4.04	1.54	1.45
3	J	4480	ADP	C2-N3	4.04	1.38	1.32
3	C	4473	ADP	C2-N3	4.05	1.38	1.32
3	C	4473	ADP	O4'-C4'	4.05	1.54	1.45
3	F	4476	ADP	C2-N3	4.05	1.38	1.32
3	D	4474	ADP	O4'-C4'	4.06	1.54	1.45
3	E	4475	ADP	C2-N3	4.06	1.38	1.32
3	G	4477	ADP	O4'-C4'	4.06	1.54	1.45
3	D	4474	ADP	C2-N3	4.07	1.38	1.32
3	F	4476	ADP	O4'-C4'	4.07	1.54	1.45
3	I	4479	ADP	C2-N3	4.07	1.39	1.32
3	A	4471	ADP	C2-N3	4.07	1.39	1.32
3	H	4478	ADP	O4'-C4'	4.07	1.54	1.45
3	A	4471	ADP	O4'-C4'	4.08	1.54	1.45
3	K	4481	ADP	O4'-C4'	4.08	1.54	1.45
3	B	4472	ADP	O4'-C4'	4.09	1.54	1.45
3	K	4481	ADP	C2-N3	4.09	1.39	1.32
3	H	4478	ADP	C2-N3	4.09	1.39	1.32
3	E	4475	ADP	O4'-C4'	4.09	1.54	1.45
3	B	4472	ADP	C2-N3	4.09	1.39	1.32
3	L	4482	ADP	C2-N3	4.10	1.39	1.32
3	L	4482	ADP	O4'-C4'	4.10	1.54	1.45
3	I	4479	ADP	O4'-C4'	4.10	1.54	1.45
3	K	4481	ADP	C4-N3	4.62	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	4472	ADP	C4-N3	4.63	1.42	1.35
3	D	4474	ADP	C4-N3	4.65	1.42	1.35
3	E	4475	ADP	C4-N3	4.66	1.42	1.35
3	A	4471	ADP	C4-N3	4.66	1.42	1.35
3	I	4479	ADP	C4-N3	4.66	1.42	1.35
3	L	4482	ADP	C4-N3	4.67	1.42	1.35
3	F	4476	ADP	C4-N3	4.67	1.42	1.35
3	H	4478	ADP	C4-N3	4.68	1.42	1.35
3	G	4477	ADP	C4-N3	4.68	1.42	1.35
3	J	4480	ADP	C4-N3	4.72	1.42	1.35
3	C	4473	ADP	C4-N3	4.72	1.42	1.35
3	B	4472	ADP	O4'-C1'	7.32	1.51	1.41
3	F	4476	ADP	O4'-C1'	7.33	1.51	1.41
3	H	4478	ADP	O4'-C1'	7.34	1.51	1.41
3	C	4473	ADP	O4'-C1'	7.35	1.51	1.41
3	A	4471	ADP	O4'-C1'	7.36	1.51	1.41
3	D	4474	ADP	O4'-C1'	7.36	1.51	1.41
3	E	4475	ADP	O4'-C1'	7.36	1.51	1.41
3	G	4477	ADP	O4'-C1'	7.37	1.51	1.41
3	I	4479	ADP	O4'-C1'	7.38	1.51	1.41
3	E	4475	ADP	PB-O3A	7.38	1.72	1.60
3	I	4479	ADP	PB-O3A	7.38	1.72	1.60
3	J	4480	ADP	O4'-C1'	7.39	1.51	1.41
3	K	4481	ADP	PB-O3A	7.39	1.72	1.60
3	B	4472	ADP	PB-O3A	7.39	1.72	1.60
3	K	4481	ADP	O4'-C1'	7.40	1.51	1.41
3	H	4478	ADP	PB-O3A	7.40	1.72	1.60
3	L	4482	ADP	O4'-C1'	7.40	1.51	1.41
3	F	4476	ADP	PB-O3A	7.41	1.72	1.60
3	A	4471	ADP	PB-O3A	7.41	1.72	1.60
3	C	4473	ADP	PB-O3A	7.41	1.72	1.60
3	L	4482	ADP	PB-O3A	7.42	1.72	1.60
3	J	4480	ADP	PB-O3A	7.42	1.72	1.60
3	G	4477	ADP	PB-O3A	7.44	1.72	1.60
3	D	4474	ADP	PB-O3A	7.44	1.72	1.60

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	4478	ADP	C4'-O4'-C1'	-8.36	100.87	109.77
3	I	4479	ADP	C4'-O4'-C1'	-8.36	100.88	109.77
