



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:12 am BST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

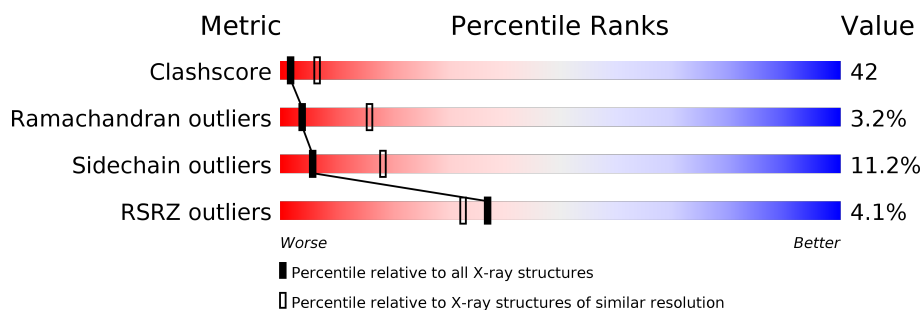
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	468	<div> <div>6%</div> <div> <div></div> <div>50%</div> <div>41%</div> <div>8%</div> </div> </div>
1	B	468	<div> <div>4%</div> <div> <div></div> <div>52%</div> <div>40%</div> <div>8%</div> </div> </div>
1	C	468	<div> <div>4%</div> <div> <div></div> <div>50%</div> <div>41%</div> <div>8%</div> </div> </div>
1	D	468	<div> <div>4%</div> <div> <div></div> <div>51%</div> <div>40%</div> <div>8%</div> </div> </div>
1	E	468	<div> <div>3%</div> <div> <div></div> <div>50%</div> <div>41%</div> <div>8%</div> </div> </div>
1	F	468	<div> <div>5%</div> <div> <div></div> <div>52%</div> <div>40%</div> <div>8%</div> </div> </div>
1	G	468	<div> <div>4%</div> <div> <div></div> <div>51%</div> <div>41%</div> <div>8%</div> </div> </div>

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

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

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

2 Entry composition

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

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

- Molecule 1 is a protein called GLUTAMINE SYNTHETASE.

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

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

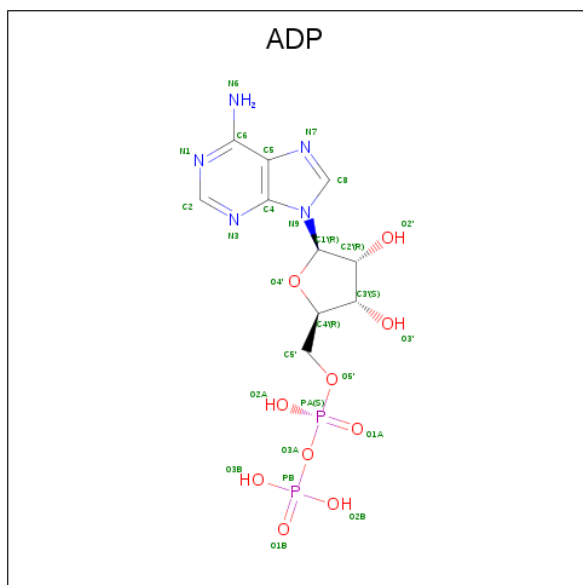
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mn	0	0
			2	2		
2	J	2	Total	Mn	0	0
			2	2		

