



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:03 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

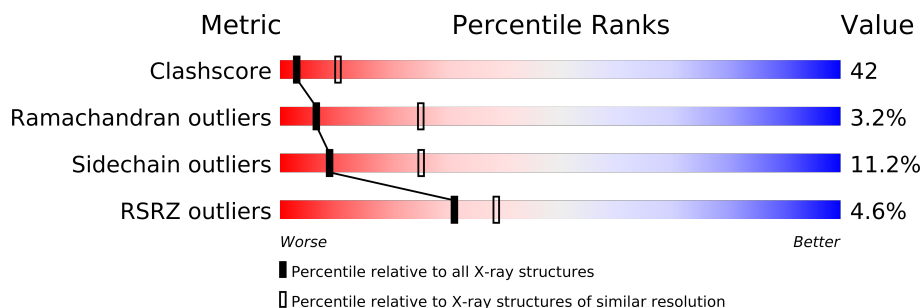
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	468	
1	B	468	
1	C	468	
1	D	468	
1	E	468	
1	F	468	
1	G	468	
1	H	468	
1	I	468	
1	J	468	
1	K	468	
1	L	468	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	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

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 47280 atoms, of which 0 are hydrogen and 0 are deuterium.

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).

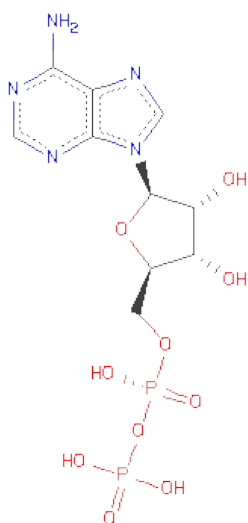
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mn	0	0
			2	2		
2	J	2	Total	Mn	0	0
			2	2		

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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: $C_{10}H_{15}N_5O_{10}P_2$).



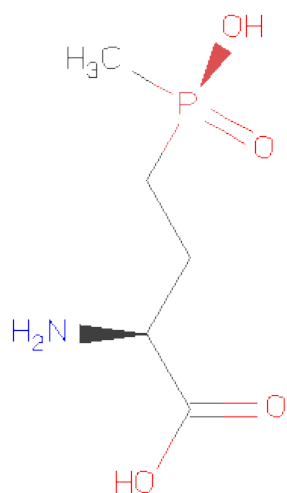
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O P	0	0
			27	10	5	10 2		

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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: C₅H₁₂NO₄P).



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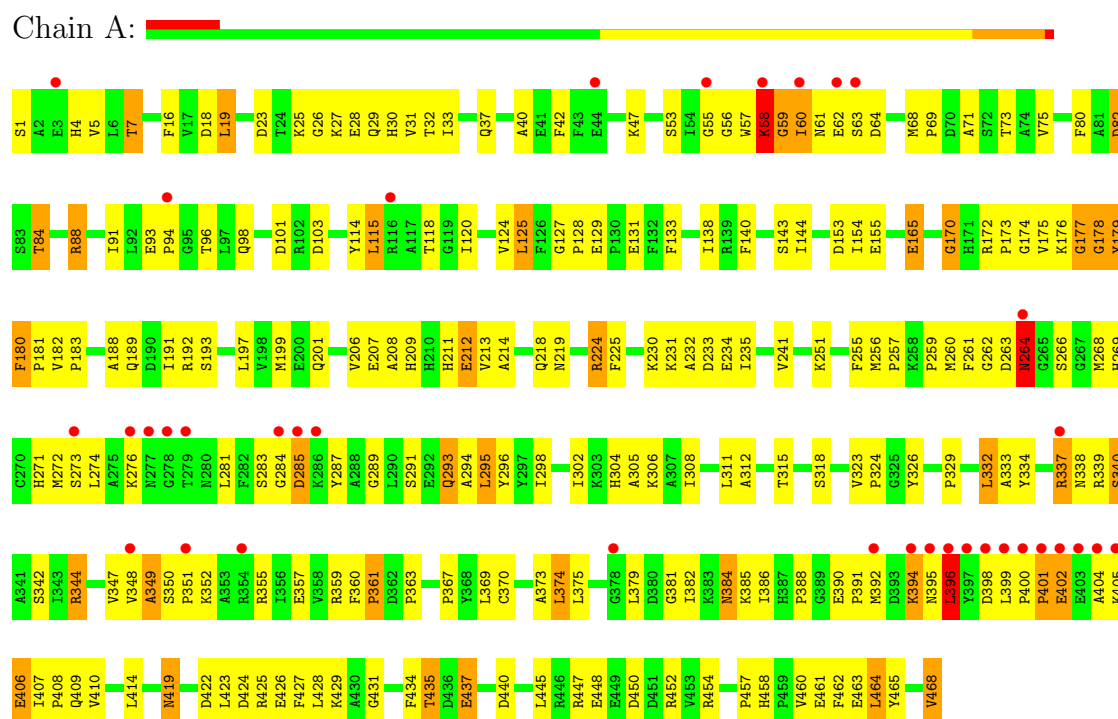
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	156	Total 156	O 156	0	0
5	J	151	Total 151	O 151	0	0
5	K	153	Total 153	O 153	0	0
5	L	153	Total 153	O 153	0	0

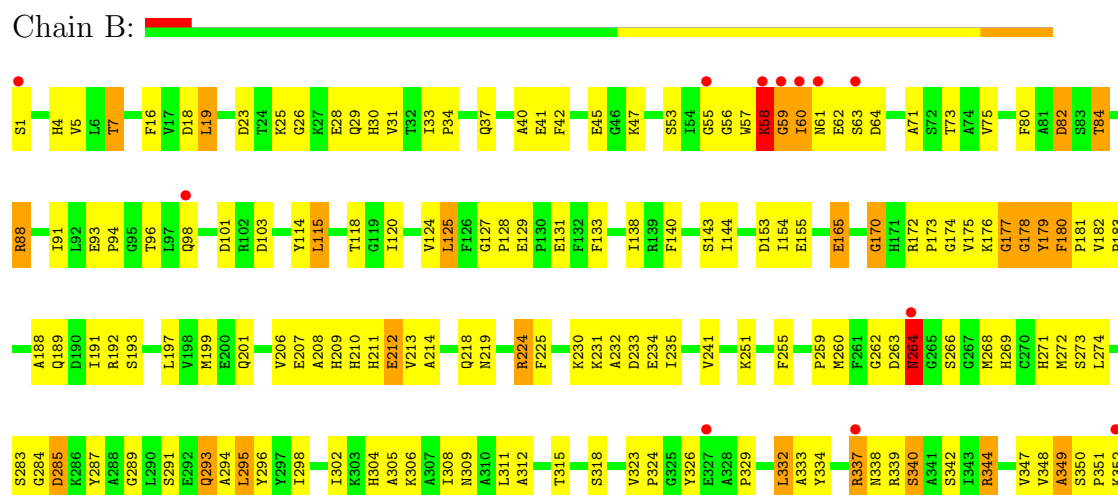
3 Residue-property plots

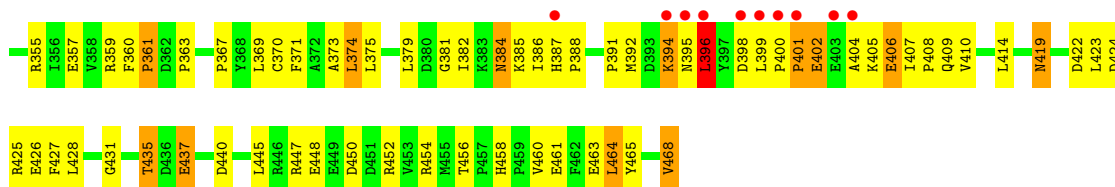
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: GLUTAMINE SYNTHETASE



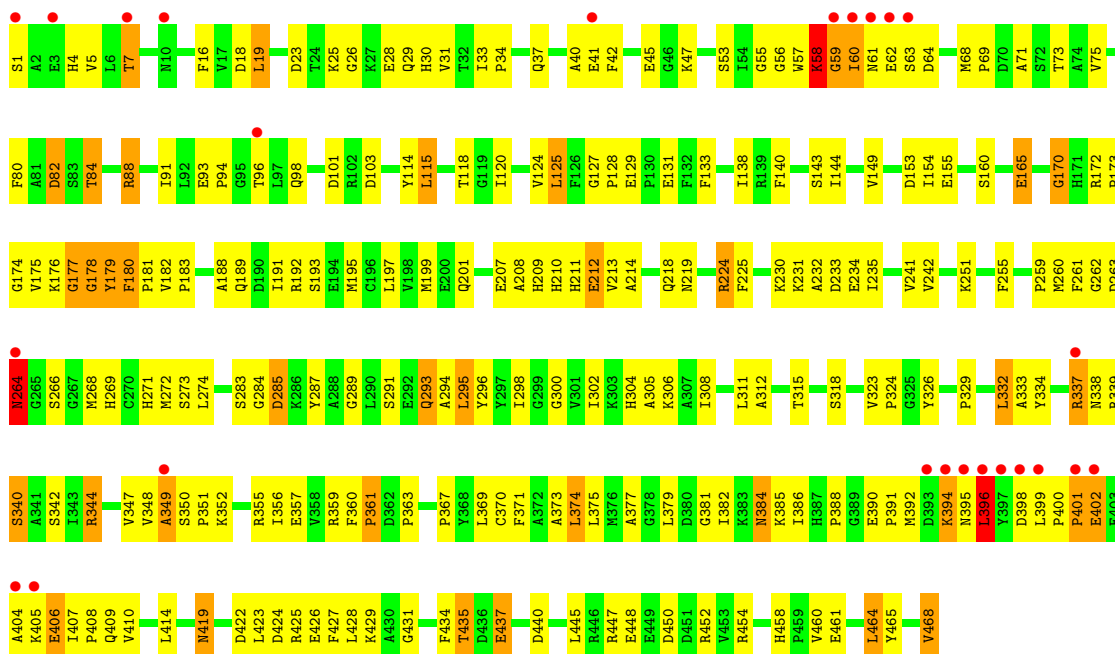
• Molecule 1: GLUTAMINE SYNTHETASE





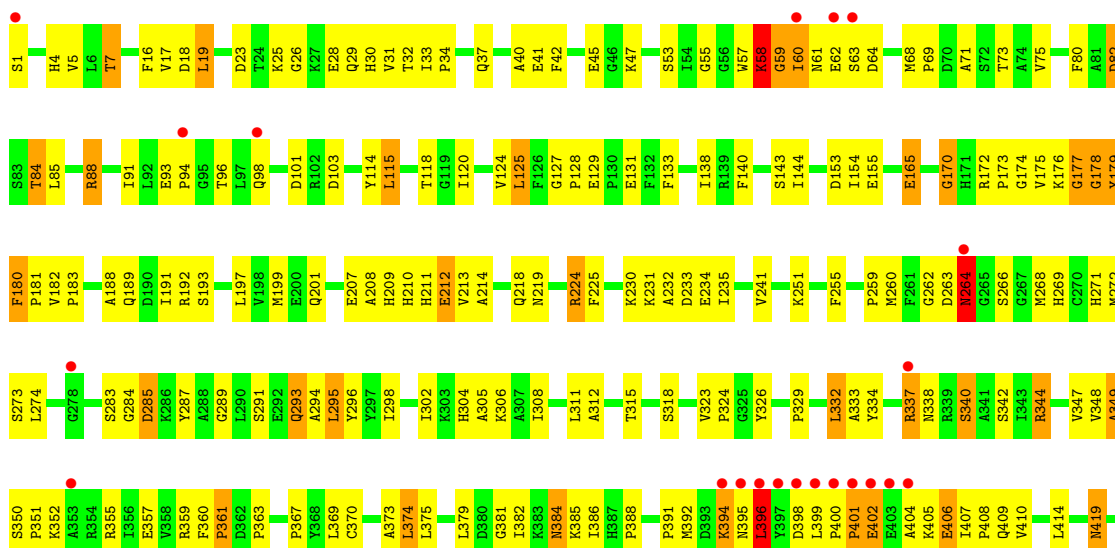
● Molecule 1: GLUTAMINE SYNTHETASE

Chain C:



● Molecule 1: GLUTAMINE SYNTHETASE

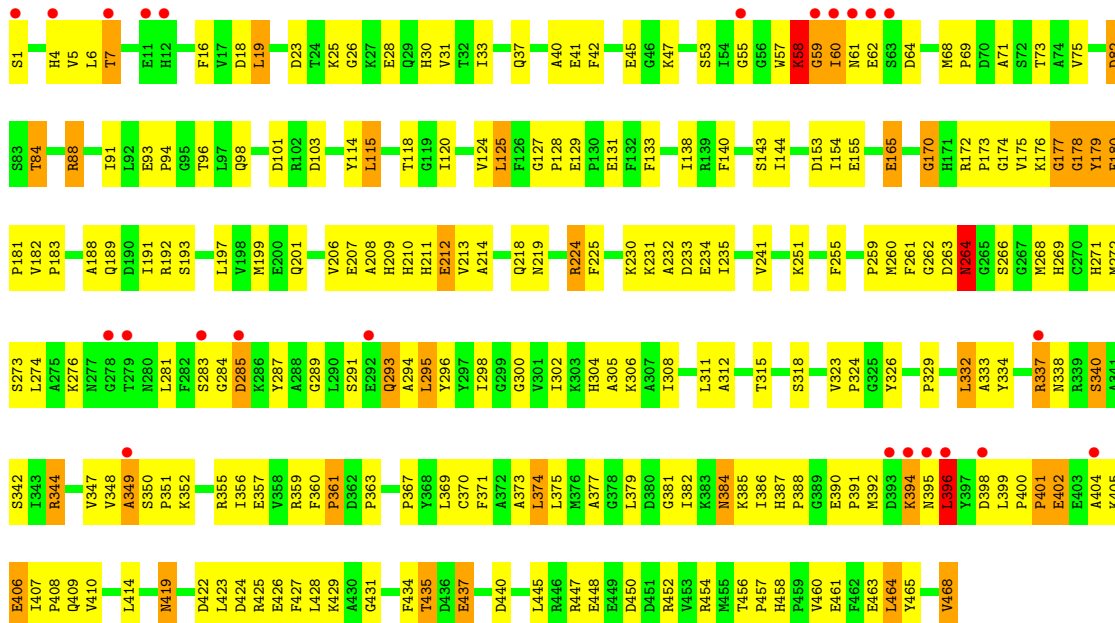
Chain D:





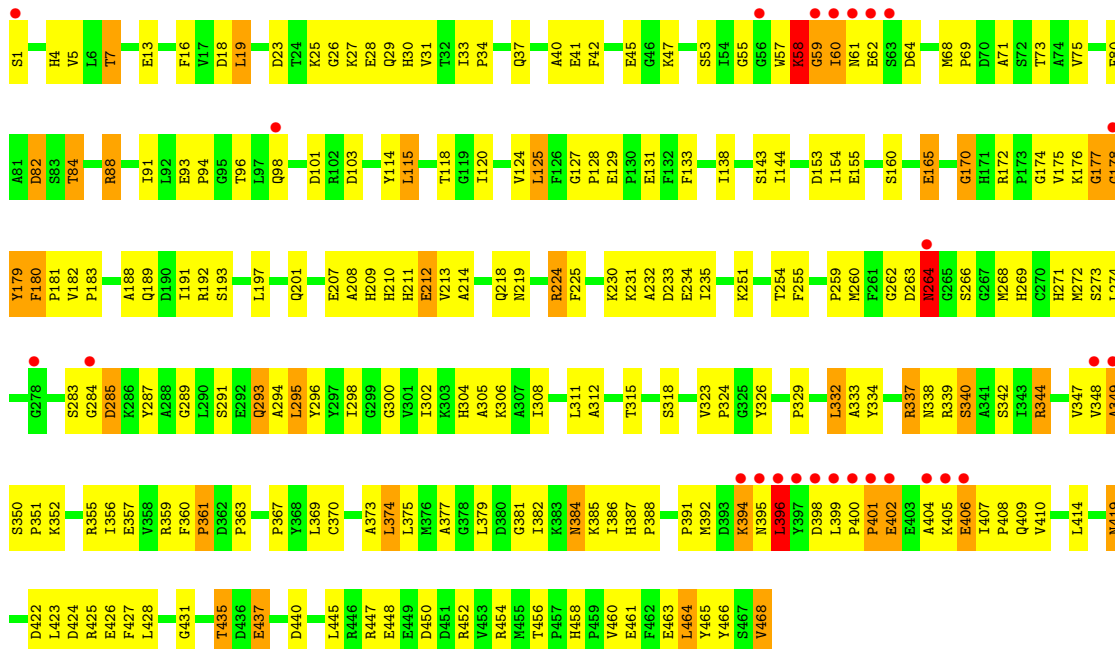
• Molecule 1: GLUTAMINE SYNTHETASE

Chain E:



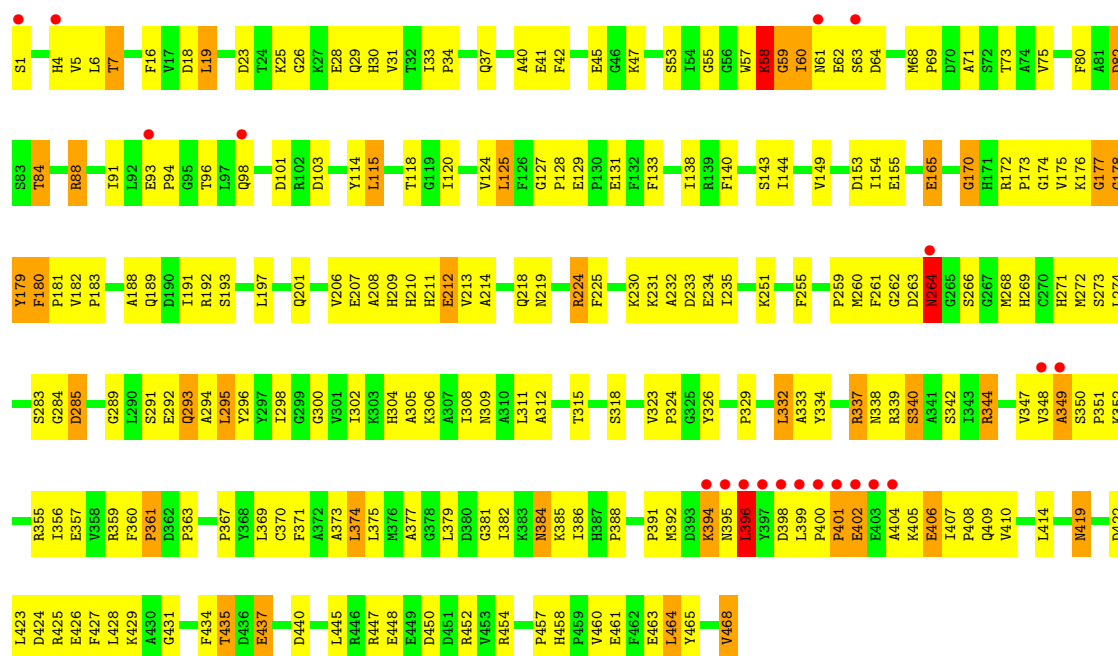
• Molecule 1: GLUTAMINE SYNTHETASE

Chain F:



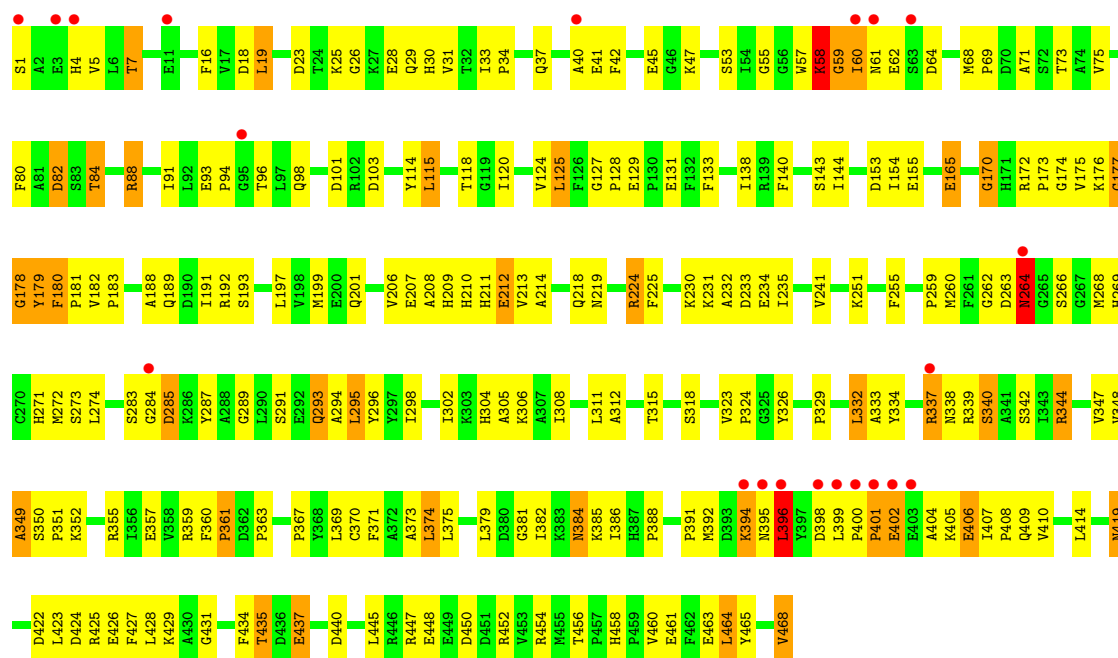
• Molecule 1: GLUTAMINE SYNTHETASE

Chain G:



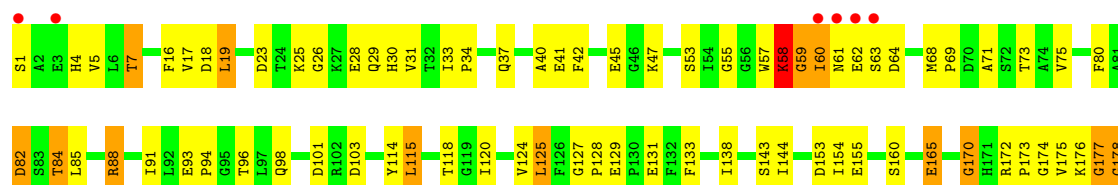
• Molecule 1: GLUTAMINE SYNTHETASE

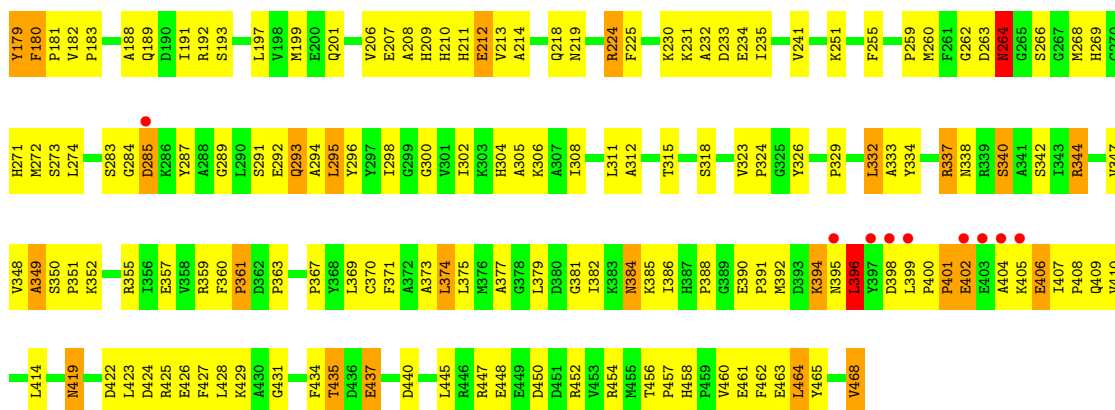
Chain H:



• Molecule 1: GLUTAMINE SYNTHETASE

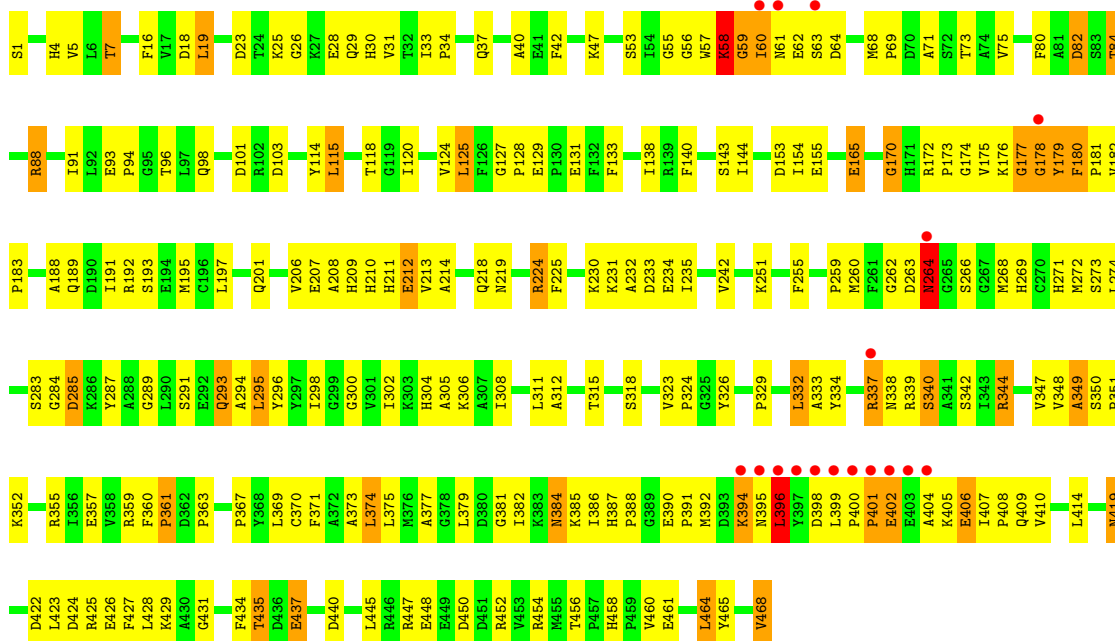
Chain I:





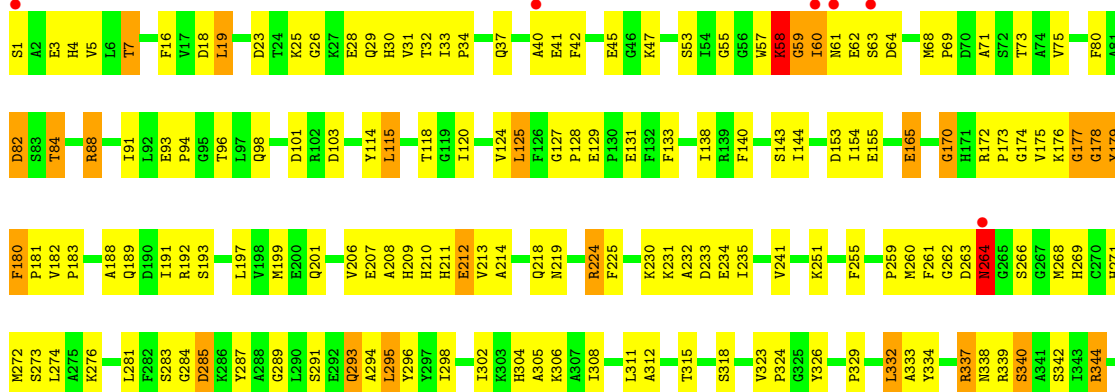
• Molecule 1: GLUTAMINE SYNTHETASE

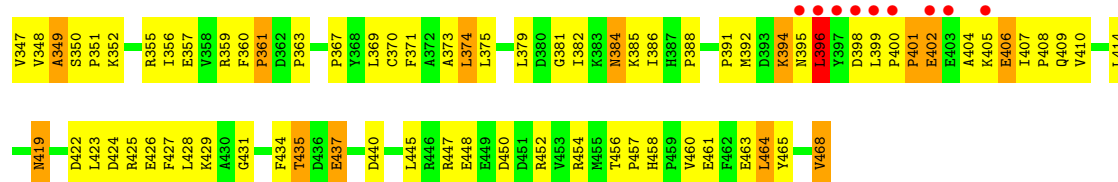
Chain J:



• Molecule 1: GLUTAMINE SYNTHETASE

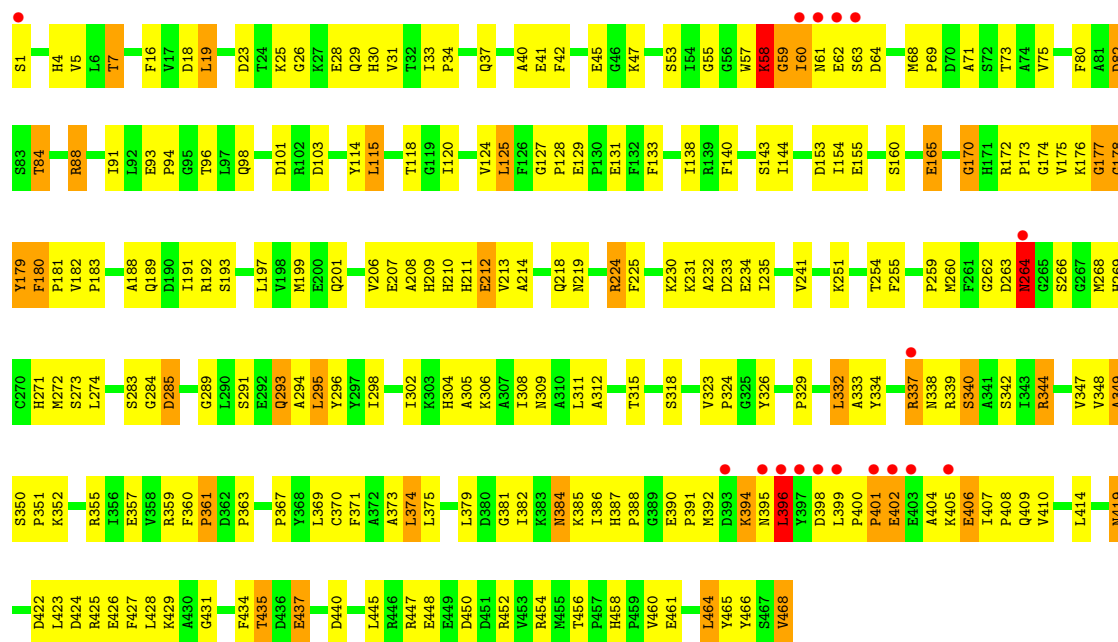
Chain K:





Molecule 1: GLUTAMINE SYNTHETASE

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	51.1	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 38.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 87421 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	47280	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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%)

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3747	0	3621	330	1
1	B	3747	0	3621	325	1
1	C	3747	0	3621	330	3
1	D	3747	0	3621	320	0
1	E	3747	0	3621	322	0
1	F	3747	0	3621	325	3
1	G	3747	0	3621	328	1
1	H	3747	0	3621	324	2
1	I	3747	0	3621	334	1
1	J	3747	0	3621	333	3
1	K	3747	0	3621	328	3
1	L	3747	0	3621	323	4
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	7
5	I	156	0	0	92	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	151	0	0	90	2
5	K	153	0	0	85	1
5	L	153	0	0	90	3
All	All	47280	0	43692	3738	18

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 42.

All (3738) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:K:211[B]:HIS:O	1:K:212[B]:GLU:HG2	1.07	1.24
1:H:211[B]:HIS:CE1	5:H:5912:HOH:O	1.91	1.24
1:D:337:ARG:HG3	1:D:338:ASN:N	1.31	1.24
1:L:337:ARG:HG3	1:L:338:ASN:N	1.31	1.23
1:G:211[B]:HIS:O	1:G: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:A:211[B]:HIS:O	1:A: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

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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:211[B]:HIS:O	1:B:212[B]:GLU:CG	1.96	1.14
1:F:211[B]:HIS:O	1:F:212[B]:GLU:CG	1.96	1.13
1:L:211[B]:HIS:O	1:L:212[B]:GLU:CG	1.96	1.13
1:D:360:PHE:CD2	1:D:361:PRO:HD3	1.83	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:K:360:PHE:CD2	1:K:361:PRO:HD3	1.83	1.13
1:H:360:PHE:CD2	1:H:361:PRO:HD3	1.83	1.13
1:A:360:PHE:CD2	1:A:361:PRO:HD3	1.83	1.13
1:G:211[B]:HIS:O	1:G:212[B]:GLU:CG	1.96	1.13
1:E:323:VAL:HG12	5:E:759:HOH:O	1.44	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: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:E:293:GLN:HB2	5:E:752:HOH:O	1.49	1.12
1:I:211[B]:HIS:O	1:I:212[B]:GLU:CG	1.96	1.12
1:E:360:PHE:CD2	1:E:361:PRO:HD3	1.83	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:J:360:PHE:CD2	1:J:361:PRO:HD3	1.83	1.12
1:C:360:PHE:CD2	1:C:361:PRO:HD3	1.84	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:I:337:ARG:CG	1:I:338:ASN:N	2.07	1.11
1:J:329:PRO:HG2	1:J:359:ARG:HD2	1.24	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:H:293:GLN:HB2	5:H:6045:HOH:O	1.49	1.10
1:D:329:PRO:HG2	1:D:359:ARG:HD2	1.24	1.10

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:G:60:ILE:HD11	5:H:6053:HOH:O	1.49	1.09
1:A:1:SER:HB2	1:A:4:HIS:HB3	1.34	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
1:I:61:ASN:HB3	1:J:337:ARG:CD	1.83	1.08
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:K:329:PRO:HG2	1:K:359:ARG:HD2	1.24	1.08
1:K:337:ARG:CG	1:K:338:ASN:N	2.07	1.08
1:G:329:PRO:HG2	1:G:359:ARG:HD2	1.24	1.08
1:F:293:GLN:HB2	5:F:6041:HOH:O	1.49	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:D:179[A]:TYR:OH	5:D:6052:HOH:O	1.70	1.08
1:J:224:ARG:HG2	1:J:224:ARG:HH21	1.19	1.08
1:D:224:ARG:HG2	1:D:224:ARG:HH21	1.19	1.07
1:G:211[B]:HIS:C	1:G:212[B]:GLU:HG2	1.75	1.07
1:E:211[B]:HIS:C	1:E: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:L:224:ARG:HH21	1:L:224:ARG:HG2	1.19	1.07
1:F:1:SER:HB2	1:F:4:HIS:HB3	1.34	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:B:211[B]:HIS:N	1:B:211[B]:HIS:CD2	2.22	1.06
1:J:211[B]:HIS:CD2	1:J:211[B]:HIS:N	2.22	1.06
1:I:224:ARG:HG2	1:I:224:ARG:HH21	1.19	1.06
1:E:1:SER:HB2	1:E:4:HIS:HB3	1.34	1.06
1:K:211[B]:HIS:C	1:K:212[B]:GLU:HG2	1.75	1.06
1:D:211[B]:HIS:C	1:D: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:J:211[B]:HIS:C	1:J:212[B]:GLU:HG2	1.75	1.06
1:I:179[A]:TYR:OH	5:I:5921:HOH:O	1.74	1.06
1:I:211[B]:HIS:C	1:I:212[B]:GLU:HG2	1.75	1.06
1:A:224:ARG:HH21	1:A:224:ARG:HG2	1.19	1.06
1:H:211[B]:HIS:C	1:H:212[B]:GLU:HG2	1.75	1.05
1:L:211[B]:HIS:C	1:L:212[B]:GLU:HG2	1.75	1.05

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:179[A]:TYR:OH	5:G:6061:HOH:O	1.74	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:H:1:SER:HB2	1:H:4:HIS:HB3	1.34	1.05
1:H:176[B]:LYS:O	1:H:178[B]:GLY:N	1.90	1.05
1:A:211[B]:HIS:CD2	1:A:211[B]:HIS:N	2.22	1.05
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:E:179[A]:TYR:OH	5:E:867:HOH:O	1.73	1.05
1:C:176[B]:LYS:O	1:C:178[B]:GLY:N	1.90	1.04
1:K:176[B]:LYS:O	1:K:178[B]:GLY:N	1.90	1.04
1:H:179[A]:TYR:OH	5:H:5917:HOH:O	1.73	1.04
1:E:176[B]:LYS:O	1:E:178[B]:GLY:N	1.90	1.04
1:G:224:ARG:HG2	1:G:224:ARG:HH21	1.19	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:I:176[B]:LYS:O	1:I:178[B]:GLY:N	1.90	1.04
1:C:1:SER:HB2	1:C:4:HIS:HB3	1.34	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:H:179[B]:TYR:CD1	1:H:212[B]:GLU:HA	1.93	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:K:211[B]:HIS:N	1:K:211[B]:HIS:CD2	2.22	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:C:179[B]:TYR:CD1	1:C:212[B]:GLU:HA	1.93	1.03
1:G:179[B]:TYR:CD1	1:G: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:F:224:ARG:HH21	1:F:224:ARG:HG2	1.19	1.03
1:F:179[B]:TYR:CD1	1:F:212[B]:GLU:HA	1.93	1.02
1:J:329:PRO:CG	1:J:359:ARG:HD2	1.89	1.02
1:H:224:ARG:HH21	1:H:224:ARG:HG2	1.19	1.02
1:F:211[B]:HIS:CD2	1:F:211[B]:HIS:N	2.22	1.02
1:E:211[B]:HIS:N	1:E:211[B]:HIS:CD2	2.22	1.02
1:B:179[A]:TYR:OH	5:B:6052:HOH:O	1.76	1.02
1:L:329:PRO:CG	1:L:359:ARG:HD2	1.89	1.02

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:329:PRO:CG	1:H: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:A:329:PRO:CG	1:A:359:ARG:HD2	1.90	1.02
1:L:176[B]:LYS:O	1:L:178[B]:GLY:N	1.90	1.02
1:L:211[B]:HIS:N	1:L:211[B]:HIS:CD2	2.22	1.02
1:B:179[B]:TYR:CD1	1:B:212[B]:GLU:HA	1.93	1.02
1:K:224:ARG:HH21	1:K:224:ARG:HG2	1.19	1.02
1:H:211[B]:HIS:N	1:H: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:I:179[B]:TYR:CD1	1:I:212[B]:GLU:HA	1.93	1.02
1:F:329:PRO:CG	1:F:359:ARG:HD2	1.90	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:CD2	1:I:211[B]:HIS:N	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:L:337:ARG:CG	1:L:338:ASN:H	1.73	0.98
1:D:285:ASP:HA	5:D:6027:HOH:O	1.60	0.98
1:J:179[A]:TYR:OH	5:J:5919:HOH:O	1.79	0.98
1:K:285:ASP:HA	5:K:1663:HOH:O	1.60	0.98
1:E:285:ASP:HA	5:E:745: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
1:F:337:ARG:CG	1:F:338:ASN:H	1.73	0.97
5:B:6040:HOH:O	1:C:60:ILE:HD11	1.62	0.97
1:B:211[B]:HIS:C	1:B:212[B]:GLU:CG	2.33	0.97

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:60:ILE:HD11	5:K:1679:HOH:O	1.65	0.97
1:L:337:ARG:HG3	1:L:338:ASN:H	0.87	0.96
1:C:406:GLU:HA	5:C:5984:HOH:O	1.66	0.96
1:H:399:LEU:H	1:H:400:PRO:HD2	1.30	0.96
1:D:192[A]:ARG:HD3	1:D:219:ASN:HD22	1.31	0.96
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:F:406:GLU:HA	5:F:5994:HOH:O	1.66	0.96
1:A:406:GLU:HA	5:A:5984:HOH:O	1.66	0.96
1:A:192[A]:ARG:HD3	1:A:219:ASN:HD22	1.31	0.96
1:F:399:LEU:H	1:F:400:PRO:HD2	1.30	0.95
1:G:337:ARG:HG3	1:G:338:ASN:H	0.87	0.95
1:B:406:GLU:HA	5:B:5985:HOH:O	1.66	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:J:399:LEU:H	1:J:400:PRO:HD2	1.30	0.95
1:C:409:GLN:HB3	5:C:6026:HOH:O	1.67	0.95
1:L:409:GLN:HB3	5:L:1818:HOH:O	1.67	0.95
1:I:337:ARG:HG3	1:I:338:ASN:H	0.87	0.94
1:H:406:GLU:HA	5:H:5998:HOH:O	1.66	0.94
1:K:406:GLU:HA	5:K:1618:HOH:O	1.66	0.94
1:F:192[A]:ARG:HD3	1:F:219:ASN:HD22	1.31	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: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:B:192[A]:ARG:HD3	1:B:219:ASN:HD22	1.31	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: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