3	E	4475	ADP	C4'-O4'-C1'	-8.36	100.88	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	4482	ADP	C4'-O4'-C1'	-8.34	100.89	109.77
3	K	4481	ADP	C4'-O4'-C1'	-8.33	100.90	109.77
3	G	4477	ADP	C4'-O4'-C1'	-8.33	100.90	109.77
3	J	4480	ADP	C4'-O4'-C1'	-8.33	100.90	109.77
3	F	4476	ADP	C4'-O4'-C1'	-8.33	100.90	109.77
3	A	4471	ADP	C4'-O4'-C1'	-8.33	100.91	109.77
3	D	4474	ADP	C4'-O4'-C1'	-8.31	100.93	109.77
3	C	4473	ADP	C4'-O4'-C1'	-8.29	100.94	109.77
3	B	4472	ADP	C4'-O4'-C1'	-8.29	100.95	109.77
3	C	4473	ADP	C5'-C4'-C3'	-3.91	100.39	115.29
3	F	4476	ADP	C5'-C4'-C3'	-3.90	100.41	115.29
3	I	4479	ADP	C5'-C4'-C3'	-3.90	100.42	115.29
3	J	4480	ADP	C5'-C4'-C3'	-3.90	100.42	115.29
3	B	4472	ADP	C5'-C4'-C3'	-3.90	100.42	115.29
3	H	4478	ADP	C5'-C4'-C3'	-3.90	100.42	115.29
3	A	4471	ADP	C5'-C4'-C3'	-3.90	100.43	115.29
3	G	4477	ADP	C5'-C4'-C3'	-3.90	100.43	115.29
3	D	4474	ADP	C5'-C4'-C3'	-3.89	100.45	115.29
3	E	4475	ADP	C5'-C4'-C3'	-3.89	100.45	115.29
3	K	4481	ADP	C5'-C4'-C3'	-3.89	100.46	115.29
3	L	4482	ADP	C5'-C4'-C3'	-3.89	100.47	115.29
3	H	4478	ADP	O5'-PA-O1A	-2.08	100.86	109.25
3	G	4477	ADP	O5'-PA-O1A	-2.08	100.86	109.25
3	K	4481	ADP	O5'-PA-O1A	-2.07	100.88	109.25
3	E	4475	ADP	O5'-PA-O1A	-2.07	100.88	109.25
3	F	4476	ADP	O5'-PA-O1A	-2.07	100.89	109.25
3	A	4471	ADP	O5'-PA-O1A	-2.07	100.89	109.25
3	L	4482	ADP	O5'-PA-O1A	-2.07	100.89	109.25
3	J	4480	ADP	O5'-PA-O1A	-2.07	100.90	109.25
3	D	4474	ADP	O5'-PA-O1A	-2.07	100.91	109.25
3	C	4473	ADP	O5'-PA-O1A	-2.07	100.92	109.25
3	B	4472	ADP	O5'-PA-O1A	-2.06	100.92	109.25
3	I	4479	ADP	O5'-PA-O1A	-2.06	100.93	109.25
3	I	4479	ADP	O3'-C3'-C2'	2.52	119.91	111.83
3	F	4476	ADP	O3'-C3'-C2'	2.53	119.93	111.83
3	A	4471	ADP	O3'-C3'-C2'	2.53	119.94	111.83
3	C	4473	ADP	O3'-C3'-C2'	2.53	119.94	111.83
3	G	4477	ADP	O3'-C3'-C2'	2.53	119.94	111.83
3	K	4481	ADP	O3'-C3'-C2'	2.53	119.94	111.83
3	L	4482	ADP	O3'-C3'-C2'	2.53	119.94	111.83
3	D	4474	ADP	O3'-C3'-C2'	2.53	119.94	111.83
3	B	4472	ADP	O3'-C3'-C2'	2.54	119.97	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	4478	ADP	O3'-C3'-C2'	2.54	119.97	111.83
3	J	4480	ADP	O3'-C3'-C2'	2.54	119.97	111.83
3	E	4475	ADP	O3'-C3'-C2'	2.54	119.97	111.83
3	L	4482	ADP	O2'-C2'-C1'	2.77	120.27	111.61
3	J	4480	ADP	O2'-C2'-C1'	2.77	120.28	111.61
3	E	4475	ADP	O2'-C2'-C1'	2.77	120.29	111.61
3	K	4481	ADP	O2'-C2'-C1'	2.78	120.30	111.61