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



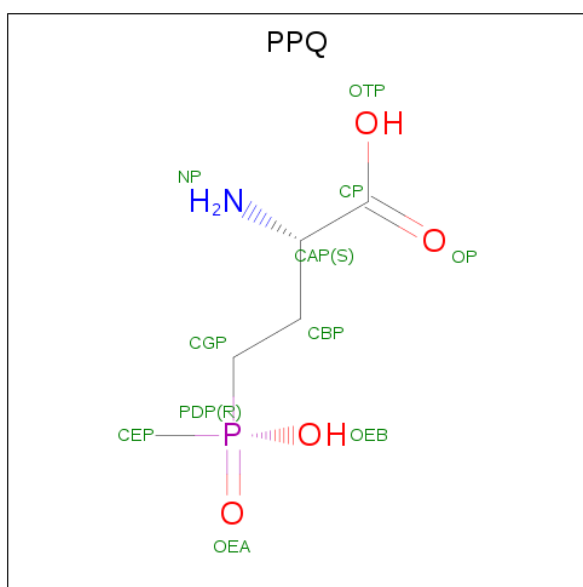
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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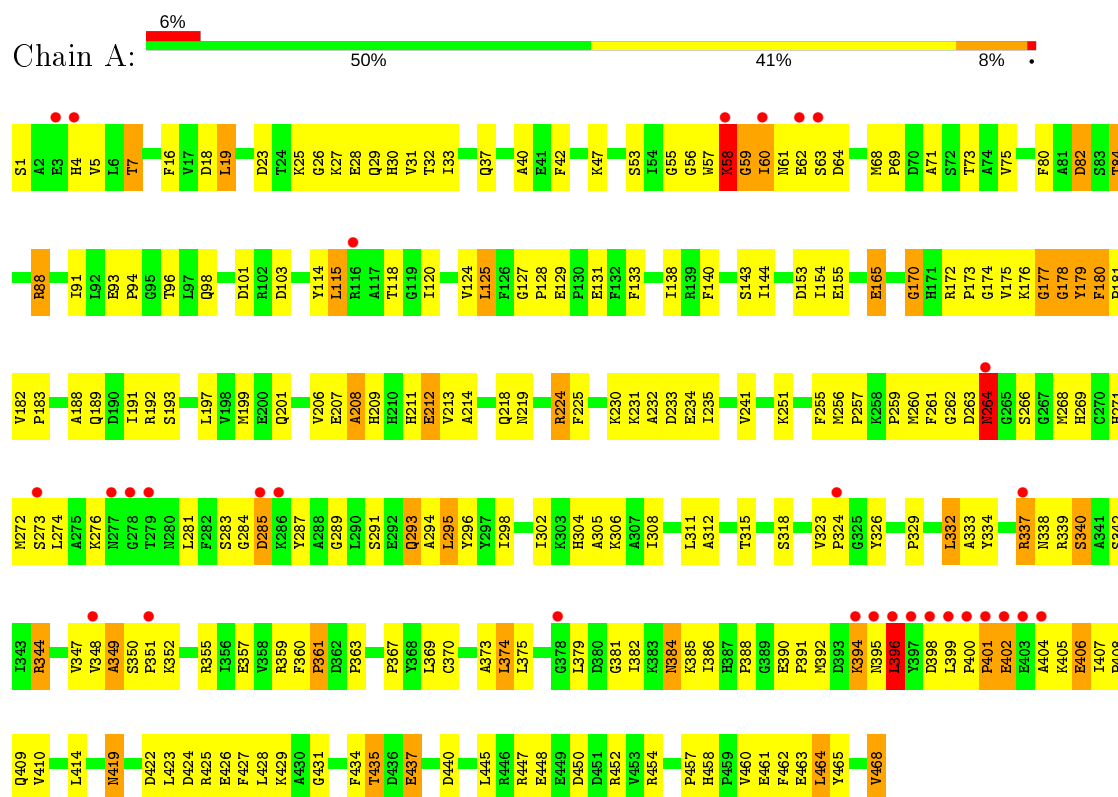
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	156	Total 156	O 156	0	0
5	J	151	Total 151	O 151	0	0
5	K	153	Total 153	O 153	0	0
5	L	153	Total 153	O 153	0	0