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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:426:GLU:HB2	5:J:5977:HOH:O	1.70	0.91
1:F:211[B]:HIS:CD2	1:F:211[B]:HIS:H	1.87	0.91
1:G:179[B]:TYR:CE2	1:G:211[B]:HIS:HB2	2.06	0.91
1:I:179[B]:TYR:CE2	1:I:211[B]:HIS:HB2	2.06	0.91
1:A:179[B]:TYR:CE2	1:A:211[B]:HIS:HB2	2.06	0.91
1:E:337:ARG:HH11	1:F:61:ASN:CB	1.83	0.91
1:G:409:GLN:HB3	5:G:6036:HOH:O	1.67	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:J:179[B]:TYR:CE2	1:J:211[B]:HIS:HB2	2.06	0.90
1:I:426:GLU:HB2	5:I:5981:HOH:O	1.70	0.90
1:K:211[B]:HIS:C	1:K:212[B]:GLU:CG	2.33	0.90
1:L:179[B]:TYR:CE2	1:L:211[B]:HIS:HB2	2.06	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: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:C:426:GLU:HB2	5:C:5960:HOH:O	1.70	0.90
1:H:179[B]:TYR:CE2	1:H: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:G:337:ARG:HD2	1:L:61:ASN:HB3	1.50	0.90
1:B:426:GLU:HB2	5:B:5961:HOH:O	1.70	0.90
1:E:337:ARG:NH1	1:F:61:ASN:HB2	1.87	0.90
1:D:211[B]:HIS:H	1:D:211[B]:HIS:CD2	1.87	0.90
1:A:323:VAL:HA	5:A:6037:HOH:O	1.72	0.90
1:K:426:GLU:HB2	5:K:1593:HOH:O	1.70	0.90
1:E:426:GLU:HB2	5:E:675:HOH:O	1.70	0.90
1:E:211[B]:HIS:H	1:E:211[B]:HIS:CD2	1.87	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:L:426:GLU:HB2	5:L:1746:HOH:O	1.70	0.90
1:F:179[B]:TYR:CE2	1:F:211[B]:HIS:HB2	2.06	0.90
1:E:179[B]:TYR:CE2	1:E: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:A:61:ASN:HB3	1:F:337:ARG:CD	2.03	0.89
1:D:302:ILE:HD13	5:D:6001:HOH:O	1.72	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:I:302:ILE:HD13	5:I:6019:HOH:O	1.72	0.89
1:E:302:ILE:HD13	5:E:717:HOH:O	1.73	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:302:ILE:HD13	5:F:6008:HOH:O	1.72	0.89
1:I:211[B]:HIS:C	1:I:212[B]:GLU:CG	2.33	0.89
1:D:323:VAL:HA	5:D:6040:HOH:O	1.72	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:L:302:ILE:HD13	5:L:1788:HOH:O	1.72	0.89
1:J:302:ILE:HD13	5:J:6015: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
3:K:4481:ADP:H3'	5:K:1609:HOH:O	1.73	0.88
1:C:337:ARG:CG	1:C:338:ASN:H	1.73	0.88
3:H:4478:ADP:H3'	5:H:5990: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
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:L:177[B]:GLY:O	1:L:178[B]:GLY:C	2.12	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: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:F:426:GLU:HB2	5:F:5970:HOH:O	1.70	0.88
1:C:177[B]:GLY:O	1:C:178[B]:GLY:O	1.92	0.88
1:J:211[B]:HIS:CD2	1:J:211[B]:HIS:H	1.87	0.88
1:C:323:VAL:HA	5:C:6037:HOH:O	1.72	0.88
1:D:177[B]:GLY:O	1:D:178[B]:GLY:O	1.92	0.88
1:A:211[B]:HIS:CD2	1:A:211[B]:HIS:H	1.87	0.88
1:I:323:VAL:HA	5:I:6058:HOH:O	1.72	0.88
1:H:340:SER:OG	1:H:396:LEU:HA	1.74	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
3:L:4482:ADP:H3'	5:L:1762:HOH:O	1.73	0.87
1:D:180[B]:PHE:CD1	1:E:31:VAL:HB	2.09	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:C:337:ARG:HG3	1:C:338:ASN:H	0.87	0.87
1:B:337:ARG:HH11	1:C:61:ASN:CB	1.86	0.87
1:L:323:VAL:HA	5:L:1830:HOH:O	1.72	0.87
1:K:302:ILE:HD13	5:K:1635:HOH:O	1.72	0.87
1:F:177[B]:GLY:O	1:F:178[B]:GLY:O	1.92	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:177[B]:GLY:O	1:I:178[B]:GLY:C	2.12	0.87
1:G:323:VAL:HA	5:G:6047:HOH:O	1.72	0.87
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
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
1:B:177[B]:GLY:O	1:B:178[B]:GLY:C	2.12	0.87
5:D:6042:HOH:O	1:E:60:ILE:HD11	1.75	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
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
3:I:4479:ADP:H3'	5:I:5997:HOH:O	1.73	0.87
1:E:323:VAL:HA	5:E:759:HOH:O	1.72	0.87
1:L:177[B]:GLY:O	1:L:178[B]:GLY:O	1.92	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: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
3:G:4477:ADP:H3'	5:G:5986:HOH:O	1.73	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
1:D:177[B]:GLY:O	1:D:178[B]:GLY:C	2.12	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:J:177[B]:GLY:O	1:J:178[B]:GLY:O	1.92	0.86
1:C:340:SER:OG	1:C:396:LEU:HA	1.74	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:H:177[B]:GLY:O	1:H:178[B]:GLY:O	1.92	0.86
1:B:337:ARG:NH1	1:C:61:ASN:HB2	1.88	0.86
1:A:340:SER:OG	1:A:396:LEU:HA	1.74	0.86
1:I:211[B]:HIS:H	1:I:211[B]:HIS:CD2	1.87	0.86
1:G:340:SER:OG	1:G:396:LEU:HA	1.74	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	Distance(Å)	Clash(Å)
1:D:337:ARG:HH11	1:E:61:ASN:CB	1.87	0.85
1:L:435:THR:HG23	5:L:1742:HOH:O	1.76	0.85
1:A:435:THR:HG23	5:A:5957:HOH:O	1.76	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: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:F:340:SER:OG	1:F:396:LEU:HA	1.74	0.85
1:B:435:THR:HG23	5:B:5958:HOH:O	1.76	0.85
1:F:344:ARG:HD2	5:F:5984:HOH:O	1.76	0.85
1:L:344:ARG:HD2	5:L:1760:HOH:O	1.76	0.85
1:G:344:ARG:HD2	5:G:5984: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: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:E:435:THR:HG23	5:E:671:HOH:O	1.76	0.84
1:J:177[B]:GLY:O	1:J:178[B]:GLY:C	2.12	0.84
1:G:165:GLU:HB2	5:G:5971:HOH:O	1.78	0.84
1:K:435:THR:HG23	5:K:1589:HOH:O	1.76	0.84
1:K:165:GLU:HB2	5:K:1594:HOH:O	1.78	0.84
1:E:165:GLU:HB2	5:E:676:HOH:O	1.78	0.84
1:G:177[B]:GLY:O	1:G:178[B]:GLY:C	2.12	0.84
1:B:337:ARG:NH1	1:C:61:ASN:CB	2.41	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:I:165:GLU:HB2	5:I:5982:HOH:O	1.78	0.83
1:D:344:ARG:HD2	5:D:5977:HOH:O	1.76	0.83
1:C:435:THR:HG23	5:C:5957:HOH:O	1.76	0.83
1:C:344:ARG:HD2	5:C:5974:HOH:O	1.76	0.83
1:C:458:HIS:HD2	1:C:460:VAL:H	1.26	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:C:165:GLU:HB2	5:C:5961:HOH:O	1.78	0.83
1:G:337:ARG:NH1	1:L:61:ASN:HB2	1.94	0.83
1:J:458:HIS:HD2	1:J:460:VAL:H	1.26	0.83
1:B:165:GLU:HB2	5:B:5962:HOH:O	1.78	0.83
1:G:435:THR:HG23	5:G:5967:HOH:O	1.76	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:458:HIS:HD2	1:B:460:VAL:H	1.26	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:L:165:GLU:HB2	5:L:1747:HOH:O	1.78	0.82
1:H:344:ARG:HD2	5:H:5988:HOH:O	1.76	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:G:337:ARG:HH11	1:L:61:ASN:CB	1.92	0.81
1:B:40:ALA:CB	5:B:5982:HOH:O	2.29	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:E:170:GLY:HA2	1:E:172:ARG:HH22	1.47	0.80
1:C:40:ALA:CB	5:C:5981:HOH:O	2.29	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
3:E:4475:ADP:N9	3:E:4475:ADP:H1'	1.96	0.80
1:B:347:VAL:HB	5:B:6003:HOH:O	1.82	0.80
1:J:31:VAL:HB	1:K:180[B]:PHE:CD1	2.17	0.80
1:A:337:ARG:NH1	1:B:61:ASN:CB	2.45	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:458:HIS:HD2	1:D:460:VAL:H	1.26	0.80
1:L:170:GLY:HA2	1:L:172:ARG:HH22	1.47	0.80
1:H:170:GLY:HA2	1:H:172:ARG:HH22	1.47	0.80
1:B:170:GLY:HA2	1:B:172:ARG:HH22	1.46	0.80
1:J:347:VAL:HB	5:J:6019:HOH:O	1.82	0.80
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:A:347:VAL:HB	5:A:6002:HOH:O	1.82	0.79
1:H:61:ASN:CB	1:I:337:ARG:HH11	1.93	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: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:I:40:ALA:CB	5:I:6002:HOH:O	2.29	0.79
1:E:40:ALA:HB3	5:E:697:HOH:O	1.83	0.79
1:A:170:GLY:HA2	1:A:172:ARG:HH22	1.47	0.79
1:H:347:VAL:HB	5:H:6016:HOH:O	1.82	0.79
1:K:347:VAL:HB	5:K:1639:HOH:O	1.82	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:H:458:HIS:HD2	1:H:460:VAL:H	1.26	0.79
1:D:347:VAL:HB	5:D:6005:HOH:O	1.82	0.79
1:J:31:VAL:HB	1:K:180[B]:PHE:CE1	2.17	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:B:180[B]:PHE:CD1	1:C:31:VAL:HB	2.16	0.79
3:L:4482:ADP:N9	3:L:4482:ADP:H1'	1.96	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
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:K:337:ARG:HG3	1:K:338:ASN:H	0.87	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:D:170:GLY:HA2	1:D:172:ARG:HH22	1.47	0.79
1:F:347:VAL:HB	5:F:6012:HOH:O	1.82	0.79
1:F:170:GLY:HA2	1:F:172:ARG:HH22	1.47	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
1:I:447:ARG:HD3	5:I:6003:HOH:O	1.83	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:170:GLY:HA2	1:G:172:ARG:HH22	1.47	0.78
1:K:40:ALA:HB3	5:K:1615:HOH:O	1.83	0.78
3:K:4481:ADP:N9	3:K:4481:ADP:H1'	1.96	0.78
1:J:447:ARG:HD3	5:J:5999:HOH:O	1.83	0.78
1:I:61:ASN:HB2	1:J:337:ARG:NH1	1.98	0.78
1:G:40:ALA:HB3	5:G:5991:HOH:O	1.83	0.78
1:F:447:ARG:HD3	5:F:5992:HOH:O	1.83	0.78
1:C:347:VAL:HB	5:C:6002:HOH:O	1.82	0.78
1:L:75:VAL:HG23	5:L:1701:HOH:O	1.84	0.78
1:C:170:GLY:HA2	1:C:172:ARG:HH22	1.47	0.78
1:J:61:ASN:CB	1:K:337:ARG:NH1	2.47	0.78
1:B:75:VAL:HG23	5:B:5917:HOH:O	1.84	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:C:40:ALA:HB3	5:C:5981:HOH:O	1.83	0.78
1:A:75:VAL:HG23	5:A:5916:HOH:O	1.84	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:L:40:ALA:HB3	5:L:1768:HOH:O	1.83	0.77
1:H:170:GLY:HA2	1:H:172:ARG:NH2	1.99	0.77
1:C:170:GLY:HA2	1:C:172:ARG:NH2	2.00	0.77
1:H:75:VAL:HG23	5:H:5932:HOH:O	1.84	0.77
1:H:447:ARG:HD3	5:H:5996:HOH:O	1.83	0.77
1:G:337:ARG:HD3	1:L:61:ASN:HB3	1.65	0.77
1:J:170:GLY:HA2	1:J:172:ARG:NH2	1.99	0.77
1:G:447:ARG:HD3	5:G:5992:HOH:O	1.84	0.77
1:B:170:GLY:HA2	1:B:172:ARG:NH2	2.00	0.77
1:K:75:VAL:HG23	5:K:1548:HOH:O	1.84	0.77
1:F:75:VAL:HG23	5:F:5927:HOH:O	1.84	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:A:61:ASN:HB3	1:F:337:ARG:HD2	1.66	0.77
3:H:4478:ADP:N9	3:H:4478:ADP:H1'	1.96	0.77
1:G:61:ASN:HB2	1:H:337:ARG:NH1	1.99	0.77
1:H:61:ASN:HB2	1:I:337:ARG:NH1	1.97	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:F:170:GLY:HA2	1:F:172:ARG:NH2	2.00	0.77
1:A:447:ARG:HD3	5:A:5982:HOH:O	1.83	0.77
1:L:170:GLY:HA2	1:L:172:ARG:NH2	1.99	0.77
1:E:75:VAL:HG23	5:E:630:HOH:O	1.84	0.77
1:B:447:ARG:HD3	5:B:5983:HOH:O	1.83	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:251:LYS:HE3	5:J:5940:HOH:O	1.85	0.77
1:E:170:GLY:HA2	1:E:172:ARG:NH2	2.00	0.77
1:D:75:VAL:HG23	5:D:5919:HOH:O	1.84	0.77
1:B:251:LYS:HE3	5:B:5923:HOH:O	1.85	0.77
1:G:31:VAL:HB	1:H:180[B]:PHE:CD1	2.20	0.77
1:F:251:LYS:HE3	5:F:5933:HOH:O	1.85	0.77
1:L:191:ILE:HG13	5:L:1743:HOH:O	1.85	0.77
1:C:447:ARG:HD3	5:C:5982:HOH:O	1.83	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: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:G:180[B]:PHE:CD1	1:L:31:VAL:HB	2.20	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:F:191:ILE:HG13	5:F:5968:HOH:O	1.85	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: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:D:447:ARG:HD3	5:D:5985:HOH:O	1.83	0.76
1:J:191:ILE:HG13	5:J:5975:HOH:O	1.85	0.76
1:K:447:ARG:HD3	5:K:1616:HOH:O	1.84	0.76
1:K:251:LYS:CE	5:K:1554:HOH:O	2.34	0.76
1:G:191:ILE:HG13	5:G:5968:HOH:O	1.85	0.76
1:C:251:LYS:HE3	5:C:5923:HOH:O	1.85	0.76
1:I:176[B]:LYS:C	1:I:178[B]:GLY:H	1.88	0.76
1:G:251:LYS:CE	5:G:5932:HOH:O	2.34	0.76
1:E:251:LYS:HE3	5:E:636:HOH:O	1.85	0.76
1:K:349:ALA:HB3	5:K:1566:HOH:O	1.86	0.76
1:I:251:LYS:HE3	5:I:5943:HOH:O	1.85	0.76
1:B:191:ILE:HG13	5:B:5959:HOH:O	1.85	0.76
1:E:349:ALA:HB3	5:E:648: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
1:I:75:VAL:HG23	5:I:5937:HOH:O	1.84	0.76
1:E:1:SER:CB	1:E:4:HIS:HB3	2.16	0.76
1:B:251:LYS:CE	5:B:5923:HOH:O	2.34	0.76
1:J:176[B]:LYS:C	1:J:178[B]:GLY:H	1.88	0.76
1:G:75:VAL:HG23	5:G:5926:HOH:O	1.84	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:251:LYS:HE3	5:L:1707:HOH:O	1.85	0.76
1:G:176[B]:LYS:C	1:G:178[B]:GLY:H	1.88	0.76
1:C:311:LEU:HD13	1:C:369:LEU:HB3	1.68	0.76
1:L:176[B]:LYS:C	1:L:178[B]:GLY:H	1.88	0.75
1:I:31:VAL:HB	1:J:180[B]:PHE:CE1	2.21	0.75
1:G:61:ASN:HB3	1:H:337:ARG:HD3	1.67	0.75
1:K:251:LYS:HE3	5:K:1554:HOH:O	1.85	0.75
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:I:61:ASN:CB	1:J:337:ARG:HH11	1.99	0.75
5:G:6052:HOH:O	1:H:176[B]:LYS:HB3	1.85	0.75
1:K:1:SER:HB2	1:K:4:HIS:CB	2.15	0.75
1:C:191:ILE:HG13	5:C:5958:HOH:O	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
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: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
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: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:211[B]:HIS:NE2	5:G:6054:HOH:O	2.07	0.75
1:K:1:SER:CB	1:K:4:HIS:HB3	2.15	0.75
1:G:180[B]:PHE:CE1	1:L:31:VAL:HB	2.22	0.75
1:E:251:LYS:CE	5:E:636:HOH:O	2.34	0.75
1:E:191:ILE:HG13	5:E:672:HOH:O	1.85	0.75
1:G:349:ALA:HB3	5:G:5944:HOH:O	1.86	0.75
1:D:176[B]:LYS:C	1:D:178[B]:GLY:H	1.88	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:F:176[B]:LYS:C	1:F:178[B]:GLY:H	1.88	0.75
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:B:224:ARG:NH2	1:B:224:ARG:HG2	1.97	0.75
1:A:170:GLY:HA2	1:A:172:ARG:NH2	2.00	0.75
1:C:176[B]:LYS:C	1:C:178[B]:GLY:H	1.88	0.75
1:K:179[A]:TYR:O	1:K:181[A]:PRO:CD	2.35	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:189:GLN:NE2	1:F:209[A]:HIS:HE1	1.85	0.75
1:L:311:LEU:HD13	1:L:369:LEU:HB3	1.69	0.75
1:G:189:GLN:NE2	1:G:209[A]:HIS:HE1	1.85	0.75
1:G:31:VAL:HB	1:H:180[B]:PHE:CE1	2.21	0.75
1:B:179[A]:TYR:O	1:B:181[A]:PRO:CD	2.34	0.75
1:H:61:ASN:HB3	1:I:337:ARG:HD2	1.66	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:E:311:LEU:HD13	1:E:369:LEU:HB3	1.69	0.75
1:I:311:LEU:HD13	1:I:369:LEU:HB3	1.68	0.75
1:B:189:GLN:NE2	1:B:209[A]:HIS:HE1	1.85	0.75
1:G:179[A]:TYR:O	1:G:181[A]:PRO:CD	2.34	0.75
1:E:176[B]:LYS:C	1:E:178[B]:GLY:H	1.88	0.75
1:J:179[A]:TYR:O	1:J:181[A]:PRO:CD	2.35	0.75
1:C:1:SER:CB	1:C:4:HIS:HB3	2.16	0.75
1:L:400:PRO:O	1:L:402:GLU:N	2.20	0.75
1:A:311:LEU:HD13	1:A:369:LEU:HB3	1.68	0.75
1:J:311:LEU:HD13	1:J:369:LEU:HB3	1.68	0.75
3:J:4480:ADP:H1'	3:J:4480:ADP:N9	1.96	0.74
1:A:179[A]:TYR:O	1:A:181[A]:PRO:CD	2.35	0.74
1:J:189:GLN:NE2	1:J:209[A]:HIS:HE1	1.85	0.74
1:H:191:ILE:HG13	5:H:5972:HOH:O	1.85	0.74
1:D:349:ALA:HB3	5:D:5937:HOH:O	1.86	0.74
1:B:349:ALA:HB3	5:B:5935:HOH:O	1.86	0.74
1:C:180[B]:PHE:CD1	1:D:31:VAL:HB	2.22	0.74
1:A:31:VAL:HB	1:F:180[B]:PHE:CD1	2.22	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:L:349:ALA:HB3	5:L:1719:HOH:O	1.86	0.74
1:D:311:LEU:HD13	1:D:369:LEU:HB3	1.69	0.74
1:D:337:ARG:HH11	1:E:61:ASN:HB3	1.52	0.74
1:K:61:ASN:CB	1:L:337:ARG:NH1	2.51	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
5:J:6059:HOH:O	1:K:176[B]:LYS:HB3	1.86	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
1:F:1:SER:CB	1:F:4:HIS:HB3	2.15	0.74
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:A:251:LYS:CE	5:A:5922:HOH:O	2.34	0.74
1:F:349:ALA:HB3	5:F:5944:HOH:O	1.86	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:189:GLN:NE2	1:E:209[A]:HIS:HE1	1.85	0.74
1:D:179[A]:TYR:O	1:D:181[A]:PRO:CD	2.34	0.74
1:I:1:SER:CB	1:I:4:HIS:HB3	2.16	0.74
1:I:189:GLN:NE2	1:I:209[A]:HIS:HE1	1.85	0.74
1:L:189:GLN:NE2	1:L:209[A]:HIS:HE1	1.85	0.74
1:K:176[B]:LYS:C	1:K:178[B]:GLY:H	1.88	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: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:I:399:LEU:H	1:I:400:PRO:CD	2.01	0.74
1:G:407:ILE:HB	1:G:408:PRO:HD2	1.70	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:F:400:PRO:O	1:F:402:GLU:N	2.20	0.73
1:L:407:ILE:HB	1:L:408:PRO:HD2	1.70	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: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:E:400:PRO:O	1:E:402:GLU:N	2.20	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:C:349:ALA:HB3	5:C:5934:HOH:O	1.86	0.73
1:K:311:LEU:HD13	1:K:369:LEU:HB3	1.68	0.73
1:K:61:ASN:CB	1:L:337:ARG:HH11	2.01	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: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:176[B]:LYS:HB3	5:F:6052:HOH:O	1.89	0.73
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:J:1:SER:CB	1:J:4:HIS:HB3	2.15	0.73
1:D:399:LEU:H	1:D:400:PRO:CD	2.01	0.73
1:F:311:LEU:HD13	1:F:369:LEU:HB3	1.68	0.73
1:C:57:TRP:O	1:C:58:LYS:O	2.07	0.73
1:E:57:TRP:O	1:E:58:LYS:O	2.07	0.73
1:H:179[B]:TYR:CE1	1:H:212[B]:GLU:CA	2.72	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:269:HIS:HE1	4:F:5905:PPQ:CEP	2.02	0.73
1:C:269:HIS:HE1	4:C:5902:PPQ:CEP	2.02	0.73
1:B:407:ILE:HB	1:B:408:PRO:HD2	1.70	0.73
1:I:407:ILE:HB	1:I:408:PRO:HD2	1.70	0.73
1:H:189:GLN:NE2	1:H:209[A]:HIS:HE1	1.85	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:D:407:ILE:HB	1:D:408:PRO:HD2	1.70	0.73
5:I:6063:HOH:O	1:J:176[B]:LYS:HB3	1.88	0.72
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: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:G:57:TRP:O	1:G:58:LYS:O	2.07	0.72
1:F:179[B]:TYR:CE1	1:F:212[B]:GLU:CA	2.72	0.72
1:K:269:HIS:HE1	4:K:5910:PPQ:CEP	2.02	0.72
1:B:57:TRP:O	1:B:58:LYS:O	2.07	0.72
1:I:57:TRP:O	1:I:58:LYS:O	2.07	0.72
1:G:179[B]:TYR:CE1	1:G:212[B]:GLU:CA	2.72	0.72
1:J:179[B]:TYR:CE1	1:J:212[B]:GLU:CA	2.72	0.72
1:I:269:HIS:HE1	4:I:5908:PPQ:CEP	2.02	0.72
1:L:1:SER:CB	1:L:4:HIS:HB3	2.15	0.72
1:A:407:ILE:HB	1:A:408:PRO:HD2	1.70	0.72
1:A:399:LEU:H	1:A:400:PRO:CD	2.01	0.72
1:C:179[B]:TYR:CE1	1:C:212[B]:GLU:CA	2.72	0.72
1:I:179[B]:TYR:CE1	1:I:212[B]:GLU:CA	2.72	0.72
1:A:179[B]:TYR:CE1	1:A:212[B]:GLU:CA	2.72	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:J:269:HIS:HE1	4:J:5909:PPQ:CEP	2.02	0.72
1:D:269:HIS:HE1	4:D:5903:PPQ:CEP	2.02	0.72
1:G:269:HIS:HE1	4:G:5906:PPQ:CEP	2.02	0.72
1:B:400:PRO:O	1:B:402:GLU:N	2.20	0.72
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:I:31:VAL:HB	1:J:180[B]:PHE:CD1	2.25	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:L:57:TRP:O	1:L:58:LYS:O	2.07	0.72
1:G:1:SER:CB	1:G:4:HIS:HB3	2.15	0.72
1:B:224:ARG:CG	1:B:224:ARG:HH21	2.01	0.72
1:K:400:PRO:O	1:K:402:GLU:N	2.20	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:A:269:HIS:HE1	4:A:5900:PPQ:CEP	2.02	0.72
1:J:399:LEU:H	1:J:400:PRO:CD	2.01	0.72
1:L:179[B]:TYR:CE1	1:L:212[B]:GLU:CA	2.72	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: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
3:C:4473:ADP:HI'	3:C:4473:ADP:N9	1.96	0.71
1:L:176[B]:LYS:HB3	5:L:1682:HOH:O	1.90	0.71
1:H:400:PRO:O	1:H:402:GLU:N	2.20	0.71
1:B:399:LEU:H	1:B:400:PRO:CD	2.01	0.71
1:H:57:TRP:O	1:H:58:LYS:O	2.07	0.71
1:C:407:ILE:HB	1:C:408:PRO:HD2	1.70	0.71
1:A:180[B]:PHE:CD1	1:B:31:VAL:HB	2.25	0.71
1:H:407:ILE:HB	1:H:408:PRO:HD2	1.70	0.71
1:G:384:ASN:HD22	1:G:384:ASN:N	1.88	0.71
1:F:57:TRP:O	1:F:58:LYS:O	2.07	0.71
1:E:399:LEU:H	1:E:400:PRO:CD	2.01	0.71
1:D:400:PRO:O	1:D:402:GLU:N	2.20	0.71
1:K:61:ASN:HB2	1:L:337:ARG:NH1	2.05	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:D:57:TRP:O	1:D:58:LYS:O	2.07	0.71
1:L:269:HIS:HE1	4:L:5911:PPQ:CEP	2.02	0.71
1:E:384:ASN:N	1:E:384:ASN:HD22	1.88	0.71
1:J:337:ARG:HG3	1:J:338:ASN:CA	2.20	0.71
1:H:31:VAL:HB	1:I:180[B]:PHE:CD1	2.25	0.71
1:F:399:LEU:H	1:F:400:PRO:CD	2.01	0.71
1:A:57:TRP:O	1:A:58:LYS:O	2.07	0.71
1:K:31:VAL:HB	1:L:180[B]:PHE:CD1	2.25	0.71
1:F:1:SER:HB2	1:F:4:HIS:CB	2.15	0.71
1:A:179[A]:TYR:O	1:A:181[A]:PRO:HD3	1.91	0.71
1:H:269:HIS:HE1	4:H:5907:PPQ:CEP	2.02	0.71
1:C:384:ASN:HD22	1:C:384:ASN:N	1.88	0.71
1:I:179[A]:TYR:O	1:I:181[A]:PRO:HD3	1.91	0.70
1:I:381:GLY:HA2	1:I:386:ILE:HG13	1.74	0.70
1:H:384:ASN:HD22	1:H:384:ASN:N	1.88	0.70
1:K:179[A]:TYR:O	1:K:181[A]:PRO:HD3	1.91	0.70
1:J:211[B]:HIS:NE2	5:J:5914:HOH:O	2.10	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:384:ASN:HD22	1:A:384:ASN:N	1.88	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:J:384:ASN:N	1:J:384:ASN:HD22	1.89	0.70
1:I:401:PRO:HA	1:I:404:ALA:HA	1.74	0.70
1:D:176[B]:LYS:HB3	5:E:764:HOH:O	1.90	0.70
1:C:337:ARG:HG3	1:C:338:ASN:CA	2.20	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:L:179[A]:TYR:O	1:L: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:E:179[A]:TYR:O	1:E:181[A]:PRO:HD3	1.92	0.70
1:I:384:ASN:HD22	1:I:384:ASN:N	1.88	0.70
1:C:381:GLY:HA2	1:C:386:ILE:HG13	1.74	0.70
1:J:179[A]:TYR:O	1:J:181[A]:PRO:HD3	1.91	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:E:224:ARG:HH21	1:E:224:ARG:CG	2.01	0.70
1:F:384:ASN:HD22	1:F:384:ASN:N	1.88	0.70
1:D:381:GLY:HA2	1:D:386:ILE:HG13	1.74	0.70
1:B:401:PRO:HA	1:B:404:ALA:HA	1.74	0.70
1:F:381:GLY:HA2	1:F:386:ILE:HG13	1.74	0.70
1:G:381:GLY:HA2	1:G:386:ILE:HG13	1.74	0.70
1:H:1:SER:HB2	1:H:4:HIS:CB	2.15	0.69
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
3:F:4476:ADP:N9	3:F:4476:ADP:H1'	1.96	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
1:B:337:ARG:HH11	1:C:61:ASN:HB3	1.56	0.69
1:C:179[A]:TYR:O	1:C:181[A]:PRO:HD3	1.91	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:B:179[A]:TYR:O	1:B:181[A]:PRO:HD3	1.91	0.69
1:L:224:ARG:HG2	1:L:224:ARG:NH2	1.97	0.69
1:D:426:GLU:HG2	5:D:5936:HOH:O	1.93	0.69
1:K:384:ASN:HD22	1:K:384:ASN:N	1.88	0.69
1:B:384:ASN:N	1:B:384:ASN:HD22	1.88	0.69
1:D:1:SER:CB	1:D:4:HIS:HB3	2.16	0.69
1:C:211[B]:HIS:NE2	5:C:6044:HOH:O	2.05	0.69
1:D:179[B]:TYR:CE1	1:D:212[B]:GLU:HA	2.27	0.69
1:G:179[B]:TYR:CE1	1:G:212[B]:GLU:HA	2.27	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:224:ARG:HH21	1:F:224:ARG:CG	2.01	0.69
1:A:426:GLU:HG2	5:A:5933:HOH:O	1.93	0.69
1:C:401:PRO:HA	1:C:404:ALA:HA	1.74	0.69
1:J:401:PRO:HA	1:J:404:ALA:HA	1.74	0.69
1:A:381:GLY:HA2	1:A:386:ILE:HG13	1.74	0.69
1:H:381:GLY:HA2	1:H:386:ILE:HG13	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:D:179[A]:TYR:O	1:D:181[A]:PRO:HD3	1.91	0.69
1:B:179[B]:TYR:CE1	1:B:212[B]:GLU:HA	2.27	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:G:211[A]:HIS:CD2	1:G:212[A]:GLU:H	2.11	0.69
1:I:211[A]:HIS:CD2	1:I:212[A]:GLU:H	2.11	0.69
1:J:231:LYS:HE2	5:J:5926:HOH:O	1.93	0.69
1:G:231:LYS:HE2	5:G:5917:HOH:O	1.93	0.69
1:K:426:GLU:HG2	5:K:1565: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:I:224:ARG:CG	1:I:224:ARG:HH21	2.01	0.69
1:B:426:GLU:HG2	5:B:5934:HOH:O	1.93	0.69
1:H:401:PRO:HA	1:H:404:ALA:HA	1.74	0.69
1:A:180[B]:PHE:CE1	1:B:31:VAL:HB	2.28	0.69
1:A:211[A]:HIS:CD2	1:A:212[A]:GLU:H	2.11	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:F:426:GLU:HG2	5:F:5943:HOH:O	1.92	0.69
1:L:381:GLY:HA2	1:L:386:ILE:HG13	1.74	0.69
1:L:211[A]:HIS:CD2	1:L:212[A]:GLU:H	2.11	0.68
1:L:179[B]:TYR:CE1	1:L:212[B]:GLU:HA	2.27	0.68
1:A:337:ARG:HG3	1:A:338:ASN:CA	2.20	0.68
1:J:427:PHE:HB2	5:J:6046:HOH:O	1.93	0.68
1:K:179[B]:TYR:CE1	1:K:212[B]:GLU:HA	2.27	0.68
1:E:179[B]:TYR:CE1	1:E:212[B]:GLU:HA	2.27	0.68
1:J:179[B]:TYR:CE1	1:J:212[B]:GLU:HA	2.27	0.68
1:B:231:LYS:HE2	5:B:5908:HOH:O	1.93	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:H:427:PHE:HB2	5:H:6043:HOH:O	1.94	0.68
1:C:180[B]:PHE:CE1	1:D:31:VAL:HB	2.29	0.68
1:I:269:HIS:HE1	4:I:5908:PPQ:HEP3	1.58	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:A:427:PHE:HB2	5:A:6029:HOH:O	1.94	0.68
1:D:427:PHE:HB2	5:D:6032:HOH:O	1.94	0.68
1:A:179[B]:TYR:CE1	1:A:212[B]:GLU:HA	2.27	0.68
1:H:337:ARG:HG3	1:H:338:ASN:CA	2.20	0.68
1:C:337:ARG:NH1	1:D:61:ASN:HB2	2.09	0.68
1:B:329:PRO:HG3	5:B:6017:HOH:O	1.94	0.68
1:A:269:HIS:HE1	4:A:5900:PPQ:HEP3	1.58	0.68
1:L:427:PHE:HB2	5:L:1821:HOH:O	1.94	0.68
1:C:114:TYR:CD2	1:C:431:GLY:HA3	2.29	0.68
1:E:211[A]:HIS:CD2	1:E:212[A]:GLU:H	2.11	0.68
1:K:269:HIS:HE1	4:K:5910:PPQ:HEP3	1.58	0.68
1:J:224:ARG:CG	1:J:224:ARG:HH21	2.01	0.68
1:A:224:ARG:HH21	1:A:224:ARG:CG	2.01	0.68
1:J:426:GLU:HG2	5:J:5950:HOH:O	1.93	0.68
1:E:426:GLU:HG2	5:E:647:HOH:O	1.92	0.68
1:J:381:GLY:HA2	1:J:386:ILE:HG13	1.74	0.68
1:J:114:TYR:CD2	1:J:431:GLY:HA3	2.29	0.68
1:C:427:PHE:HB2	5:C:6029:HOH:O	1.94	0.68
1:K:211[A]:HIS:CD2	1:K:212[A]:GLU:H	2.11	0.68
1:I:61:ASN:CB	1:J:337:ARG:NH1	2.56	0.68
1:H:179[B]:TYR:CE1	1:H:212[B]:GLU:HA	2.27	0.68
1:L:337:ARG:HG3	1:L:338:ASN:CA	2.20	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:B:269:HIS:HE1	4:B:5901:PPQ:HEP3	1.58	0.68
1:G:114:TYR:CD2	1:G:431:GLY:HA3	2.29	0.68
1:E:114:TYR:CD2	1:E:431:GLY:HA3	2.29	0.68
1:L:401:PRO:HA	1:L:404:ALA:HA	1.74	0.68
1:F:401:PRO:HA	1:F:404:ALA:HA	1.74	0.68
1:H:211[A]:HIS:CD2	1:H:212[A]:GLU:H	2.11	0.68
1:D:337:ARG:HG3	1:D:338:ASN:CA	2.20	0.68
1:I:337:ARG:HG3	1:I:338:ASN:CA	2.20	0.68
1:I:231:LYS:HE2	5:I:5928:HOH:O	1.93	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:K:114:TYR:CD2	1:K:431:GLY:HA3	2.29	0.68
1:K:337:ARG:HG3	1:K:338:ASN:CA	2.20	0.68
1:K:323:VAL:CG1	5:K:1677:HOH:O	2.20	0.68
1:A:231:LYS:HE2	5:A:5907:HOH:O	1.93	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:224:ARG:HG2	1:I:224:ARG:NH2	1.97	0.68
1:K:427:PHE:HB2	5:K:1668:HOH:O	1.93	0.68
1:G:401:PRO:HA	1:G:404:ALA:HA	1.74	0.68
1:A:114:TYR:CD2	1:A:431:GLY:HA3	2.29	0.68
1:L:360:PHE:CE2	1:L:361:PRO:HD3	2.29	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:F:211[A]:HIS:CD2	1:F:212[A]:GLU:H	2.11	0.67
1:D:211[A]:HIS:CD2	1:D:212[A]:GLU:H	2.11	0.67
1:G:212[A]:GLU:HG3	1:G:218:GLN:NE2	2.10	0.67
1:B:427:PHE:HB2	5:B:6030:HOH:O	1.94	0.67
1:C:211[A]:HIS:CD2	1:C:212[A]:GLU:H	2.11	0.67
1:L:269:HIS:HE1	4:L:5911:PPQ:HEP3	1.58	0.67
1:J:360:PHE:CE2	1:J:361:PRO:HD3	2.29	0.67
1:I:360:PHE:CE2	1:I:361:PRO:HD3	2.29	0.67
1:L:114:TYR:CD2	1:L:431:GLY:HA3	2.29	0.67
1:F:114:TYR:CD2	1:F:431:GLY:HA3	2.29	0.67
1:D:212[A]:GLU:HG3	1:D:218:GLN:NE2	2.10	0.67
1:I:61:ASN:CB	1:J:337:ARG:CD	2.67	0.67
1:C:337:ARG:HH11	1:D:61:ASN:CB	2.08	0.67
1:C:231:LYS:HE2	5:C:5909:HOH:O	1.93	0.67
1:A:329:PRO:HG3	5:A:6016:HOH:O	1.94	0.67
1:K:224:ARG:HH21	1:K:224:ARG:CG	2.01	0.67
1:C:426:GLU:HG2	5:C:5933:HOH:O	1.93	0.67
1:B:114:TYR:CD2	1:B:431:GLY:HA3	2.29	0.67
1:F:211[B]:HIS:NE2	5:F:5906:HOH:O	2.08	0.67
1:H:212[A]:GLU:HG3	1:H:218:GLN:NE2	2.10	0.67
1:G:329:PRO:HG3	5:G:6026:HOH:O	1.94	0.67
1:L:384:ASN:N	1:L:384:ASN:HD22	1.88	0.67
1:K:212[A]:GLU:HG3	1:K:218:GLN:NE2	2.10	0.67
1:A:212[A]:GLU:HG3	1:A:218:GLN:NE2	2.10	0.67
1:J:212[A]:GLU:HG3	1:J:218:GLN:NE2	2.10	0.67
1:L:231:LYS:HE2	5:L:1692:HOH:O	1.93	0.67
1:C:337:ARG:HD3	1:D:61:ASN:HB3	1.75	0.67
1:F:329:PRO:HG3	5:F:6026:HOH:O	1.94	0.67
1:H:329:PRO:HG3	5:H:6030:HOH:O	1.94	0.67
1:F:360:PHE:CE2	1:F:361:PRO:HD3	2.29	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:A:224:ARG:NH2	1:A:224:ARG:HG2	1.97	0.67
1:I:426:GLU:HG2	5:I:5954:HOH:O	1.92	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:401:PRO:HA	1:E:404:ALA:HA	1.74	0.67
1:I:212[A]:GLU:HG3	1:I:218:GLN:NE2	2.10	0.67
1:H:269:HIS:HE1	4:H:5907:PPQ:HEP3	1.58	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:176[B]:LYS:C	1:H:178[B]:GLY:N	2.47	0.67
1:B:211[A]:HIS:CD2	1:B:212[A]:GLU:H	2.11	0.67
1:C:269:HIS:HE1	4:C:5902:PPQ:HEP3	1.58	0.67
1:E:360:PHE:CE2	1:E:361:PRO:HD3	2.29	0.67
1:B:360:PHE:CE2	1:B:361:PRO:HD3	2.29	0.67
1:E:399:LEU:N	1:E:400:PRO:HD2	2.09	0.67
1:L:426:GLU:HG2	5:L:1718:HOH:O	1.93	0.67
1:D:114:TYR:CD2	1:D:431:GLY:HA3	2.29	0.67
1:I:427:PHE:HB2	5:I:6050:HOH:O	1.94	0.67
1:E:212[A]:GLU:HG3	1:E:218:GLN:NE2	2.10	0.67
1:H:211[B]:HIS:NE2	5:H:5912:HOH:O	2.11	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: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:K:179[A]:TYR:C	1:K:181[A]:PRO:HD2	2.16	0.66
1:H:179[A]:TYR:C	1:H:181[A]:PRO:HD2	2.16	0.66
1:J:179[A]:TYR:C	1:J:181[A]:PRO:HD2	2.16	0.66
1:I:329:PRO:HG3	5:I:6037:HOH:O	1.94	0.66
1:E:427:PHE:HB2	5:E:750:HOH:O	1.94	0.66
1:E:315:THR:O	1:E:318:SER:HB2	1.96	0.66
1:D:179[A]:TYR:C	1:D:181[A]:PRO:HD2	2.16	0.66
1:G:179[A]:TYR:C	1:G:181[A]:PRO:HD2	2.16	0.66
1:D:360:PHE:CE2	1:D:361:PRO:HD3	2.29	0.66
1:H:360:PHE:CE2	1:H:361:PRO:HD3	2.29	0.66
1:B:323:VAL:CG1	5:B:6038:HOH:O	2.20	0.66
1:I:385:LYS:HE2	5:I:5992:HOH:O	1.95	0.66
1:A:82:ASP:HB3	5:A:5943:HOH:O	1.96	0.66
1:K:315:THR:O	1:K:318:SER:HB2	1.96	0.66
1:C:82:ASP:HB3	5:C:5943:HOH:O	1.96	0.66
1:E:179[A]:TYR:C	1:E:181[A]:PRO:HD2	2.16	0.66
1:J:329:PRO:HG3	5:J:6033:HOH:O	1.94	0.66
1:G:385:LYS:HE2	5:G:5981:HOH:O	1.95	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:L:329:PRO:HG3	5:L:1808:HOH:O	1.94	0.66
1:K:360:PHE:CE2	1:K:361:PRO:HD3	2.29	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:L:82:ASP:HB3	5:L:1728:HOH:O	1.96	0.66
1:K:211[B]:HIS:NE2	5:K:1381:HOH:O	2.04	0.66
1:A:179[B]:TYR:CD1	1:A:212[B]:GLU:CA	2.77	0.66
1:A:61:ASN:HB3	1:F:337:ARG:HD3	1.76	0.66
1:H:231:LYS:HE2	5:H:5924:HOH:O	1.93	0.66
1:K:298:ILE:O	1:K:302:ILE:HG13	1.96	0.66
1:C:385:LYS:HE2	5:C:5971:HOH:O	1.95	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:F:385:LYS:HE2	5:F:5981:HOH:O	1.95	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:C:298:ILE:O	1:C:302:ILE:HG13	1.96	0.66
1:I:399:LEU:N	1:I:400:PRO:HD2	2.09	0.66
1:D:25:LYS:HD3	5:D:5949:HOH:O	1.96	0.66
1:F:212[A]:GLU:HG3	1:F:218:GLN:NE2	2.10	0.66
1:A:360:PHE:CE2	1:A:361:PRO:HD3	2.29	0.66
1:J:269:HIS:HE1	4:J:5909:PPQ:HEP3	1.58	0.66
1:B:82:ASP:HB3	5:B:5944:HOH:O	1.96	0.66
1:K:385:LYS:HE2	5:K:1604:HOH:O	1.95	0.66
1:L:385:LYS:HE2	5:L:1757:HOH:O	1.95	0.66
1:L:315:THR:O	1:L:318:SER:HB2	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:I:298:ILE:O	1:I:302:ILE:HG13	1.96	0.66
1:G:427:PHE:HB2	5:G:6039:HOH:O	1.94	0.66
1:F:179[A]:TYR:C	1:F:181[A]:PRO:HD2	2.16	0.66
1:L:176[B]:LYS:C	1:L:178[B]:GLY:N	2.47	0.66
1:B:176[B]:LYS:C	1:B:178[B]:GLY:N	2.47	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:J:82:ASP:HB3	5:J:5960:HOH:O	1.95	0.66
1:L:334:TYR:CD1	5:L:1764:HOH:O	2.49	0.66
1:I:25:LYS:HD3	5:I:5967:HOH:O	1.96	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:A:334:TYR:CD1	5:A:5978: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:I:211[B]:HIS:NE2	5:I:5913:HOH:O	2.09	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:B:206:VAL:O	1:C:34:PRO:HG2	1.97	0.65
1:I:308:ILE:HG21	1:I:374:LEU:HD13	1.78	0.65
1:A:315:THR:O	1:A:318:SER:HB2	1.96	0.65
1:J:385:LYS:HE2	5:J:5988:HOH:O	1.96	0.65
1:H:55:GLY:HA3	5:H:5961:HOH:O	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:C:315:THR:O	1:C:318:SER:HB2	1.96	0.65
1:J:315:THR:O	1:J:318:SER:HB2	1.95	0.65
1:J:25:LYS:HD3	5:J:5963:HOH:O	1.96	0.65
1:J:55:GLY:HA3	5:J:5963:HOH:O	1.96	0.65
1:C:25:LYS:HD3	5:C:5946:HOH:O	1.96	0.65
1:F:82:ASP:HB3	5:F:5953:HOH:O	1.96	0.65
1:G:298:ILE:O	1:G:302:ILE:HG13	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:K:55:GLY:HA3	5:K:1578:HOH:O	1.96	0.65
1:I:82:ASP:HB3	5:I:5964:HOH:O	1.96	0.65
1:I:334:TYR:CD1	5:I:5999:HOH:O	2.49	0.65
1:D:315:THR:O	1:D:318:SER:HB2	1.96	0.65
1:E:179[B]:TYR:CD1	1:E:212[B]:GLU:CA	2.77	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:C:25:LYS:CD	5:C:5946:HOH:O	2.45	0.65
1:B:308:ILE:HG21	1:B:374:LEU:HD13	1.78	0.65
1:H:82:ASP:HB3	5:H:5958:HOH:O	1.96	0.65
1:C:308:ILE:HG21	1:C:374:LEU:HD13	1.78	0.65
1:F:334:TYR:CD1	5:F:5988:HOH:O	2.49	0.65
1:K:61:ASN:HB3	1:L:337:ARG:HD3	1.78	0.65
1:I:179[A]:TYR:C	1:I:181[A]:PRO:HD2	2.16	0.65
1:A:323:VAL:CG1	5:A:6037:HOH:O	2.20	0.65
1:J:298:ILE:O	1:J:302:ILE:HG13	1.96	0.65
1:C:334:TYR:CD1	5:C:5978:HOH:O	2.49	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:25:LYS:HD3	5:F:5956:HOH:O	1.96	0.65
1:J:61:ASN:HB3	1:K:337:ARG:HH11	1.61	0.65
1:A:61:ASN:CB	1:F:337:ARG:HH11	2.10	0.65
1:F:224:ARG:NH2	1:F:224:ARG:HG2	1.97	0.65
1:H:298:ILE:O	1:H:302:ILE:HG13	1.96	0.65
1:F:201:GLN:HA	5:F:6013:HOH:O	1.97	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:D:59:GLY:C	1:D:61:ASN:H	2.01	0.65
1:B:298:ILE:O	1:B:302:ILE:HG13	1.96	0.65
1:I:201:GLN:HA	5:I:6024:HOH:O	1.97	0.65
1:L:25:LYS:HD3	5:L:1731:HOH:O	1.96	0.65
1:E:82:ASP:HB3	5:E:657:HOH:O	1.96	0.65
1:J:334:TYR:CD1	5:J:5995:HOH:O	2.49	0.65
1:H:385:LYS:HE2	5:H:5985:HOH:O	1.95	0.65
1:F:179[B]:TYR:CD1	1:F:212[B]:GLU:CA	2.77	0.65
1:L:179[B]:TYR:CD1	1:L:212[B]:GLU:CA	2.77	0.65
1:I:323:VAL:CG1	5:I:6058:HOH:O	2.20	0.65
1:D:399:LEU:N	1:D:400:PRO:HD2	2.09	0.65
1:D:25:LYS:CD	5:D:5949:HOH:O	2.45	0.65
1:E:55:GLY:HA3	5:E:660:HOH:O	1.96	0.65
1:B:334:TYR:CD1	5:B:5979:HOH:O	2.49	0.65
1:I:176[B]:LYS:C	1:I:178[B]:GLY:N	2.47	0.64
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
1:F:399:LEU:N	1:F:400:PRO:HD2	2.09	0.64
1:K:25:LYS:CD	5:K:1578:HOH:O	2.45	0.64
1:F:25:LYS:CD	5:F:5956:HOH:O	2.45	0.64
1:H:308:ILE:HG21	1:H:374:LEU:HD13	1.78	0.64
1:F:308:ILE:HG21	1:F:374:LEU:HD13	1.78	0.64
1:G:82:ASP:HB3	5:G:5953:HOH:O	1.95	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: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:A:55:GLY:HA3	5:A:5946:HOH:O	1.96	0.64
1:L:201:GLN:HA	5:L:1793:HOH:O	1.97	0.64
1:G:25:LYS:HD3	5:G:5956:HOH:O	1.96	0.64
1:A:31:VAL:HB	1:F:180[B]:PHE:CE1	2.31	0.64
1:H:25:LYS:HD3	5:H:5961:HOH:O	1.96	0.64
1:L:25:LYS:CD	5:L:1731:HOH:O	2.45	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:334:TYR:CD1	5:E:693:HOH:O	2.49	0.64
1:J:308:ILE:HG21	1:J:374:LEU:HD13	1.78	0.64
1:E:201:GLN:HA	5:E:722:HOH:O	1.97	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:A:25:LYS:HD3	5:A:5946:HOH:O	1.96	0.64
1:D:201:GLN:HA	5:D:6006:HOH:O	1.97	0.64
1:A:308:ILE:HG21	1:A:374:LEU:HD13	1.78	0.64
1:E:308:ILE:HG21	1:E:374:LEU:HD13	1.78	0.64
5:H:6056:HOH:O	1:I:176[B]:LYS:HB3	1.96	0.64
1:B:59:GLY:C	1:B:61:ASN:H	2.01	0.64
1:B:399:LEU:N	1:B:400:PRO:HD2	2.09	0.64
1:L:458:HIS:CD2	1:L:460:VAL:H	2.14	0.64
1:D:55:GLY:HA3	5:D:5949:HOH:O	1.96	0.64
1:I:25:LYS:CD	5:I:5967:HOH:O	2.45	0.64
1:D:82:ASP:HB3	5:D:5946:HOH:O	1.96	0.64
1:D:385:LYS:HE2	5:D:5974:HOH:O	1.95	0.64
1:A:385:LYS:HE2	5:A:5971:HOH:O	1.95	0.64
1:F:176[B]:LYS:C	1:F:178[B]:GLY:N	2.47	0.64
1:J:59:GLY:C	1:J:61:ASN:H	2.01	0.64
1:B:25:LYS:CD	5:B:5947:HOH:O	2.45	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:G:59:GLY:C	1:G:61:ASN:H	2.01	0.64
1:D:308:ILE:HG21	1:D:374:LEU:HD13	1.78	0.64
1:A:201:GLN:HA	5:A:6003:HOH:O	1.97	0.64
1:L:308:ILE:HG21	1:L:374:LEU:HD13	1.78	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: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:L:82:ASP:O	1:L:84:THR:HG22	1.98	0.64
1:I:82:ASP:O	1:I:84:THR:HG22	1.98	0.64
1:F:174[B]:GLY:O	1:F:177[B]:GLY:N	2.31	0.64
1:I:61:ASN:CB	1:J:337:ARG:HD3	2.27	0.64
1:H:155:GLU:OE1	1:H:211[A]:HIS:HE1	1.82	0.64
1:F:59:GLY:C	1:F:61:ASN:H	2.01	0.64
1:K:458:HIS:CD2	1:K:460:VAL:H	2.14	0.64
1:H:25:LYS:CD	5:H:5961:HOH:O	2.45	0.64
1:J:201:GLN:HA	5:J:6020:HOH:O	1.97	0.64
1:B:201:GLN:HA	5:B:6004:HOH:O	1.97	0.64
1:K:176[B]:LYS:C	1:K:178[B]:GLY:N	2.47	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:55:GLY:HA3	5:L:1731:HOH:O	1.96	0.63
1:G:55:GLY:HA3	5:G:5956:HOH:O	1.96	0.63
1:G:308:ILE:HG21	1:G:374:LEU:HD13	1.78	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
1:D:165:GLU:CB	5:D:5964:HOH:O	2.43	0.63
1:K:334:TYR:CD1	5:K:1611:HOH:O	2.49	0.63
1:D:334:TYR:CD1	5:D:5981:HOH:O	2.49	0.63
5:I:5969:HOH:O	1:J:182:VAL:HG23	1.97	0.63
1:C:174[B]:GLY:O	1:C:177[B]:GLY:N	2.31	0.63
1:K:174[B]:GLY:O	1:K:177[B]:GLY:N	2.31	0.63
1:G:155:GLU:OE1	1:G:211[A]:HIS:HE1	1.81	0.63
1:E:155:GLU:OE1	1:E:211[A]:HIS:HE1	1.81	0.63
1:J:224:ARG:HG2	1:J:224:ARG:NH2	1.97	0.63
1:C:82:ASP:O	1:C:84:THR:HG22	1.98	0.63
1:E:82:ASP:O	1:E:84:THR:HG22	1.98	0.63
1:D:82:ASP:O	1:D:84:THR:HG22	1.98	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:D:458:HIS:CD2	1:D:460:VAL:H	2.14	0.63
1:K:59:GLY:C	1:K:61:ASN:H	2.01	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
1:I:155:GLU:OE1	1:I:211[A]:HIS:HE1	1.81	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:L:155:GLU:OE1	1:L:211[A]:HIS:HE1	1.81	0.63
1:F:155:GLU:OE1	1:F:211[A]:HIS:HE1	1.81	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:B:165:GLU:CB	5:B:5962:HOH:O	2.43	0.62
1:I:174[B]:GLY:O	1:I:177[B]:GLY:N	2.31	0.62
1:C:155:GLU:OE1	1:C:211[A]:HIS:HE1	1.81	0.62
1:A:176[B]:LYS:HB3	5:B:6043:HOH:O	1.99	0.62
1:G:61:ASN:CB	1:H:337:ARG:CD	2.73	0.62
1:E:25:LYS:HD3	5:E:660:HOH:O	1.96	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:J:174[B]:GLY:O	1:J:177[B]:GLY:N	2.32	0.62
1:K:269:HIS:CE1	4:K:5910:PPQ:HEP3	2.35	0.62
1:J:82:ASP:O	1:J:84:THR:HG22	1.98	0.62
1:F:82:ASP:O	1:F:84:THR:HG22	1.98	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:155:GLU:OE1	1:D:211[A]:HIS:HE1	1.82	0.62
1:B:174[B]:GLY:O	1:B:177[B]:GLY:N	2.31	0.62
1:F:269:HIS:CE1	4:F:5905:PPQ:HEP3	2.35	0.62
1:I:269:HIS:CE1	4:I:5908:PPQ:HEP3	2.35	0.62
1:G:360:PHE:CG	1:G:361:PRO:HD3	2.34	0.62
1:B:269:HIS:CE1	4:B:5901:PPQ:HEP3	2.35	0.62
1:D:269:HIS:CE1	4:D:5903:PPQ:HEP3	2.35	0.62
1:H:399:LEU:N	1:H:400:PRO:CD	2.62	0.62
1:A:452:ARG:HA	5:A:6015:HOH:O	2.00	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:K:82:ASP:O	1:K:84:THR:HG22	1.98	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:61:ASN:HB3	1:L:337:ARG:HH11	1.65	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:C:165:GLU:CB	5:C:5961:HOH:O	2.43	0.62
1:B:82:ASP:O	1:B:84:THR:HG22	1.98	0.62
1:L:452:ARG:HA	5:L:1807: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:C:360:PHE:CG	1:C:361:PRO:HD3	2.34	0.62
1:B:128:PRO:HD2	5:B:5908:HOH:O	2.00	0.62
1:K:437:GLU:HA	5:K:1656:HOH:O	2.00	0.62
1:C:452:ARG:HA	5:C:6015: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:C:128:PRO:HD2	5:C:5909:HOH:O	2.00	0.62
1:A:437:GLU:HA	5:A:6017:HOH:O	2.00	0.62
1:G:452:ARG:HA	5:G:6025:HOH:O	2.00	0.62
1:C:437:GLU:HA	5:C:6017: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: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:F:452:ARG:HA	5:F:6025:HOH:O	2.00	0.61
1:B:452:ARG:HA	5:B:6016:HOH:O	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:437:GLU:HA	5:D:6020:HOH:O	2.00	0.61
1:D:174[B]:GLY:O	1:D:177[B]:GLY:N	2.31	0.61
1:L:269:HIS:CE1	4:L:5911:PPQ:HEP3	2.35	0.61
1:E:128:PRO:HD2	5:E:621:HOH:O	2.00	0.61
1:D:224:ARG:HG2	1:D:224:ARG:NH2	1.97	0.61
1:J:437:GLU:HA	5:J:6034: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:B:437:GLU:HA	5:B:6018:HOH:O	2.00	0.61
1:E:269:HIS:CE1	4:E:5904:PPQ:HEP3	2.35	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:437:GLU:HA	5:E:738:HOH:O	2.00	0.61
1:C:350:SER:HB2	1:C:351:PRO:HD2	1.83	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: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:D:360:PHE:CG	1:D:361:PRO:HD3	2.34	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:L:165:GLU:CB	5:L:1747:HOH:O	2.43	0.61
1:G:458:HIS:CD2	1:G:460:VAL:H	2.14	0.61
1:F:458:HIS:CD2	1:F:460:VAL:H	2.14	0.61
1:F:437:GLU:HA	5:F:6027:HOH:O	2.00	0.61
1:K:42:PHE:HA	5:K:1622:HOH:O	2.01	0.61
1:B:182:VAL:HG23	5:C:5948:HOH:O	2.00	0.61
1:L:174[B]:GLY:O	1:L:177[B]:GLY:N	2.31	0.61
1:A:61:ASN:CB	1:F:337:ARG:NH1	2.64	0.61
1:L:329:PRO:CG	1:L:359:ARG:CD	2.75	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:360:PHE:CG	1:L:361:PRO:HD3	2.34	0.61
1:A:128:PRO:HD2	5:A:5907:HOH:O	2.00	0.61
1:C:269:HIS:CE1	4:C:5902:PPQ:HEP3	2.35	0.61
1:A:269:HIS:CE1	4:A:5900:PPQ:HEP3	2.35	0.61
1:K:128:PRO:HD2	5:K:1539:HOH:O	2.00	0.61
1:E:458:HIS:CD2	1:E:460:VAL:H	2.14	0.61
1:E:42:PHE:HA	5:E:704:HOH:O	2.01	0.61
1:H:350:SER:HB2	1:H:351:PRO:HD2	1.83	0.61
1:K:179[B]:TYR:CD1	1:K:212[B]:GLU:CA	2.77	0.61
1:I:63:SER:N	1:J:339:ARG:HH12	1.98	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:J:350:SER:HB2	1:J:351:PRO:HD2	1.83	0.61
1:L:128:PRO:HD2	5:L:1692:HOH:O	2.00	0.60
1:J:323:VAL:CG1	5:J:6054:HOH:O	2.20	0.60
1:F:360:PHE:CG	1:F:361:PRO:HD3	2.34	0.60
1:L:192[A]:ARG:HD3	1:L:219:ASN:ND2	2.11	0.60
1:I:399:LEU:N	1:I:400:PRO:CD	2.62	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:K:452:ARG:HA	5:K:1654:HOH:O	2.00	0.60
1:F:350:SER:HB2	1:F: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:I:29[A]:GLN:HB3	1:J:180[A]:PHE:HB3	1.83	0.60
1:E:350:SER:HB2	1:E:351:PRO:HD2	1.83	0.60
1:A:350:SER:HB2	1:A:351:PRO:HD2	1.83	0.60
1:C:211[B]:HIS:HD2	1:C:211[B]:HIS:N	1.96	0.60
1:H:458:HIS:CD2	1:H:460:VAL:H	2.14	0.60
1:B:42:PHE:HA	5:B:5989:HOH:O	2.01	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:A:192[A]:ARG:HD3	1:A:219:ASN:ND2	2.11	0.60
1:K:350:SER:HB2	1:K:351:PRO:HD2	1.83	0.60
1:H:179[B]:TYR:CD1	1:H:212[B]:GLU:CA	2.77	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:L:323:VAL:CG1	5:L:1830:HOH:O	2.20	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:B:350:SER:HB2	1:B:351:PRO:HD2	1.83	0.60
1:A:42:PHE:HA	5:A:5988:HOH:O	2.01	0.60
1:G:63:SER:N	1:H:339:ARG:HH12	1.99	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:D:350:SER:HB2	1:D:351:PRO:HD2	1.83	0.60
1:H:452:ARG:HA	5:H:6029:HOH:O	2.00	0.60
1:E:211[B]:HIS:N	1:E:211[B]:HIS:HD2	1.96	0.60
1:G:337:ARG:HH11	1:L:61:ASN:HB3	1.65	0.60
1:B:458:HIS:CD2	1:B:460:VAL:H	2.14	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:26:GLY:HA3	5:K:1592:HOH:O	2.02	0.60
1:D:465:TYR:O	1:D:468:VAL:HB	2.02	0.60
1:F:42:PHE:HA	5:F:5998:HOH:O	2.01	0.60
1:A:465:TYR:O	1:A:468:VAL:HB	2.02	0.60
1:F:465:TYR:O	1:F:468:VAL:HB	2.02	0.60
1:I:350:SER:HB2	1:I:351:PRO:HD2	1.83	0.60
1:H:42:PHE:HA	5:H:6002:HOH:O	2.01	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: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:K:251:LYS:HE2	5:K:1554:HOH:O	2.01	0.59
1:J:42:PHE:HA	5:J:6005:HOH:O	2.01	0.59
1:D:42:PHE:HA	5:D:5991:HOH:O	2.01	0.59
1:A:26:GLY:HA3	5:A:5959:HOH:O	2.02	0.59
1:G:42:PHE:HA	5:G:5998:HOH:O	2.01	0.59
1:L:26:GLY:HA3	5:L:1745:HOH:O	2.02	0.59
1:C:465:TYR:O	1:C:468:VAL:HB	2.02	0.59
1:H:28:GLU:HB2	5:H:5945:HOH:O	2.03	0.59
1:D:452:ARG:HA	5:D:6018:HOH:O	2.00	0.59
3:J:4480:ADP:C3'	5:J:5993:HOH:O	2.43	0.59
1:A:30[A]:HIS:CE1	1:F:183:PRO:HD3	2.37	0.59
1:G:350:SER:HB2	1:G:351:PRO:HD2	1.83	0.59
1:B:465:TYR:O	1:B:468:VAL:HB	2.02	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:D:183:PRO:HB2	5:E:684:HOH:O	2.01	0.59
1:A:28:GLU:HB2	5:A:5930:HOH:O	2.03	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: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:G:4477:ADP:C3'	5:G:5986:HOH:O	2.43	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:L:42:PHE:HA	5:L:1775:HOH:O	2.01	0.59
1:G:26:GLY:HA3	5:G:5969:HOH:O	2.02	0.59
1:I:26:GLY:HA3	5:I:5980:HOH:O	2.02	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:G:212[A]:GLU:HG3	1:G:218:GLN:HE21	1.68	0.59
1:C:192[A]:ARG:HD3	1:C:219:ASN:ND2	2.11	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:D:28:GLU:HB2	5:D:5933: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:F:212[A]:GLU:HG3	1:F:218:GLN:HE21	1.68	0.58
1:A:176[B]:LYS:C	1:A:178[B]:GLY:N	2.47	0.58
1:H:329:PRO:CG	1:H:359:ARG:CD	2.75	0.58
1:K:131:GLU:OE2	4:K:5910:PPQ:NP	2.36	0.58
1:I:165:GLU:CB	5:I:5982:HOH:O	2.43	0.58
1:I:212[A]:GLU:HG3	1:I:218:GLN:HE21	1.68	0.58
1:G:337:ARG:HD3	1:L:61:ASN:CB	2.33	0.58
1:E:131:GLU:OE2	4:E:5904:PPQ:NP	2.36	0.58
1:D:131:GLU:OE2	4:D:5903:PPQ:NP	2.36	0.58
1:A:63:SER:N	1:F:339:ARG:HH12	2.01	0.58
1:K:285:ASP:CA	5:K:1663:HOH:O	2.35	0.58
1:F:285:ASP:CA	5:F:6034:HOH:O	2.35	0.58
1:J:399:LEU:N	1:J:400:PRO:HD2	2.09	0.58
1:E:419:ASN:O	1:E:422:ASP:HB3	2.03	0.58
1:I:42:PHE:HA	5:I:6009:HOH:O	2.01	0.58
1:A:182:VAL:HG23	5:B:5949:HOH:O	2.01	0.58
3:B:4472:ADP:C8	3:B:4472:ADP:C1'	2.81	0.58
1:C:178[A]:GLY:O	1:C:212[A]:GLU:C	2.42	0.58
1:B:337:ARG:HD3	1:C:61:ASN:HB3	1.81	0.58
1:G:131:GLU:OE2	4:G:5906:PPQ:NP	2.36	0.58
1:A:285:ASP:CA	5:A:6024:HOH:O	2.35	0.58
1:H:165:GLU:CB	5:H:5975:HOH:O	2.43	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:I:419:ASN:O	1:I:422:ASP:HB3	2.03	0.58
1:C:26:GLY:HA3	5:C:5959:HOH:O	2.02	0.58
1:C:212[A]:GLU:HG3	1:C:218:GLN:HE21	1.68	0.58
1:K:211[B]:HIS:N	1:K:211[B]:HIS:HD2	1.96	0.58
1:H:211[B]:HIS:N	1:H:211[B]:HIS:HD2	1.96	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:399:LEU:N	1:C:400:PRO:HD2	2.09	0.58
1:H:465:TYR:O	1:H:468:VAL:HB	2.02	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:251:LYS:HE2	5:J:5940:HOH:O	2.00	0.58
1:L:419:ASN:O	1:L:422:ASP:HB3	2.03	0.58
1:F:28:GLU:HB2	5:F:5940:HOH:O	2.03	0.58
1:H:26:GLY:HA3	5:H:5973:HOH:O	2.02	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:J:178[A]:GLY:O	1:J:212[A]:GLU:C	2.42	0.58
1:L:212[A]:GLU:HG3	1:L:218:GLN:HE21	1.68	0.58
1:F:329:PRO:CG	1:F:359:ARG:CD	2.75	0.58
1:C:131:GLU:OE2	4:C:5902:PPQ:NP	2.36	0.58
1:B:131:GLU:OE2	4:B:5901:PPQ:NP	2.36	0.58
1:J:131:GLU:OE2	4:J:5909:PPQ:NP	2.36	0.58
1:G:419:ASN:O	1:G:422:ASP:HB3	2.03	0.58
1:D:26:GLY:HA3	5:D:5962:HOH:O	2.02	0.58
1:K:419:ASN:O	1:K:422:ASP:HB3	2.03	0.58
1:I:211[B]:HIS:HD2	1:I:211[B]:HIS:N	1.96	0.58
1:E:211[B]:HIS:NE2	5:E:769:HOH:O	2.10	0.58
1:B:178[A]:GLY:O	1:B:212[A]:GLU:C	2.42	0.58
1:I:131:GLU:OE2	4:I:5908:PPQ:NP	2.36	0.58
1:C:360:PHE:CD2	1:C:361:PRO:CD	2.75	0.58
1:A:131:GLU:OE2	4:A:5900:PPQ:NP	2.36	0.58
1:G:285:ASP:CA	5:G:6034:HOH:O	2.35	0.58
1:B:192[A]:ARG:HD3	1:B:219:ASN:ND2	2.11	0.58
1:K:192[A]:ARG:HD3	1:K:219:ASN:ND2	2.11	0.58
1:B:189:GLN:HG3	1:C:80:PHE:CZ	2.39	0.58
1:J:114:TYR:HD2	1:J:431:GLY:HA3	1.69	0.58
1:H:419:ASN:O	1:H:422:ASP:HB3	2.03	0.58
1:C:42:PHE:HA	5:C:5988:HOH:O	2.01	0.58
1:J:419:ASN:O	1:J:422:ASP:HB3	2.03	0.58
1:C:28:GLU:HB2	5:C:5930:HOH:O	2.03	0.58
1:H:178[A]:GLY:O	1:H:212[A]:GLU:C	2.42	0.58
1:A:178[A]:GLY:O	1:A:212[A]:GLU:C	2.42	0.58
1:G:360:PHE:CD2	1:G:361:PRO:CD	2.75	0.58
1:C:224:ARG:NH2	1:C:224:ARG:HG2	1.97	0.58
1:F:399:LEU:N	1:F:400:PRO:CD	2.63	0.58
1:E:192[A]:ARG:HD3	1:E:219:ASN:ND2	2.11	0.58
1:L:114:TYR:HD2	1:L:431:GLY:HA3	1.69	0.58
1:J:28:GLU:HB2	5:J:5947:HOH:O	2.03	0.58
1:E:183:PRO:HB2	5:F:5979:HOH:O	2.03	0.58
1:B:26:GLY:HA3	5:B:5960:HOH:O	2.02	0.58
3:A:4471:ADP:C8	3:A:4471:ADP:C1'	2.81	0.58
1:D:211[B]:HIS:NE2	5:D:6046:HOH:O	2.20	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:178[A]:GLY:O	1:D:212[A]:GLU:C	2.42	0.58