3	B	4472	ADP	O2'-C2'-C1'	2.78	120.31	111.61
3	H	4478	ADP	O2'-C2'-C1'	2.78	120.31	111.61
3	G	4477	ADP	O2'-C2'-C1'	2.78	120.31	111.61
3	C	4473	ADP	O2'-C2'-C1'	2.78	120.32	111.61
3	A	4471	ADP	O2'-C2'-C1'	2.78	120.33	111.61
3	D	4474	ADP	O2'-C2'-C1'	2.78	120.33	111.61
3	I	4479	ADP	O2'-C2'-C1'	2.79	120.33	111.61
3	F	4476	ADP	O2'-C2'-C1'	2.80	120.36	111.61
3	I	4479	ADP	O4'-C4'-C5'	3.51	121.26	109.40
3	L	4482	ADP	O4'-C4'-C5'	3.53	121.31	109.40
3	C	4473	ADP	O4'-C4'-C5'	3.53	121.31	109.40
3	D	4474	ADP	O4'-C4'-C5'	3.53	121.33	109.40
3	A	4471	ADP	O4'-C4'-C5'	3.53	121.33	109.40
3	K	4481	ADP	O4'-C4'-C5'	3.53	121.33	109.40
3	H	4478	ADP	O4'-C4'-C5'	3.53	121.33	109.40
3	F	4476	ADP	O4'-C4'-C5'	3.54	121.34	109.40
3	E	4475	ADP	O4'-C4'-C5'	3.54	121.35	109.40
3	G	4477	ADP	O4'-C4'-C5'	3.54	121.35	109.40
3	B	4472	ADP	O4'-C4'-C5'	3.54	121.35	109.40
3	J	4480	ADP	O4'-C4'-C5'	3.54	121.36	109.40
3	D	4474	ADP	C4-C5-N7	5.09	114.32	109.41
3	E	4475	ADP	C4-C5-N7	5.09	114.32	109.41
3	H	4478	ADP	C4-C5-N7	5.10	114.33	109.41
3	F	4476	ADP	C4-C5-N7	5.10	114.34	109.41
3	J	4480	ADP	C4-C5-N7	5.10	114.34	109.41
3	D	4474	ADP	C1'-N9-C4	5.12	135.48	126.64
3	I	4479	ADP	C4-C5-N7	5.12	114.36	109.41
3	I	4479	ADP	C1'-N9-C4	5.12	135.48	126.64
3	H	4478	ADP	C1'-N9-C4	5.12	135.48	126.64
3	F	4476	ADP	C1'-N9-C4	5.12	135.48	126.64
3	L	4482	ADP	C1'-N9-C4	5.13	135.49	126.64
3	B	4472	ADP	C1'-N9-C4	5.13	135.50	126.64
3	J	4480	ADP	C1'-N9-C4	5.13	135.50	126.64
3	A	4471	ADP	C1'-N9-C4	5.13	135.50	126.64
3	C	4473	ADP	C4-C5-N7	5.13	114.37	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4471	ADP	C4-C5-N7	5.14	114.37	109.41
3	K	4481	ADP	C1'-N9-C4	5.14	135.52	126.64
3	C	4473	ADP	C1'-N9-C4	5.15	135.53	126.64
3	E	4475	ADP	C1'-N9-C4	5.15	135.53	126.64
3	G	4477	ADP	C4-C5-N7	5.15	114.39	109.41
3	G	4477	ADP	C1'-N9-C4	5.15	135.53	126.64
3	B	4472	ADP	C4-C5-N7	5.17	114.40	109.41
3	K	4481	ADP	C4-C5-N7	5.18	114.41	109.41
3	L	4482	ADP	C4-C5-N7	5.18	114.41	109.41
4	F	5905	PPQ	CEP-PDP-CGP	6.81	119.70	107.57
4	G	5906	PPQ	CEP-PDP-CGP	6.82	119.73	107.57
4	I	5908	PPQ	CEP-PDP-CGP	6.82	119.73	107.57
4	K	5910	PPQ	CEP-PDP-CGP	6.83	119.74	107.57
4	A	5900	PPQ	CEP-PDP-CGP	6.83	119.75	107.57
4	E	5904	PPQ	CEP-PDP-CGP	6.83	119.75	107.57
4	H	5907	PPQ	CEP-PDP-CGP	6.83	119.75	107.57