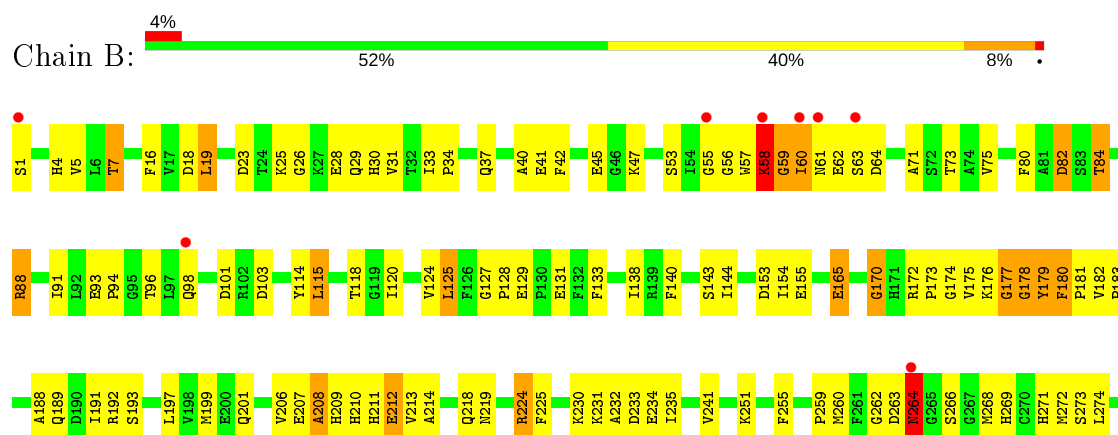
3 Residue-property plots

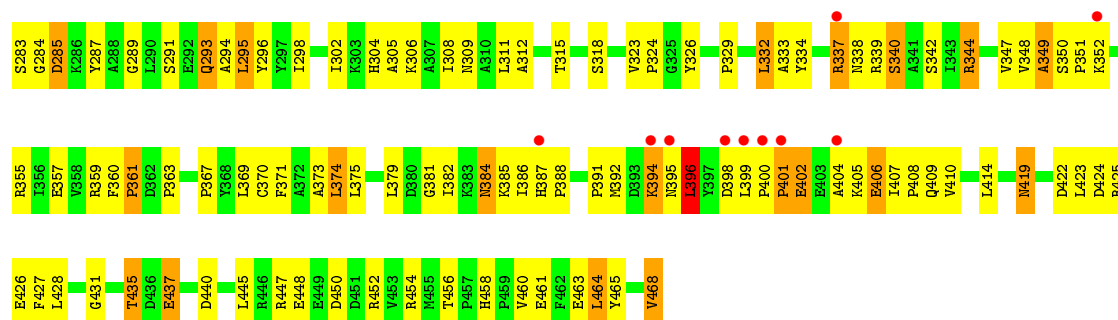
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: GLUTAMINE SYNTHETASE