1:L:211[B]:HIS:HD2	1:L:211[B]:HIS:N	1.96	0.58
1:A:212[A]:GLU:HG3	1:A:218:GLN:HE21	1.68	0.58
1:L:131:GLU:OE2	4:L:5911:PPQ:NP	2.36	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
3:G:4477:ADP:C1'	3:G:4477:ADP:C8	2.81	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:D:192[A]:ARG:HD3	1:D:219:ASN:ND2	2.11	0.58
1:G:399:LEU:N	1:G:400:PRO:HD2	2.09	0.58
1:B:419:ASN:O	1:B:422:ASP:HB3	2.03	0.58
1:I:28:GLU:HB2	5:I:5951:HOH:O	2.03	0.58
3:I:4479:ADP:C3'	5:I:5997:HOH:O	2.42	0.57
1:D:114:TYR:HD2	1:D:431:GLY:HA3	1.69	0.57
1:J:26:GLY:HA3	5:J:5976:HOH:O	2.02	0.57
1:E:178[A]:GLY:O	1:E:212[A]:GLU:C	2.42	0.57
1:G:399:LEU:N	1:G:400:PRO:CD	2.63	0.57
1:F:458:HIS:HD2	1:F:460:VAL:N	2.01	0.57
1:B:251:LYS:HE2	5:B:5923:HOH:O	2.00	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:B:360:PHE:CD2	1:B:361:PRO:CD	2.75	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:F:178[A]:GLY:O	1:F:212[A]:GLU:C	2.42	0.57
1:K:29[A]:GLN:HB3	1:L:180[A]:PHE:HB3	1.87	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:I:114:TYR:HD2	1:I:431:GLY:HA3	1.69	0.57
5:B:5946:HOH:O	1:C:84:THR:HG21	2.05	0.57
1:B:291:SER:O	1:B:295:LEU:HD12	2.05	0.57
1:B:28:GLU:HB2	5:B:5931:HOH:O	2.03	0.57
3:I:4479:ADP:C8	3:I:4479:ADP:C1'	2.81	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
1:B:312:ALA:HB2	1:B:370:CYS:SG	2.45	0.57
3:L:4482:ADP:C3'	5:L:1762:HOH:O	2.43	0.57
1:L:178[A]:GLY:O	1:L:212[A]:GLU:C	2.42	0.57
1:E:323:VAL:CG1	5:E:759:HOH:O	2.20	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:285:ASP:CA	5:H:6038:HOH:O	2.35	0.57
1:G:165:GLU:CB	5:G:5971:HOH:O	2.43	0.57
1:D:311:LEU:HD12	1:D:373:ALA:HB2	1.87	0.57
1:F:201:GLN:CA	5:F:6013:HOH:O	2.53	0.57
1:C:312:ALA:HB2	1:C:370:CYS:SG	2.45	0.57
1:K:312:ALA:HB2	1:K:370:CYS:SG	2.45	0.57
1:B:212[A]:GLU:HG3	1:B:218:GLN:HE21	1.68	0.57
1:H:458:HIS:HD2	1:H:460:VAL:N	2.01	0.57
1:H:311:LEU:HD12	1:H:373:ALA:HB2	1.87	0.57
1:A:311:LEU:HD12	1:A:373:ALA:HB2	1.87	0.57
1:H:291:SER:O	1:H:295:LEU:HD12	2.05	0.57
1:G:312:ALA:HB2	1:G:370:CYS:SG	2.45	0.57
1:A:312:ALA:HB2	1:A:370:CYS:SG	2.45	0.57
1:D:419:ASN:O	1:D:422:ASP:HB3	2.03	0.57
1:C:180[A]:PHE:HB3	1:D:29[A]:GLN:HB3	1.86	0.57
1:A:337:ARG:HH11	1:B:61:ASN:HB3	1.68	0.57
1:L:360:PHE:CD2	1:L:361:PRO:CD	2.75	0.57
1:B:285:ASP:CA	5:B:6025:HOH:O	2.35	0.57
1:G:347:VAL:HA	5:G:5966:HOH:O	2.04	0.57
1:L:311:LEU:HD12	1:L:373:ALA:HB2	1.87	0.57
1:G:114:TYR:HD2	1:G:431:GLY:HA3	1.69	0.57
1:I:291:SER:O	1:I:295:LEU:HD12	2.05	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:419:ASN:O	1:F:422:ASP:HB3	2.03	0.57
1:F:291:SER:O	1:F:295:LEU:HD12	2.05	0.57
1:H:312:ALA:HB2	1:H:370:CYS:SG	2.45	0.57
1:G:61:ASN:CB	1:H:337:ARG:HD3	2.33	0.57
1:E:165:GLU:CB	5:E:676:HOH:O	2.43	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:A:114:TYR:HD2	1:A:431:GLY:HA3	1.69	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:I:312:ALA:HB2	1:I:370:CYS:SG	2.45	0.57
5:G:5958:HOH:O	1:H:182:VAL:HG23	2.04	0.57
3:A:4471:ADP:C3'	5:A:5976:HOH:O	2.43	0.56
1:K:1:SER:C	1:K:71:ALA:HB1	2.25	0.56
1:B:1:SER:C	1:B:71:ALA:HB1	2.25	0.56
1:F:1:SER:C	1:F:71:ALA:HB1	2.26	0.56
1:A:347:VAL:HA	5:A:5956:HOH:O	2.04	0.56
1:K:347:VAL:HA	5:K:1588:HOH:O	2.04	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:114:TYR:HD2	1:K:431:GLY:HA3	1.69	0.56
1:C:291:SER:O	1:C:295:LEU:HD12	2.05	0.56
1:J:230:LYS:O	1:J:233:ASP:HB2	2.05	0.56
1:B:180[A]:PHE:HB3	1:C:29[A]:GLN:HB3	1.88	0.56
1:I:360:PHE:CD2	1:I:361:PRO:CD	2.75	0.56
1:B:399:LEU:N	1:B:400:PRO:CD	2.62	0.56
1:K:311:LEU:HD12	1:K:373:ALA:HB2	1.87	0.56
1:F:57:TRP:C	1:F:58:LYS:O	2.42	0.56
1:J:291:SER:O	1:J:295:LEU:HD12	2.05	0.56
1:F:264[B]:ASN:HA	1:F:326:TYR:HB3	1.87	0.56
1:H:264[B]:ASN:HA	1:H:326:TYR:HB3	1.87	0.56
1:H:212[A]:GLU:HG3	1:H:218:GLN:HE21	1.68	0.56
1:H:61:ASN:HB3	1:I:337:ARG:NH1	2.14	0.56
1:E:360:PHE:CD2	1:E:361:PRO:CD	2.75	0.56
1:H:1:SER:C	1:H:71:ALA:HB1	2.26	0.56
1:G:1:SER:C	1:G:71:ALA:HB1	2.26	0.56
1:C:347:VAL:HA	5:C:5956:HOH:O	2.04	0.56
1:C:251:LYS:HE2	5:C:5923:HOH:O	2.01	0.56
1:G:189:GLN:NE2	1:G:209[A]:HIS:CE1	2.72	0.56
1:E:311:LEU:HD12	1:E:373:ALA:HB2	1.87	0.56
1:J:80:PHE:CZ	1:K:189:GLN:HG3	2.40	0.56
1:K:57:TRP:C	1:K:58:LYS:O	2.42	0.56
1:H:57:TRP:C	1:H:58:LYS:O	2.42	0.56
1:C:114:TYR:HD2	1:C:431:GLY:HA3	1.69	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:C:264[B]:ASN:HA	1:C:326:TYR:HB3	1.87	0.56
1:E:230:LYS:O	1:E:233:ASP:HB2	2.05	0.56
1:H:230:LYS:O	1:H:233:ASP:HB2	2.05	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:J:264[B]:ASN:HA	1:J:326:TYR:HB3	1.87	0.56
3:E:4475:ADP:C3'	5:E:691:HOH:O	2.43	0.56
1:I:61:ASN:O	1:J:337:ARG:O	2.23	0.56
1:E:212[A]:GLU:HG3	1:E:218:GLN:HE21	1.68	0.56
1:A:1:SER:C	1:A:71:ALA:HB1	2.26	0.56
1:C:1:SER:C	1:C:71:ALA:HB1	2.26	0.56
1:A:165:GLU:CB	5:A:5961:HOH:O	2.43	0.56
1:I:347:VAL:HA	5:I:5977:HOH:O	2.04	0.56
1:B:311:LEU:HD12	1:B:373:ALA:HB2	1.87	0.56
1:E:312:ALA:HB2	1:E:370:CYS:SG	2.45	0.56
3:H:4478:ADP:C8	3:H:4478:ADP:C1'	2.81	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:360:PHE:CD2	1:J:361:PRO:CD	2.75	0.56
1:E:1:SER:C	1:E:71:ALA:HB1	2.26	0.56
1:J:399:LEU:N	1:J:400:PRO:CD	2.63	0.56
1:G:192[A]:ARG:HD3	1:G:219:ASN:ND2	2.11	0.56
1:C:458:HIS:CD2	1:C:460:VAL:H	2.14	0.56
1:J:347:VAL:HA	5:J:5973:HOH:O	2.04	0.56
1:D:347:VAL:HA	5:D:5959:HOH:O	2.04	0.56
1:F:311:LEU:HD12	1:F:373:ALA:HB2	1.87	0.56
1:K:264[B]:ASN:HA	1:K:326:TYR:HB3	1.87	0.56
1:J:29[A]:GLN:HB3	1:K:180[A]:PHE:HB3	1.87	0.56
1:C:329:PRO:CG	1:C:359:ARG:CD	2.75	0.56
1:I:1:SER:C	1:I:71:ALA:HB1	2.25	0.56
1:L:347:VAL:HA	5:L:1741:HOH:O	2.04	0.56
1:B:57:TRP:C	1:B:58:LYS:O	2.42	0.56
1:G:201:GLN:CA	5:G:6013:HOH:O	2.53	0.56
1:B:264[B]:ASN:HA	1:B:326:TYR:HB3	1.87	0.56
3:L:4482:ADP:C1'	3:L:4482:ADP:C8	2.81	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:J:1:SER:C	1:J:71:ALA:HB1	2.26	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: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
1:I:182:VAL:HG23	5:I:5916:HOH:O	2.05	0.56
1:H:179[A]:TYR:O	1:H:181[A]:PRO:HD2	2.05	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:C:311:LEU:HD12	1:C:373:ALA:HB2	1.87	0.56
1:E:57:TRP:C	1:E:58:LYS:O	2.42	0.56
1:G:57:TRP:C	1:G:58:LYS:O	2.42	0.56
1:H:201:GLN:CA	5:H:6017:HOH:O	2.53	0.56
1:F:230:LYS:O	1:F:233:ASP:HB2	2.05	0.56
1:A:291:SER:O	1:A:295:LEU:HD12	2.05	0.56
3:F:4476:ADP:C1'	3:F:4476:ADP:C8	2.81	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:I:179[A]:TYR:C	1:I:181[A]:PRO:CD	2.75	0.56
1:C:269:HIS:CD2	1:C:359:ARG:HG3	2.41	0.56
1:H:251:LYS:HE2	5:H:5938:HOH:O	2.00	0.56
1:K:201:GLN:CA	5:K:1640:HOH:O	2.53	0.56
3:H:4478:ADP:C3'	5:H:5990:HOH:O	2.43	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:179[A]:TYR:O	1:K:181[A]:PRO:HD2	2.05	0.56
1:H:29[A]:GLN:HB3	1:I:180[A]:PHE:HB3	1.88	0.56
1:J:269:HIS:CD2	1:J:359:ARG:HG3	2.41	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:K:399:LEU:N	1:K:400:PRO:HD2	2.09	0.56
1:I:458:HIS:HB3	1:I:461:GLU:HG3	1.88	0.56
1:B:347:VAL:HA	5:B:5957:HOH:O	2.04	0.56
1:I:251:LYS:HE2	5:I:5943:HOH:O	2.01	0.56
1:G:311:LEU:HD12	1:G:373:ALA:HB2	1.87	0.56
5:J:5965:HOH:O	1:K:182:VAL:HG23	2.06	0.56
1:I:269:HIS:CD2	1:I:359:ARG:HG3	2.41	0.55
1:L:1:SER:C	1:L:71:ALA:HB1	2.26	0.55
1:A:458:HIS:HB3	1:A:461:GLU:HG3	1.88	0.55
1:I:57:TRP:C	1:I:58:LYS:O	2.42	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: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: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:G:269:HIS:CD2	1:G:359:ARG:HG3	2.41	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:G:458:HIS:HD2	1:G:460:VAL:N	2.01	0.55
1:L:458:HIS:HB3	1:L:461:GLU:HG3	1.88	0.55
1:D:458:HIS:HB3	1:D:461:GLU:HG3	1.88	0.55
1:D:251:LYS:HE2	5:D:5925:HOH:O	2.01	0.55
1:C:57:TRP:C	1:C:58:LYS:O	2.42	0.55
1:G:334:TYR:HD1	5:G:5988:HOH:O	1.88	0.55
1:A:230:LYS:O	1:A:233:ASP:HB2	2.05	0.55
1:E:91:ILE:HB	1:E:103:ASP:HB2	1.89	0.55
1:B:179[A]:TYR:C	1:B:181[A]:PRO:CD	2.75	0.55
1:G:337:ARG:CD	1:L:61:ASN:CB	2.72	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:A:264[B]:ASN:HA	1:A:326:TYR:HB3	1.87	0.55
1:K:230:LYS:O	1:K:233:ASP:HB2	2.05	0.55
1:E:179[A]:TYR:O	1:E:181[A]:PRO:HD2	2.05	0.55
1:K:360:PHE:CD2	1:K:361:PRO:CD	2.75	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:1:SER:C	1:D:71:ALA:HB1	2.26	0.55
1:J:458:HIS:HD2	1:J:460:VAL:N	2.01	0.55
1:J:189:GLN:NE2	1:J:209[A]:HIS:CE1	2.72	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:C:183:PRO:HD3	1:D:30[A]:HIS:CE1	2.41	0.55
1:A:29[A]:GLN:HB3	1:F:180[A]:PHE:HB3	1.88	0.55
1:A:179[A]:TYR:O	1:A:181[A]:PRO:HD2	2.05	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:J:91:ILE:HB	1:J:103:ASP:HB2	1.88	0.55
1:E:264[B]:ASN:HA	1:E:326:TYR:HB3	1.87	0.55
1:H:179[A]:TYR:C	1:H:181[A]:PRO:CD	2.75	0.55
1:B:179[A]:TYR:O	1:B:181[A]:PRO:HD2	2.05	0.55
1:F:323:VAL:CG1	5:F:6047:HOH:O	2.20	0.55
1:H:323:VAL:CG1	5:H:6051:HOH:O	2.20	0.55
1:E:189:GLN:HG3	1:F:80:PHE:CZ	2.41	0.55
1:D:264[B]:ASN:HA	1:D:326:TYR:HB3	1.87	0.55
1:D:291:SER:O	1:D:295:LEU:HD12	2.05	0.55
1:I:179[A]:TYR:O	1:I:181[A]:PRO:HD2	2.05	0.55
1:J:211[B]:HIS:HD2	1:J:211[B]:HIS:N	1.96	0.55
1:F:269:HIS:CD2	1:F:359:ARG:HG3	2.41	0.55
1:B:458:HIS:HD2	1:B:460:VAL:N	2.01	0.55
1:J:201:GLN:CA	5:J:6020:HOH:O	2.53	0.55
1:G:230:LYS:O	1:G:233:ASP:HB2	2.05	0.55
1:L:91:ILE:HB	1:L:103:ASP:HB2	1.88	0.55
1:H:269:HIS:CD2	1:H:359:ARG:HG3	2.41	0.55
1:E:269:HIS:CD2	1:E:359:ARG:HG3	2.41	0.55
1:K:399:LEU:N	1:K:400:PRO:CD	2.62	0.55
1:B:458:HIS:HB3	1:B:461:GLU:HG3	1.88	0.55
1:A:334:TYR:HD1	5:A:5978:HOH:O	1.88	0.55
1:K:334:TYR:HD1	5:K:1611:HOH:O	1.88	0.55
1:H:91:ILE:HB	1:H:103:ASP:HB2	1.88	0.55
1:F:179[A]:TYR:C	1:F:181[A]:PRO:CD	2.75	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: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
3:C:4473:ADP:C3'	5:C:5976:HOH:O	2.43	0.55
1:C:176[B]:LYS:C	1:C:178[B]:GLY:N	2.47	0.55
1:L:269:HIS:CD2	1:L:359:ARG:HG3	2.41	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:458:HIS:HD2	1:E:460:VAL:N	2.01	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:I:91:ILE:HB	1:I:103:ASP:HB2	1.89	0.55
1:K:211[B]:HIS:O	1:K:212[B]:GLU:CB	2.54	0.54
1:D:360:PHE:CD2	1:D:361:PRO:CD	2.75	0.54
1:K:458:HIS:HB3	1:K:461:GLU:HG3	1.88	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:E:201:GLN:CA	5:E:722:HOH:O	2.53	0.54
1:D:201:GLN:CA	5:D:6006:HOH:O	2.53	0.54
1:C:454:ARG:HB3	1:C:454:ARG:NH2	2.22	0.54
1:D:230:LYS:O	1:D:233:ASP:HB2	2.05	0.54
1:C:179[A]:TYR:C	1:C:181[A]:PRO:CD	2.75	0.54
1:E:337:ARG:NH1	1:F:61:ASN:HB3	2.12	0.54
1:B:269:HIS:CD2	1:B:359:ARG:HG3	2.41	0.54
1:A:269:HIS:CD2	1:A:359:ARG:HG3	2.41	0.54
1:K:329:PRO:CG	1:K:359:ARG:CD	2.75	0.54
1:H:458:HIS:HB3	1:H:461:GLU:HG3	1.88	0.54
1:D:91:ILE:HB	1:D:103:ASP:HB2	1.89	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:C:458:HIS:HB3	1:C:461:GLU:HG3	1.88	0.54
1:F:458:HIS:HB3	1:F:461:GLU:HG3	1.88	0.54
1:J:311:LEU:HD12	1:J:373:ALA:HB2	1.87	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:H:114:TYR:HD2	1:H:431:GLY:HA3	1.69	0.54
1:F:334:TYR:HD1	5:F:5988:HOH:O	1.89	0.54
1:A:91:ILE:HB	1:A:103:ASP:HB2	1.89	0.54
1:G:183:PRO:HB2	5:L:1755:HOH:O	2.06	0.54
1:E:206:VAL:O	1:F:34:PRO:HG2	2.08	0.54
1:I:129:GLU:HA	5:I:5925:HOH:O	2.08	0.54
1:F:211[A]:HIS:CD2	1:F:212[A]:GLU:N	2.76	0.54
1:K:179[A]:TYR:C	1:K:181[A]:PRO:CD	2.75	0.54
1:F:189:GLN:NE2	1:F:209[A]:HIS:CE1	2.72	0.54
1:D:57:TRP:O	1:D:58:LYS:C	2.46	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:57:TRP:C	1:D:58:LYS:O	2.42	0.54
1:D:454:ARG:HB3	1:D:454:ARG:NH2	2.22	0.54
1:E:454:ARG:NH2	1:E:454:ARG:HB3	2.22	0.54
1:L:454:ARG:NH2	1:L:454:ARG:HB3	2.22	0.54
1:F:454:ARG:HB3	1:F:454:ARG:NH2	2.22	0.54
1:L:129:GLU:HA	5:L:1689:HOH:O	2.08	0.54
1:G:182:VAL:HG23	5:L:1733:HOH:O	2.07	0.54
1:I:59:GLY:O	1:I:61:ASN:N	2.41	0.54
1:H:84:THR:HG21	5:I:5966:HOH:O	2.08	0.54
1:J:454:ARG:HB3	1:J:454:ARG:NH2	2.22	0.54
1:G:454:ARG:HB3	1:G:454:ARG:NH2	2.23	0.54
1:H:454:ARG:NH2	1:H:454:ARG:HB3	2.22	0.54
1:B:91:ILE:HB	1:B:103:ASP:HB2	1.88	0.54
1:D:211[A]:HIS:CD2	1:D:212[A]:GLU:N	2.76	0.54
1:D:211[B]:HIS:O	1:D:212[B]:GLU:CB	2.54	0.54
1:G:211[A]:HIS:CD2	1:G:212[A]:GLU:N	2.76	0.54
1:C:399:LEU:N	1:C:400:PRO:CD	2.62	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:F:57:TRP:O	1:F:58:LYS:C	2.46	0.54
1:C:211[A]:HIS:CD2	1:C:212[A]:GLU:N	2.76	0.54
1:F:211[B]:HIS:O	1:F:212[B]:GLU:CB	2.54	0.54
1:K:211[A]:HIS:CD2	1:K: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:A:211[A]:HIS:CD2	1:A:212[A]:GLU:N	2.76	0.54
1:G:251:LYS:HE2	5:G:5932:HOH:O	2.01	0.54
1:A:251:LYS:HE2	5:A:5922:HOH:O	2.00	0.54
1:J:57:TRP:C	1:J:58:LYS:O	2.42	0.54
1:B:57:TRP:O	1:B:58:LYS:C	2.46	0.54
1:E:334:TYR:CE2	1:E:391:PRO:HG3	2.43	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:D:268:MET:HB2	1:D:363:PRO:HD3	1.90	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:A:57:TRP:O	1:A:58:LYS:C	2.46	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:D:189:GLN:HE22	1:D:209[A]:HIS:CE1	2.26	0.54
1:L:268:MET:HB2	1:L:363:PRO:HD3	1.90	0.54
1:F:268:MET:HB2	1:F:363:PRO:HD3	1.90	0.54
1:D:337:ARG:NH1	1:E:61:ASN:HB3	2.16	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:332:LEU:HD22	1:G:409:GLN:C	2.29	0.53
1:L:334:TYR:HD1	5:L:1764:HOH:O	1.88	0.53
1:E:334:TYR:HD1	5:E:693:HOH:O	1.88	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
3:B:4472:ADP:C3'	5:B:5977:HOH:O	2.43	0.53
1:E:176[B]:LYS:C	1:E:178[B]:GLY:N	2.47	0.53
1:C:332:LEU:HD22	1:C:409:GLN:C	2.29	0.53
1:B:332:LEU:HD22	1:B:409:GLN:C	2.29	0.53
1:G:57:TRP:O	1:G:58:LYS:C	2.46	0.53
1:B:308:ILE:HG21	1:B:374:LEU:CD1	2.39	0.53
1:G:308:ILE:HG21	1:G:374:LEU:CD1	2.39	0.53
1:F:91:ILE:HB	1:F:103:ASP:HB2	1.89	0.53
1:L:332:LEU:HD22	1:L:409:GLN:C	2.29	0.53
1:J:332:LEU:HD22	1:J:409:GLN:C	2.29	0.53
1:F:332:LEU:HD22	1:F:409:GLN:C	2.29	0.53
1:E:189:GLN:NE2	1:E:209[A]:HIS:CE1	2.72	0.53
1:C:189:GLN:NE2	1:C:209[A]:HIS:CE1	2.72	0.53
1:J:57:TRP:O	1:J:58:LYS:C	2.46	0.53
1:F:334:TYR:CE2	1:F:391:PRO:HG3	2.43	0.53
1:J:334:TYR:CE2	1:J:391:PRO:HG3	2.43	0.53
1:K:334:TYR:CE2	1:K:391:PRO:HG3	2.43	0.53
1:F:129:GLU:HA	5:F:5916:HOH:O	2.08	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: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:K:129:GLU:HA	5:K:1536:HOH:O	2.08	0.53
1:L:179[A]:TYR:C	1:L:181[A]:PRO:CD	2.75	0.53
1:E:189:GLN:HE22	1:E:209[A]:HIS:CE1	2.26	0.53
1:B:334:TYR:CE2	1:B:391:PRO:HG3	2.43	0.53
1:B:129:GLU:HA	5:B:5905:HOH:O	2.08	0.53
1:G:268:MET:HB2	1:G:363:PRO:HD3	1.90	0.53
1:C:118:THR:OG1	1:C:120:ILE:HG13	2.09	0.53
1:J:118:THR:OG1	1:J:120:ILE:HG13	2.09	0.53
1:H:211[A]:HIS:CD2	1:H:212[A]:GLU:N	2.76	0.53
1:B:211[A]:HIS:CD2	1:B:212[A]:GLU:N	2.76	0.53
1:A:60:ILE:CD1	5:F:6049:HOH:O	2.35	0.53
1:A:399:LEU:N	1:A:400:PRO:CD	2.62	0.53
1:B:189:GLN:HE22	1:B:209[A]:HIS:CE1	2.26	0.53
1:K:189:GLN:HE22	1:K:209[A]:HIS:CE1	2.26	0.53
1:H:189:GLN:HE22	1:H:209[A]:HIS:CE1	2.26	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:A:334:TYR:CE2	1:A:391:PRO:HG3	2.43	0.53
1:H:334:TYR:CE2	1:H:391:PRO:HG3	2.43	0.53
1:D:308:ILE:HG21	1:D:374:LEU:CD1	2.38	0.53
1:J:268:MET:HB2	1:J:363:PRO:HD3	1.90	0.53
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:I:332:LEU:HD22	1:I:409:GLN:C	2.29	0.53
1:F:251:LYS:HE2	5:F:5933:HOH:O	2.01	0.53
1:L:189:GLN:HE22	1:L:209[A]:HIS:CE1	2.26	0.53
1:K:57:TRP:O	1:K:58:LYS:C	2.46	0.53
1:H:57:TRP:O	1:H:58:LYS:C	2.46	0.53
5:E:659:HOH:O	1:F:84:THR:HG21	2.08	0.53
1:C:308:ILE:HG21	1:C:374:LEU:CD1	2.38	0.53
1:H:308:ILE:HG21	1:H:374:LEU:CD1	2.39	0.53
1:I:211[A]:HIS:CD2	1:I:212[A]:GLU:N	2.76	0.53
1:A:337:ARG:CD	1:A:338:ASN:N	2.72	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:K:189:GLN:HE22	1:K:209[A]:HIS:HE1	1.57	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:A:19:LEU:O	1:A:30[A]:HIS:HA	2.09	0.53
1:L:47:LYS:HD3	5:L:1827:HOH:O	2.09	0.53
1:H:255:PHE:O	1:H:363:PRO:HB2	2.09	0.53
1:C:255:PHE:O	1:C:363:PRO:HB2	2.09	0.53
1:J:19:LEU:O	1:J:30[A]:HIS:HA	2.09	0.53
1:F:337:ARG:CD	1:F:338:ASN:N	2.72	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:57:TRP:O	1:E:58:LYS:C	2.46	0.53
1:I:308:ILE:HG21	1:I:374:LEU:CD1	2.38	0.53
1:F:255:PHE:O	1:F:363:PRO:HB2	2.09	0.53
1:K:255:PHE:O	1:K:363:PRO:HB2	2.09	0.53
1:E:129:GLU:HA	5:E:618:HOH:O	2.08	0.53
1:K:30[A]:HIS:CE1	1:L:183:PRO:HD3	2.44	0.53
1:K:118:THR:OG1	1:K:120:ILE:HG13	2.09	0.53
1:F:118:THR:OG1	1:F:120:ILE:HG13	2.09	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
1:J:211[A]:HIS:CD2	1:J:212[A]:GLU:N	2.76	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:285:ASP:CA	5:C:6024:HOH:O	2.35	0.53
1:E:332:LEU:HD22	1:E:409:GLN:C	2.29	0.53
1:I:189:GLN:HE22	1:I:209[A]:HIS:CE1	2.26	0.53
1:B:114:TYR:HD2	1:B:431:GLY:HA3	1.69	0.53
1:C:334:TYR:CE2	1:C:391:PRO:HG3	2.43	0.53
1:A:308:ILE:HG21	1:A:374:LEU:CD1	2.39	0.53
1:L:19:LEU:O	1:L:30[A]:HIS:HA	2.09	0.53
1:B:255:PHE:O	1:B:363:PRO:HB2	2.09	0.53
1:A:47:LYS:HD3	5:A:6035:HOH:O	2.09	0.53
1:H:47:LYS:HD3	5:H:6049:HOH:O	2.09	0.53
1:K:59:GLY:O	1:K:61:ASN:N	2.41	0.53
1:G:329:PRO:CG	1:G:359:ARG:CD	2.75	0.53
1:K:399:LEU:HB3	1:K:400:PRO:HD3	1.91	0.53
1:G:189:GLN:HE22	1:G:209[A]:HIS:CE1	2.26	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:G:255:PHE:O	1:G:363:PRO:HB2	2.09	0.53
1:E:118:THR:OG1	1:E:120:ILE:HG13	2.09	0.53
1:A:268:MET:HB2	1:A:363:PRO:HD3	1.90	0.53
1:H:399:LEU:HB3	1:H:400:PRO:HD3	1.91	0.52
1:D:332:LEU:HD22	1:D:409:GLN:C	2.29	0.52
1:L:334:TYR:CE2	1:L:391:PRO:HG3	2.43	0.52
1:I:334:TYR:CE2	1:I:391:PRO:HG3	2.43	0.52
1:F:308:ILE:HG21	1:F:374:LEU:CD1	2.39	0.52
1:E:19:LEU:O	1:E:30[A]:HIS:HA	2.09	0.52
1:J:255:PHE:O	1:J:363:PRO:HB2	2.09	0.52
1:C:268:MET:HB2	1:C:363:PRO:HD3	1.90	0.52
1:E:255:PHE:O	1:E:363:PRO:HB2	2.09	0.52
1:I:118:THR:OG1	1:I:120:ILE:HG13	2.09	0.52
1:H:19:LEU:O	1:H:30[A]:HIS:HA	2.09	0.52
1:G:329:PRO:CD	1:G:359:ARG:CD	2.87	0.52
1:L:285:ASP:CA	5:L:1816:HOH:O	2.35	0.52
1:D:189:GLN:HE22	1:D:209[A]:HIS:HE1	1.57	0.52
1:I:255:PHE:O	1:I:363:PRO:HB2	2.09	0.52
1:D:129:GLU:HA	5:D:5907:HOH:O	2.08	0.52
1:C:129:GLU:HA	5:C:5906:HOH:O	2.08	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: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:K:329:PRO:CD	1:K:359:ARG:CD	2.87	0.52
1:H:332:LEU:HD22	1:H:409:GLN:C	2.29	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:332:LEU:HD22	1:K:409:GLN:C	2.29	0.52
1:C:458:HIS:HD2	1:C:460:VAL:N	2.01	0.52
1:I:334:TYR:HD1	5:I:5999:HOH:O	1.88	0.52
1:E:308:ILE:HG21	1:E:374:LEU:CD1	2.39	0.52
1:I:295:LEU:HB3	1:I:388:PRO:HG3	1.91	0.52
1:L:255:PHE:O	1:L:363:PRO:HB2	2.09	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
1:D:118:THR:OG1	1:D:120:ILE:HG13	2.09	0.52
1:B:47:LYS:HD3	5:B:6036:HOH:O	2.09	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:A:189:GLN:HE22	1:A:209[A]:HIS:CE1	2.26	0.52
1:E:295:LEU:HB3	1:E:388:PRO:HG3	1.92	0.52
1:D:255:PHE:O	1:D:363:PRO:HB2	2.09	0.52
1:H:268:MET:HB2	1:H:363:PRO:HD3	1.90	0.52
1:E:268:MET:HB2	1:E:363:PRO:HD3	1.90	0.52
1:L:211[A]:HIS:CD2	1:L:212[A]:GLU:N	2.76	0.52
1:E:337:ARG:CD	1:E:338:ASN:N	2.72	0.52
1:F:329:PRO:CD	1:F:359:ARG:CD	2.87	0.52
1:E:329:PRO:CD	1:E:359:ARG:CD	2.87	0.52
1:J:329:PRO:CD	1:J:359:ARG:CD	2.87	0.52
1:D:189:GLN:NE2	1:D:209[A]:HIS:CE1	2.72	0.52
1:H:334:TYR:HD1	5:H:5992:HOH:O	1.88	0.52
1:F:19:LEU:O	1:F:30[A]:HIS:HA	2.09	0.52
1:H:295:LEU:HB3	1:H:388:PRO:HG3	1.91	0.52
1:J:129:GLU:HA	5:J:5923:HOH:O	2.08	0.52
1:F:47:LYS:HD3	5:F:6045:HOH:O	2.09	0.52
1:G:59:GLY:O	1:G:61:ASN:N	2.41	0.52
1:B:329:PRO:CD	1:B:359:ARG:CD	2.87	0.52
1:A:329:PRO:CD	1:A:359:ARG:CD	2.87	0.52
1:L:399:LEU:HB3	1:L:400:PRO:HD3	1.91	0.52
1:F:189:GLN:HE22	1:F:209[A]:HIS:CE1	2.26	0.52
1:B:189:GLN:NE2	1:B:209[A]:HIS:CE1	2.72	0.52
1:K:308:ILE:HG21	1:K:374:LEU:CD1	2.39	0.52
1:F:437:GLU:CA	5:F:6027:HOH:O	2.58	0.52
1:B:295:LEU:HB3	1:B:388:PRO:HG3	1.91	0.52
1:L:295:LEU:HB3	1:L:388:PRO:HG3	1.92	0.52
1:H:129:GLU:HA	5:H:5921:HOH:O	2.08	0.52
1:A:129:GLU:HA	5:A:5904:HOH:O	2.08	0.52
1:J:47:LYS:HD3	5:J:6052:HOH:O	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:47:LYS:HD3	5:C:6035:HOH:O	2.09	0.52
1:H:211[B]:HIS:O	1:H:212[B]:GLU:CB	2.54	0.52
1:J:179[A]:TYR:O	1:J:181[A]:PRO:HD2	2.05	0.52
1:A:59:GLY:O	1:A:61:ASN:N	2.41	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:J:334:TYR:HD1	5:J:5995:HOH:O	1.88	0.52
1:I:437:GLU:CA	5:I:6038:HOH:O	2.58	0.52
1:D:295:LEU:HB3	1:D:388:PRO:HG3	1.92	0.52
1:G:118:THR:OG1	1:G:120:ILE:HG13	2.09	0.52
1:I:60:ILE:CD1	5:J:6056:HOH:O	2.25	0.52
1:D:329:PRO:CD	1:D:359:ARG:CD	2.87	0.52
1:D:28:GLU:CB	5:D:5933:HOH:O	2.58	0.52
1:K:19:LEU:O	1:K:30[A]:HIS:HA	2.09	0.52
1:G:47:LYS:HD3	5:G:6045:HOH:O	2.09	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:H:189:GLN:NE2	1:H:209[A]:HIS:CE1	2.72	0.52
1:C:295:LEU:HB3	1:C:388:PRO:HG3	1.91	0.52
1:B:118:THR:OG1	1:B:120:ILE:HG13	2.09	0.52
1:H:337:ARG:CD	1:H:338:ASN:N	2.72	0.52
1:F:360:PHE:CD2	1:F:361:PRO:CD	2.75	0.52
1:A:329:PRO:CG	1:A:359:ARG:CD	2.75	0.52
1:E:399:LEU:HB3	1:E:400:PRO:HD3	1.91	0.52
1:C:334:TYR:HD1	5:C:5978:HOH:O	1.89	0.52
1:L:308:ILE:HG21	1:L:374:LEU:CD1	2.39	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:D:235:ILE:HG21	1:D:367:PRO:HG3	1.92	0.52
1:A:457:PRO:HD3	1:G:261[A]:PHE:HB2	1.92	0.52
1:A:235:ILE:HG21	1:A:367:PRO:HG3	1.92	0.52
1:I:337:ARG:CD	1:I:338:ASN:N	2.72	0.51
1:I:329:PRO:CD	1:I:359:ARG:CD	2.87	0.51
1:E:33:ILE:HG23	1:E:37:GLN:HB2	1.92	0.51
1:A:414:LEU:HD23	1:A:450:ASP:HB2	1.93	0.51
1:I:19:LEU:O	1:I:30[A]:HIS:HA	2.09	0.51
1:H:59:GLY:O	1:H:61:ASN:N	2.41	0.51
1:G:399:LEU:HB3	1:G:400:PRO:HD3	1.91	0.51
1:J:189:GLN:HE22	1:J:209[A]:HIS:HE1	1.57	0.51
1:G:437:GLU:CA	5:G:6027:HOH:O	2.58	0.51
1:A:255:PHE:O	1:A:363:PRO:HB2	2.09	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:47:LYS:HA	5:E:756:HOH:O	2.10	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:F:414:LEU:HD23	1:F:450:ASP:HB2	1.92	0.51
1:B:33:ILE:HG23	1:B:37:GLN:HB2	1.92	0.51
1:I:414:LEU:HD23	1:I:450:ASP:HB2	1.93	0.51
1:B:211[B]:HIS:O	1:B:212[B]:GLU:CB	2.54	0.51
1:L:329:PRO:CD	1:L:359:ARG:CD	2.87	0.51
1:A:360:PHE:CD2	1:A:361:PRO:CD	2.75	0.51
1:J:189:GLN:HE22	1:J:209[A]:HIS:CE1	2.26	0.51
1:D:334:TYR:HD1	5:D:5981:HOH:O	1.88	0.51
1:L:414:LEU:HD23	1:L:450:ASP:HB2	1.93	0.51
1:L:235:ILE:HG21	1:L:367:PRO:HG3	1.92	0.51
1:A:211[B]:HIS:N	1:A:211[B]:HIS:HD2	1.96	0.51
1:E:399:LEU:N	1:E:400:PRO:CD	2.62	0.51
1:A:437:GLU:CA	5:A:6017:HOH:O	2.58	0.51
1:K:295:LEU:HB3	1:K:388:PRO:HG3	1.92	0.51
1:K:47:LYS:HD3	5:K:1674:HOH:O	2.09	0.51
1:G:33:ILE:HG23	1:G:37:GLN:HB2	1.92	0.51
1:K:115:LEU:HD23	1:K:379:LEU:HD21	1.93	0.51
1:J:414:LEU:HD23	1:J:450:ASP:HB2	1.93	0.51
1:C:179[B]:TYR:CE1	1:C:212[B]:GLU:N	2.79	0.51
1:H:179[B]:TYR:CE1	1:H:212[B]:GLU:N	2.79	0.51
1:J:179[B]:TYR:CE1	1:J:212[B]:GLU:N	2.79	0.51
1:A:4:HIS:O	1:A:7:THR:HG23	2.11	0.51
1:E:4:HIS:O	1:E:7:THR:HG23	2.11	0.51
1:A:28:GLU:CB	5:A:5930:HOH:O	2.58	0.51
1:K:268:MET:HB2	1:K:363:PRO:HD3	1.90	0.51
1:F:47:LYS:HA	5:F:6045:HOH:O	2.10	0.51
1:A:115:LEU:HD23	1:A:379:LEU:HD21	1.93	0.51
1:G:414:LEU:HD23	1:G:450:ASP:HB2	1.93	0.51
1:F:115:LEU:HD23	1:F:379:LEU:HD21	1.93	0.51
1:D:414:LEU:HD23	1:D:450:ASP:HB2	1.93	0.51
1:G:206:VAL:O	1:L:34:PRO:HG2	2.11	0.51
1:I:33:ILE:HG23	1:I:37:GLN:HB2	1.92	0.51
1:F:179[B]:TYR:CE1	1:F:212[B]:GLU:N	2.79	0.51
1:J:337:ARG:CD	1:J:338:ASN:N	2.72	0.51
1:A:179[B]:TYR:CE1	1:A:212[B]:GLU:N	2.79	0.51
1:A:180[A]:PHE:HB3	1:B:29[A]:GLN:HB3	1.92	0.51
1:E:179[B]:TYR:CE1	1:E:212[B]:GLU:N	2.79	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:4:HIS:O	1:L:7:THR:HG23	2.11	0.51
1:F:399:LEU:HB3	1:F:400:PRO:HD3	1.91	0.51
1:B:399:LEU:HB3	1:B:400:PRO:HD3	1.91	0.51
1:K:188:ALA:HA	5:K:1590:HOH:O	2.11	0.51
1:A:295:LEU:HB3	1:A:388:PRO:HG3	1.91	0.51
1:K:414:LEU:HD23	1:K:450:ASP:HB2	1.93	0.51
1:H:235:ILE:HG21	1:H:367:PRO:HG3	1.92	0.51
1:B:179[B]:TYR:CE1	1:B:212[B]:GLU:N	2.79	0.51
1:H:394:LYS:HD3	1:H:395:ASN:H	1.76	0.51
1:L:251:LYS:HE2	5:L:1707:HOH:O	2.01	0.51
1:D:384:ASN:N	1:D:384:ASN:ND2	2.59	0.51
1:D:183:PRO:HD3	1:E:30[A]:HIS:CE1	2.46	0.51
1:L:28:GLU:CB	5:L:1715:HOH:O	2.58	0.51
1:D:115:LEU:HD23	1:D:379:LEU:HD21	1.93	0.51
1:J:115:LEU:HD23	1:J:379:LEU:HD21	1.93	0.51
1:C:19:LEU:O	1:C:30[A]:HIS:HA	2.09	0.51
1:L:179[B]:TYR:CE1	1:L:212[B]:GLU:N	2.79	0.51
1:I:179[B]:TYR:CE1	1:I:212[B]:GLU:N	2.79	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:C:394:LYS:HD3	1:C:395:ASN:H	1.76	0.51
1:L:189:GLN:NE2	1:L:209[A]:HIS:CE1	2.72	0.51
1:B:25:LYS:HD2	5:B:5947:HOH:O	2.10	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:L:47:LYS:HA	5:L:1827:HOH:O	2.10	0.51
1:J:445:LEU:O	1:J:448:GLU:HG2	2.11	0.51
1:I:115:LEU:HD23	1:I:379:LEU:HD21	1.93	0.51
1:C:115:LEU:HD23	1:C:379:LEU:HD21	1.93	0.51
1:I:445:LEU:O	1:I:448:GLU:HG2	2.11	0.51
1:G:115:LEU:HD23	1:G:379:LEU:HD21	1.93	0.51
1:G:179[B]:TYR:CE1	1:G:212[B]:GLU:N	2.79	0.51
1:J:211[B]:HIS:O	1:J:212[B]:GLU:CB	2.54	0.51
1:J:4:HIS:O	1:J:7:THR:HG23	2.11	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:I:189:GLN:HE22	1:I:209[A]:HIS:HE1	1.57	0.51
1:A:189:GLN:HE22	1:A:209[A]:HIS:HE1	1.57	0.51
1:L:384:ASN:N	1:L:384:ASN:ND2	2.59	0.51
1:J:28:GLU:CB	5:J:5947:HOH:O	2.58	0.51
1:C:264[B]:ASN:CA	1:C:326:TYR:HB3	2.41	0.51
1:K:264[B]:ASN:CA	1:K:326:TYR:HB3	2.41	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:47:LYS:HA	5:D:6038:HOH:O	2.10	0.51
1:H:445:LEU:O	1:H:448:GLU:HG2	2.11	0.51
1:B:179[B]:TYR:CD1	1:B:212[B]:GLU:CA	2.77	0.51
1:J:399:LEU:HB3	1:J:400:PRO:HD3	1.91	0.51
1:A:394:LYS:HD3	1:A:395:ASN:H	1.76	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:B:264[B]:ASN:CA	1:B:326:TYR:HB3	2.41	0.51
1:D:264[B]:ASN:CA	1:D:326:TYR:HB3	2.41	0.51
5:J:5986:HOH:O	1:K:183:PRO:HB2	2.11	0.51
1:B:47:LYS:HA	5:B:6036:HOH:O	2.10	0.51
1:D:33:ILE:HG23	1:D:37:GLN:HB2	1.92	0.51
1:L:445:LEU:O	1:L:448:GLU:HG2	2.11	0.51
1:D:73:THR:HG21	1:D:88:ARG:HB3	1.93	0.51
1:A:33:ILE:HG23	1:A:37:GLN:HB2	1.92	0.51
1:B:183:PRO:HB2	5:C:5969:HOH:O	2.10	0.51
1:I:235:ILE:HG21	1:I:367:PRO:HG3	1.92	0.51
1:D:445:LEU:O	1:D:448:GLU:HG2	2.11	0.51
1:I:59:GLY:O	1:J:339:ARG:NH1	2.42	0.50
1:I:211[B]:HIS:O	1:I:212[B]:GLU:CB	2.54	0.50
5:C:6039:HOH:O	1:D:60:ILE:CD1	2.33	0.50
1:I:4:HIS:O	1:I:7:THR:HG23	2.11	0.50
1:K:394:LYS:HD3	1:K:395:ASN:H	1.76	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
1:H:33:ILE:HG23	1:H:37:GLN:HB2	1.92	0.50
1:I:264[B]:ASN:CA	1:I:326:TYR:HB3	2.41	0.50
1:A:47:LYS:HA	5:A:6035:HOH:O	2.10	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
3:F:4476:ADP:C3'	5:F:5986:HOH:O	2.43	0.50
1:K:179[B]:TYR:CE1	1:K:212[B]:GLU:N	2.79	0.50
1:L:337:ARG:CD	1:L:338:ASN:N	2.72	0.50
1:K:460:VAL:HG12	1:K:464:LEU:HD22	1.94	0.50
1:H:460:VAL:HG12	1:H:464:LEU:HD22	1.93	0.50
1:D:188:ALA:HA	5:D:5961:HOH:O	2.11	0.50
1:H:334:TYR:CZ	1:H:391:PRO:HG3	2.47	0.50
1:G:264[B]:ASN:CA	1:G:326:TYR:HB3	2.41	0.50
1:F:445:LEU:O	1:F:448:GLU:HG2	2.11	0.50
1:A:445:LEU:O	1:A:448:GLU:HG2	2.11	0.50
1:E:125:LEU:O	1:E:272:MET:HA	2.12	0.50
1:C:445:LEU:O	1:C:448:GLU:HG2	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:F:394:LYS:HD3	1:F:395:ASN:H	1.76	0.50
1:D:460:VAL:HG12	1:D:464:LEU:HD22	1.94	0.50
1:I:80:PHE:CZ	1:J:189:GLN:HG3	2.46	0.50
1:K:334:TYR:CZ	1:K:391:PRO:HG3	2.47	0.50
1:A:264[B]:ASN:CA	1:A:326:TYR:HB3	2.41	0.50
1:J:47:LYS:HA	5:J:6052:HOH:O	2.10	0.50
1:H:73:THR:HG21	1:H:88:ARG:HB3	1.93	0.50
1:K:235:ILE:HG21	1:K:367:PRO:HG3	1.92	0.50
1:J:59:GLY:C	1:J:61:ASN:N	2.65	0.50
1:F:460:VAL:HG12	1:F:464:LEU:HD22	1.94	0.50
1:L:188:ALA:HA	5:L:1743:HOH:O	2.11	0.50
1:B:188:ALA:HA	5:B:5959:HOH:O	2.11	0.50
5:I:5990:HOH:O	1:J:183:PRO:HB2	2.11	0.50
1:J:33:ILE:HG23	1:J:37:GLN:HB2	1.92	0.50
1:J:264[B]:ASN:CA	1:J:326:TYR:HB3	2.41	0.50
1:D:125:LEU:O	1:D:272:MET:HA	2.12	0.50
1:H:125:LEU:O	1:H:272:MET:HA	2.12	0.50
1:J:125:LEU:O	1:J:272:MET:HA	2.12	0.50
1:G:176[B]:LYS:C	1:G:178[B]:GLY:N	2.47	0.50
1:K:337:ARG:CD	1:K:338:ASN:N	2.72	0.50
1:H:4:HIS:O	1:H:7:THR:HG23	2.11	0.50
1:G:394:LYS:HD3	1:G:395:ASN:H	1.76	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:L:334:TYR:CZ	1:L:391:PRO:HG3	2.46	0.50
1:H:25:LYS:HD2	5:H:5961:HOH:O	2.10	0.50
1:J:25:LYS:HD2	5:J:5963:HOH:O	2.11	0.50
1:A:25:LYS:HD2	5:A:5946:HOH:O	2.10	0.50
1:K:28:GLU:CB	5:K:1562:HOH:O	2.58	0.50
1:C:28:GLU:CB	5:C:5930:HOH:O	2.58	0.50
1:H:264[B]:ASN:CA	1:H:326:TYR:HB3	2.41	0.50
1:E:445:LEU:O	1:E:448:GLU:HG2	2.11	0.50
1:C:125:LEU:O	1:C:272:MET:HA	2.12	0.50
1:J:235:ILE:HG21	1:J:367:PRO:HG3	1.92	0.50
1:L:33:ILE:HG23	1:L:37:GLN:HB2	1.92	0.50
1:F:179[A]:TYR:O	1:F:181[A]:PRO:HD2	2.05	0.50
1:G:337:ARG:CD	1:G:338:ASN:N	2.72	0.50
1:F:59:GLY:C	1:F:61:ASN:N	2.65	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:4:HIS:O	1:G:7:THR:HG23	2.11	0.50
1:A:334:TYR:CZ	1:A:391:PRO:HG3	2.47	0.50
1:L:25:LYS:HD2	5:L:1731:HOH:O	2.10	0.50
1:B:334:TYR:CZ	1:B:391:PRO:HG3	2.47	0.50
1:G:28:GLU:CB	5:G:5940:HOH:O	2.58	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:I:73:THR:HG21	1:I:88:ARG:HB3	1.93	0.50
1:G:235:ILE:HG21	1:G:367:PRO:HG3	1.92	0.50
1:F:235:ILE:HG21	1:F:367:PRO:HG3	1.92	0.50
1:D:59:GLY:C	1:D:61:ASN:N	2.65	0.50
1:H:59:GLY:C	1:H:61:ASN:N	2.65	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:A:460:VAL:HG12	1:A:464:LEU:HD22	1.94	0.50
1:A:188:ALA:HA	5:A:5958:HOH:O	2.11	0.50
1:J:384:ASN:ND2	1:J:384:ASN:N	2.59	0.50
1:I:334:TYR:CZ	1:I:391:PRO:HG3	2.46	0.50
1:F:334:TYR:CZ	1:F:391:PRO:HG3	2.47	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:J:295:LEU:HB3	1:J:388:PRO:HG3	1.91	0.50
1:H:47:LYS:HA	5:H:6049:HOH:O	2.10	0.50
1:H:272:MET:O	1:H:355:ARG:HB2	2.12	0.50
1:K:272:MET:O	1:K:355:ARG:HB2	2.12	0.50
1:I:47:LYS:HD3	5:I:6056:HOH:O	2.09	0.50
1:C:235:ILE:HG21	1:C:367:PRO:HG3	1.92	0.50
1:L:59:GLY:C	1:L:61:ASN:N	2.65	0.50
1:K:4:HIS:O	1:K:7:THR:HG23	2.11	0.50
1:F:4:HIS:O	1:F:7:THR:HG23	2.11	0.50
1:J:394:LYS:HD3	1:J:395:ASN:H	1.76	0.50
1:I:458:HIS:HD2	1:I:460:VAL:N	2.01	0.50
1:L:460:VAL:HG12	1:L:464:LEU:HD22	1.93	0.50
1:E:384:ASN:N	1:E:384:ASN:ND2	2.59	0.50
1:I:384:ASN:N	1:I:384:ASN:ND2	2.59	0.50
1:C:334:TYR:CZ	1:C:391:PRO:HG3	2.47	0.50
1:A:25:LYS:NZ	5:A:5919:HOH:O	2.45	0.50
1:I:47:LYS:HA	5:I:6056:HOH:O	2.10	0.50
1:K:445:LEU:O	1:K:448:GLU:HG2	2.11	0.50
1:J:63:SER:N	1:K:339:ARG:HH12	2.09	0.50
1:L:115:LEU:HD23	1:L:379:LEU:HD21	1.93	0.50
1:B:414:LEU:HD23	1:B:450:ASP:HB2	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:414:LEU:HD23	1:C:450:ASP:HB2	1.93	0.50
1:F:211[B]:HIS:N	1:F:211[B]:HIS:HD2	1.96	0.50
1:E:59:GLY:O	1:E:61:ASN:N	2.41	0.50
1:L:59:GLY:O	1:L:61:ASN:N	2.41	0.50
1:C:59:GLY:C	1:C:61:ASN:N	2.65	0.50
1:G:59:GLY:C	1:G:61:ASN:N	2.65	0.50
1:E:460:VAL:HG12	1:E:464:LEU:HD22	1.94	0.50
1:J:188:ALA:HA	5:J:5975:HOH:O	2.11	0.50
1:L:264[B]:ASN:CA	1:L:326:TYR:HB3	2.41	0.50
1:K:125:LEU:O	1:K:272:MET:HA	2.12	0.50
1:I:125:LEU:O	1:I:272:MET:HA	2.12	0.50
1:B:125:LEU:O	1:B:272:MET:HA	2.12	0.50
1:F:272:MET:O	1:F:355:ARG:HB2	2.12	0.50
1:I:60:ILE:HG23	1:I:60:ILE:O	2.12	0.49
1:H:179[B]:TYR:CD2	1:H:211[B]:HIS:HB2	2.47	0.49
1:D:394:LYS:HD3	1:D:395:ASN:H	1.76	0.49
1:F:188:ALA:HA	5:F:5968:HOH:O	2.11	0.49
1:G:334:TYR:CZ	1:G:391:PRO:HG3	2.47	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:G:272:MET:O	1:G:355:ARG:HB2	2.12	0.49
1:B:235:ILE:HG21	1:B:367:PRO:HG3	1.92	0.49
1:L:125:LEU:O	1:L:272:MET:HA	2.12	0.49
1:G:73:THR:HG21	1:G:88:ARG:HB3	1.93	0.49
1:K:59:GLY:C	1:K:61:ASN:N	2.65	0.49
1:B:394:LYS:HD3	1:B:395:ASN:H	1.76	0.49
1:L:394:LYS:HD3	1:L:395:ASN:H	1.76	0.49
1:I:188:ALA:HA	5:I:5979:HOH:O	2.11	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
3:K:4481:ADP:C3'	5:K:1609:HOH:O	2.42	0.49
1:K:175[B]:VAL:HG12	1:K:175[B]:VAL:O	2.13	0.49
1:L:179[B]:TYR:CD2	1:L:211[B]:HIS:HB2	2.47	0.49
1:L:178[A]:GLY:O	1:L:212[A]:GLU:O	2.31	0.49
1:E:59:GLY:C	1:E:61:ASN:N	2.65	0.49
1:B:175[B]:VAL:O	1:B:175[B]:VAL:HG12	2.13	0.49
1:J:178[A]:GLY:O	1:J:212[A]:GLU:O	2.31	0.49
1:J:460:VAL:HG12	1:J:464:LEU:HD22	1.94	0.49
1:B:460:VAL:HG12	1:B:464:LEU:HD22	1.93	0.49
1:D:75:VAL:CG2	5:D:5919:HOH:O	2.53	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:188:ALA:HA	5:E:672:HOH:O	2.11	0.49
1:A:384:ASN:ND2	1:A:384:ASN:N	2.59	0.49
1:J:25:LYS:NZ	5:J:5937:HOH:O	2.45	0.49
1:E:334:TYR:CZ	1:E:391:PRO:HG3	2.47	0.49
1:I:272:MET:O	1:I:355:ARG:HB2	2.12	0.49
1:B:272:MET:O	1:B:355:ARG:HB2	2.12	0.49
1:F:125:LEU:O	1:F:272:MET:HA	2.12	0.49
1:C:124:VAL:HA	1:C:274:LEU:HD23	1.95	0.49
1:B:445:LEU:O	1:B:448:GLU:HG2	2.11	0.49
1:H:414:LEU:HD23	1:H:450:ASP:HB2	1.93	0.49
1:F:73:THR:HG21	1:F:88:ARG:HB3	1.93	0.49
1:D:178[A]:GLY:O	1:D:212[A]:GLU:O	2.31	0.49
1:H:175[B]:VAL:O	1:H:175[B]:VAL:HG12	2.13	0.49
1:A:59:GLY:C	1:A:61:ASN:N	2.65	0.49
1:L:60:ILE:O	1:L:60:ILE:HG23	2.12	0.49
1:L:458:HIS:HD2	1:L:460:VAL:N	2.01	0.49
1:C:384:ASN:ND2	1:C:384:ASN:N	2.59	0.49
1:E:25:LYS:HD2	5:E:660:HOH:O	2.10	0.49
1:J:334:TYR:CZ	1:J:391:PRO:HG3	2.47	0.49
1:G:125:LEU:O	1:G:272:MET:HA	2.12	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:K:73:THR:HG21	1:K:88:ARG:HB3	1.93	0.49
1:C:178[A]:GLY:O	1:C:212[A]:GLU:O	2.31	0.49
1:F:178[A]:GLY:O	1:F: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:G:178[A]:GLY:O	1:G:212[A]:GLU:O	2.31	0.49
1:G:60:ILE:O	1:G:60:ILE:HG23	2.12	0.49
1:B:4:HIS:O	1:B:7:THR:HG23	2.11	0.49
1:H:60:ILE:HG23	1:H:60:ILE:O	2.12	0.49
1:C:188:ALA:HA	5:C:5958:HOH:O	2.11	0.49
1:E:28:GLU:CB	5:E:644:HOH:O	2.58	0.49
1:F:264[B]:ASN:CA	1:F:326:TYR:HB3	2.41	0.49
1:E:272:MET:O	1:E:355:ARG:HB2	2.12	0.49
1:J:73:THR:HG21	1:J:88:ARG:HB3	1.93	0.49
1:B:259:PRO:HG2	1:B:260[A]:MET:H	1.78	0.49
1:C:179[B]:TYR:CD2	1:C:211[B]:HIS:HB2	2.47	0.49
1:B:178[A]:GLY:O	1:B:212[A]:GLU:O	2.31	0.49
1:J:59:GLY:O	1:J:61:ASN:N	2.41	0.49
1:K:60:ILE:O	1:K:60:ILE:HG23	2.12	0.49
1:J:33:ILE:CD1	1:K:208:ALA:HB2	2.42	0.49
1:A:463:GLU:HA	1:G:140:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:182:VAL:HG23	5:F:5958:HOH:O	2.11	0.49
1:C:73:THR:HG21	1:C:88:ARG:HB3	1.93	0.49
1:C:259:PRO:HG2	1:C:260[A]:MET:H	1.77	0.49
1:L:73:THR:HG21	1:L:88:ARG:HB3	1.93	0.49
1:I:124:VAL:HA	1:I:274:LEU:HD23	1.95	0.49
1:F:179[B]:TYR:CD2	1:F:211[B]:HIS:HB2	2.47	0.49
1:E:175[B]:VAL:HG12	1:E:175[B]:VAL:O	2.13	0.49
1:G:329:PRO:CD	1:G:359:ARG:HD2	2.42	0.49
1:E:60:ILE:HG23	1:E:60:ILE:O	2.12	0.49
1:F:60:ILE:HG23	1:F:60:ILE:O	2.12	0.49
1:L:75:VAL:CG2	5:L:1701:HOH:O	2.53	0.49
1:B:348:VAL:HG22	5:B:5935:HOH:O	2.13	0.49
1:G:25:LYS:NZ	5:G:5929:HOH:O	2.45	0.49
1:D:334:TYR:CZ	1:D:391:PRO:HG3	2.47	0.49
1:E:264[B]:ASN:CA	1:E:326:TYR:HB3	2.41	0.49
1:K:124:VAL:HA	1:K:274:LEU:HD23	1.95	0.49
1:D:175[B]:VAL:O	1:D:175[B]:VAL:HG12	2.12	0.49
1:I:178[A]:GLY:O	1:I:212[A]:GLU:O	2.31	0.49
1:A:178[A]:GLY:O	1:A: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:C:460:VAL:HG12	1:C:464:LEU:HD22	1.94	0.49
1:D:348:VAL:HG22	5:D:5937:HOH:O	2.13	0.49
1:A:183:PRO:HB2	5:B:5970:HOH:O	2.12	0.49
1:K:437:GLU:CA	5:K:1656:HOH:O	2.58	0.49
1:H:437:GLU:CA	5:H:6031:HOH:O	2.58	0.49
1:B:28:GLU:CB	5:B:5931:HOH:O	2.58	0.49
1:I:179[B]:TYR:CD2	1:I:211[B]:HIS:HB2	2.47	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:C:25:LYS:HD2	5:C:5946:HOH:O	2.10	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:73:THR:HG21	1:A:88:ARG:HB3	1.93	0.49
1:A:272:MET:O	1:A:355:ARG:HB2	2.12	0.49
1:J:259:PRO:HG2	1:J:260[A]:MET:H	1.78	0.49
1:I:174[B]:GLY:O	1:I:177[B]:GLY:HA2	2.13	0.49
1:A:60:ILE:HG23	1:A:60:ILE:O	2.12	0.49
1:K:348:VAL:HG22	5:K:1566:HOH:O	2.13	0.49
1:A:32:THR:OG1	1:F:189:GLN:NE2	2.46	0.49
1:D:25:LYS:HD2	5:D:5949:HOH:O	2.11	0.49
1:H:25:LYS:NZ	5:H:5935:HOH:O	2.45	0.49
1:E:259:PRO:HG2	1:E:260[A]:MET:H	1.78	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:124:VAL:HA	1:A:274:LEU:HD23	1.95	0.49
1:D:174[B]:GLY:O	1:D:177[B]:GLY:HA2	2.13	0.48
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:J:61:ASN:CB	1:K:337:ARG:CD	2.84	0.48
1:F:329:PRO:CD	1:F:359:ARG:HD2	2.42	0.48
1:H:231:LYS:CE	5:H:5924:HOH:O	2.59	0.48
1:J:60:ILE:HG23	1:J:60:ILE:O	2.12	0.48
1:G:460:VAL:HG12	1:G:464:LEU:HD22	1.94	0.48
1:I:348:VAL:HG22	5:I:5955:HOH:O	2.13	0.48
1:D:25:LYS:NZ	5:D:5922:HOH:O	2.45	0.48
1:C:25:LYS:NZ	5:C:5920:HOH:O	2.45	0.48
1:F:25:LYS:NZ	5:F:5930:HOH:O	2.45	0.48
1:F:259:PRO:HG2	1:F:260[A]:MET:H	1.78	0.48
5:K:1580:HOH:O	1:L:182:VAL:HG23	2.13	0.48
1:K:174[B]:GLY:O	1:K:177[B]:GLY:HA2	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:L:437:GLU:CA	5:L:1809:HOH:O	2.58	0.48
1:H:259:PRO:HG2	1:H:260[A]:MET:H	1.77	0.48
1:L:174[B]:GLY:O	1:L:177[B]:GLY:HA2	2.13	0.48
1:H:178[A]:GLY:O	1:H:212[A]:GLU:O	2.31	0.48
1:G:175[B]:VAL:O	1:G:175[B]:VAL:HG12	2.13	0.48
1:C:337:ARG:HH11	1:D:61:ASN:HB3	1.78	0.48
1:H:348:VAL:HG22	5:H:5949:HOH:O	2.13	0.48
1:B:25:LYS:NZ	5:B:5920:HOH:O	2.45	0.48
1:I:25:LYS:HD2	5:I:5967:HOH:O	2.10	0.48
1:L:230:LYS:HG2	5:L:1749:HOH:O	2.14	0.48
1:J:272:MET:O	1:J:355:ARG:HB2	2.12	0.48
1:A:125:LEU:O	1:A:272:MET:HA	2.12	0.48
1:B:124:VAL:HA	1:B:274:LEU:HD23	1.95	0.48
1:F:124:VAL:HA	1:F:274:LEU:HD23	1.95	0.48
1:G:124:VAL:HA	1:G:274:LEU:HD23	1.95	0.48
1:A:61:ASN:HB3	1:F:337:ARG:HH11	1.79	0.48
1:J:329:PRO:HG2	1:J:359:ARG:CD	2.18	0.48
1:L:348:VAL:HG22	5:L:1719:HOH:O	2.13	0.48
1:I:25:LYS:NZ	5:I:5940:HOH:O	2.45	0.48
1:B:334:TYR:HD1	5:B:5979:HOH:O	1.88	0.48
1:G:25:LYS:HD2	5:G:5956:HOH:O	2.10	0.48
1:K:259:PRO:HG2	1:K:260[A]:MET:H	1.78	0.48
1:C:154:ILE:HG13	5:C:5977:HOH:O	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:E:4475:ADP:H5'1	5:E:691:HOH:O	2.14	0.48
1:K:178[A]:GLY:O	1:K:212[A]:GLU:O	2.31	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:L:175[B]:VAL:O	1:L:175[B]:VAL:HG12	2.13	0.48
1:B:59:GLY:C	1:B:61:ASN:N	2.65	0.48
1:E:360:PHE:CG	1:E:361:PRO:CD	2.97	0.48
1:J:410:VAL:HG22	5:J:6043:HOH:O	2.14	0.48
1:G:384:ASN:ND2	1:G:384:ASN:N	2.59	0.48
1:H:28:GLU:CB	5:H:5945:HOH:O	2.58	0.48
1:L:272:MET:O	1:L:355:ARG:HB2	2.12	0.48
1:L:259:PRO:HG2	1:L:260[A]:MET:H	1.78	0.48
1:H:154:ILE:HG13	5:H:5991:HOH:O	2.13	0.48
1:D:124:VAL:HA	1:D:274:LEU:HD23	1.95	0.48
1:I:259:PRO:HG2	1:I:260[A]:MET:H	1.78	0.48
1:F:174[B]:GLY:O	1:F:177[B]:GLY:HA2	2.13	0.48
1:E:211[B]:HIS:O	1:E:212[B]:GLU:CB	2.54	0.48
1:B:179[B]:TYR:CD2	1:B:211[B]:HIS:HB2	2.47	0.48
1:D:60:ILE:O	1:D:60:ILE:HG23	2.12	0.48
1:G:329:PRO:HG2	1:G:359:ARG:CD	2.18	0.48
1:A:399:LEU:N	1:A:400:PRO:HD2	2.09	0.48
1:F:410:VAL:HG22	5:F:6036:HOH:O	2.14	0.48
1:B:437:GLU:CA	5:B:6018:HOH:O	2.58	0.48
1:C:175[B]:VAL:O	1:C:175[B]:VAL:HG12	2.13	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:A:174[B]:GLY:O	1:A:177[B]:GLY:HA2	2.13	0.48
1:J:175[B]:VAL:HG12	1:J:175[B]:VAL:O	2.13	0.48
1:A:329:PRO:CD	1:A:359:ARG:HD2	2.42	0.48
1:D:285:ASP:CA	5:D:6027:HOH:O	2.35	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:A:259:PRO:HG2	1:A:260[A]:MET:H	1.78	0.48
1:J:124:VAL:HA	1:J:274:LEU:HD23	1.95	0.48
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:H:75:VAL:CG2	5:H:5932:HOH:O	2.53	0.48
1:E:348:VAL:HG22	5:E:648:HOH:O	2.13	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:D:329:PRO:CD	1:D:359:ARG:HD2	2.42	0.48
1:L:410:VAL:HG22	5:L:1818:HOH:O	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:25:LYS:NZ	5:E:633:HOH:O	2.45	0.48
1:E:230:LYS:HG2	5:E:678:HOH:O	2.14	0.48
1:C:183:PRO:HB2	5:D:5972:HOH:O	2.14	0.48
1:E:124:VAL:HA	1:E:274:LEU:HD23	1.95	0.48
1:D:259:PRO:HG2	1:D:260[A]:MET:H	1.78	0.48
1:H:174[B]:GLY:O	1:H:177[B]:GLY:HA2	2.13	0.48
1:G:174[B]:GLY:O	1:G:177[B]:GLY:HA2	2.13	0.48
1:L:128:PRO:CD	5:L:1692:HOH:O	2.61	0.48
1:K:360:PHE:CG	1:K:361:PRO:CD	2.97	0.48
1:L:360:PHE:CG	1:L:361:PRO:CD	2.97	0.48
1:B:410:VAL:HG22	5:B:6027:HOH:O	2.14	0.48
1:E:180[A]:PHE:HB3	1:F:29[A]:GLN:HB3	1.96	0.48
1:D:456:THR:O	1:J:458:HIS:HE1	1.97	0.48
1:K:25:LYS:HD2	5:K:1578:HOH:O	2.11	0.48
1:C:304:HIS:O	1:C:308:ILE:HG13	2.14	0.48
1:H:304:HIS:O	1:H:308:ILE:HG13	2.14	0.48
1:A:206:VAL:O	1:B:34:PRO:HG2	2.13	0.48
1:H:124:VAL:HA	1:H:274:LEU:HD23	1.95	0.48
1:J:154:ILE:HG13	5:J:5994:HOH:O	2.14	0.48
1:H:463:GLU:OE1	5:H:5909:HOH:O	2.20	0.48
3:H:4478:ADP:H5'1	5:H:5990:HOH:O	2.14	0.47
3:G:4477:ADP:H5'1	5:G:5986:HOH:O	2.14	0.47
1:I:269:HIS:CE1	4:I:5908:PPQ:CEP	2.92	0.47
1:D:329:PRO:HB2	1:D:342:SER:HA	1.96	0.47
1:B:60:ILE:O	1:B:60:ILE:HG23	2.12	0.47
1:A:348:VAL:HG22	5:A:5934:HOH:O	2.13	0.47
1:G:189:GLN:HE22	1:G:209[A]:HIS:HE1	1.57	0.47
1:A:304:HIS:O	1:A:308:ILE:HG13	2.14	0.47
1:D:304:HIS:O	1:D:308:ILE:HG13	2.14	0.47
1:G:230:LYS:HG2	5:G:5973:HOH:O	2.14	0.47
1:I:68:MET:HA	1:I:69:PRO:HD2	1.78	0.47
1:I:154:ILE:HG13	5:I:5998:HOH:O	2.14	0.47
1:L:124:VAL:HA	1:L:274:LEU:HD23	1.95	0.47
1:I:175[B]:VAL:O	1:I:175[B]:VAL:HG12	2.12	0.47
1:F:329:PRO:HB2	1:F:342:SER:HA	1.97	0.47
1:H:360:PHE:CG	1:H:361:PRO:CD	2.97	0.47
1:C:360:PHE:CG	1:C:361:PRO:CD	2.97	0.47
1:I:224:ARG:CG	1:I:224:ARG:NH2	2.69	0.47
1:F:304:HIS:O	1:F:308:ILE:HG13	2.14	0.47
1:J:437:GLU:CA	5:J:6034:HOH:O	2.58	0.47
1:H:230:LYS:HG2	5:H:5977:HOH:O	2.14	0.47
1:A:230:LYS:HG2	5:A:5963:HOH:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:34:PRO:HG2	1:L:206:VAL:O	2.14	0.47
1:E:154:ILE:HG13	5:E:692:HOH:O	2.14	0.47
1:G:259:PRO:HG2	1:G:260[A]:MET:H	1.78	0.47
1:F:68:MET:HA	1:F:69:PRO:HD2	1.78	0.47
1:E:174[B]:GLY:O	1:E:177[B]:GLY:HA2	2.13	0.47
1:J:174[B]:GLY:O	1:J:177[B]:GLY:HA2	2.13	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:D:410:VAL:HG22	5:D:6029:HOH:O	2.14	0.47
1:F:230:LYS:HG2	5:F:5973:HOH:O	2.14	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:G:154:ILE:HG13	5:G:5987:HOH:O	2.14	0.47
1:B:154:ILE:HG13	5:B:5978:HOH:O	2.14	0.47
1:D:154:ILE:HG13	5:D:5980:HOH:O	2.14	0.47
1:C:261[A]:PHE:HB2	1:I:457:PRO:HD3	1.97	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:K:179[B]:TYR:CD2	1:K:211[B]:HIS:HB2	2.47	0.47
1:I:231:LYS:CE	5:I:5928:HOH:O	2.59	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
1:D:128:PRO:CD	5:D:5910:HOH:O	2.61	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:A:128:PRO:CD	5:A:5907:HOH:O	2.61	0.47
1:K:304:HIS:O	1:K:308:ILE:HG13	2.14	0.47
1:K:84:THR:HG21	5:L:1730:HOH:O	2.12	0.47
1:C:232:ALA:HB1	1:C:367:PRO:HB2	1.97	0.47
1:A:154:ILE:HG13	5:A:5977:HOH:O	2.14	0.47
1:D:68:MET:HA	1:D:69:PRO:HD2	1.78	0.47
1:C:140:PHE:CE1	1:I:463:GLU:HA	2.49	0.47
1:B:174[B]:GLY:O	1:B:177[B]:GLY:CA	2.63	0.47
1:H:329:PRO:CD	1:H:359:ARG:HD2	2.42	0.47
1:E:329:PRO:HB2	1:E:342:SER:HA	1.96	0.47
1:K:231:LYS:CE	5:K:1539:HOH:O	2.59	0.47
1:G:165:GLU:N	5:G:5971:HOH:O	2.46	0.47
1:C:165:GLU:N	5:C:5961:HOH:O	2.46	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:H:207:GLU:O	1:H:208:ALA:HB2	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:154:ILE:HG13	5:F:5987:HOH:O	2.14	0.47
1:C:207:GLU:O	1:C:208:ALA:HB2	2.15	0.47
1:A:296:TYR:HB3	1:A:382:ILE:HA	1.97	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:C:174[B]:GLY:O	1:C:177[B]:GLY:CA	2.63	0.47
1:F:174[B]:GLY:O	1:F:177[B]:GLY:CA	2.63	0.47
1:L:174[B]:GLY:O	1:L:177[B]:GLY:CA	2.63	0.47
1:I:174[B]:GLY:O	1:I:177[B]:GLY:CA	2.63	0.47
1:A:339:ARG:NH1	1:B:59:GLY:O	2.44	0.47
1:J:174[B]:GLY:O	1:J:177[B]:GLY:CA	2.63	0.47
1:G:60:ILE:O	1:H:339:ARG:HB2	2.15	0.47
1:F:128:PRO:CD	5:F:5919:HOH:O	2.61	0.47
1:D:360:PHE:CG	1:D:361:PRO:CD	2.97	0.47
1:J:360:PHE:CG	1:J:361:PRO:CD	2.97	0.47
1:I:360:PHE:CG	1:I:361:PRO:CD	2.97	0.47
1:F:1:SER:N	1:F:71:ALA:CB	2.78	0.47
1:G:1:SER:N	1:G:71:ALA:CB	2.78	0.47
1:G:1:SER:O	1:G:5:VAL:HG23	2.15	0.47
1:D:332:LEU:O	5:D:6001:HOH:O	2.20	0.47
1:I:410:VAL:HG22	5:I:6047:HOH:O	2.14	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:J:75:VAL:CG2	5:J:5934:HOH:O	2.53	0.47
1:G:447:ARG:HD2	5:G:6019:HOH:O	2.15	0.47
1:J:348:VAL:HG22	5:J:5951:HOH:O	2.13	0.47
1:C:348:VAL:HG22	5:C:5934:HOH:O	2.13	0.47
1:A:401:PRO:HA	1:A:404:ALA:CA	2.44	0.47
1:J:304:HIS:O	1:J:308:ILE:HG13	2.14	0.47
1:I:28:GLU:CB	5:I:5951:HOH:O	2.58	0.47
1:H:230:LYS:O	1:H:234:GLU:HG3	2.15	0.47
1:B:230:LYS:HG2	5:B:5964:HOH:O	2.14	0.47
1:A:230:LYS:O	1:A:234:GLU:HG3	2.15	0.47
1:E:232:ALA:HB1	1:E:367:PRO:HB2	1.97	0.47
1:H:296:TYR:HB3	1:H:382:ILE:HA	1.97	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:K:296:TYR:HB3	1:K:382:ILE:HA	1.97	0.47
1:G:34:PRO:HG2	1:H:206:VAL:O	2.15	0.47
1:J:329:PRO:HB2	1:J:342:SER:HA	1.96	0.47
1:H:1:SER:O	1:H:5:VAL:HG23	2.15	0.47
1:A:332:LEU:O	5:A:5998:HOH:O	2.20	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:230:LYS:HG2	5:J:5980:HOH:O	2.14	0.47
1:D:230:LYS:O	1:D:234:GLU:HG3	2.15	0.47
1:L:232:ALA:HB1	1:L:367:PRO:HB2	1.97	0.47
1:I:207:GLU:O	1:I:208:ALA:HB2	2.15	0.47
1:F:207:GLU:O	1:F:208:ALA:HB2	2.15	0.47
1:C:273:SER:OG	3:C:4473:ADP:N6	2.48	0.47
3:C:4473:ADP:H5'1	5:C:5976:HOH:O	2.14	0.47
1:J:273:SER:OG	3:J:4480:ADP:N6	2.48	0.47
1:G:174[B]:GLY:O	1:G:177[B]:GLY:CA	2.63	0.47
1:H:329:PRO:HB2	1:H:342:SER:HA	1.97	0.47
1:K:1:SER:O	1:K:5:VAL:HG23	2.15	0.47
1:C:1:SER:N	1:C:71:ALA:CB	2.78	0.47
1:B:165:GLU:N	5:B:5962:HOH:O	2.46	0.47
1:B:208:ALA:HB2	1:C:33:ILE:CD1	2.44	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:A:232:ALA:HB1	1:A:367:PRO:HB2	1.97	0.47
1:G:232:ALA:HB1	1:G:367:PRO:HB2	1.97	0.47
1:A:261[A]:PHE:HB2	1:G:457:PRO:HD3	1.96	0.47
1:L:207:GLU:O	1:L:208:ALA:HB2	2.15	0.47
1:B:273:SER:OG	3:B:4472:ADP:N6	2.48	0.47