4	C	5902	PPQ	CEP-PDP-CGP	6.83	119.75	107.57
4	D	5903	PPQ	CEP-PDP-CGP	6.84	119.75	107.57
4	L	5911	PPQ	CEP-PDP-CGP	6.84	119.76	107.57
4	B	5901	PPQ	CEP-PDP-CGP	6.85	119.78	107.57
4	J	5909	PPQ	CEP-PDP-CGP	6.87	119.81	107.57
3	B	4472	ADP	O5'-C5'-C4'	8.08	137.63	109.00
3	J	4480	ADP	O5'-C5'-C4'	8.08	137.65	109.00
3	C	4473	ADP	O5'-C5'-C4'	8.08	137.65	109.00
3	H	4478	ADP	O5'-C5'-C4'	8.08	137.66	109.00
3	F	4476	ADP	O5'-C5'-C4'	8.08	137.67	109.00
3	G	4477	ADP	O5'-C5'-C4'	8.08	137.67	109.00
3	E	4475	ADP	O5'-C5'-C4'	8.09	137.68	109.00
3	A	4471	ADP	O5'-C5'-C4'	8.09	137.68	109.00
3	D	4474	ADP	O5'-C5'-C4'	8.09	137.69	109.00
3	L	4482	ADP	O5'-C5'-C4'	8.09	137.70	109.00
3	I	4479	ADP	O5'-C5'-C4'	8.09	137.70	109.00
3	K	4481	ADP	O5'-C5'-C4'	8.09	137.70	109.00
4	J	5909	PPQ	PDP-CGP-CBP	9.88	132.63	114.53
4	K	5910	PPQ	PDP-CGP-CBP	9.89	132.63	114.53
4	C	5902	PPQ	PDP-CGP-CBP	9.89	132.65	114.53
4	D	5903	PPQ	PDP-CGP-CBP	9.90	132.66	114.53
4	B	5901	PPQ	PDP-CGP-CBP	9.90	132.66	114.53
4	A	5900	PPQ	PDP-CGP-CBP	9.90	132.67	114.53
4	L	5911	PPQ	PDP-CGP-CBP	9.91	132.67	114.53
4	E	5904	PPQ	PDP-CGP-CBP	9.91	132.68	114.53
4	I	5908	PPQ	PDP-CGP-CBP	9.92	132.70	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	5905	PPQ	PDP-CGP-CBP	9.92	132.70	114.53
4	G	5906	PPQ	PDP-CGP-CBP	9.93	132.71	114.53
4	H	5907	PPQ	PDP-CGP-CBP	9.93	132.71	114.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 172 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4471	ADP	8	0
4	A	5900	PPQ	7	0
3	B	4472	ADP	8	0
4	B	5901	PPQ	7	0
3	C	4473	ADP	8	0
4	C	5902	PPQ	6	0
3	D	4474	ADP	8	0
4	D	5903	PPQ	6	0
3	E	4475	ADP	8	0
4	E	5904	PPQ	6	0
3	F	4476	ADP	8	0
4	F	5905	PPQ	7	0
3	G	4477	ADP	8	0
4	G	5906	PPQ	6	0
3	H	4478	ADP	8	0
4	H	5907	PPQ	7	0
3	I	4479	ADP	8	0
4	I	5908	PPQ	6	0
3	J	4480	ADP	8	0
4	J	5909	PPQ	6	0
3	K	4481	ADP	8	0
4	K	5910	PPQ	5	0
3	L	4482	ADP	8	0
4	L	5911	PPQ	7	0

## 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, 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(Å²)	Q<0.9
1	A	468/468 (100%)	0.10	30 (6%)	20	15	20, 47, 80, 100	94 (20%)
1	B	468/468 (100%)	-0.15	18 (3%)	41	35	20, 47, 80, 100	94 (20%)
1	C	468/468 (100%)	-0.19	18 (3%)	41	35	20, 47, 80, 100	94 (20%)
1	D	468/468 (100%)	-0.29	21 (4%)	34	29	20, 47, 80, 100	94 (20%)
1	E	468/468 (100%)	-0.22	17 (3%)	43	37	20, 47, 80, 100	94 (20%)