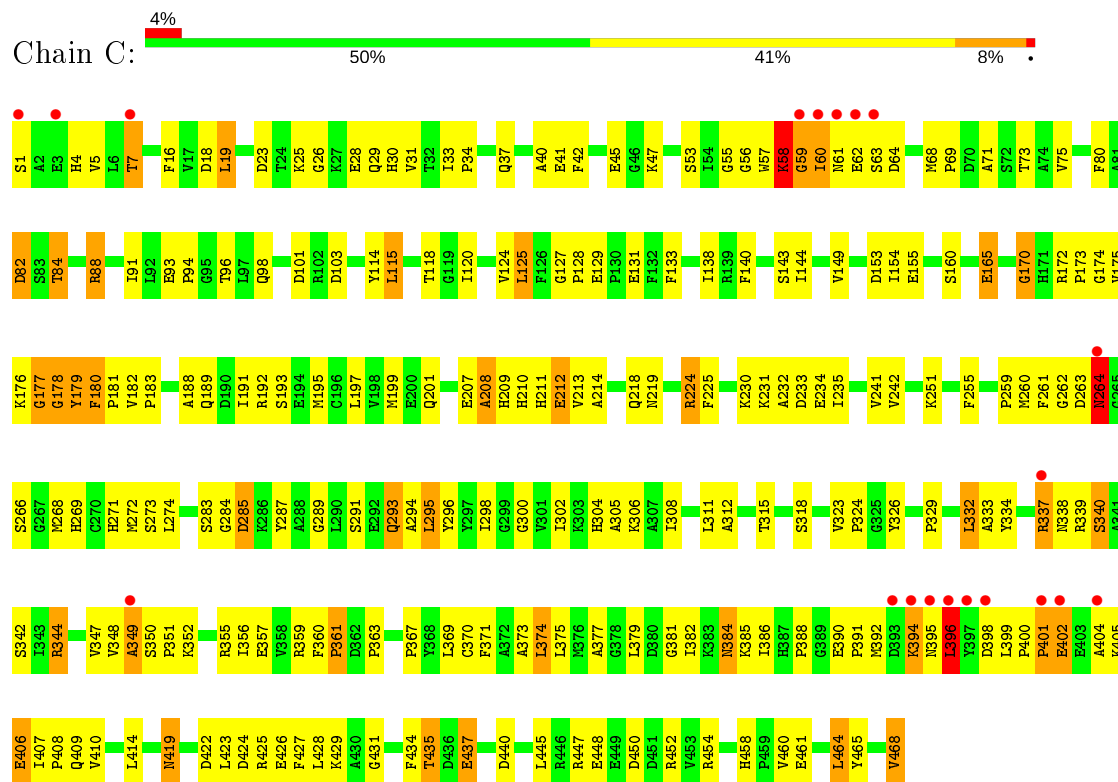


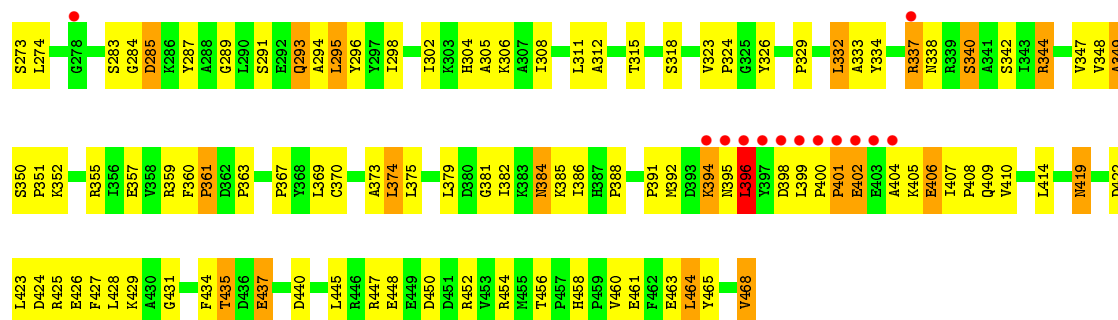
• Molecule 1: GLUTAMINE SYNTHETASE



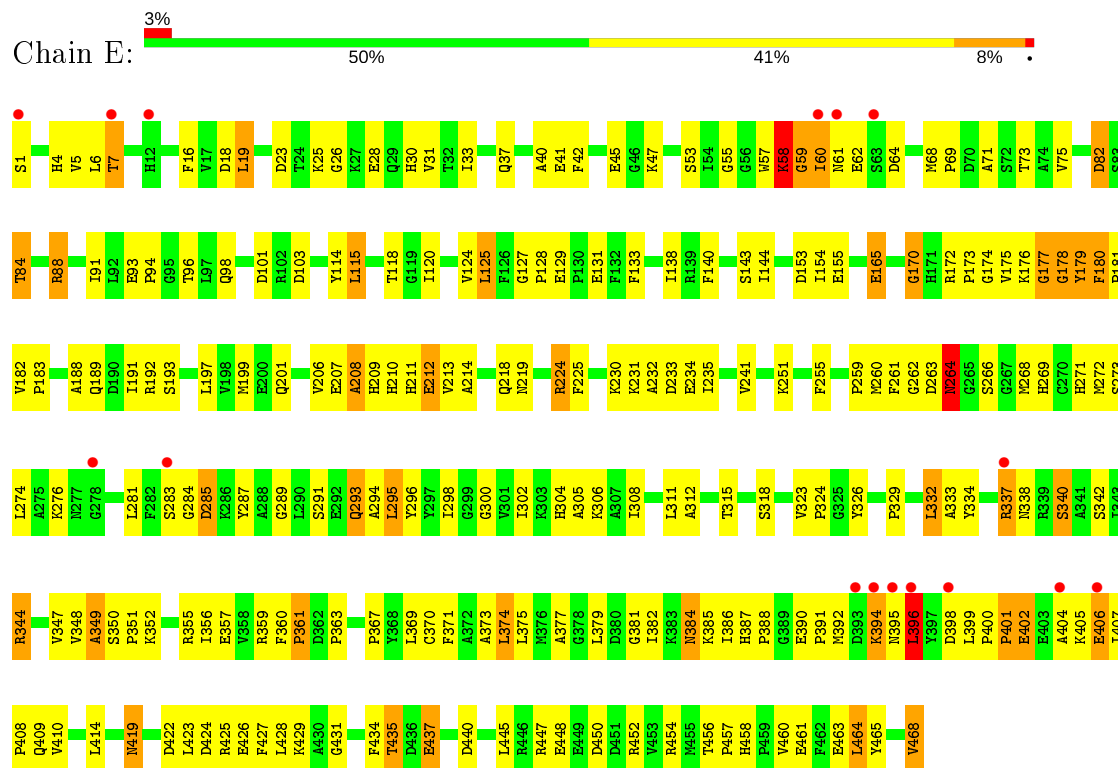