1:D:273:SER:OG	3:D:4474:ADP:N6	2.48	0.47
1:D:133:PHE:CE2	1:D:218:GLN:HB2	2.50	0.47
1:K:61:ASN:HB3	1:L:337:ARG:NH1	2.27	0.47
1:G:133:PHE:CE2	1:G:218:GLN:HB2	2.50	0.47
1:A:211[B]:HIS:O	1:A:212[B]:GLU:CB	2.54	0.47
1:A:337:ARG:CZ	1:B:61:ASN:HB2	2.44	0.47
1:I:329:PRO:HG2	1:I:359:ARG:CD	2.18	0.47
1:C:329:PRO:CD	1:C:359:ARG:HD2	2.42	0.47
1:B:360:PHE:CG	1:B:361:PRO:CD	2.97	0.47
1:L:1:SER:O	1:L:5:VAL:HG23	2.15	0.47
1:K:1:SER:N	1:K:71:ALA:CB	2.78	0.47
1:F:1:SER:O	1:F:5:VAL:HG23	2.15	0.47
1:E:1:SER:O	1:E:5:VAL:HG23	2.15	0.47
1:C:1:SER:O	1:C:5:VAL:HG23	2.15	0.47
1:A:410:VAL:HG22	5:A:6026:HOH:O	2.14	0.47
1:G:410:VAL:HG22	5:G:6036:HOH:O	2.14	0.47
1:A:447:ARG:HD2	5:A:6009:HOH:O	2.15	0.47
1:B:447:ARG:HD2	5:B:6010:HOH:O	2.15	0.47
1:G:348:VAL:HG22	5:G:5944:HOH:O	2.13	0.47
1:G:304:HIS:O	1:G:308:ILE:HG13	2.14	0.47
1:I:232:ALA:HB1	1:I:367:PRO:HB2	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:296:TYR:HB3	1:B:382:ILE:HA	1.97	0.47
1:L:273:SER:OG	3:L:4482:ADP:N6	2.48	0.46
3:D:4474:ADP:H5'1	5:D:5979:HOH:O	2.14	0.46
1:E:273:SER:OG	3:E:4475:ADP:N6	2.48	0.46
1:D:174[B]:GLY:O	1:D:177[B]:GLY:CA	2.63	0.46
1:B:133:PHE:CE2	1:B:218:GLN:HB2	2.50	0.46
1:L:329:PRO:HB2	1:L:342:SER:HA	1.97	0.46
1:I:128:PRO:CD	5:I:5928:HOH:O	2.61	0.46
1:E:329:PRO:HG2	1:E:359:ARG:CD	2.18	0.46
1:A:1:SER:N	1:A:71:ALA:CB	2.78	0.46
1:J:1:SER:N	1:J:71:ALA:CB	2.78	0.46
1:B:1:SER:N	1:B:71:ALA:CB	2.78	0.46
1:K:329:PRO:HG2	1:K:359:ARG:CD	2.18	0.46
1:A:224:ARG:NH2	1:A:224:ARG:CG	2.69	0.46
1:G:75:VAL:CG2	5:G:5926:HOH:O	2.53	0.46
1:E:304:HIS:O	1:E:308:ILE:HG13	2.14	0.46
1:L:230:LYS:O	1:L:234:GLU:HG3	2.15	0.46
1:H:232:ALA:HB1	1:H:367:PRO:HB2	1.97	0.46
1:K:232:ALA:HB1	1:K:367:PRO:HB2	1.97	0.46
1:J:232:ALA:HB1	1:J:367:PRO:HB2	1.97	0.46
1:B:339:ARG:HH12	1:C:63:SER:N	2.13	0.46
1:E:296:TYR:HB3	1:E:382:ILE:HA	1.97	0.46
3:I:4479:ADP:H5'1	5:I:5997:HOH:O	2.14	0.46
3:A:4471:ADP:H5'1	5:A:5976:HOH:O	2.14	0.46
1:G:360:PHE:CG	1:G:361:PRO:CD	2.97	0.46
1:K:329:PRO:HB2	1:K:342:SER:HA	1.96	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
1:B:207:GLU:O	1:B:208:ALA:HB2	2.15	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:K:273:SER:OG	3:K:4481:ADP:N6	2.48	0.46
1:C:133:PHE:CE2	1:C:218:GLN:HB2	2.50	0.46
1:H:133:PHE:CE2	1:H:218:GLN:HB2	2.50	0.46
1:E:174[B]:GLY:O	1:E:177[B]:GLY:CA	2.63	0.46
1:L:1:SER:N	1:L:71:ALA:CB	2.78	0.46
1:B:1:SER:O	1:B:5:VAL:HG23	2.15	0.46
1:D:1:SER:N	1:D:71:ALA:CB	2.78	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:B:304:HIS:O	1:B:308:ILE:HG13	2.14	0.46
1:F:230:LYS:O	1:F:234:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:230:LYS:HG2	5:D:5966:HOH:O	2.14	0.46
1:G:273:SER:OG	3:G:4477:ADP:N6	2.48	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:I:133:PHE:CE2	1:I:218:GLN:HB2	2.50	0.46
1:C:329:PRO:HB2	1:C:342:SER:HA	1.96	0.46
1:J:1:SER:O	1:J:5:VAL:HG23	2.15	0.46
1:E:1:SER:N	1:E:71:ALA:CB	2.78	0.46
1:I:1:SER:N	1:I:71:ALA:CB	2.78	0.46
1:F:332:LEU:O	5:F:6008:HOH:O	2.20	0.46
1:I:447:ARG:HD2	5:I:6030:HOH:O	2.15	0.46
1:H:447:ARG:HD2	5:H:6023:HOH:O	2.15	0.46
1:L:401:PRO:HA	1:L:404:ALA:CA	2.44	0.46
1:K:207:GLU:O	1:K:208:ALA:HB2	2.15	0.46
1:E:230:LYS:O	1:E:234:GLU:HG3	2.15	0.46
3:L:4482:ADP:H5'1	5:L:1762:HOH:O	2.14	0.46
1:H:273:SER:OG	3:H:4478:ADP:N6	2.48	0.46
1:F:273:SER:OG	3:F:4476:ADP:N6	2.48	0.46
1:I:332:LEU:O	5:I:6019:HOH:O	2.20	0.46
1:E:410:VAL:HG22	5:E:747:HOH:O	2.14	0.46
1:C:447:ARG:HD2	5:C:6009:HOH:O	2.15	0.46
1:K:401:PRO:HA	1:K:404:ALA:CA	2.44	0.46
1:I:84:THR:HG21	5:J:5962:HOH:O	2.16	0.46
1:F:18:ASP:OD2	1:F:30[A]:HIS:HD2	1.99	0.46
1:G:18:ASP:OD2	1:G:30[A]:HIS:HD2	1.99	0.46
1:I:33:ILE:CD1	1:J:208:ALA:HB2	2.45	0.46
1:J:207:GLU:O	1:J:208:ALA:HB2	2.15	0.46
1:E:333:ALA:HB1	1:E:392:MET:HG2	1.97	0.46
1:E:207:GLU:O	1:E:208:ALA:HB2	2.15	0.46
1:I:333:ALA:HB1	1:I:392:MET:HG2	1.97	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:C:410:VAL:HG22	5:C:6026:HOH:O	2.14	0.46
1:K:410:VAL:HG22	5:K:1665:HOH:O	2.14	0.46
1:L:447:ARG:HD2	5:L:1800:HOH:O	2.15	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:E:390:GLU:HA	1:E:391:PRO:HD3	1.84	0.46
1:D:183:PRO:CB	5:E:684:HOH:O	2.62	0.46
1:B:232:ALA:HB1	1:B:367:PRO:HB2	1.97	0.46
1:D:182:VAL:HG23	5:E:662:HOH:O	2.16	0.46
1:L:296:TYR:HB3	1:L:382:ILE:HA	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:4476:ADP:H5'1	5:F:5986:HOH:O	2.14	0.46
1:F:133:PHE:CE2	1:F:218:GLN:HB2	2.51	0.46
1:I:63:SER:N	1:J:339:ARG:NH1	2.62	0.46
1:J:133:PHE:CE2	1:J:218:GLN:HB2	2.50	0.46
1:A:269:HIS:CE1	4:A:5900:PPQ:CEP	2.92	0.46
1:D:1:SER:O	1:D:5:VAL:HG23	2.15	0.46
1:L:332:LEU:O	5:L:1788:HOH:O	2.20	0.46
1:J:447:ARG:HD2	5:J:6026:HOH:O	2.15	0.46
1:C:437:GLU:CA	5:C:6017:HOH:O	2.58	0.46
1:J:230:LYS:O	1:J:234:GLU:HG3	2.15	0.46
1:J:18:ASP:OD2	1:J:30[A]:HIS:HD2	1.99	0.46
1:D:232:ALA:HB1	1:D:367:PRO:HB2	1.97	0.46
1:E:306:LYS:HE2	5:E:751:HOH:O	2.16	0.46
1:A:333:ALA:HB1	1:A:392:MET:HG2	1.97	0.46
1:I:1:SER:O	1:I:5:VAL:HG23	2.15	0.46
1:D:395:ASN:HB2	1:D:399:LEU:HD12	1.98	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:E:447:ARG:HD2	5:E:729:HOH:O	2.15	0.46
1:I:401:PRO:HA	1:I:404:ALA:CA	2.44	0.46
1:A:207:GLU:O	1:A:208:ALA:HB2	2.15	0.46
1:I:296:TYR:HB3	1:I:382:ILE:HA	1.97	0.46
1:D:333:ALA:HB1	1:D:392:MET:HG2	1.97	0.46
1:D:207:GLU:O	1:D:208:ALA:HB2	2.15	0.46
1:B:333:ALA:HB1	1:B:392:MET:HG2	1.97	0.46
1:I:273:SER:OG	3:I:4479:ADP:N6	2.48	0.46
1:A:273:SER:OG	3:A:4471:ADP:N6	2.48	0.46
1:I:294:ALA:O	1:I:298:ILE:HG13	2.16	0.46
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:K:18:ASP:OD2	1:K:30[A]:HIS:HD2	1.99	0.46
1:C:18:ASP:OD2	1:C:30[A]:HIS:HD2	1.99	0.46
1:B:140:PHE:CE1	1:H:463:GLU:HA	2.51	0.46
1:K:154:ILE:HG13	5:K:1610:HOH:O	2.14	0.46
1:I:61:ASN:HB3	1:J:337:ARG:HH11	1.79	0.46
1:H:174[B]:GLY:O	1:H:177[B]:GLY:CA	2.63	0.46
1:E:210[A]:HIS:ND1	1:E:211[A]:HIS:O	2.47	0.46
1:G:337:ARG:CZ	1:L:61:ASN:HB2	2.45	0.46
1:H:1:SER:N	1:H:71:ALA:CB	2.78	0.46
1:F:395:ASN:HB2	1:F:399:LEU:HD12	1.98	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:172:ARG:HA	1:H:173[A]:PRO:HD3	1.80	0.46
1:C:189:GLN:NE2	1:D:32:THR:OG1	2.48	0.46
1:G:235:ILE:HA	1:G:235:ILE:HD13	1.80	0.46
1:C:68:MET:HA	1:C:69:PRO:HD2	1.78	0.46
1:C:333:ALA:HB1	1:C:392:MET:HG2	1.97	0.46
1:C:180[A]:PHE:O	1:D:29[A]:GLN:HA	2.16	0.45
1:L:133:PHE:CE2	1:L:218:GLN:HB2	2.51	0.45
1:E:133:PHE:CE2	1:E:218:GLN:HB2	2.50	0.45
1:D:231:LYS:CE	5:D:5910:HOH:O	2.59	0.45
1:A:1:SER:O	1:A:5:VAL:HG23	2.15	0.45
1:J:332:LEU:O	5:J:6015:HOH:O	2.20	0.45
1:H:294:ALA:O	1:H:298:ILE:HG13	2.16	0.45
1:E:165:GLU:N	5:E:676:HOH:O	2.46	0.45
1:J:165:GLU:N	5:J:5978:HOH:O	2.46	0.45
1:A:18:ASP:OD2	1:A:30[A]:HIS:HD2	1.99	0.45
1:K:230:LYS:O	1:K:234:GLU:HG3	2.15	0.45
1:G:125:LEU:HA	1:G:125:LEU:HD12	1.79	0.45
1:B:306:LYS:HE2	5:B:6031:HOH:O	2.16	0.45
1:G:339:ARG:HH12	1:L:63:SER:N	2.14	0.45
1:J:333:ALA:HB1	1:J:392:MET:HG2	1.97	0.45
1:L:333:ALA:HB1	1:L:392:MET:HG2	1.97	0.45
1:K:210[A]:HIS:ND1	1:K:211[A]:HIS:O	2.47	0.45
1:L:294:ALA:O	1:L:298:ILE:HG13	2.16	0.45
1:E:294:ALA:O	1:E:298:ILE:HG13	2.16	0.45
1:I:165:GLU:N	5:I:5982:HOH:O	2.46	0.45
1:G:80:PHE:CZ	1:H:189:GLN:HG3	2.51	0.45
1:C:230:LYS:O	1:C:234:GLU:HG3	2.15	0.45
1:L:18:ASP:OD2	1:L:30[A]:HIS:HD2	1.99	0.45
1:F:232:ALA:HB1	1:F:367:PRO:HB2	1.97	0.45
1:G:155:GLU:OE1	1:G:211[A]:HIS:CE1	2.68	0.45
1:E:269:HIS:CE1	4:E:5904:PPQ:CEP	2.92	0.45
1:J:128:PRO:CD	5:J:5926:HOH:O	2.61	0.45
1:A:329:PRO:HB2	1:A:342:SER:HA	1.96	0.45
1:K:128:PRO:CD	5:K:1539:HOH:O	2.61	0.45
1:J:294:ALA:O	1:J:298:ILE:HG13	2.16	0.45
1:K:294:ALA:O	1:K:298:ILE:HG13	2.16	0.45
1:H:401:PRO:HA	1:H:404:ALA:CA	2.44	0.45
1:B:230:LYS:O	1:B:234:GLU:HG3	2.15	0.45
1:A:47:LYS:CD	5:A:6035:HOH:O	2.65	0.45
1:D:47:LYS:CD	5:D:6038:HOH:O	2.65	0.45
1:J:47:LYS:CD	5:J:6052:HOH:O	2.65	0.45
1:C:296:TYR:HB3	1:C:382:ILE:HA	1.97	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:296:TYR:HB3	1:J:382:ILE:HA	1.97	0.45
1:H:333:ALA:HB1	1:H:392:MET:HG2	1.97	0.45
1:F:296:TYR:HB3	1:F:382:ILE:HA	1.97	0.45
1:G:172:ARG:HA	1:G:173[A]:PRO:HD3	1.80	0.45
1:E:18:ASP:OD2	1:E:30[A]:HIS:HD2	1.99	0.45
1:H:18:ASP:OD2	1:H:30[A]:HIS:HD2	1.99	0.45
1:C:182:VAL:HG23	5:D:5951:HOH:O	2.16	0.45
1:G:296:TYR:HB3	1:G:382:ILE:HA	1.97	0.45
1:A:329:PRO:HD2	1:A:359:ARG:HG2	1.99	0.45
1:I:395:ASN:HB2	1:I:399:LEU:HD12	1.98	0.45
1:L:395:ASN:HB2	1:L:399:LEU:HD12	1.98	0.45
1:F:344:ARG:HE	1:F:344:ARG:HB3	1.59	0.45
1:A:165:GLU:N	5:A:5961:HOH:O	2.46	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:G:153:ASP:OD1	1:G:251:LYS:NZ	2.50	0.45
1:F:333:ALA:HB1	1:F:392:MET:HG2	1.97	0.45
1:H:306:LYS:HE2	5:H:6044:HOH:O	2.16	0.45
1:G:333:ALA:HB1	1:G:392:MET:HG2	1.97	0.45
1:K:333:ALA:HB1	1:K:392:MET:HG2	1.97	0.45
1:C:128:PRO:CD	5:C:5909:HOH:O	2.61	0.45
1:H:395:ASN:HB2	1:H:399:LEU:HD12	1.98	0.45
1:B:395:ASN:HB2	1:B:399:LEU:HD12	1.98	0.45
1:E:172:ARG:HA	1:E:173[A]:PRO:HD3	1.80	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:L:329:PRO:HD2	1:L:359:ARG:HG2	1.99	0.45
1:H:329:PRO:HD2	1:H:359:ARG:HG2	1.99	0.45
1:F:294:ALA:O	1:F:298:ILE:HG13	2.16	0.45
1:G:294:ALA:O	1:G:298:ILE:HG13	2.16	0.45
1:K:165:GLU:N	5:K:1594:HOH:O	2.46	0.45
1:A:189:GLN:HG3	1:B:80:PHE:CZ	2.51	0.45
1:G:183:PRO:CB	5:L:1755:HOH:O	2.62	0.45
1:G:306:LYS:HE2	5:G:6040:HOH:O	2.16	0.45
1:I:306:LYS:HE2	5:I:6051:HOH:O	2.16	0.45
1:C:306:LYS:HE2	5:C:6030:HOH:O	2.16	0.45
1:J:306:LYS:HE2	5:J:6047:HOH:O	2.16	0.45
1:K:306:LYS:HE2	5:K:1669:HOH:O	2.16	0.45
1:K:29[A]:GLN:HA	1:L:180[A]:PHE:O	2.17	0.45
1:G:63:SER:N	1:H:339:ARG:NH1	2.62	0.45
1:E:128:PRO:CD	5:E:621:HOH:O	2.61	0.45
1:D:329:PRO:HD2	1:D:359:ARG:HG2	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:4:HIS:CE1	5:A:5986:HOH:O	2.70	0.45
1:G:332:LEU:O	5:G:6008:HOH:O	2.20	0.45
1:I:40:ALA:HB2	5:I:6002:HOH:O	2.10	0.45
1:A:153:ASP:OD1	1:A:251:LYS:NZ	2.50	0.45
1:F:210[A]:HIS:ND1	1:F:211[A]:HIS:O	2.47	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:K:395:ASN:HB2	1:K:399:LEU:HD12	1.98	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:B:18:ASP:OD2	1:B:30[A]:HIS:HD2	1.99	0.45
1:J:401:PRO:CA	1:J:404:ALA:HA	2.46	0.45
1:F:401:PRO:HA	1:F:404:ALA:CA	2.44	0.45
1:K:193:SER:O	1:K:197:LEU:HG	2.17	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:B:183:PRO:CB	5:C:5969:HOH:O	2.65	0.45
1:F:306:LYS:HE2	5:F:6040:HOH:O	2.16	0.45
1:B:269:HIS:HE1	4:B:5901:PPQ:HEP2	1.82	0.45
1:D:359:ARG:HH11	1:D:359:ARG:HD3	1.65	0.45
1:C:294:ALA:O	1:C:298:ILE:HG13	2.16	0.45
1:A:395:ASN:HB2	1:A:399:LEU:HD12	1.98	0.45
1:D:458:HIS:HE1	1:J:456:THR:O	2.00	0.45
1:H:153:ASP:OD1	1:H:251:LYS:NZ	2.50	0.45
1:K:447:ARG:HG3	1:K:447:ARG:HH21	1.83	0.45
1:H:193:SER:O	1:H:197:LEU:HG	2.17	0.45
1:E:47:LYS:CD	5:E:756:HOH:O	2.65	0.45
1:L:306:LYS:HE2	5:L:1822:HOH:O	2.16	0.45
1:F:155:GLU:OE1	1:F:211[A]:HIS:CE1	2.68	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:E:447:ARG:HG3	1:E:447:ARG:HH21	1.82	0.44
1:G:447:ARG:HH21	1:G:447:ARG:HG3	1.82	0.44
1:J:401:PRO:HA	1:J:404:ALA:CA	2.44	0.44
1:F:25:LYS:HD2	5:F:5956:HOH:O	2.10	0.44
1:L:387:HIS:HA	1:L:388:PRO:HD2	1.85	0.44
1:D:284:GLY:HA3	1:D:291:SER:HA	1.99	0.44
1:C:268:MET:N	1:C:363:PRO:HD3	2.33	0.44
1:G:47:LYS:CD	5:G:6045:HOH:O	2.65	0.44
1:C:149:VAL:HG21	1:I:462:PHE:CE1	2.52	0.44
1:L:210[A]:HIS:ND1	1:L:211[A]:HIS:O	2.47	0.44
1:B:337:ARG:HD3	1:C:61:ASN:CB	2.46	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:339:ARG:HB2	1:D:60:ILE:O	2.18	0.44
1:A:447:ARG:HG3	1:A:447:ARG:HH21	1.82	0.44
1:K:153:ASP:OD1	1:K:251:LYS:NZ	2.50	0.44
1:C:153:ASP:OD1	1:C:251:LYS:NZ	2.50	0.44
1:B:401:PRO:HA	1:B:404:ALA:CA	2.44	0.44
1:B:193:SER:O	1:B:197:LEU:HG	2.17	0.44
1:I:268:MET:N	1:I:363:PRO:HD3	2.33	0.44
1:E:115:LEU:CD2	1:E:379:LEU:HD21	2.48	0.44
1:B:115:LEU:CD2	1:B:379:LEU:HD21	2.48	0.44
1:A:462:PHE:CE1	1:G:149:VAL:HG21	2.52	0.44
1:I:329:PRO:HD2	1:I:359:ARG:HG2	1.99	0.44
1:F:360:PHE:CG	1:F:361:PRO:CD	2.97	0.44
1:J:4:HIS:CE1	5:J:6003:HOH:O	2.70	0.44
1:A:231:LYS:CE	5:A:5907:HOH:O	2.59	0.44
1:K:329:PRO:HD2	1:K:359:ARG:HG2	1.99	0.44
1:A:60:ILE:O	1:F:339:ARG:HB2	2.17	0.44
1:D:289:GLY:HA2	5:D:6027:HOH:O	2.18	0.44
1:E:289:GLY:HA2	5:E:745:HOH:O	2.18	0.44
1:I:447:ARG:HH21	1:I:447:ARG:HG3	1.82	0.44
1:J:447:ARG:HG3	1:J:447:ARG:HH21	1.82	0.44
1:F:75:VAL:CG2	5:F:5927:HOH:O	2.53	0.44
1:D:153:ASP:OD1	1:D:251:LYS:NZ	2.50	0.44
1:D:401:PRO:HA	1:D:404:ALA:CA	2.44	0.44
1:B:401:PRO:CA	1:B:404:ALA:HA	2.47	0.44
1:H:401:PRO:CA	1:H:404:ALA:HA	2.47	0.44
1:H:268:MET:N	1:H:363:PRO:HD3	2.33	0.44
1:K:68:MET:HA	1:K:69:PRO:HD2	1.78	0.44
1:C:210[A]:HIS:ND1	1:C:211[A]:HIS:O	2.47	0.44
1:H:4:HIS:CE1	5:H:6000:HOH:O	2.70	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:H:447:ARG:HH21	1:H:447:ARG:HG3	1.82	0.44
1:B:447:ARG:HG3	1:B:447:ARG:HH21	1.82	0.44
1:E:153:ASP:OD1	1:E:251:LYS:NZ	2.50	0.44
1:J:284:GLY:HA3	1:J:291:SER:HA	1.99	0.44
1:F:268:MET:N	1:F:363:PRO:HD3	2.33	0.44
1:B:268:MET:N	1:B:363:PRO:HD3	2.33	0.44
1:K:63:SER:N	1:L:339:ARG:HH12	2.15	0.44
1:H:324:PRO:N	5:H:6034:HOH:O	2.51	0.44
1:C:324:PRO:N	5:C:6020:HOH:O	2.51	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:289:GLY:HA2	5:G:6034:HOH:O	2.18	0.44
1:J:153:ASP:OD1	1:J:251:LYS:NZ	2.50	0.44
1:I:153:ASP:OD1	1:I:251:LYS:NZ	2.50	0.44
1:F:193:SER:O	1:F:197:LEU:HG	2.17	0.44
1:E:193:SER:O	1:E:197:LEU:HG	2.18	0.44
1:F:284:GLY:HA3	1:F:291:SER:HA	1.99	0.44
1:C:337:ARG:O	1:D:61:ASN:O	2.35	0.44
1:J:231:LYS:CE	5:J:5926:HOH:O	2.59	0.44
1:K:359:ARG:HH11	1:K:359:ARG:HD3	1.65	0.44
1:H:289:GLY:HA2	5:H:6038:HOH:O	2.18	0.44
1:L:447:ARG:HH21	1:L:447:ARG:HG3	1.82	0.44
1:G:193:SER:O	1:G:197:LEU:HG	2.17	0.44
1:D:193:SER:O	1:D:197:LEU:HG	2.17	0.44
1:K:284:GLY:HA3	1:K:291:SER:HA	1.99	0.44
1:A:268:MET:N	1:A:363:PRO:HD3	2.33	0.44
1:K:47:LYS:CD	5:K:1674:HOH:O	2.65	0.44
1:D:115:LEU:CD2	1:D:379:LEU:HD21	2.48	0.44
1:L:324:PRO:N	5:L:1812:HOH:O	2.51	0.44
1:A:306:LYS:HE2	5:A:6030:HOH:O	2.16	0.44
1:D:306:LYS:HE2	5:D:6033:HOH:O	2.16	0.44
1:K:178[A]:GLY:O	1:K:211[A]:HIS:HD2	2.01	0.44
1:G:210[A]:HIS:ND1	1:G:211[A]:HIS:O	2.47	0.44
1:F:329:PRO:HD2	1:F:359:ARG:HG2	1.99	0.44
1:C:269:HIS:HE1	4:C:5902:PPQ:HEP2	1.82	0.44
1:F:4:HIS:CE1	5:F:5996:HOH:O	2.70	0.44
1:E:401:PRO:HA	1:E:404:ALA:CA	2.44	0.44
1:I:193:SER:O	1:I:197:LEU:HG	2.17	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:D:268:MET:N	1:D:363:PRO:HD3	2.33	0.44
1:G:268:MET:N	1:G:363:PRO:HD3	2.33	0.44
1:J:115:LEU:CD2	1:J:379:LEU:HD21	2.48	0.44
1:F:352:LYS:HE2	1:F:352:LYS:HA	2.00	0.44
1:G:68:MET:HA	1:G:69:PRO:HD2	1.78	0.44
1:A:68:MET:HA	1:A:69:PRO:HD2	1.78	0.44
1:B:231:LYS:CE	5:B:5908:HOH:O	2.59	0.44
1:K:4:HIS:CE1	5:K:1620:HOH:O	2.70	0.44
1:K:344:ARG:HB3	1:K:344:ARG:HE	1.59	0.44
1:A:40:ALA:HB2	5:A:5981:HOH:O	2.10	0.44
1:L:153:ASP:OD1	1:L:251:LYS:NZ	2.50	0.44
1:G:208:ALA:HB2	1:L:33:ILE:CD1	2.48	0.44
1:E:324:PRO:N	5:E:741:HOH:O	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:61:ASN:CB	1:F:337:ARG:HD3	2.46	0.44
1:L:231:LYS:CE	5:L:1692:HOH:O	2.59	0.44
1:L:128:PRO:HA	1:L:269:HIS:O	2.18	0.44
1:L:269:HIS:CE1	4:L:5911:PPQ:CEP	2.92	0.44
1:F:128:PRO:HA	1:F:269:HIS:O	2.18	0.44
1:H:323:VAL:O	5:H:5936:HOH:O	2.21	0.44
1:L:4:HIS:CE1	5:L:1773:HOH:O	2.70	0.44
1:G:269:HIS:CE1	4:G:5906:PPQ:CEP	2.92	0.44
1:C:4:HIS:CE1	5:C:5986:HOH:O	2.70	0.44
1:K:289:GLY:HA2	5:K:1663:HOH:O	2.18	0.44
1:K:401:PRO:CA	1:K:404:ALA:HA	2.47	0.44
1:E:284:GLY:HA3	1:E:291:SER:HA	1.99	0.44
1:H:230:LYS:CG	5:H:5977:HOH:O	2.66	0.44
1:G:230:LYS:CG	5:G:5973:HOH:O	2.66	0.44
1:K:115:LEU:CD2	1:K:379:LEU:HD21	2.48	0.44
1:H:115:LEU:CD2	1:H:379:LEU:HD21	2.48	0.44
1:G:324:PRO:N	5:G:6030:HOH:O	2.51	0.44
1:J:324:PRO:N	5:J:6037:HOH:O	2.51	0.44
1:C:211[B]:HIS:O	1:C:212[B]:GLU:CB	2.54	0.43
1:D:178[A]:GLY:O	1:D:211[A]:HIS:HD2	2.01	0.43
1:L:210[B]:HIS:C	1:L:211[B]:HIS:CD2	2.89	0.43
1:J:61:ASN:CB	1:K:337:ARG:HD3	2.47	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
1:L:289:GLY:HA2	5:L:1816:HOH:O	2.18	0.43
1:G:401:PRO:HA	1:G:404:ALA:CA	2.44	0.43
1:K:16:PHE:HB2	1:K:84:THR:HB	2.00	0.43
1:C:193:SER:O	1:C:197:LEU:HG	2.18	0.43
1:L:193:SER:O	1:L:197:LEU:HG	2.18	0.43
1:A:193:SER:O	1:A:197:LEU:HG	2.17	0.43
1:C:230:LYS:CG	5:C:5963:HOH:O	2.66	0.43
1:F:230:LYS:CG	5:F:5973:HOH:O	2.66	0.43
1:K:268:MET:N	1:K:363:PRO:HD3	2.33	0.43
1:J:268:MET:N	1:J:363:PRO:HD3	2.33	0.43
1:D:235:ILE:HD13	1:D:235:ILE:HA	1.80	0.43
1:C:178[A]:GLY:O	1:C:211[A]:HIS:HD2	2.01	0.43
1:L:323:VAL:O	5:L:1705:HOH:O	2.21	0.43
1:D:323:VAL:O	5:D:5923:HOH:O	2.21	0.43
1:I:128:PRO:HA	1:I:269:HIS:O	2.18	0.43
1:C:128:PRO:HA	1:C:269:HIS:O	2.18	0.43
1:E:323:VAL:O	5:E:634:HOH:O	2.21	0.43
1:E:231:LYS:CE	5:E:621:HOH:O	2.59	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:128:PRO:CD	5:B:5908:HOH:O	2.61	0.43
1:E:4:HIS:CE1	5:E:702:HOH:O	2.70	0.43
1:G:4:HIS:CE1	5:G:5996:HOH:O	2.70	0.43
1:G:395:ASN:HB2	1:G:399:LEU:HD12	1.98	0.43
1:L:172:ARG:HA	1:L:173[A]:PRO:HD3	1.80	0.43
1:G:16:PHE:HB2	1:G:84:THR:HB	2.00	0.43
1:A:374:LEU:HD12	1:A:374:LEU:HA	1.91	0.43
1:H:30[A]:HIS:CE1	1:I:183:PRO:HD3	2.54	0.43
1:I:47:LYS:CD	5:I:6056:HOH:O	2.65	0.43
1:H:68:MET:HA	1:H:69:PRO:HD2	1.78	0.43
1:K:127:GLY:HA3	3:K:4481:ADP:H1'	2.00	0.43
1:F:178[A]:GLY:O	1:F:211[A]:HIS:HD2	2.01	0.43
1:D:155:GLU:OE1	1:D:211[A]:HIS:CE1	2.68	0.43
1:L:178[A]:GLY:O	1:L:211[A]:HIS:HD2	2.01	0.43
1:C:339:ARG:NH1	1:D:63:SER:N	2.65	0.43
1:K:323:VAL:O	5:K:1552:HOH:O	2.21	0.43
1:E:128:PRO:HA	1:E:269:HIS:O	2.18	0.43
1:B:323:VAL:O	5:B:5921:HOH:O	2.21	0.43
1:E:395:ASN:HB2	1:E:399:LEU:HD12	1.98	0.43
1:A:16:PHE:HB2	1:A:84:THR:HB	2.00	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:G:183:PRO:HD3	1:L:30[A]:HIS:CE1	2.52	0.43
1:F:47:LYS:CD	5:F:6045:HOH:O	2.65	0.43
1:I:115:LEU:CD2	1:I:379:LEU:HD21	2.48	0.43
1:L:352:LYS:HA	1:L:352:LYS:HE2	2.00	0.43
1:F:324:PRO:N	5:F:6030:HOH:O	2.51	0.43
1:D:423:LEU:C	1:D:425:ARG:H	2.22	0.43
1:E:463:GLU:HA	1:K:140:PHE:CE1	2.53	0.43
1:J:29[A]:GLN:HA	1:K:180[A]:PHE:O	2.18	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:D:344:ARG:HB3	1:D:344:ARG:HE	1.58	0.43
1:B:456:THR:O	1:H:458:HIS:HE1	2.00	0.43
1:F:447:ARG:HG3	1:F:447:ARG:HH21	1.82	0.43
1:A:390:GLU:HA	1:A:391:PRO:HD3	1.84	0.43
1:J:193:SER:O	1:J:197:LEU:HG	2.17	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:L:115:LEU:CD2	1:L:379:LEU:HD21	2.48	0.43
1:B:56:GLY:N	5:B:5994:HOH:O	2.40	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:423:LEU:C	1:A:425:ARG:H	2.22	0.43
1:L:68:MET:HA	1:L:69:PRO:HD2	1.78	0.43
1:B:127:GLY:HA3	3:B:4472:ADP:H1'	2.00	0.43
1:H:178[A]:GLY:O	1:H:211[A]:HIS:HD2	2.01	0.43
1:I:178[A]:GLY:O	1:I:211[A]:HIS:HD2	2.01	0.43
1:B:180[A]:PHE:O	1:C:29[A]:GLN:HA	2.19	0.43
1:J:178[A]:GLY:O	1:J:211[A]:HIS:HD2	2.01	0.43
1:H:269:HIS:HE1	4:H:5907:PPQ:HEP2	1.82	0.43
1:B:128:PRO:HA	1:B:269:HIS:O	2.18	0.43
1:J:329:PRO:HD2	1:J:359:ARG:HG2	1.99	0.43
1:D:128:PRO:HA	1:D:269:HIS:O	2.18	0.43
1:A:289:GLY:HA2	5:A:6024:HOH:O	2.18	0.43
1:I:75:VAL:CG2	5:I:5937:HOH:O	2.53	0.43
1:K:32:THR:OG1	1:L:189:GLN:NE2	2.50	0.43
1:E:401:PRO:CA	1:E:404:ALA:HA	2.47	0.43
1:I:16:PHE:HB2	1:I:84:THR:HB	2.00	0.43
1:G:284:GLY:HA3	1:G:291:SER:HA	1.99	0.43
1:E:230:LYS:CG	5:E:678:HOH:O	2.66	0.43
1:G:30[A]:HIS:CE1	1:H:183:PRO:HD3	2.54	0.43
1:D:33:ILE:HA	1:D:34:PRO:HD3	1.90	0.43
1:K:125:LEU:HA	1:K:125:LEU:HD12	1.79	0.43
1:F:423:LEU:C	1:F:425:ARG:H	2.22	0.43
1:F:269:HIS:CE1	4:F:5905:PPQ:CEP	2.91	0.43
1:C:231:LYS:CE	5:C:5909:HOH:O	2.59	0.43
1:E:1:SER:N	1:E:71:ALA:HB3	2.34	0.43
1:B:289:GLY:HA2	5:B:6025:HOH:O	2.18	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:G:40:ALA:HB2	5:G:5991:HOH:O	2.10	0.43
1:B:16:PHE:HB2	1:B:84:THR:HB	2.00	0.43
1:C:33:ILE:HA	1:C:34:PRO:HD3	1.90	0.43
1:F:16:PHE:HB2	1:F:84:THR:HB	2.00	0.43
1:F:82:ASP:O	1:F:84:THR:CG2	2.67	0.43
1:D:16:PHE:HB2	1:D:84:THR:HB	2.00	0.43
1:J:230:LYS:CG	5:J:5980:HOH:O	2.66	0.43
1:C:230:LYS:HE2	1:C:230:LYS:HB2	1.85	0.43
1:A:284:GLY:HA3	1:A:291:SER:HA	1.99	0.43
1:A:230:LYS:CG	5:A:5963:HOH:O	2.66	0.43
1:J:30[A]:HIS:CE1	1:K:183:PRO:HD3	2.53	0.43
1:G:115:LEU:CD2	1:G:379:LEU:HD21	2.48	0.43
1:G:144:ILE:HG22	5:G:5922:HOH:O	2.19	0.43
1:A:324:PRO:N	5:A:6020:HOH:O	2.51	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:261[A]:PHE:HB2	1:K:457:PRO:HD3	2.01	0.43
1:A:140:PHE:CE1	1:G:463:GLU:HA	2.54	0.43
1:G:423:LEU:C	1:G:425:ARG:H	2.22	0.43
1:E:140:PHE:CE1	1:K:463:GLU:HA	2.54	0.43
1:G:271:HIS:CD2	1:G:357:GLU:HB2	2.54	0.43
1:C:271:HIS:CD2	1:C:357:GLU:HB2	2.54	0.43
1:A:29[A]:GLN:HA	1:F:180[A]:PHE:O	2.18	0.43
1:A:339:ARG:HH12	1:B:63:SER:N	2.16	0.43
1:J:210[A]:HIS:ND1	1:J:211[A]:HIS:O	2.47	0.43
1:E:337:ARG:CD	1:F:61:ASN:CB	2.84	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:C:359:ARG:HH12	4:C:5902:PPQ:HEP2	1.84	0.43
1:E:192[A]:ARG:HH21	1:E:219:ASN:ND2	2.17	0.43
1:C:458:HIS:HE1	1:I:456:THR:O	2.02	0.43
1:E:16:PHE:HB2	1:E:84:THR:HB	2.00	0.43
1:J:390:GLU:HA	1:J:391:PRO:HD3	1.84	0.43
1:E:268:MET:N	1:E:363:PRO:HD3	2.33	0.43
1:D:352:LYS:HE2	1:D:352:LYS:HA	2.00	0.43
1:L:423:LEU:C	1:L:425:ARG:H	2.22	0.43
1:K:271:HIS:CD2	1:K:357:GLU:HB2	2.54	0.43
1:H:423:LEU:C	1:H:425:ARG:H	2.22	0.43
1:F:144:ILE:HG22	5:F:5923:HOH:O	2.19	0.43
1:A:155:GLU:OE1	1:A:211[A]:HIS:CE1	2.68	0.43
1:I:323:VAL:O	5:I:5941:HOH:O	2.21	0.43
1:H:1:SER:N	1:H:71:ALA:HB3	2.34	0.43
1:H:305:ALA:CB	1:H:332:LEU:HD21	2.49	0.43
1:C:16:PHE:HB2	1:C:84:THR:HB	2.00	0.43
5:A:5945:HOH:O	1:B:84:THR:HG21	2.18	0.43
1:H:201:GLN:N	5:H:6017:HOH:O	2.52	0.43
1:I:230:LYS:CG	5:I:5984:HOH:O	2.66	0.43
1:F:115:LEU:CD2	1:F:379:LEU:HD21	2.48	0.43
1:K:423:LEU:C	1:K:425:ARG:H	2.22	0.43
1:C:144:ILE:HG22	5:C:5913:HOH:O	2.19	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:E:127:GLY:HA3	3:E:4475:ADP:H1'	2.00	0.43
1:B:210[B]:HIS:C	1:B:211[B]:HIS:CD2	2.90	0.43
1:B:178[A]:GLY:O	1:B:211[A]:HIS:HD2	2.01	0.43
1:E:329:PRO:HD2	1:E:359:ARG:HG2	1.99	0.43
1:J:128:PRO:HA	1:J:269:HIS:O	2.18	0.43
1:B:1:SER:N	1:B:71:ALA:HB3	2.34	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:192[A]:ARG:HH21	1:D:219:ASN:ND2	2.17	0.43
1:A:192[A]:ARG:HH21	1:A:219:ASN:ND2	2.17	0.43
1:C:305:ALA:CB	1:C:332:LEU:HD21	2.49	0.43
1:G:192[A]:ARG:HH21	1:G:219:ASN:ND2	2.17	0.43
1:I:305:ALA:CB	1:I:332:LEU:HD21	2.49	0.43
1:K:305:ALA:CB	1:K:332:LEU:HD21	2.49	0.43
1:B:305:ALA:CB	1:B:332:LEU:HD21	2.49	0.43
1:I:172:ARG:HA	1:I:173[A]:PRO:HD3	1.80	0.43
1:C:447:ARG:HH21	1:C:447:ARG:HG3	1.82	0.43
1:C:401:PRO:CA	1:C:404:ALA:HA	2.47	0.43
1:F:401:PRO:CA	1:F:404:ALA:HA	2.46	0.43
1:C:201:GLN:N	5:C:6003:HOH:O	2.52	0.43
1:L:201:GLN:N	5:L:1793:HOH:O	2.52	0.43
1:K:201:GLN:N	5:K:1640:HOH:O	2.52	0.43
5:J:5986:HOH:O	1:K:183:PRO:CB	2.66	0.43
1:A:115:LEU:CD2	1:A:379:LEU:HD21	2.48	0.43
1:A:140:PHE:CE1	1:F:160:SER:HB2	2.54	0.43
1:I:423:LEU:C	1:I:425:ARG:H	2.22	0.43
1:J:423:LEU:C	1:J:425:ARG:H	2.22	0.43
1:F:127:GLY:HA3	3:F:4476:ADP:H1'	2.00	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:G:210[B]:HIS:C	1:G:211[B]:HIS:CD2	2.89	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:J:289:GLY:HA2	5:J:6041:HOH:O	2.18	0.43
1:F:289:GLY:HA2	5:F:6034:HOH:O	2.18	0.43
1:F:192[A]:ARG:HH21	1:F:219:ASN:ND2	2.17	0.43
1:D:305:ALA:CB	1:D:332:LEU:HD21	2.49	0.43
1:K:192[A]:ARG:HH21	1:K:219:ASN:ND2	2.17	0.43
1:E:332:LEU:O	5:E:717:HOH:O	2.20	0.43
1:C:40:ALA:HB2	5:C:5981:HOH:O	2.10	0.43
1:K:197:LEU:O	1:K:201:GLN:HG3	2.19	0.43
1:I:452:ARG:HG2	5:I:6036:HOH:O	2.19	0.43
1:H:324:PRO:HA	5:H:6034:HOH:O	2.19	0.43
1:K:352:LYS:HA	1:K:352:LYS:HE2	2.00	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:I:144:ILE:HG22	5:I:5933:HOH:O	2.19	0.43
1:A:271:HIS:CD2	1:A:357:GLU:HB2	2.54	0.43
1:L:127:GLY:HA3	3:L:4482:ADP:H1'	2.00	0.42
1:D:127:GLY:HA3	3:D:4474:ADP:H1'	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:210[B]:HIS:C	1:F:211[B]:HIS:CD2	2.89	0.42
1:D:175[B]:VAL:O	1:D:176[B]:LYS:HB2	2.20	0.42
1:I:29[A]:GLN:HA	1:J:180[A]:PHE:O	2.19	0.42
1:I:359:ARG:HH12	4:I:5908:PPQ:HEP2	1.84	0.42
1:D:359:ARG:HH12	4:D:5903:PPQ:HEP2	1.84	0.42
1:K:1:SER:N	1:K:71:ALA:HB3	2.34	0.42
1:I:192[A]:ARG:HH21	1:I:219:ASN:ND2	2.17	0.42
1:E:305:ALA:CB	1:E:332:LEU:HD21	2.49	0.42
1:L:16:PHE:HB2	1:L:84:THR:HB	2.00	0.42
1:L:452:ARG:HG2	5:L:1807:HOH:O	2.19	0.42
5:G:5979:HOH:O	1:H:183:PRO:CB	2.66	0.42
1:B:309:ASN:HA	1:B:309:ASN:HD22	1.71	0.42
1:G:93:GLU:OE2	1:G:94:PRO:HD2	2.20	0.42
1:I:324:PRO:N	5:I:6041:HOH:O	2.51	0.42
1:D:324:PRO:N	5:D:6023:HOH:O	2.51	0.42
1:H:210[B]:HIS:C	1:H:211[B]:HIS:CD2	2.89	0.42
1:A:178[A]:GLY:O	1:A:211[A]:HIS:HD2	2.01	0.42
1:E:178[A]:GLY:O	1:E:211[A]:HIS:HD2	2.01	0.42
1:J:323:VAL:O	5:J:5938:HOH:O	2.21	0.42
1:A:128:PRO:HA	1:A:269:HIS:O	2.18	0.42
1:C:289:GLY:HA2	5:C:6024:HOH:O	2.18	0.42
1:F:197:LEU:O	1:F:201:GLN:HG3	2.19	0.42
1:J:197:LEU:O	1:J:201:GLN:HG3	2.20	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:H:47:LYS:CD	5:H:6049:HOH:O	2.65	0.42
1:B:47:LYS:CD	5:B:6036:HOH:O	2.65	0.42
1:E:125:LEU:HA	1:E:125:LEU:HD12	1.79	0.42
1:B:271:HIS:CD2	1:B:357:GLU:HB2	2.54	0.42
1:J:144:ILE:HG22	5:J:5930:HOH:O	2.19	0.42
1:E:93:GLU:OE2	1:E:94:PRO:HD2	2.19	0.42
1:G:127:GLY:HA3	3:G:4477:ADP:H1'	2.00	0.42
1:G:175[B]:VAL:O	1:G:176[B]:LYS:HB2	2.20	0.42
1:I:175[B]:VAL:O	1:I:176[B]:LYS:HB2	2.20	0.42
1:E:337:ARG:HD3	1:F:61:ASN:CB	2.49	0.42
1:B:359:ARG:HH12	4:B:5901:PPQ:HEP2	1.84	0.42
1:D:269:HIS:HE1	4:D:5903:PPQ:HEP2	1.82	0.42
1:L:192[A]:ARG:HH21	1:L:219:ASN:ND2	2.17	0.42
1:J:305:ALA:CB	1:J:332:LEU:HD21	2.49	0.42
1:F:458:HIS:HE1	1:L:456:THR:O	2.02	0.42
1:I:201:GLN:N	5:I:6024:HOH:O	2.52	0.42
1:F:374:LEU:HA	1:F:374:LEU:HD12	1.91	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:183:PRO:HD3	1:F:30[A]:HIS:CE1	2.54	0.42
1:G:352:LYS:HE2	1:G:352:LYS:HA	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:C:160:SER:HB2	1:D:140:PHE:CE1	2.54	0.42
1:I:271:HIS:CD2	1:I:357:GLU:HB2	2.54	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:G:1:SER:N	1:G:71:ALA:HB3	2.34	0.42
1:A:82:ASP:O	1:A:84:THR:CG2	2.67	0.42
1:G:197:LEU:O	1:G:201:GLN:HG3	2.19	0.42
1:A:197:LEU:O	1:A:201:GLN:HG3	2.20	0.42
1:D:230:LYS:CG	5:D:5966:HOH:O	2.66	0.42
1:L:47:LYS:CD	5:L:1827:HOH:O	2.65	0.42
1:A:324:PRO:HA	5:A:6020:HOH:O	2.19	0.42
1:D:324:PRO:HA	5:D:6023:HOH:O	2.19	0.42
1:G:309:ASN:HA	1:G:309:ASN:HD22	1.71	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
1:F:271:HIS:CD2	1:F:357:GLU:HB2	2.54	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:A:127:GLY:HA3	3:A:4471:ADP:H1'	2.00	0.42
1:C:155:GLU:OE1	1:C:211[A]:HIS:CE1	2.68	0.42
1:A:175[B]:VAL:O	1:A:176[B]:LYS:HB2	2.20	0.42
1:E:175[B]:VAL:O	1:E:176[B]:LYS:HB2	2.20	0.42
1:J:155:GLU:OE1	1:J:211[A]:HIS:CE1	2.68	0.42
1:C:323:VAL:O	5:C:5921:HOH:O	2.21	0.42
1:H:359:ARG:HH12	4:H:5907:PPQ:HEP2	1.84	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:J:359:ARG:HH12	4:J:5909:PPQ:HEP2	1.84	0.42
1:A:1:SER:N	1:A:71:ALA:HB3	2.34	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:C:192[A]:ARG:HH21	1:C:219:ASN:ND2	2.17	0.42
1:A:172:ARG:HA	1:A:173[A]:PRO:HD3	1.80	0.42
1:A:183:PRO:HD3	1:B:30[A]:HIS:CE1	2.54	0.42
1:G:401:PRO:CA	1:G:404:ALA:HA	2.47	0.42
1:E:201:GLN:N	5:E:722:HOH:O	2.52	0.42
1:D:374:LEU:HA	1:D:374:LEU:HD12	1.91	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:452:ARG:HG2	5:A:6015:HOH:O	2.19	0.42
1:H:324:PRO:CA	5:H:6034:HOH:O	2.68	0.42
1:E:324:PRO:CA	5:E:741:HOH:O	2.68	0.42
1:J:271:HIS:CD2	1:J:357:GLU:HB2	2.54	0.42
1:I:352:LYS:HE2	1:I:352:LYS:HA	2.00	0.42
1:A:93:GLU:OE2	1:A:94:PRO:HD2	2.19	0.42
1:L:144:ILE:HG22	5:L:1697:HOH:O	2.19	0.42
1:B:324:PRO:N	5:B:6021:HOH:O	2.51	0.42
1:I:93:GLU:OE2	1:I:94:PRO:HD2	2.19	0.42
1:K:93:GLU:OE2	1:K:94:PRO:HD2	2.19	0.42
1:C:127:GLY:HA3	3:C:4473:ADP:H1'	2.00	0.42
1:I:127:GLY:HA3	3:I:4479:ADP:H1'	2.00	0.42
1:F:231:LYS:CE	5:F:5919:HOH:O	2.59	0.42
1:D:1:SER:N	1:D:71:ALA:HB3	2.34	0.42
1:C:1:SER:N	1:C:71:ALA:HB3	2.34	0.42
1:I:1:SER:N	1:I:71:ALA:HB3	2.34	0.42
1:H:192[A]:ARG:HH21	1:H:219:ASN:ND2	2.17	0.42
1:E:332:LEU:HD12	1:E:332:LEU:HA	1.90	0.42
1:D:172:ARG:HA	1:D:173[A]:PRO:HD3	1.80	0.42
1:F:201:GLN:N	5:F:6013:HOH:O	2.52	0.42
1:E:197:LEU:O	1:E:201:GLN:HG3	2.20	0.42
1:J:33:ILE:HA	1:J:34:PRO:HD3	1.90	0.42
1:G:324:PRO:CA	5:G:6030:HOH:O	2.68	0.42
1:L:93:GLU:OE2	1:L:94:PRO:HD2	2.19	0.42
1:E:352:LYS:HA	1:E:352:LYS:HE2	2.00	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:C:93:GLU:OE2	1:C:94:PRO:HD2	2.19	0.42
1:J:127:GLY:HA3	3:J:4480:ADP:H1'	2.00	0.42
1:E:210[B]:HIS:C	1:E:211[B]:HIS:CD2	2.89	0.42
1:L:359:ARG:HH12	4:L:5911:PPQ:HEP2	1.84	0.42
1:G:359:ARG:HH12	4:G:5906:PPQ:HEP2	1.84	0.42
1:J:192[A]:ARG:HH21	1:J:219:ASN:ND2	2.17	0.42
1:H:332:LEU:O	5:H:6012:HOH:O	2.20	0.42
1:J:16:PHE:HB2	1:J:84:THR:HB	2.00	0.42
1:H:16:PHE:HB2	1:H:84:THR:HB	2.00	0.42
1:C:197:LEU:O	1:C:201:GLN:HG3	2.19	0.42
1:I:197:LEU:O	1:I:201:GLN:HG3	2.19	0.42
1:B:197:LEU:O	1:B:201:GLN:HG3	2.20	0.42
1:H:197:LEU:O	1:H:201:GLN:HG3	2.19	0.42
1:J:33:ILE:HD12	1:K:208:ALA:CB	2.49	0.42
1:C:47:LYS:CD	5:C:6035:HOH:O	2.65	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:J:324:PRO:HA	5:J:6037:HOH:O	2.19	0.42
1:F:324:PRO:CA	5:F:6030:HOH:O	2.68	0.42
1:K:140:PHE:CE1	1:L:160:SER:HB2	2.55	0.42
1:A:352:LYS:HE2	1:A:352:LYS:HA	2.00	0.42
1:E:457:PRO:HD3	1:K:261[A]:PHE:HB2	2.01	0.42
1:J:56:GLY:N	5:J:6010:HOH:O	2.40	0.42
5:A:5948:HOH:O	1:F:182:VAL:HG23	2.20	0.42
1:K:175[B]:VAL:O	1:K:176[B]:LYS:HB2	2.20	0.42
1:D:210[B]:HIS:C	1:D:211[B]:HIS:CD2	2.89	0.42
1:L:175[B]:VAL:O	1:L:176[B]:LYS:HB2	2.20	0.42
1:H:175[B]:VAL:O	1:H:176[B]:LYS:HB2	2.20	0.42
1:E:155:GLU:OE1	1:E:211[A]:HIS:CE1	2.68	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:L:305:ALA:CB	1:L:332:LEU:HD21	2.49	0.42
1:B:192[A]:ARG:HH21	1:B:219:ASN:ND2	2.17	0.42
1:G:305:ALA:CB	1:G:332:LEU:HD21	2.49	0.42
1:F:456:THR:O	1:L:458:HIS:HE1	2.02	0.42
1:H:447:ARG:CD	5:H:6023:HOH:O	2.68	0.42
1:C:401:PRO:HA	1:C:404:ALA:CA	2.44	0.42
1:E:452:ARG:HG2	5:E:736:HOH:O	2.19	0.42
1:K:230:LYS:CG	5:K:1596:HOH:O	2.66	0.42
1:J:125:LEU:HD12	1:J:125:LEU:HA	1.79	0.42
1:F:125:LEU:HD12	1:F:125:LEU:HA	1.79	0.42
1:B:210[A]:HIS:ND1	1:B:211[A]:HIS:O	2.47	0.42
1:G:59:GLY:O	1:H:339:ARG:NH1	2.47	0.42
1:L:1:SER:N	1:L:71:ALA:HB3	2.34	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:E:456:THR:O	1:K:458:HIS:HE1	2.03	0.42
1:D:447:ARG:CD	5:D:6012:HOH:O	2.68	0.42
1:I:401:PRO:CA	1:I:404:ALA:HA	2.46	0.42
1:G:201:GLN:N	5:G:6013:HOH:O	2.52	0.42
1:J:201:GLN:N	5:J:6020:HOH:O	2.52	0.42
1:E:387:HIS:HA	1:E:388:PRO:HD2	1.85	0.42
1:C:324:PRO:HA	5:C:6020:HOH:O	2.19	0.42
1:F:93:GLU:OE2	1:F:94:PRO:HD2	2.20	0.42
1:H:93:GLU:OE2	1:H:94:PRO:HD2	2.20	0.42
1:A:440:ASP:HB2	5:A:6028:HOH:O	2.20	0.42
1:B:463:GLU:HA	1:H:140:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:144:ILE:HG22	5:E:626:HOH:O	2.19	0.42
1:G:323:VAL:O	5:G:5930:HOH:O	2.21	0.42
1:A:332:LEU:HA	1:A:332:LEU:HD12	1.90	0.42
1:L:401:PRO:CA	1:L:404:ALA:HA	2.47	0.42
1:B:208:ALA:CB	1:C:33:ILE:HD12	2.50	0.42
1:B:201:GLN:N	5:B:6004:HOH:O	2.52	0.42
1:J:129:GLU:O	1:J:268:MET:HA	2.20	0.42
1:B:125:LEU:HA	1:B:125:LEU:HD12	1.79	0.42
1:L:324:PRO:HA	5:L:1812:HOH:O	2.19	0.42
1:K:324:PRO:CA	5:K:1659:HOH:O	2.68	0.42
1:E:423:LEU:C	1:E:425:ARG:H	2.22	0.42
1:H:144:ILE:HG22	5:H:5928:HOH:O	2.19	0.42
1:C:175[B]:VAL:O	1:C:176[B]:LYS:HB2	2.20	0.41
1:C:210[B]:HIS:C	1:C:211[B]:HIS:CD2	2.90	0.41
1:F:175[B]:VAL:O	1:F:176[B]:LYS:HB2	2.20	0.41
1:K:210[B]:HIS:C	1:K:211[B]:HIS:CD2	2.89	0.41
1:H:29[A]:GLN:HA	1:I:180[A]:PHE:O	2.20	0.41
1:A:61:ASN:O	1:F:337:ARG:O	2.38	0.41
1:A:323:VAL:O	5:A:5920:HOH:O	2.21	0.41
1:H:165:GLU:N	5:H:5975:HOH:O	2.46	0.41
1:J:172:ARG:HA	1:J:173[A]:PRO:HD3	1.80	0.41
1:E:447:ARG:CD	5:E:729:HOH:O	2.68	0.41
1:C:82:ASP:O	1:C:84:THR:CG2	2.67	0.41
1:I:390:GLU:HA	1:I:391:PRO:HD3	1.84	0.41
1:C:390:GLU:HA	1:C:391:PRO:HD3	1.84	0.41
1:L:197:LEU:O	1:L:201:GLN:HG3	2.20	0.41
1:C:452:ARG:HG2	5:C:6015:HOH:O	2.19	0.41
1:F:452:ARG:HG2	5:F:6025:HOH:O	2.19	0.41
1:D:452:ARG:HG2	5:D:6018:HOH:O	2.19	0.41
1:H:129:GLU:O	1:H:268:MET:HA	2.20	0.41
1:I:324:PRO:CA	5:I:6041:HOH:O	2.68	0.41
1:J:440:ASP:HB2	5:J:6045:HOH:O	2.20	0.41
1:L:440:ASP:HB2	5:L:1820:HOH:O	2.20	0.41
1:C:195:MET:HE1	1:C:242:VAL:HG13	2.02	0.41
1:D:214:ALA:HA	1:D:263[A]:ASP:OD2	2.21	0.41
1:C:179[B]:TYR:CD1	1:C:212[B]:GLU:CA	2.77	0.41
1:J:176[B]:LYS:C	1:J:178[B]:GLY:N	2.47	0.41
1:G:128:PRO:CD	5:G:5917:HOH:O	2.61	0.41
1:G:461:GLU:O	1:G:465:TYR:N	2.50	0.41
1:I:461:GLU:O	1:I:465:TYR:N	2.50	0.41
1:I:447:ARG:CD	5:I:6030:HOH:O	2.68	0.41
1:A:401:PRO:CA	1:A:404:ALA:HA	2.46	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:82:ASP:O	1:L:84:THR:CG2	2.67	0.41
1:I:82:ASP:O	1:I:84:THR:CG2	2.67	0.41
1:A:201:GLN:N	5:A:6003:HOH:O	2.52	0.41
1:H:283:SER:O	1:H:291:SER:HB3	2.21	0.41
1:F:129:GLU:O	1:F:268:MET:HA	2.20	0.41
1:G:129:GLU:O	1:G:268:MET:HA	2.20	0.41
1:F:324:PRO:HA	5:F:6030:HOH:O	2.19	0.41
1:H:140:PHE:CE1	1:I:160:SER:HB2	2.55	0.41
1:H:138:ILE:O	1:H:138:ILE:HG23	2.21	0.41
1:D:138:ILE:HG23	1:D:138:ILE:O	2.20	0.41
1:K:440:ASP:HB2	5:K:1667:HOH:O	2.20	0.41
1:C:423:LEU:C	1:C:425:ARG:H	2.22	0.41
1:A:56:GLY:N	5:A:5993:HOH:O	2.40	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:J:1:SER:N	1:J:71:ALA:HB3	2.34	0.41
1:K:359:ARG:HH12	4:K:5910:PPQ:HEP2	1.84	0.41
1:A:80:PHE:CZ	1:F:189:GLN:HG3	2.55	0.41
1:F:384:ASN:ND2	1:F:384:ASN:N	2.59	0.41
1:G:452:ARG:HG2	5:G:6025:HOH:O	2.19	0.41
1:E:283:SER:O	1:E:291:SER:HB3	2.20	0.41
1:C:129:GLU:O	1:C:268:MET:HA	2.20	0.41
1:E:129:GLU:O	1:E:268:MET:HA	2.20	0.41
1:C:125:LEU:HG	1:C:225:PHE:CD2	2.56	0.41
1:L:125:LEU:HG	1:L:225:PHE:CD2	2.56	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:A:144:ILE:HG22	5:A:5912:HOH:O	2.19	0.41
1:F:440:ASP:HB2	5:F:6038:HOH:O	2.20	0.41
1:J:93:GLU:OE2	1:J:94:PRO:HD2	2.19	0.41
1:C:210[A]:HIS:HB3	1:D:31:VAL:HG23	2.02	0.41
1:J:175[B]:VAL:O	1:J:176[B]:LYS:HB2	2.20	0.41
1:C:359:ARG:HH11	1:C:359:ARG:HD3	1.65	0.41
1:B:1:SER:OG	1:B:1:SER:O	2.39	0.41
1:J:224:ARG:NH2	1:J:224:ARG:CG	2.69	0.41
1:B:302:ILE:CD1	5:B:5999:HOH:O	2.49	0.41
1:K:75:VAL:CG2	5:K:1548:HOH:O	2.53	0.41
1:A:447:ARG:CD	5:A:6009:HOH:O	2.68	0.41
5:I:5990:HOH:O	1:J:183:PRO:CB	2.68	0.41
1:J:452:ARG:HG2	5:J:6032:HOH:O	2.19	0.41
1:B:419:ASN:ND2	5:B:5993:HOH:O	2.42	0.41
1:J:283:SER:O	1:J:291:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:129:GLU:O	1:L:268:MET:HA	2.20	0.41
1:H:125:LEU:HG	1:H:225:PHE:CD2	2.56	0.41
1:G:125:LEU:HG	1:G:225:PHE:CD2	2.56	0.41
1:J:324:PRO:CA	5:J:6037:HOH:O	2.68	0.41
1:B:138:ILE:O	1:B:138:ILE:HG23	2.20	0.41
1:B:214:ALA:HA	1:B:263[A]:ASP:OD2	2.21	0.41
1:D:93:GLU:OE2	1:D:94:PRO:HD2	2.19	0.41
1:C:211[B]:HIS:HE1	5:C:6044:HOH:O	1.60	0.41
1:D:175[B]:VAL:O	1:D:176[B]:LYS:CB	2.69	0.41
1:L:155:GLU:OE1	1:L:211[A]:HIS:CE1	2.68	0.41
1:F:323:VAL:O	5:F:5931:HOH:O	2.21	0.41
1:A:359:ARG:HH12	4:A:5900:PPQ:HEP2	1.84	0.41
1:F:447:ARG:CD	5:F:6019:HOH:O	2.68	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:B:230:LYS:CG	5:B:5964:HOH:O	2.66	0.41
1:K:129:GLU:O	1:K:268:MET:HA	2.20	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:A:125:LEU:HG	1:A:225:PHE:CD2	2.56	0.41
1:I:324:PRO:HA	5:I:6041:HOH:O	2.19	0.41
1:K:199:MET:HG3	1:K:241:VAL:HG11	2.03	0.41
1:I:138:ILE:HG23	1:I:138:ILE:O	2.20	0.41
1:B:371:PHE:CD2	1:B:371:PHE:N	2.89	0.41
1:B:93:GLU:OE2	1:B:94:PRO:HD2	2.19	0.41
1:C:429:LYS:HA	1:C:434:PHE:O	2.21	0.41
1:H:214:ALA:HA	1:H:263[A]:ASP:OD2	2.21	0.41
1:C:175[B]:VAL:O	1:C:176[B]:LYS:CB	2.69	0.41
1:K:175[B]:VAL:O	1:K:176[B]:LYS:CB	2.69	0.41
1:I:61:ASN:C	1:J:337:ARG:HD3	2.41	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:G:344:ARG:HE	1:G:344:ARG:HB3	1.58	0.41
1:K:461:GLU:O	1:K:465:TYR:N	2.50	0.41
1:J:82:ASP:O	1:J:84:THR:CG2	2.67	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:A:283:SER:O	1:A:291:SER:HB3	2.20	0.41
1:I:129:GLU:O	1:I:268:MET:HA	2.20	0.41
1:D:129:GLU:O	1:D:268:MET:HA	2.20	0.41
1:B:129:GLU:O	1:B:268:MET:HA	2.20	0.41
1:H:235:ILE:HD13	1:H:235:ILE:HA	1.80	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:324:PRO:CA	5:L:1812:HOH:O	2.68	0.41
1:E:324:PRO:HA	5:E:741:HOH:O	2.19	0.41
1:G:324:PRO:HA	5:G:6030:HOH:O	2.19	0.41
1:B:324:PRO:HA	5:B:6021:HOH:O	2.19	0.41
1:E:429:LYS:HA	1:E:434:PHE:O	2.21	0.41
1:K:138:ILE:HG23	1:K:138:ILE:O	2.20	0.41
1:L:138:ILE:O	1:L:138:ILE:HG23	2.21	0.41
1:L:214:ALA:HA	1:L:263[A]:ASP:OD2	2.21	0.41
1:J:214:ALA:HA	1:J:263[A]:ASP:OD2	2.21	0.41
1:I:199:MET:HG3	1:I:241:VAL:HG11	2.03	0.41
1:K:144:ILE:HG22	5:K:1544:HOH:O	2.19	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:F:302:ILE:CD1	5:F:6008:HOH:O	2.49	0.41
1:A:75:VAL:CG2	5:A:5916:HOH:O	2.53	0.41
1:D:401:PRO:CA	1:D:404:ALA:HA	2.47	0.41
1:K:287:TYR:CD1	1:K:391:PRO:HG2	2.56	0.41
1:B:452:ARG:HG2	5:B:6016:HOH:O	2.19	0.41
1:A:235:ILE:HD13	1:A:235:ILE:HA	1.80	0.41
1:K:33:ILE:HA	1:K:34:PRO:HD3	1.90	0.41
1:A:324:PRO:CA	5:A:6020:HOH:O	2.68	0.41
1:D:324:PRO:CA	5:D:6023:HOH:O	2.68	0.41
1:A:138:ILE:HG23	1:A:138:ILE:O	2.20	0.41
1:A:27:LYS:HD2	1:A:27:LYS:HA	1.95	0.41
1:C:56:GLY:N	5:C:5993:HOH:O	2.40	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:B:199:MET:HG3	1:B:241:VAL:HG11	2.03	0.41
1:D:179[B]:TYR:HB3	1:D:180[B]:PHE:CD2	2.56	0.41
1:K:61:ASN:CB	1:L:337:ARG:HD3	2.50	0.41
1:F:269:HIS:HE1	4:F:5905:PPQ:HEP2	1.82	0.41
1:B:172:ARG:HA	1:B:173[A]:PRO:HD3	1.80	0.41
1:H:82:ASP:CB	5:H:5958:HOH:O	2.64	0.41
1:H:287:TYR:CD1	1:H:391:PRO:HG2	2.56	0.41
1:K:283:SER:O	1:K:291:SER:HB3	2.21	0.41
1:B:387:HIS:HA	1:B:388:PRO:HD2	1.85	0.41
1:L:283:SER:O	1:L:291:SER:HB3	2.21	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:6:LEU:HD13	1:E:6:LEU:HA	1.93	0.41
1:C:138:ILE:O	1:C:138:ILE:HG23	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:138:ILE:O	1:J:138:ILE:HG23	2.21	0.41
1:L:429:LYS:HA	1:L:434:PHE:O	2.21	0.41
1:A:199:MET:HG3	1:A:241:VAL:HG11	2.03	0.41
1:K:41:GLU:O	1:K:45:GLU:HG2	2.21	0.41
1:E:276:LYS:HB3	1:E:281:LEU:HD11	2.03	0.41
1:A:429:LYS:HA	1:A:434:PHE:O	2.21	0.41
1:I:440:ASP:HB2	5:I:6049:HOH:O	2.20	0.41
1:D:199:MET:HG3	1:D:241:VAL:HG11	2.03	0.41
1:H:199:MET:HG3	1:H:241:VAL:HG11	2.03	0.41
1:L:211[A]:HIS:HD2	1:L:212[A]:GLU:O	2.04	0.41
1:L:179[B]:TYR:HB3	1:L:180[B]:PHE:CD2	2.56	0.41
1:G:175[B]:VAL:O	1:G:176[B]:LYS:CB	2.69	0.41
1:I:211[A]:HIS:HD2	1:I:212[A]:GLU:O	2.04	0.41
1:A:211[A]:HIS:HD2	1:A:212[A]:GLU:O	2.04	0.41
1:H:128:PRO:CD	5:H:5924:HOH:O	2.61	0.41
1:B:329:PRO:HG2	1:B:359:ARG:CD	2.18	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:E:1:SER:O	1:E:1:SER:OG	2.39	0.41
1:A:332:LEU:HB2	1:A:408:PRO:O	2.21	0.41
1:D:332:LEU:HB2	1:D:408:PRO:O	2.21	0.41
1:L:426:GLU:CB	5:L:1746:HOH:O	2.49	0.41
1:G:447:ARG:CD	5:G:5992:HOH:O	2.58	0.41
1:B:447:ARG:CD	5:B:6010:HOH:O	2.68	0.41
1:K:452:ARG:HG2	5:K:1654:HOH:O	2.20	0.41
1:B:283:SER:O	1:B:291:SER:HB3	2.21	0.41
1:L:264[B]:ASN:N	1:L:326:TYR:HD2	2.19	0.41
1:I:264[B]:ASN:N	1:I:326:TYR:HD2	2.19	0.41
1:A:264[B]:ASN:N	1:A:326:TYR:HD2	2.19	0.41
5:K:1602:HOH:O	1:L:183:PRO:HB2	2.21	0.41
1:G:33:ILE:CD1	1:H:208:ALA:HB2	2.51	0.41
1:D:125:LEU:HG	1:D:225:PHE:CD2	2.56	0.41
1:I:125:LEU:HG	1:I:225:PHE:CD2	2.56	0.41
1:K:324:PRO:HA	5:K:1659:HOH:O	2.19	0.41
1:G:138:ILE:O	1:G:138:ILE:HG23	2.20	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:L:199:MET:HG3	1:L:241:VAL:HG11	2.03	0.41
1:K:276:LYS:HB3	1:K:281:LEU:HD11	2.03	0.41
1:A:256:MET:HA	1:A:257:PRO:HD2	1.89	0.41
1:H:440:ASP:HB2	5:H:6042:HOH:O	2.20	0.41
1:B:41:GLU:O	1:B:45:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:371:PHE:N	1:I:371:PHE:CD2	2.89	0.41
1:K:371:PHE:CD2	1:K:371:PHE:N	2.89	0.41
1:L:371:PHE:CD2	1:L:371:PHE:N	2.89	0.41
1:L:309:ASN:HA	1:L:309:ASN:HD22	1.71	0.41
1:D:41:GLU:O	1:D:45:GLU:HG2	2.21	0.41
1:E:41:GLU:O	1:E:45:GLU:HG2	2.21	0.41
1:I:429:LYS:HA	1:I:434:PHE:O	2.21	0.41
1:K:214:ALA:HA	1:K:263[A]:ASP:OD2	2.21	0.41
1:E:214:ALA:HA	1:E:263[A]:ASP:OD2	2.21	0.41
1:D:144:ILE:HG22	5:D:5915:HOH:O	2.19	0.41
1:C:440:ASP:HB2	5:C:6028:HOH:O	2.20	0.41
1:F:214:ALA:HA	1:F:263[A]:ASP:OD2	2.21	0.41
1:D:210[A]:HIS:ND1	1:D:211[A]:HIS:O	2.47	0.41
1:D:211[A]:HIS:HD2	1:D:212[A]:GLU:O	2.04	0.41
1:L:175[B]:VAL:O	1:L:176[B]:LYS:CB	2.69	0.41
1:H:179[B]:TYR:HB3	1:H:180[B]:PHE:CD2	2.56	0.41
1:B:175[B]:VAL:O	1:B:176[B]:LYS:CB	2.69	0.41
1:I:29[A]:GLN:HB3	1:J:180[A]:PHE:CB	2.49	0.41
1:E:359:ARG:HH11	1:E:359:ARG:HD3	1.65	0.41
1:J:1:SER:OG	1:J:1:SER:O	2.39	0.41
1:J:302:ILE:CD1	5:J:6015:HOH:O	2.49	0.41
1:L:447:ARG:CD	5:L:1800: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:J:287:TYR:CD1	1:J:391:PRO:HG2	2.56	0.41
1:G:283:SER:O	1:G:291:SER:HB3	2.20	0.41
1:I:283:SER:O	1:I:291:SER:HB3	2.20	0.41
1:K:264[B]:ASN:N	1:K:326:TYR:HD2	2.19	0.41
1:B:264[B]:ASN:N	1:B:326:TYR:HD2	2.19	0.41
1:D:283:SER:O	1:D:291:SER:HB3	2.20	0.41
1:G:271:HIS:HA	1:G:356:ILE:O	2.21	0.41
1:C:271:HIS:HA	1:C:356:ILE:O	2.21	0.41
1:B:324:PRO:CA	5:B:6021:HOH:O	2.68	0.41
1:D:440:ASP:HB2	5:D:6031:HOH:O	2.20	0.41
1:C:371:PHE:N	1:C:371:PHE:CD2	2.89	0.41
1:G:6:LEU:HA	1:G:6:LEU:HD13	1.93	0.41
1:E:138:ILE:O	1:E:138:ILE:HG23	2.20	0.41
1:G:429:LYS:HA	1:G:434:PHE:O	2.21	0.41
1:F:463:GLU:HA	1:L:140:PHE:CE1	2.56	0.41
1:A:276:LYS:HB3	1:A:281:LEU:HD11	2.03	0.41
1:J:195:MET:HE1	1:J:242:VAL:HG13	2.03	0.41
1:F:175[B]:VAL:O	1:F:176[B]:LYS:CB	2.69	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:155:GLU:OE1	1:H:211[A]:HIS:CE1	2.68	0.40
1:B:179[B]:TYR:HB3	1:B:180[B]:PHE:CD2	2.56	0.40
1:J:179[B]:TYR:HB3	1:J:180[B]:PHE:CD2	2.56	0.40
1:C:339:ARG:NH1	1:D:59:GLY:O	2.53	0.40
1:H:61:ASN:CB	1:I:337:ARG:HD3	2.50	0.40
1:K:332:LEU:HB2	1:K:408:PRO:O	2.21	0.40
1:E:458:HIS:HE1	1:K:456:THR:O	2.04	0.40
1:K:172:ARG:HA	1:K:173[A]:PRO:HD3	1.80	0.40
1:H:461:GLU:O	1:H:465:TYR:N	2.50	0.40
1:I:287:TYR:CD1	1:I:391:PRO:HG2	2.56	0.40
1:G:82:ASP:CB	5:G:5953:HOH:O	2.64	0.40
1:D:287:TYR:CD1	1:D:391:PRO:HG2	2.56	0.40
1:A:129:GLU:O	1:A:268:MET:HA	2.20	0.40
1:K:125:LEU:HG	1:K:225:PHE:CD2	2.56	0.40
1:I:41:GLU:O	1:I:45:GLU:HG2	2.21	0.40
1:I:214:ALA:HA	1:I:263[A]:ASP:OD2	2.21	0.40
1:C:300:GLY:HA3	1:C:377:ALA:O	2.21	0.40
1:K:429:LYS:HA	1:K:434:PHE:O	2.21	0.40
1:C:41:GLU:O	1:C:45:GLU:HG2	2.21	0.40
1:C:199:MET:HG3	1:C:241:VAL:HG11	2.03	0.40
1:D:429:LYS:HA	1:D:434:PHE:O	2.21	0.40
1:A:31:VAL:HG23	1:F:210[A]:HIS:HB3	2.03	0.40
1:A:179[B]:TYR:HB3	1:A:180[B]:PHE:CD2	2.56	0.40
1:G:231:LYS:CE	5:G:5917:HOH:O	2.59	0.40
1:F:1:SER:O	1:F:1:SER:OG	2.39	0.40
1:A:63:SER:N	1:F:339:ARG:NH1	2.67	0.40
1:L:332:LEU:HB2	1:L:408:PRO:O	2.21	0.40
1:F:332:LEU:HB2	1:F:408:PRO:O	2.21	0.40
1:E:447:ARG:CD	5:E:698:HOH:O	2.58	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:I:82:ASP:CB	5:I:5964:HOH:O	2.64	0.40
1:L:230:LYS:HB2	1:L:230:LYS:HE2	1.85	0.40
1:J:264[B]:ASN:N	1:J:326:TYR:HD2	2.19	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:J:429:LYS:HA	1:J:434:PHE:O	2.21	0.40
1:F:179[B]:TYR:HB3	1:F:180[B]:PHE:CD2	2.56	0.40
1:I:60:ILE:HG12	1:J:339:ARG:HB2	2.03	0.40
1:I:175[B]:VAL:O	1:I:176[B]:LYS:CB	2.69	0.40
1:H:61:ASN:HB2	1:I:337:ARG:CZ	2.51	0.40
1:A:302:ILE:CD1	5:A:5998:HOH:O	2.49	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:332:LEU:HB2	1:E:408:PRO:O	2.21	0.40
1:A:344:ARG:HE	1:A:344:ARG:HB3	1.59	0.40
1:F:287:TYR:CD1	1:F:391:PRO:HG2	2.56	0.40
1:H:452:ARG:HG2	5:H:6029:HOH:O	2.19	0.40
1:F:283:SER:O	1:F:291:SER:HB3	2.20	0.40
1:B:125:LEU:HG	1:B:225:PHE:CD2	2.56	0.40
1:G:440:ASP:HB2	5:G:6038:HOH:O	2.20	0.40
1:L:41:GLU:O	1:L:45:GLU:HG2	2.21	0.40
1:F:41:GLU:O	1:F:45:GLU:HG2	2.21	0.40
1:A:214:ALA:HA	1:A:263[A]:ASP:OD2	2.21	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:F:300:GLY:HA3	1:F:377:ALA:O	2.21	0.40
1:H:41:GLU:O	1:H:45:GLU:HG2	2.21	0.40
1:C:179[B]:TYR:HB3	1:C:180[B]:PHE:CD2	2.56	0.40
1:G:29[A]:GLN:HA	1:H:180[A]:PHE:O	2.21	0.40
1:I:210[A]:HIS:ND1	1:I:211[A]:HIS:O	2.47	0.40
1:B:211[A]:HIS:HD2	1:B:212[A]:GLU:O	2.04	0.40
1:J:175[B]:VAL:O	1:J:176[B]:LYS:CB	2.69	0.40
1:K:329:PRO:CD	1:K:359:ARG:HD2	2.42	0.40
1:I:80:PHE:HE2	5:I:5990:HOH:O	2.04	0.40
1:A:287:TYR:CD1	1:A:391:PRO:HG2	2.56	0.40
1:H:82:ASP:O	1:H:84:THR:CG2	2.67	0.40
1:G:264[B]:ASN:N	1:G:326:TYR:HD2	2.19	0.40
1:J:125:LEU:HG	1:J:225:PHE:CD2	2.56	0.40
1:F:271:HIS:HA	1:F:356:ILE:O	2.21	0.40
1:J:371:PHE:N	1:J:371:PHE:CD2	2.89	0.40
1:I:300:GLY:HA3	1:I:377:ALA:O	2.21	0.40
1:J:68:MET:HA	1:J:69:PRO:HD2	1.78	0.40
1:D:17:VAL:HA	1:D:85:LEU:O	2.22	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:F:176[B]:LYS:CB	5:F:5912:HOH:O	2.55	0.40
1:K:179[B]:TYR:HB3	1:K:180[B]:PHE:CD2	2.56	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
1:I:1:SER:OG	1:I:5:VAL:HG23	2.22	0.40
1:H:332:LEU:HB2	1:H:408:PRO:O	2.21	0.40
1:C:172:ARG:HA	1:C:173[A]:PRO:HD3	1.80	0.40
1:H:82:ASP:OD2	5:H:5937:HOH:O	2.22	0.40
1:B:287:TYR:CD1	1:B:391:PRO:HG2	2.56	0.40
1:E:287:TYR:CD1	1:E:391:PRO:HG2	2.56	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:5945:HOH:O	1:D:84:THR:HG21	2.21	0.40
1:E:419:ASN:ND2	5:E:709:HOH:O	2.42	0.40
1:C:283:SER:O	1:C:291:SER:HB3	2.21	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
1:E:271:HIS:HA	1:E:356:ILE:O	2.21	0.40
1:F:27:LYS:HA	1:F:27:LYS:HD2	1.95	0.40
1:J:300:GLY:HA3	1:J:377:ALA:O	2.21	0.40
1:I:17:VAL:HA	1:I:85:LEU:O	2.22	0.40
1:C:214:ALA:HA	1:C:263[A]:ASP:OD2	2.21	0.40