1	F	468/468 (100%)	-0.16	24 (5%)	29	24	20, 47, 80, 100	94 (20%)
1	G	468/468 (100%)	-0.30	18 (3%)	41	35	20, 47, 80, 100	94 (20%)
1	H	468/468 (100%)	-0.25	19 (4%)	38	32	20, 47, 80, 100	94 (20%)
1	I	468/468 (100%)	-0.36	15 (3%)	48	42	20, 47, 80, 100	94 (20%)
1	J	468/468 (100%)	-0.26	18 (3%)	41	35	20, 47, 80, 100	94 (20%)
1	K	468/468 (100%)	-0.35	12 (2%)	56	51	20, 47, 80, 100	94 (20%)
1	L	468/468 (100%)	-0.30	17 (3%)	43	37	20, 47, 80, 100	94 (20%)
All	All	5616/5616 (100%)	-0.23	227 (4%)	39	34	20, 47, 81, 100	1128 (20%)

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	396	LEU	10.1
1	F	396	LEU	8.5
1	L	396	LEU	7.6
1	J	398	ASP	7.3
1	J	60	ILE	7.3
1	D	395	ASN	7.2
1	I	63	SER	7.0
1	A	404	ALA	7.0
1	H	337	ARG	6.2
1	J	396	LEU	6.2
1	C	396	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
1	E	63	SER	5.9
1	F	398	ASP	5.7
1	C	63	SER	5.6
1	A	395	ASN	5.6
1	K	395	ASN	5.5
1	F	401	PRO	5.5
1	F	63	SER	5.5
1	L	397	TYR	5.5
1	C	395	ASN	5.4
1	C	398	ASP	5.4
1	F	404	ALA	5.2
1	B	404	ALA	5.2
1	E	395	ASN	5.1
1	G	63	SER	5.1
1	G	401	PRO	5.0
1	J	399	LEU	5.0
1	J	403	GLU	5.0
1	A	60	ILE	5.0
1	A	399	LEU	5.0
1	B	399	LEU	5.0
1	D	398	ASP	4.9
1	H	60	ILE	4.9
1	A	277	ASN	4.9
1	G	398	ASP	4.9
1	H	402	GLU	4.8
1	K	63	SER	4.7
1	J	402	GLU	4.7
1	C	61	ASN	4.6
1	K	398	ASP	4.6
1	F	402	GLU	4.6
1	A	285	ASP	4.5
1	H	398	ASP	4.5
1	L	402	GLU	4.4
1	L	395	ASN	4.3
1	H	401	PRO	4.2
1	G	395	ASN	4.2
1	A	396	LEU	4.2
1	C	402	GLU	4.1
1	K	397	TYR	4.1
1	A	400	PRO	4.1
1	F	395	ASN	4.1
1	D	60	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	394	LYS	4.0
1	K	1	SER	4.0
1	E	1	SER	4.0
1	D	399	LEU	4.0
1	A	398	ASP	4.0
1	E	398	ASP	3.9
1	L	398	ASP	3.9
1	A	403	GLU	3.9
1	G	397	TYR	3.9
1	G	404	ALA	3.9
1	A	402	GLU	3.9
1	J	337	ARG	3.9
1	D	394	LYS	3.9
1	I	61	ASN	3.9
1	D	396	LEU	3.8
1	D	400	PRO	3.8
1	H	264[A]	ASN	3.7
1	J	397	TYR	3.7
1	F	400	PRO	3.7
1	F	62	GLU	3.7
1	B	1	SER	3.6
1	F	264[A]	ASN	3.6
1	D	401	PRO	3.6
1	G	402	GLU	3.6
1	H	396	LEU	3.6
1	K	60	ILE	3.6
1	I	398	ASP	3.6
1	L	401	PRO	3.6
1	D	404	ALA	3.6
1	E	396	LEU	3.5
1	F	1	SER	3.5
1	B	400	PRO	3.5
1	K	402	GLU	3.5
1	F	349	ALA	3.5
1	H	61	ASN	3.5
1	I	1	SER	3.4
1	L	63	SER	3.4
1	B	337	ARG	3.4
1	G	396	LEU	3.4
1	G	403	GLU	3.4
1	L	61	ASN	3.4
1	A	62	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	395	ASN	3.4
1	G	399	LEU	3.3
1	A	63	SER	3.3
1	H	395	ASN	3.3