All (18) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:390:GLU:CD	5:H:6021:HOH:O[1_545]	0.95	1.25
1:J:390:GLU:CD	5:L:1798:HOH:O[3_555]	1.20	1.00
1:L:390:GLU:CG	5:H:6021:HOH:O[1_545]	1.23	0.97
1:J:390:GLU:OE2	5:L:1798:HOH:O[3_555]	1.25	0.95
1:L:390:GLU:OE2	5:H:6021:HOH:O[1_545]	1.29	0.91
1:H:285:ASP:OD2	5:J:6024:HOH:O[3_455]	1.32	0.88
1:I:292:GLU:OE1	5:K:1646:HOH:O[1_565]	1.44	0.76
1:C:1:SER:CB	1:F:13:GLU:OE2[4_454]	1.62	0.58
1:C:1:SER:CA	1:F:13:GLU:OE2[4_454]	1.67	0.53
1:J:390:GLU:CG	5:L:1798:HOH:O[3_555]	1.69	0.51
1:G:292:GLU:OE1	5:I:6029:HOH:O[3_445]	1.83	0.37
1:A:351:PRO:CG	1:B:41:GLU:OE1[2_454]	1.90	0.30
1:K:3:GLU:OE2	5:H:6014:HOH:O[4_445]	2.00	0.20
1:K:3:GLU:OE1	5:H:6017:HOH:O[4_445]	2.05	0.15
1:K:3:GLU:OE2	5:H:6017:HOH:O[4_445]	2.13	0.07
1:H:285:ASP:CG	5:J:6024:HOH:O[3_455]	2.16	0.04
1:L:390:GLU:OE1	5:H:6021:HOH:O[1_545]	2.16	0.04
1:C:1:SER:N	1:F:13:GLU:OE2[4_454]	2.20	0.00