1	L	62	GLU	3.3
1	K	403	GLU	3.3
1	F	397	TYR	3.3
1	C	59	GLY	3.3
1	D	402	GLU	3.3
1	A	378	GLY	3.3
1	A	351	PRO	3.3
1	J	401	PRO	3.2
1	G	264[A]	ASN	3.2
1	I	402	GLU	3.2
1	L	264[A]	ASN	3.2
1	E	283	SER	3.2
1	I	60	ILE	3.2
1	F	394	LYS	3.2
1	B	398	ASP	3.1
1	L	1	SER	3.1
1	C	397	TYR	3.1
1	H	400	PRO	3.1
1	E	404	ALA	3.1
1	E	61	ASN	3.1
1	G	349	ALA	3.1
1	C	264[A]	ASN	3.1
1	A	401	PRO	3.0
1	D	337	ARG	3.0
1	A	348	VAL	3.0
1	A	3	GLU	3.0
1	G	98	GLN	3.0
1	J	395	ASN	2.9
1	C	404	ALA	2.9
1	I	404	ALA	2.9
1	C	1	SER	2.9
1	H	4	HIS	2.9
1	E	337	ARG	2.9
1	H	1	SER	2.8
1	A	116	ARG	2.8
1	C	60	ILE	2.8
1	D	63	SER	2.8
1	F	348	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	61	ASN	2.8
1	F	61	ASN	2.8
1	I	62	GLU	2.8
1	B	63	SER	2.8
1	B	98	GLN	2.8
1	I	397	TYR	2.8
1	H	63	SER	2.7
1	I	399	LEU	2.7
1	I	285	ASP	2.7
1	E	394	LYS	2.7
1	B	61	ASN	2.7
1	J	63	SER	2.6
1	C	3	GLU	2.6
1	A	394	LYS	2.6
1	J	178[A]	GLY	2.6
1	F	60	ILE	2.6
1	C	62	GLU	2.6
1	B	55	GLY	2.6
1	E	393	ASP	2.6
1	A	58	LYS	2.6
1	B	352	LYS	2.6
1	A	397	TYR	2.6
1	A	278	GLY	2.5
1	A	286	LYS	2.5
1	D	264[A]	ASN	2.5
1	I	403	GLU	2.5
1	L	399	LEU	2.5
1	G	400	PRO	2.5
1	D	278	GLY	2.5
1	F	59	GLY	2.5
1	B	60	ILE	2.5
1	B	401	PRO	2.5
1	L	60	ILE	2.5
1	A	337	ARG	2.5
1	F	284	GLY	2.5
1	F	406	GLU	2.5
1	A	273	SER	2.4
1	I	395	ASN	2.4
1	L	337	ARG	2.4
1	A	264[A]	ASN	2.4
1	H	11	GLU	2.4
1	E	278	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	94	PRO	2.4
1	D	397	TYR	2.4
1	G	61	ASN	2.4
1	C	337	ARG	2.4
1	E	7	THR	2.4
1	G	394	LYS	2.4
1	D	1	SER	2.4
1	E	60	ILE	2.3
1	F	56	GLY	2.3
1	E	12	HIS	2.3
1	J	61	ASN	2.3
1	J	400	PRO	2.3
1	J	404	ALA	2.3
1	B	387	HIS	2.3
1	H	403	GLU	2.3
1	L	405	LYS	2.3
1	D	62	GLU	2.3
1	L	393	ASP	2.2
1	D	98	GLN	2.2
1	G	348	VAL	2.2
1	J	394	LYS	2.2
1	G	1	SER	2.2
1	H	394	LYS	2.2
1	C	7	THR	2.2
1	H	399	LEU	2.2
1	C	401	PRO	2.2
1	F	390	GLU	2.2
1	B	264[A]	ASN	2.2
1	I	405	LYS	2.2
1	A	324	PRO	2.2
1	B	394	LYS	2.2
1	D	403	GLU	2.2
1	K	264[A]	ASN	2.2
1	F	405	LYS	2.2
1	H	284	GLY	2.1
1	I	396	LEU	2.1
1	H	3	GLU	2.1
1	J	1	SER	2.1
1	K	40	ALA	2.1
1	F	399	LEU	2.1
1	D	7	THR	2.1
1	A	55	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	58	LYS	2.0
1	E	62	GLU	2.0
1	A	1	SER	2.0
1	J	264[A]	ASN	2.0
1	E	406	GLU	2.0
1	L	59	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ADP	L	4482	27/27	0.73	0.42	4.99	42,80,100,100	27
3	ADP	F	4476	27/27	0.82	0.41	4.58	42,80,100,100	27