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	4	15
1	B	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	4	15
1	C	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	4	15
1	D	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	4	15
1	E	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	4	15
1	F	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	4	15
1	G	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	4	15
1	H	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	4	15
1	I	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	4	15
1	J	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	4	15
1	K	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	4	15
1	L	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	4	15
All	All	5784/5616 (103%)	4932 (85%)	600 (10%)	252 (4%)	6	15

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	8	24
1	B	395/384 (103%)	350 (89%)	45 (11%)	8	24
1	C	395/384 (103%)	350 (89%)	45 (11%)	8	24
1	D	395/384 (103%)	350 (89%)	45 (11%)	8	24
1	E	395/384 (103%)	350 (89%)	45 (11%)	8	24
1	F	395/384 (103%)	350 (89%)	45 (11%)	8	24
1	G	395/384 (103%)	350 (89%)	45 (11%)	8	24
1	H	395/384 (103%)	350 (89%)	45 (11%)	8	24
1	I	395/384 (103%)	350 (89%)	45 (11%)	8	24
1	J	395/384 (103%)	350 (89%)	45 (11%)	8	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	395/384 (103%)	350 (89%)	45 (11%)	8	24
1	L	395/384 (103%)	350 (89%)	45 (11%)	8	24
All	All	4740/4608 (103%)	4200 (89%)	540 (11%)	9	24

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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

5.3.3 RNA ⓘ

There are no RNA chains 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	29,29,29	3.59	13 (44%)	45,45,45	3.94	17 (37%)
4	PPQ	A	5900	2	10,10,10	1.37	1 (10%)	14,14,14	3.89	3 (21%)
3	ADP	B	4472	2	29,29,29	3.59	13 (44%)	45,45,45	3.94	17 (37%)
4	PPQ	B	5901	2	10,10,10	1.36	1 (10%)	14,14,14	3.89	3 (21%)
3	ADP	C	4473	2	29,29,29	3.59	13 (44%)	45,45,45	3.94	17 (37%)
4	PPQ	C	5902	2	10,10,10	1.36	1 (10%)	14,14,14	3.89	3 (21%)
3	ADP	D	4474	2	29,29,29	3.59	13 (44%)	45,45,45	3.94	17 (37%)
4	PPQ	D	5903	2	10,10,10	1.37	1 (10%)	14,14,14	3.89	3 (21%)
3	ADP	E	4475	2	29,29,29	3.59	13 (44%)	45,45,45	3.94	17 (37%)
4	PPQ	E	5904	2	10,10,10	1.38	1 (10%)	14,14,14	3.90	3 (21%)
3	ADP	F	4476	2	29,29,29	3.59	13 (44%)	45,45,45	3.94	17 (37%)
4	PPQ	F	5905	2	10,10,10	1.36	1 (10%)	14,14,14	3.89	3 (21%)
3	ADP	G	4477	2	29,29,29	3.59	13 (44%)	45,45,45	3.94	16 (35%)
4	PPQ	G	5906	2	10,10,10	1.37	1 (10%)	14,14,14	3.90	3 (21%)
3	ADP	H	4478	2	29,29,29	3.59	13 (44%)	45,45,45	3.94	17 (37%)
4	PPQ	H	5907	2	10,10,10	1.37	1 (10%)	14,14,14	3.90	3 (21%)
3	ADP	I	4479	2	29,29,29	3.60	13 (44%)	45,45,45	3.94	17 (37%)
4	PPQ	I	5908	2	10,10,10	1.37	2 (20%)	14,14,14	3.89	3 (21%)
3	ADP	J	4480	2	29,29,29	3.59	13 (44%)	45,45,45	3.94	17 (37%)
4	PPQ	J	5909	2	10,10,10	1.36	1 (10%)	14,14,14	3.89	3 (21%)
3	ADP	K	4481	2	29,29,29	3.59	13 (44%)	45,45,45	3.95	17 (37%)
4	PPQ	K	5910	2	10,10,10	1.36	1 (10%)	14,14,14	3.88	3 (21%)
3	ADP	L	4482	2	29,29,29	3.60	13 (44%)	45,45,45	3.94	17 (37%)
4	PPQ	L	5911	2	10,10,10	1.38	1 (10%)	14,14,14	3.90	3 (21%)

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	-	0/16/32/32	0/1/3/3
4	PPQ	A	5900	2	-	0/10/10/10	0/0/0/0
3	ADP	B	4472	2	-	0/16/32/32	0/1/3/3
4	PPQ	B	5901	2	-	0/10/10/10	0/0/0/0
3	ADP	C	4473	2	-	0/16/32/32	0/1/3/3
4	PPQ	C	5902	2	-	0/10/10/10	0/0/0/0
3	ADP	D	4474	2	-	0/16/32/32	0/1/3/3
4	PPQ	D	5903	2	-	0/10/10/10	0/0/0/0
3	ADP	E	4475	2	-	0/16/32/32	0/1/3/3
4	PPQ	E	5904	2	-	0/10/10/10	0/0/0/0
3	ADP	F	4476	2	-	0/16/32/32	0/1/3/3
4	PPQ	F	5905	2	-	0/10/10/10	0/0/0/0
3	ADP	G	4477	2	-	0/16/32/32	0/1/3/3
4	PPQ	G	5906	2	-	0/10/10/10	0/0/0/0
3	ADP	H	4478	2	-	0/16/32/32	0/1/3/3
4	PPQ	H	5907	2	-	0/10/10/10	0/0/0/0
3	ADP	I	4479	2	-	0/16/32/32	0/1/3/3
4	PPQ	I	5908	2	-	0/10/10/10	0/0/0/0
3	ADP	J	4480	2	-	0/16/32/32	0/1/3/3
4	PPQ	J	5909	2	-	0/10/10/10	0/0/0/0
3	ADP	K	4481	2	-	0/16/32/32	0/1/3/3
4	PPQ	K	5910	2	-	0/10/10/10	0/0/0/0
3	ADP	L	4482	2	-	0/16/32/32	0/1/3/3
4	PPQ	L	5911	2	-	0/10/10/10	0/0/0/0