3	ADP	H	4478	27/27	0.81	0.32	4.09	42,80,100,100	27
3	ADP	I	4479	27/27	0.78	0.36	3.94	42,80,100,100	27
3	ADP	C	4473	27/27	0.76	0.36	3.69	42,80,100,100	27
3	ADP	K	4481	27/27	0.78	0.35	3.61	42,80,100,100	27
3	ADP	E	4475	27/27	0.79	0.39	3.49	42,80,100,100	27
3	ADP	G	4477	27/27	0.84	0.28	2.08	42,80,100,100	27
3	ADP	D	4474	27/27	0.88	0.34	1.92	42,80,100,100	27
3	ADP	J	4480	27/27	0.84	0.30	1.76	42,80,100,100	27
3	ADP	A	4471	27/27	0.85	0.34	1.33	42,80,100,100	27
3	ADP	B	4472	27/27	0.82	0.31	1.04	42,80,100,100	27
4	PPQ	I	5908	11/11	0.93	0.22	0.21	16,36,70,83	11
4	PPQ	L	5911	11/11	0.95	0.21	-0.07	16,36,70,83	11
4	PPQ	H	5907	11/11	0.93	0.20	-0.12	16,36,70,83	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PPQ	F	5905	11/11	0.92	0.20	-0.17	16,36,70,83	11
4	PPQ	B	5901	11/11	0.91	0.19	-0.17	16,36,70,83	11
4	PPQ	D	5903	11/11	0.93	0.19	-0.22	16,36,70,83	11
4	PPQ	K	5910	11/11	0.94	0.17	-0.39	16,36,70,83	11
4	PPQ	J	5909	11/11	0.95	0.19	-0.39	16,36,70,83	11
4	PPQ	G	5906	11/11	0.94	0.17	-0.42	16,36,70,83	11
4	PPQ	C	5902	11/11	0.94	0.17	-0.42	16,36,70,83	11
4	PPQ	E	5904	11/11	0.94	0.16	-0.57	16,36,70,83	11
4	PPQ	A	5900	11/11	0.95	0.16	-0.87	16,36,70,83	11
2	MN	K	469	1/1	0.97	0.11	-1.35	41,41,41,41	0
2	MN	J	469	1/1	0.99	0.07	-1.85	41,41,41,41	0
2	MN	L	469	1/1	0.98	0.11	-1.90	41,41,41,41	0
2	MN	H	469	1/1	0.97	0.10	-1.98	41,41,41,41	0
2	MN	D	469	1/1	0.93	0.07	-2.02	41,41,41,41	0
2	MN	G	469	1/1	0.92	0.08	-2.36	41,41,41,41	0
2	MN	I	469	1/1	0.99	0.06	-2.84	41,41,41,41	0
2	MN	A	469	1/1	0.97	0.06	-3.07	41,41,41,41	0
2	MN	E	469	1/1	0.95	0.03	-3.70	41,41,41,41	0
2	MN	B	469	1/1	0.98	0.04	-4.09	41,41,41,41	0
2	MN	F	469	1/1	0.97	0.06	-4.36	41,41,41,41	0
2	MN	C	469	1/1	0.92	0.06	-4.61	41,41,41,41	0
2	MN	D	470	1/1	0.98	0.08	-	43,43,43,43	0
2	MN	C	470	1/1	0.98	0.03	-	43,43,43,43	0
2	MN	A	470	1/1	0.98	0.03	-	43,43,43,43	0
2	MN	I	470	1/1	0.99	0.04	-	43,43,43,43	0
2	MN	F	470	1/1	0.98	0.06	-	43,43,43,43	0
2	MN	B	470	1/1	0.98	0.05	-	43,43,43,43	0
2	MN	H	470	1/1	0.90	0.07	-	43,43,43,43	0
2	MN	G	470	1/1	0.99	0.04	-	43,43,43,43	0
2	MN	E	470	1/1	0.97	0.06	-	43,43,43,43	0
2	MN	J	470	1/1	0.99	0.02	-	43,43,43,43	0
2	MN	L	470	1/1	0.98	0.05	-	43,43,43,43	0
2	MN	K	470	1/1	0.98	0.04	-	43,43,43,43	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.