All (169) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	4479	ADP	PA-O3A	7.50	1.73	1.59
3	J	4480	ADP	PA-O3A	7.49	1.73	1.59
3	B	4472	ADP	PA-O3A	7.48	1.73	1.59
3	A	4471	ADP	PA-O3A	7.47	1.73	1.59
3	L	4482	ADP	PA-O3A	7.47	1.73	1.59
3	C	4473	ADP	PA-O3A	7.47	1.73	1.59
3	D	4474	ADP	PA-O3A	7.46	1.73	1.59
3	G	4477	ADP	PA-O3A	7.46	1.73	1.59
3	K	4481	ADP	PA-O3A	7.45	1.73	1.59
3	E	4475	ADP	PA-O3A	7.45	1.73	1.59
3	H	4478	ADP	PA-O3A	7.45	1.73	1.59
3	F	4476	ADP	PA-O3A	7.44	1.73	1.59
3	C	4473	ADP	C8-N9	7.13	1.47	1.36
3	E	4475	ADP	C8-N9	7.12	1.47	1.36
3	I	4479	ADP	C8-N9	7.11	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4476	ADP	C8-N9	7.09	1.47	1.36
3	L	4482	ADP	C8-N9	7.08	1.47	1.36
3	A	4471	ADP	C8-N9	7.08	1.47	1.36
3	G	4477	ADP	C8-N9	7.08	1.47	1.36
3	K	4481	ADP	C8-N9	7.07	1.47	1.36
3	D	4474	ADP	C8-N9	7.06	1.47	1.36
3	B	4472	ADP	C8-N9	7.05	1.47	1.36
3	H	4478	ADP	C8-N9	7.05	1.47	1.36
3	F	4476	ADP	C1'-N9	7.03	1.70	1.48
3	H	4478	ADP	C1'-N9	7.03	1.70	1.48
3	E	4475	ADP	C1'-N9	7.02	1.70	1.48
3	J	4480	ADP	C1'-N9	7.02	1.70	1.48
3	J	4480	ADP	C8-N9	7.02	1.47	1.36
3	A	4471	ADP	C1'-N9	7.01	1.70	1.48
3	L	4482	ADP	C1'-N9	7.01	1.70	1.48
3	B	4472	ADP	C1'-N9	7.01	1.70	1.48
3	G	4477	ADP	C1'-N9	7.01	1.70	1.48
3	I	4479	ADP	C1'-N9	7.01	1.70	1.48
3	D	4474	ADP	C1'-N9	7.00	1.70	1.48
3	C	4473	ADP	C1'-N9	7.00	1.70	1.48
3	K	4481	ADP	C1'-N9	6.99	1.70	1.48
3	D	4474	ADP	PB-O3A	6.85	1.72	1.60
3	G	4477	ADP	PB-O3A	6.84	1.72	1.60
3	J	4480	ADP	PB-O3A	6.83	1.72	1.60
3	L	4482	ADP	PB-O3A	6.83	1.72	1.60
3	C	4473	ADP	PB-O3A	6.82	1.72	1.60
3	A	4471	ADP	PB-O3A	6.82	1.72	1.60
3	F	4476	ADP	PB-O3A	6.82	1.72	1.60
3	H	4478	ADP	PB-O3A	6.81	1.72	1.60
3	B	4472	ADP	PB-O3A	6.81	1.72	1.60
3	K	4481	ADP	PB-O3A	6.80	1.72	1.60
3	I	4479	ADP	PB-O3A	6.79	1.72	1.60
3	E	4475	ADP	PB-O3A	6.79	1.72	1.60
3	L	4482	ADP	O4'-C1'	6.60	1.51	1.41
3	K	4481	ADP	O4'-C1'	6.60	1.51	1.41
3	J	4480	ADP	O4'-C1'	6.59	1.51	1.41
3	I	4479	ADP	O4'-C1'	6.58	1.51	1.41
3	G	4477	ADP	O4'-C1'	6.58	1.51	1.41
3	E	4475	ADP	O4'-C1'	6.56	1.51	1.41
3	D	4474	ADP	O4'-C1'	6.56	1.51	1.41
3	A	4471	ADP	O4'-C1'	6.56	1.51	1.41
3	C	4473	ADP	O4'-C1'	6.55	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	4478	ADP	O4'-C1'	6.54	1.51	1.41
3	F	4476	ADP	O4'-C1'	6.54	1.51	1.41
3	B	4472	ADP	O4'-C1'	6.52	1.51	1.41
3	K	4481	ADP	C4-N9	5.18	1.45	1.37
3	D	4474	ADP	C4-N9	5.16	1.45	1.37
3	H	4478	ADP	C4-N9	5.15	1.45	1.37
3	G	4477	ADP	C4-N9	5.14	1.45	1.37
3	L	4482	ADP	C4-N9	5.14	1.45	1.37
3	E	4475	ADP	C4-N9	5.14	1.45	1.37
3	A	4471	ADP	C4-N9	5.14	1.45	1.37
3	I	4479	ADP	C4-N9	5.13	1.45	1.37
3	F	4476	ADP	C4-N9	5.13	1.45	1.37
3	J	4480	ADP	C4-N9	5.12	1.45	1.37
3	B	4472	ADP	C4-N9	5.12	1.45	1.37
3	C	4473	ADP	C4-N9	5.12	1.45	1.37
3	C	4473	ADP	C4-N3	4.52	1.42	1.35
3	J	4480	ADP	C4-N3	4.52	1.42	1.35
3	G	4477	ADP	C4-N3	4.48	1.42	1.35
3	H	4478	ADP	C4-N3	4.47	1.42	1.35
3	F	4476	ADP	C4-N3	4.47	1.42	1.35
3	L	4482	ADP	C4-N3	4.46	1.42	1.35
3	I	4479	ADP	C4-N3	4.46	1.42	1.35
3	A	4471	ADP	C4-N3	4.46	1.42	1.35
3	E	4475	ADP	C4-N3	4.45	1.42	1.35
3	D	4474	ADP	C4-N3	4.45	1.42	1.35
3	B	4472	ADP	C4-N3	4.43	1.42	1.35
3	K	4481	ADP	C4-N3	4.42	1.42	1.35
3	H	4478	ADP	PB-O3B	4.09	1.69	1.54
3	I	4479	ADP	PB-O3B	4.09	1.69	1.54
3	J	4480	ADP	PB-O3B	4.09	1.69	1.54
3	C	4473	ADP	PB-O3B	4.09	1.69	1.54
3	L	4482	ADP	PB-O3B	4.09	1.69	1.54
3	K	4481	ADP	PB-O3B	4.08	1.69	1.54
3	B	4472	ADP	PB-O3B	4.08	1.69	1.54
3	A	4471	ADP	PB-O3B	4.08	1.69	1.54
3	D	4474	ADP	PB-O3B	4.08	1.69	1.54
3	G	4477	ADP	PB-O3B	4.07	1.69	1.54
3	E	4475	ADP	PB-O3B	4.07	1.69	1.54
3	F	4476	ADP	PB-O3B	4.06	1.69	1.54
3	I	4479	ADP	O4'-C4'	3.95	1.54	1.45
3	L	4482	ADP	O4'-C4'	3.95	1.54	1.45
3	E	4475	ADP	O4'-C4'	3.94	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	4472	ADP	O4'-C4'	3.94	1.54	1.45
3	K	4481	ADP	O4'-C4'	3.94	1.54	1.45
3	A	4471	ADP	O4'-C4'	3.93	1.54	1.45
3	H	4478	ADP	O4'-C4'	3.93	1.54	1.45
3	I	4479	ADP	C6-N6	-3.92	1.22	1.35
3	F	4476	ADP	O4'-C4'	3.92	1.54	1.45
3	E	4475	ADP	C6-N6	-3.92	1.22	1.35
3	D	4474	ADP	C6-N6	-3.92	1.22	1.35
3	G	4477	ADP	O4'-C4'	3.91	1.54	1.45
3	J	4480	ADP	C6-N6	-3.91	1.22	1.35
3	D	4474	ADP	O4'-C4'	3.91	1.54	1.45
3	B	4472	ADP	C6-N6	-3.91	1.22	1.35
3	L	4482	ADP	C6-N6	-3.91	1.22	1.35
3	A	4471	ADP	C6-N6	-3.91	1.22	1.35
3	H	4478	ADP	C6-N6	-3.90	1.22	1.35
3	F	4476	ADP	C6-N6	-3.90	1.22	1.35
3	C	4473	ADP	O4'-C4'	3.90	1.54	1.45
3	G	4477	ADP	C6-N6	-3.90	1.22	1.35
3	K	4481	ADP	C6-N6	-3.90	1.22	1.35
3	C	4473	ADP	C6-N6	-3.90	1.22	1.35
3	J	4480	ADP	O4'-C4'	3.89	1.54	1.45
3	L	4482	ADP	C2-N3	3.45	1.39	1.32
3	B	4472	ADP	C2-N3	3.45	1.39	1.32
3	K	4481	ADP	C2-N3	3.44	1.39	1.32
3	H	4478	ADP	C2-N3	3.44	1.39	1.32
3	A	4471	ADP	C2-N3	3.43	1.39	1.32
3	I	4479	ADP	C2-N3	3.43	1.39	1.32
3	D	4474	ADP	C2-N3	3.43	1.38	1.32
3	E	4475	ADP	C2-N3	3.42	1.38	1.32
3	F	4476	ADP	C2-N3	3.41	1.38	1.32
3	J	4480	ADP	C2-N3	3.41	1.38	1.32
3	C	4473	ADP	C2-N3	3.41	1.38	1.32
3	G	4477	ADP	C2-N3	3.40	1.38	1.32
4	L	5911	PPQ	PDP-CEP	-2.79	1.75	1.78
4	G	5906	PPQ	PDP-CEP	-2.70	1.75	1.78
4	D	5903	PPQ	PDP-CEP	-2.69	1.75	1.78
4	K	5910	PPQ	PDP-CEP	-2.69	1.75	1.78
4	J	5909	PPQ	PDP-CEP	-2.69	1.75	1.78
4	C	5902	PPQ	PDP-CEP	-2.69	1.75	1.78
4	A	5900	PPQ	PDP-CEP	-2.68	1.75	1.78
4	E	5904	PPQ	PDP-CEP	-2.68	1.75	1.78
4	B	5901	PPQ	PDP-CEP	-2.67	1.75	1.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	5908	PPQ	PDP-CEP	-2.64	1.75	1.78
4	F	5905	PPQ	PDP-CEP	-2.64	1.75	1.78
4	H	5907	PPQ	PDP-CEP	-2.64	1.75	1.78
3	H	4478	ADP	C3'-C4'	-2.16	1.47	1.53
3	L	4482	ADP	C3'-C4'	-2.15	1.47	1.53
3	J	4480	ADP	C3'-C4'	-2.15	1.47	1.53
3	B	4472	ADP	C3'-C4'	-2.14	1.47	1.53
3	A	4471	ADP	C3'-C4'	-2.14	1.47	1.53
3	G	4477	ADP	C3'-C4'	-2.14	1.47	1.53
3	I	4479	ADP	C3'-C4'	-2.13	1.47	1.53
3	K	4481	ADP	C3'-C4'	-2.13	1.47	1.53
3	D	4474	ADP	C3'-C4'	-2.13	1.47	1.53
3	F	4476	ADP	C3'-C4'	-2.13	1.47	1.53
3	E	4475	ADP	C3'-C4'	-2.13	1.47	1.53
3	C	4473	ADP	C3'-C4'	-2.12	1.47	1.53
3	I	4479	ADP	C5-C4	2.10	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	H	4478	ADP	C5-C4	2.08	1.45	1.40
3	F	4476	ADP	C5-C4	2.07	1.45	1.40
3	K	4481	ADP	C5-C4	2.07	1.45	1.40
3	L	4482	ADP	C5-C4	2.07	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	G	4477	ADP	C5-C4	2.06	1.45	1.40
3	E	4475	ADP	C5-C4	2.06	1.45	1.40
3	J	4480	ADP	C5-C4	2.05	1.45	1.40
4	I	5908	PPQ	PDP-OEA	-2.03	1.46	1.50

All (239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4474	ADP	O4'-C1'-N9	14.55	121.97	108.44
3	B	4472	ADP	O4'-C1'-N9	14.54	121.96	108.44
3	I	4479	ADP	O4'-C1'-N9	14.52	121.94	108.44
3	C	4473	ADP	O4'-C1'-N9	14.52	121.94	108.44
3	F	4476	ADP	O4'-C1'-N9	14.51	121.94	108.44
3	L	4482	ADP	O4'-C1'-N9	14.51	121.93	108.44
3	K	4481	ADP	O4'-C1'-N9	14.50	121.93	108.44
3	A	4471	ADP	O4'-C1'-N9	14.50	121.92	108.44
3	J	4480	ADP	O4'-C1'-N9	14.49	121.92	108.44
3	H	4478	ADP	O4'-C1'-N9	14.48	121.91	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	4477	ADP	O4'-C1'-N9	14.48	121.90	108.44
3	E	4475	ADP	O4'-C1'-N9	14.47	121.90	108.44
4	H	5907	PPQ	PDP-CGP-CBP	11.26	132.71	114.51
4	G	5906	PPQ	PDP-CGP-CBP	11.26	132.71	114.51
4	I	5908	PPQ	PDP-CGP-CBP	11.25	132.70	114.51
4	F	5905	PPQ	PDP-CGP-CBP	11.25	132.70	114.51
4	E	5904	PPQ	PDP-CGP-CBP	11.24	132.68	114.51
4	L	5911	PPQ	PDP-CGP-CBP	11.24	132.67	114.51
4	A	5900	PPQ	PDP-CGP-CBP	11.23	132.67	114.51
4	B	5901	PPQ	PDP-CGP-CBP	11.23	132.66	114.51
4	D	5903	PPQ	PDP-CGP-CBP	11.23	132.66	114.51
4	C	5902	PPQ	PDP-CGP-CBP	11.22	132.65	114.51
4	K	5910	PPQ	PDP-CGP-CBP	11.21	132.63	114.51
4	J	5909	PPQ	PDP-CGP-CBP	11.21	132.63	114.51
3	J	4480	ADP	O4'-C1'-C2'	-10.21	91.13	106.77
3	L	4482	ADP	O4'-C1'-C2'	-10.20	91.13	106.77
3	C	4473	ADP	O4'-C1'-C2'	-10.20	91.14	106.77
3	K	4481	ADP	O4'-C1'-C2'	-10.19	91.15	106.77
3	B	4472	ADP	O4'-C1'-C2'	-10.19	91.15	106.77
3	A	4471	ADP	O4'-C1'-C2'	-10.19	91.15	106.77
3	D	4474	ADP	O4'-C1'-C2'	-10.19	91.15	106.77
3	G	4477	ADP	O4'-C1'-C2'	-10.19	91.15	106.77
3	E	4475	ADP	O4'-C1'-C2'	-10.18	91.16	106.77
3	H	4478	ADP	O4'-C1'-C2'	-10.18	91.17	106.77
3	I	4479	ADP	O4'-C1'-C2'	-10.18	91.17	106.77
3	F	4476	ADP	O4'-C1'-C2'	-10.17	91.19	106.77
3	E	4475	ADP	C8-N9-C4	-9.39	99.73	106.90
3	K	4481	ADP	C8-N9-C4	-9.38	99.74	106.90
3	C	4473	ADP	C8-N9-C4	-9.36	99.75	106.90
3	J	4480	ADP	C8-N9-C4	-9.35	99.76	106.90
3	G	4477	ADP	C8-N9-C4	-9.35	99.76	106.90
3	I	4479	ADP	C8-N9-C4	-9.34	99.77	106.90
3	A	4471	ADP	C8-N9-C4	-9.33	99.78	106.90
3	H	4478	ADP	C8-N9-C4	-9.33	99.78	106.90
3	F	4476	ADP	C8-N9-C4	-9.32	99.78	106.90
3	B	4472	ADP	C8-N9-C4	-9.32	99.78	106.90
3	D	4474	ADP	C8-N9-C4	-9.32	99.79	106.90
3	L	4482	ADP	C8-N9-C4	-9.31	99.79	106.90
3	H	4478	ADP	C4'-O4'-C1'	-8.17	100.87	109.75
3	I	4479	ADP	C4'-O4'-C1'	-8.17	100.88	109.75
3	E	4475	ADP	C4'-O4'-C1'	-8.17	100.88	109.75
3	L	4482	ADP	C4'-O4'-C1'	-8.16	100.89	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	4481	ADP	C4'-O4'-C1'	-8.15	100.90	109.75
3	G	4477	ADP	C4'-O4'-C1'	-8.15	100.90	109.75
3	J	4480	ADP	C4'-O4'-C1'	-8.15	100.90	109.75
3	F	4476	ADP	C4'-O4'-C1'	-8.15	100.90	109.75
3	A	4471	ADP	C4'-O4'-C1'	-8.14	100.91	109.75
3	D	4474	ADP	C4'-O4'-C1'	-8.12	100.93	109.75
3	C	4473	ADP	C4'-O4'-C1'	-8.11	100.94	109.75
3	B	4472	ADP	C4'-O4'-C1'	-8.10	100.95	109.75
3	I	4479	ADP	O5'-C5'-C4'	7.84	137.70	108.94
3	K	4481	ADP	O5'-C5'-C4'	7.84	137.70	108.94
3	L	4482	ADP	O5'-C5'-C4'	7.84	137.70	108.94
3	D	4474	ADP	O5'-C5'-C4'	7.83	137.69	108.94
3	A	4471	ADP	O5'-C5'-C4'	7.83	137.68	108.94
3	E	4475	ADP	O5'-C5'-C4'	7.83	137.68	108.94
3	F	4476	ADP	O5'-C5'-C4'	7.83	137.67	108.94
3	G	4477	ADP	O5'-C5'-C4'	7.83	137.67	108.94
3	H	4478	ADP	O5'-C5'-C4'	7.83	137.66	108.94
3	J	4480	ADP	O5'-C5'-C4'	7.82	137.65	108.94
3	C	4473	ADP	O5'-C5'-C4'	7.82	137.65	108.94
3	B	4472	ADP	O5'-C5'-C4'	7.82	137.63	108.94
4	J	5909	PPQ	CEP-PDP-CGP	6.87	119.81	107.57
4	B	5901	PPQ	CEP-PDP-CGP	6.85	119.78	107.57
4	L	5911	PPQ	CEP-PDP-CGP	6.84	119.76	107.57
4	D	5903	PPQ	CEP-PDP-CGP	6.84	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	A	5900	PPQ	CEP-PDP-CGP	6.83	119.75	107.57
4	K	5910	PPQ	CEP-PDP-CGP	6.83	119.74	107.57
4	I	5908	PPQ	CEP-PDP-CGP	6.82	119.73	107.57
4	G	5906	PPQ	CEP-PDP-CGP	6.82	119.73	107.57
4	F	5905	PPQ	CEP-PDP-CGP	6.81	119.70	107.57
4	E	5904	PPQ	OEB-PDP-OEA	-5.87	106.03	113.00
4	L	5911	PPQ	OEB-PDP-OEA	-5.86	106.04	113.00
4	J	5909	PPQ	OEB-PDP-OEA	-5.85	106.05	113.00
4	G	5906	PPQ	OEB-PDP-OEA	-5.85	106.06	113.00
4	B	5901	PPQ	OEB-PDP-OEA	-5.85	106.06	113.00
4	A	5900	PPQ	OEB-PDP-OEA	-5.84	106.07	113.00
4	D	5903	PPQ	OEB-PDP-OEA	-5.84	106.07	113.00
4	C	5902	PPQ	OEB-PDP-OEA	-5.82	106.09	113.00
4	H	5907	PPQ	OEB-PDP-OEA	-5.82	106.09	113.00
4	I	5908	PPQ	OEB-PDP-OEA	-5.82	106.10	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	5910	PPQ	OEB-PDP-OEA	-5.81	106.10	113.00
4	F	5905	PPQ	OEB-PDP-OEA	-5.81	106.11	113.00
3	L	4482	ADP	C4-C5-N7	5.71	114.41	109.52
3	K	4481	ADP	C4-C5-N7	5.71	114.41	109.52
3	B	4472	ADP	C4-C5-N7	5.70	114.40	109.52
3	G	4477	ADP	C4-C5-N7	5.68	114.39	109.52
3	A	4471	ADP	C4-C5-N7	5.66	114.37	109.52
3	C	4473	ADP	C4-C5-N7	5.66	114.37	109.52
3	I	4479	ADP	C4-C5-N7	5.64	114.36	109.52
3	J	4480	ADP	C4-C5-N7	5.63	114.34	109.52
3	F	4476	ADP	C4-C5-N7	5.62	114.34	109.52
3	H	4478	ADP	C4-C5-N7	5.62	114.33	109.52
3	D	4474	ADP	C4-C5-N7	5.61	114.32	109.52
3	E	4475	ADP	C4-C5-N7	5.61	114.32	109.52
3	G	4477	ADP	C1'-N9-C4	5.15	135.53	126.64
3	E	4475	ADP	C1'-N9-C4	5.15	135.53	126.64
3	C	4473	ADP	C1'-N9-C4	5.15	135.53	126.64
3	K	4481	ADP	C1'-N9-C4	5.14	135.52	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	B	4472	ADP	C1'-N9-C4	5.13	135.50	126.64
3	L	4482	ADP	C1'-N9-C4	5.13	135.49	126.64
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	D	4474	ADP	C1'-N9-C4	5.12	135.48	126.64
3	C	4473	ADP	C5'-C4'-C3'	-3.70	100.39	115.21
3	F	4476	ADP	C5'-C4'-C3'	-3.70	100.41	115.21
3	I	4479	ADP	C5'-C4'-C3'	-3.69	100.42	115.21
3	B	4472	ADP	C5'-C4'-C3'	-3.69	100.42	115.21
3	J	4480	ADP	C5'-C4'-C3'	-3.69	100.42	115.21
3	H	4478	ADP	C5'-C4'-C3'	-3.69	100.42	115.21
3	A	4471	ADP	C5'-C4'-C3'	-3.69	100.43	115.21
3	G	4477	ADP	C5'-C4'-C3'	-3.69	100.43	115.21
3	D	4474	ADP	C5'-C4'-C3'	-3.69	100.45	115.21
3	E	4475	ADP	C5'-C4'-C3'	-3.69	100.45	115.21
3	K	4481	ADP	C5'-C4'-C3'	-3.68	100.46	115.21
3	L	4482	ADP	C5'-C4'-C3'	-3.68	100.47	115.21
3	H	4478	ADP	C3'-C2'-C1'	-3.49	95.45	100.91
3	E	4475	ADP	C3'-C2'-C1'	-3.49	95.45	100.91
3	K	4481	ADP	C3'-C2'-C1'	-3.47	95.47	100.91
3	F	4476	ADP	C3'-C2'-C1'	-3.47	95.48	100.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4474	ADP	C3'-C2'-C1'	-3.46	95.49	100.91
3	B	4472	ADP	C3'-C2'-C1'	-3.46	95.49	100.91
3	A	4471	ADP	C3'-C2'-C1'	-3.46	95.49	100.91
3	G	4477	ADP	C3'-C2'-C1'	-3.46	95.49	100.91
3	J	4480	ADP	C3'-C2'-C1'	-3.45	95.50	100.91
3	C	4473	ADP	C3'-C2'-C1'	-3.45	95.51	100.91
3	I	4479	ADP	C3'-C2'-C1'	-3.45	95.51	100.91
3	L	4482	ADP	C3'-C2'-C1'	-3.44	95.52	100.91
3	J	4480	ADP	O4'-C4'-C5'	3.36	121.36	109.36
3	B	4472	ADP	O4'-C4'-C5'	3.36	121.35	109.36
3	G	4477	ADP	O4'-C4'-C5'	3.36	121.35	109.36
3	E	4475	ADP	O4'-C4'-C5'	3.36	121.35	109.36
3	F	4476	ADP	O4'-C4'-C5'	3.36	121.34	109.36
3	K	4481	ADP	O4'-C4'-C5'	3.35	121.33	109.36
3	D	4474	ADP	O4'-C4'-C5'	3.35	121.33	109.36
3	A	4471	ADP	O4'-C4'-C5'	3.35	121.33	109.36
3	H	4478	ADP	O4'-C4'-C5'	3.35	121.33	109.36
3	C	4473	ADP	O4'-C4'-C5'	3.35	121.31	109.36
3	L	4482	ADP	O4'-C4'-C5'	3.35	121.31	109.36
3	I	4479	ADP	O4'-C4'-C5'	3.33	121.26	109.36
3	F	4476	ADP	O2'-C2'-C1'	3.02	120.36	111.23
3	I	4479	ADP	O2'-C2'-C1'	3.01	120.33	111.23
3	D	4474	ADP	O2'-C2'-C1'	3.01	120.33	111.23
3	A	4471	ADP	O2'-C2'-C1'	3.01	120.33	111.23
3	C	4473	ADP	O2'-C2'-C1'	3.01	120.32	111.23
3	H	4478	ADP	O2'-C2'-C1'	3.00	120.31	111.23
3	G	4477	ADP	O2'-C2'-C1'	3.00	120.31	111.23
3	B	4472	ADP	O2'-C2'-C1'	3.00	120.31	111.23
3	K	4481	ADP	O2'-C2'-C1'	3.00	120.30	111.23
3	J	4480	ADP	O2'-C2'-C1'	2.99	120.28	111.23
3	E	4475	ADP	O2'-C2'-C1'	3.00	120.29	111.23
3	L	4482	ADP	O2'-C2'-C1'	2.99	120.27	111.23
3	D	4474	ADP	N3-C4-N9	2.81	130.51	125.43
3	I	4479	ADP	N3-C4-N9	2.81	130.51	125.43
3	B	4472	ADP	N3-C4-N9	2.81	130.51	125.43
3	F	4476	ADP	N3-C4-N9	2.81	130.50	125.43
3	A	4471	ADP	N3-C4-N9	2.81	130.50	125.43
3	L	4482	ADP	N3-C4-N9	2.80	130.50	125.43
3	J	4480	ADP	N3-C4-N9	2.80	130.50	125.43
3	H	4478	ADP	N3-C4-N9	2.79	130.48	125.43
3	C	4473	ADP	N3-C4-N9	2.79	130.47	125.43
3	E	4475	ADP	N3-C4-N9	2.79	130.47	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	4477	ADP	N3-C4-N9	2.79	130.47	125.43
3	K	4481	ADP	N3-C4-N9	2.79	130.47	125.43
3	K	4481	ADP	PA-O3A-PB	2.63	139.41	131.68
3	B	4472	ADP	PA-O3A-PB	2.62	139.38	131.68
3	L	4482	ADP	PA-O3A-PB	2.62	139.37	131.68
3	J	4480	ADP	PA-O3A-PB	2.62	139.36	131.68
3	F	4476	ADP	PA-O3A-PB	2.62	139.35	131.68
3	E	4475	ADP	PA-O3A-PB	2.62	139.35	131.68
3	A	4471	ADP	PA-O3A-PB	2.61	139.35	131.68
3	H	4478	ADP	PA-O3A-PB	2.61	139.35	131.68
3	C	4473	ADP	PA-O3A-PB	2.61	139.35	131.68
3	D	4474	ADP	PA-O3A-PB	2.61	139.34	131.68
3	I	4479	ADP	PA-O3A-PB	2.61	139.33	131.68
3	G	4477	ADP	PA-O3A-PB	2.60	139.31	131.68
3	I	4479	ADP	PA-O5'-C5'	2.51	140.11	122.03
3	B	4472	ADP	PA-O5'-C5'	2.52	140.12	122.03
3	K	4481	ADP	PA-O5'-C5'	2.51	140.11	122.03
3	L	4482	ADP	PA-O5'-C5'	2.51	140.10	122.03
3	D	4474	ADP	PA-O5'-C5'	2.51	140.09	122.03
3	C	4473	ADP	PA-O5'-C5'	2.51	140.10	122.03
3	A	4471	ADP	PA-O5'-C5'	2.51	140.08	122.03
3	J	4480	ADP	PA-O5'-C5'	2.51	140.07	122.03
3	H	4478	ADP	PA-O5'-C5'	2.51	140.06	122.03
3	G	4477	ADP	PA-O5'-C5'	2.51	140.07	122.03
3	F	4476	ADP	PA-O5'-C5'	2.51	140.06	122.03
3	E	4475	ADP	PA-O5'-C5'	2.51	140.05	122.03
3	B	4472	ADP	O3'-C3'-C2'	2.50	119.97	111.83
3	J	4480	ADP	O3'-C3'-C2'	2.50	119.97	111.83
3	H	4478	ADP	O3'-C3'-C2'	2.50	119.97	111.83
3	E	4475	ADP	O3'-C3'-C2'	2.50	119.97	111.83
3	D	4474	ADP	O3'-C3'-C2'	2.49	119.94	111.83
3	K	4481	ADP	O3'-C3'-C2'	2.49	119.94	111.83
3	L	4482	ADP	O3'-C3'-C2'	2.49	119.94	111.83
3	A	4471	ADP	O3'-C3'-C2'	2.49	119.94	111.83
3	C	4473	ADP	O3'-C3'-C2'	2.49	119.94	111.83
3	G	4477	ADP	O3'-C3'-C2'	2.49	119.94	111.83
3	F	4476	ADP	O3'-C3'-C2'	2.49	119.93	111.83
3	I	4479	ADP	O3'-C3'-C2'	2.48	119.91	111.83
3	H	4478	ADP	O5'-PA-O1A	-2.17	100.86	109.37
3	G	4477	ADP	O5'-PA-O1A	-2.17	100.86	109.37
3	K	4481	ADP	O5'-PA-O1A	-2.17	100.88	109.37
3	E	4475	ADP	O5'-PA-O1A	-2.17	100.88	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4471	ADP	O5'-PA-O1A	-2.17	100.89	109.37
3	F	4476	ADP	O5'-PA-O1A	-2.17	100.89	109.37
3	L	4482	ADP	O5'-PA-O1A	-2.17	100.89	109.37
3	J	4480	ADP	O5'-PA-O1A	-2.16	100.90	109.37
3	D	4474	ADP	O5'-PA-O1A	-2.16	100.91	109.37
3	C	4473	ADP	O5'-PA-O1A	-2.16	100.92	109.37
3	B	4472	ADP	O5'-PA-O1A	-2.16	100.92	109.37
3	I	4479	ADP	O5'-PA-O1A	-2.15	100.93	109.37
3	K	4481	ADP	O2B-PB-O3A	2.02	114.71	105.14
3	J	4480	ADP	O2B-PB-O3A	2.01	114.70	105.14
3	I	4479	ADP	O2B-PB-O3A	2.01	114.68	105.14
3	H	4478	ADP	O2B-PB-O3A	2.01	114.68	105.14
3	C	4473	ADP	O2B-PB-O3A	2.01	114.68	105.14
3	F	4476	ADP	O2B-PB-O3A	2.01	114.67	105.14
3	L	4482	ADP	O2B-PB-O3A	2.01	114.66	105.14
3	A	4471	ADP	O2B-PB-O3A	2.01	114.66	105.14
3	E	4475	ADP	O2B-PB-O3A	2.01	114.66	105.14
3	B	4472	ADP	O2B-PB-O3A	2.01	114.65	105.14
3	D	4474	ADP	O2B-PB-O3A	2.00	114.63	105.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	468/468 (100%)	0.16	36 (7%)	13	16	20, 47, 80, 100	94 (20%)
1	B	468/468 (100%)	-0.13	22 (4%)	30	37	20, 47, 80, 100	94 (20%)
1	C	468/468 (100%)	-0.16	25 (5%)	25	31	20, 47, 80, 100	94 (20%)
1	D	468/468 (100%)	-0.29	21 (4%)	32	39	20, 47, 80, 100	94 (20%)
1	E	468/468 (100%)	-0.18	24 (5%)	27	33	20, 47, 80, 100	94 (20%)
1	F	468/468 (100%)	-0.12	26 (5%)	24	28	20, 47, 80, 100	94 (20%)
1	G	468/468 (100%)	-0.30	20 (4%)	34	40	20, 47, 80, 100	94 (20%)
1	H	468/468 (100%)	-0.23	21 (4%)	32	39	20, 47, 80, 100	94 (20%)
1	I	468/468 (100%)	-0.36	15 (3%)	45	54	20, 47, 80, 100	94 (20%)
1	J	468/468 (100%)	-0.25	17 (3%)	41	48	20, 47, 80, 100	94 (20%)
1	K	468/468 (100%)	-0.33	15 (3%)	45	54	20, 47, 80, 100	94 (20%)
1	L	468/468 (100%)	-0.30	17 (3%)	41	48	20, 47, 80, 100	94 (20%)
All	All	5616/5616 (100%)	-0.21	259 (4%)	31	38	20, 47, 81, 100	1128 (20%)

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	396	LEU	10.5
1	K	396	LEU	10.4
1	J	398	ASP	8.4
1	L	396	LEU	8.0
1	A	404	ALA	7.6
1	F	398	ASP	7.5
1	J	396	LEU	7.1
1	I	63	SER	7.1
1	J	60	ILE	6.8
1	D	395	ASN	6.6
1	K	395	ASN	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	60	ILE	6.3
1	C	398	ASP	6.2
1	L	397	TYR	6.1
1	B	404	ALA	6.1
1	E	63	SER	6.0
1	C	396	LEU	6.0
1	F	401	PRO	6.0
1	A	395	ASN	6.0
1	C	63	SER	5.9
1	H	337	ARG	5.7
1	H	398	ASP	5.7
1	D	398	ASP	5.6
1	E	395	ASN	5.6
1	J	403	GLU	5.6
1	F	404	ALA	5.5
1	J	399	LEU	5.5
1	C	395	ASN	5.5
1	G	63	SER	5.5
1	C	61	ASN	5.4
1	F	63	SER	5.4
1	D	399	LEU	5.4
1	A	285	ASP	5.2
1	H	402	GLU	5.2
1	G	401	PRO	5.1
1	A	399	LEU	5.1
1	H	60	ILE	4.9
1	B	399	LEU	4.9
1	A	277	ASN	4.9
1	K	398	ASP	4.9
1	A	403	GLU	4.7
1	L	402	GLU	4.6
1	G	398	ASP	4.6
1	J	402	GLU	4.5
1	F	395	ASN	4.5
1	F	402	GLU	4.5
1	C	394	LYS	4.5
1	A	400	PRO	4.4
1	K	397	TYR	4.4
1	H	61	ASN	4.4
1	J	337	ARG	4.4
1	F	400	PRO	4.4
1	G	399	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	H	395	ASN	4.3
1	B	400	PRO	4.3
1	G	395	ASN	4.3
1	J	397	TYR	4.3
1	I	398	ASP	4.2
1	D	60	ILE	4.2
1	G	396	LEU	4.2
1	G	404	ALA	4.2
1	D	400	PRO	4.2
1	E	396	LEU	4.2
1	A	402	GLU	4.1
1	K	1	SER	4.1
1	A	398	ASP	4.0
1	E	1	SER	4.0
1	I	399	LEU	4.0
1	G	397	TYR	4.0
1	F	397	TYR	3.9
1	B	337	ARG	3.9
1	K	63	SER	3.8
1	L	398	ASP	3.8
1	F	394	LYS	3.8
1	L	395	ASN	3.8
1	H	399	LEU	3.8
1	F	62	GLU	3.8
1	E	398	ASP	3.8
1	D	394	LYS	3.8
1	A	396	LEU	3.7
1	D	401	PRO	3.7
1	F	349	ALA	3.7
1	C	59	GLY	3.7
1	L	401	PRO	3.7
1	J	401	PRO	3.7
1	I	61	ASN	3.7
1	D	396	LEU	3.7
1	D	63	SER	3.6
1	E	61	ASN	3.6
1	D	404	ALA	3.6
1	F	264[A]	ASN	3.6
1	G	402	GLU	3.6
1	K	402	GLU	3.6
1	G	349	ALA	3.5
1	B	55	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	404	ALA	3.5
1	H	264[A]	ASN	3.5
1	H	396	LEU	3.5
1	A	63	SER	3.4
1	C	1	SER	3.4
1	L	62	GLU	3.4
1	F	61	ASN	3.4
1	E	337	ARG	3.4
1	F	284	GLY	3.4
1	H	400	PRO	3.4
1	I	402	GLU	3.4
1	B	395	ASN	3.3
1	G	403	GLU	3.3
1	C	402	GLU	3.3
1	D	278	GLY	3.3
1	H	63	SER	3.3
1	A	378	GLY	3.3
1	E	60	ILE	3.3
1	D	402	GLU	3.3
1	E	404	ALA	3.3
1	H	1	SER	3.2
1	A	337	ARG	3.2
1	C	397	TYR	3.2
1	I	404	ALA	3.2
1	I	60	ILE	3.2
1	L	1	SER	3.2
1	K	403	GLU	3.2
1	L	399	LEU	3.2
1	A	401	PRO	3.2
1	A	62	GLU	3.2
1	G	264[A]	ASN	3.2
1	D	1	SER	3.2
1	C	60	ILE	3.2
1	E	59	GLY	3.2
1	L	264[A]	ASN	3.1
1	L	63	SER	3.1
1	A	394	LYS	3.0
1	I	62	GLU	3.0
1	A	351	PRO	3.0
1	I	397	TYR	3.0
1	D	403	GLU	3.0
1	B	394	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	401	PRO	3.0
1	A	3	GLU	3.0
1	F	59	GLY	3.0
1	D	337	ARG	3.0
1	J	395	ASN	3.0
1	L	61	ASN	3.0
1	C	3	GLU	3.0
1	B	1	SER	2.9
1	C	264[A]	ASN	2.9
1	A	348	VAL	2.9
1	B	398	ASP	2.9
1	F	399	LEU	2.9
1	J	400	PRO	2.9
1	H	4	HIS	2.9
1	E	283	SER	2.9
1	F	60	ILE	2.9
1	B	63	SER	2.9
1	F	1	SER	2.8
1	G	394	LYS	2.8
1	B	98	GLN	2.8
1	H	403	GLU	2.8
1	D	94	PRO	2.8
1	L	337	ARG	2.8
1	E	62	GLU	2.8
1	F	406	GLU	2.7
1	A	116	ARG	2.7
1	B	60	ILE	2.7
1	K	60	ILE	2.7
1	E	7	THR	2.7
1	I	1	SER	2.7
1	I	405	LYS	2.7
1	F	348	VAL	2.7
1	K	61	ASN	2.7
1	G	1	SER	2.7
1	F	56	GLY	2.7
1	L	405	LYS	2.6
1	L	60	ILE	2.6
1	A	276	LYS	2.6
1	A	264[A]	ASN	2.6
1	A	55	GLY	2.6
1	J	178[A]	GLY	2.6
1	C	41	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	58	LYS	2.6
1	L	393	ASP	2.6
1	G	4	HIS	2.6
1	E	12	HIS	2.6
1	G	400	PRO	2.5
1	A	286	LYS	2.5
1	J	63	SER	2.5
1	L	403	GLU	2.5
1	K	399	LEU	2.5
1	A	44	GLU	2.5
1	A	354	ARG	2.5
1	E	394	LYS	2.5
1	G	98	GLN	2.5
1	D	397	TYR	2.5
1	B	61	ASN	2.5
1	B	58	LYS	2.5
1	F	405	LYS	2.5
1	E	279	THR	2.4
1	E	4	HIS	2.4
1	D	264[A]	ASN	2.4
1	G	348	VAL	2.4
1	H	95	GLY	2.4
1	H	284	GLY	2.4
1	B	59	GLY	2.4
1	E	11	GLU	2.4
1	A	284	GLY	2.4
1	E	393	ASP	2.4
1	B	396	LEU	2.4
1	I	395	ASN	2.4
1	E	55	GLY	2.3
1	F	98	GLN	2.3
1	D	62	GLU	2.3
1	H	11	GLU	2.3
1	E	349	ALA	2.3
1	A	397	TYR	2.3
1	B	352	LYS	2.3
1	A	405	LYS	2.3
1	G	61	ASN	2.3
1	J	61	ASN	2.3
1	I	285	ASP	2.3
1	I	3	GLU	2.3
1	C	349	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	404	ALA	2.3
1	H	3	GLU	2.3
1	H	40	ALA	2.3
1	J	264[A]	ASN	2.2
1	C	401	PRO	2.2
1	C	10	ASN	2.2
1	B	387	HIS	2.2
1	C	62	GLU	2.2
1	C	399	LEU	2.2
1	J	394	LYS	2.2
1	K	405	LYS	2.2
1	C	337	ARG	2.2
1	I	403	GLU	2.2
1	K	264[A]	ASN	2.2
1	A	278	GLY	2.2
1	B	401	PRO	2.2
1	G	93	GLU	2.2
1	E	278	GLY	2.2
1	A	273	SER	2.1
1	E	292	GLU	2.1
1	D	353	ALA	2.1
1	B	327	GLU	2.1
1	C	393	ASP	2.1
1	K	40	ALA	2.1
1	C	96	THR	2.1
1	A	392	MET	2.1
1	K	400	PRO	2.1
1	B	264[A]	ASN	2.1
1	F	178[A]	GLY	2.1
1	C	7	THR	2.1
1	B	403	GLU	2.1
1	E	285	ASP	2.0
1	F	278	GLY	2.0
1	A	94	PRO	2.0
1	A	279	THR	2.0
1	D	98	GLN	2.0
1	C	405	LYS	2.0
1	H	394	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ADP	L	4482	27/27	0.42	5.26	42,80,100,100	27
3	ADP	F	4476	27/27	0.41	4.74	42,80,100,100	27
3	ADP	K	4481	27/27	0.35	3.87	42,80,100,100	27
3	ADP	H	4478	27/27	0.31	3.50	42,80,100,100	27
3	ADP	C	4473	27/27	0.35	3.46	42,80,100,100	27
3	ADP	E	4475	27/27	0.37	3.02	42,80,100,100	27
3	ADP	I	4479	27/27	0.32	2.86	42,80,100,100	27
3	ADP	G	4477	27/27	0.27	2.03	42,80,100,100	27
3	ADP	D	4474	27/27	0.34	1.98	42,80,100,100	27
3	ADP	J	4480	27/27	0.28	1.80	42,80,100,100	27
3	ADP	B	4472	27/27	0.29	1.08	42,80,100,100	27
3	ADP	A	4471	27/27	0.32	0.99	42,80,100,100	27
4	PPQ	I	5908	11/11	0.21	0.33	16,36,70,83	11
4	PPQ	L	5911	11/11	0.20	-0.01	16,36,70,83	11
4	PPQ	B	5901	11/11	0.19	-0.10	16,36,70,83	11
4	PPQ	D	5903	11/11	0.18	-0.25	16,36,70,83	11
4	PPQ	F	5905	11/11	0.19	-0.29	16,36,70,83	11
4	PPQ	J	5909	11/11	0.19	-0.29	16,36,70,83	11
4	PPQ	H	5907	11/11	0.18	-0.33	16,36,70,83	11
4	PPQ	K	5910	11/11	0.17	-0.37	16,36,70,83	11
4	PPQ	G	5906	11/11	0.16	-0.40	16,36,70,83	11
4	PPQ	C	5902	11/11	0.16	-0.45	16,36,70,83	11
4	PPQ	A	5900	11/11	0.16	-0.86	16,36,70,83	11
4	PPQ	E	5904	11/11	0.13	-0.96	16,36,70,83	11
2	MN	K	469	1/1	0.12	-1.02	41,41,41,41	0
2	MN	D	470	1/1	0.07	-1.30	43,43,43,43	0
2	MN	J	469	1/1	0.07	-2.04	41,41,41,41	0
2	MN	L	469	1/1	0.10	-2.09	41,41,41,41	0
2	MN	D	469	1/1	0.07	-2.11	41,41,41,41	0
2	MN	L	470	1/1	0.05	-2.13	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MN	H	469	1/1	0.10	-2.17	41,41,41,41	0
2	MN	G	470	1/1	0.03	-2.53	43,43,43,43	0
2	MN	I	469	1/1	0.06	-2.53	41,41,41,41	0
2	MN	A	469	1/1	0.06	-2.54	41,41,41,41	0
2	MN	E	470	1/1	0.06	-2.59	43,43,43,43	0
2	MN	I	470	1/1	0.05	-2.65	43,43,43,43	0
2	MN	K	470	1/1	0.05	-2.70	43,43,43,43	0
2	MN	G	469	1/1	0.06	-2.73	41,41,41,41	0
2	MN	J	470	1/1	0.02	-2.83	43,43,43,43	0
2	MN	F	470	1/1	0.06	-2.88	43,43,43,43	0
2	MN	H	470	1/1	0.06	-2.98	43,43,43,43	0
2	MN	A	470	1/1	0.03	-3.34	43,43,43,43	0
2	MN	B	470	1/1	0.05	-3.48	43,43,43,43	0
2	MN	E	469	1/1	0.03	-3.62	41,41,41,41	0
2	MN	C	469	1/1	0.05	-4.27	41,41,41,41	0
2	MN	B	469	1/1	0.04	-4.66	41,41,41,41	0
2	MN	C	470	1/1	0.03	-4.92	43,43,43,43	0
2	MN	F	469	1/1	0.05	-4.95	41,41,41,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.