• Molecule 1: GLUTAMINE SYNTHETASE

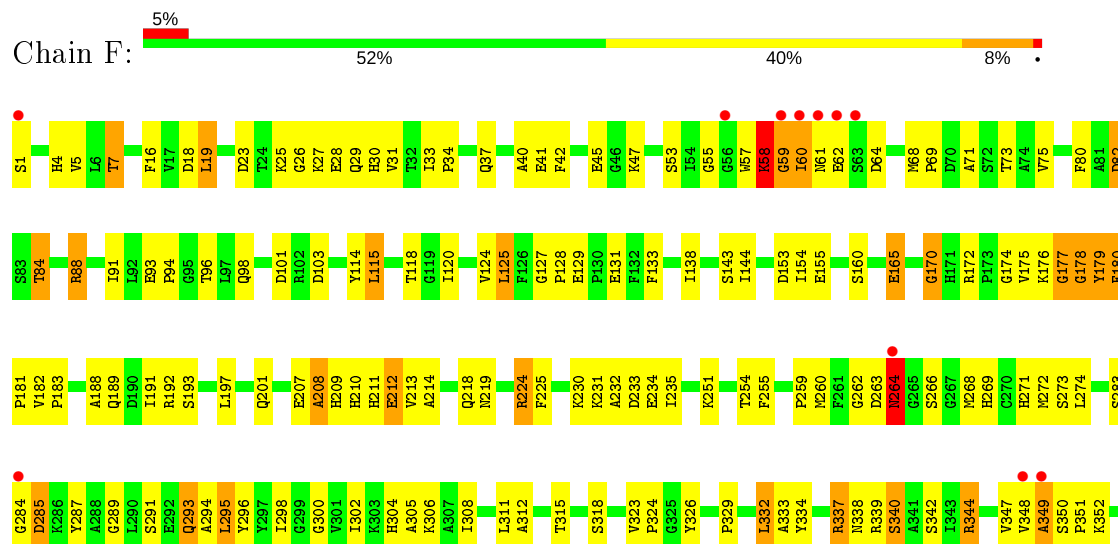


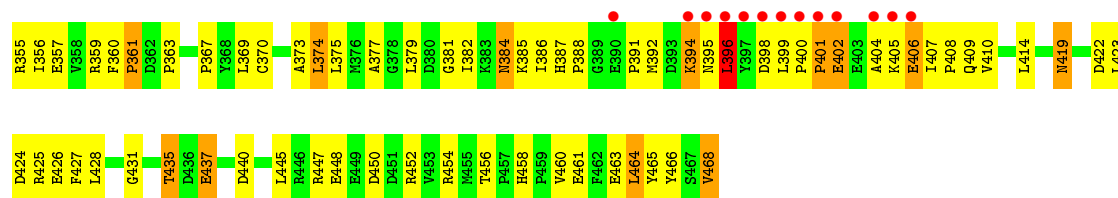


• Molecule 1: GLUTAMINE SYNTHETASE

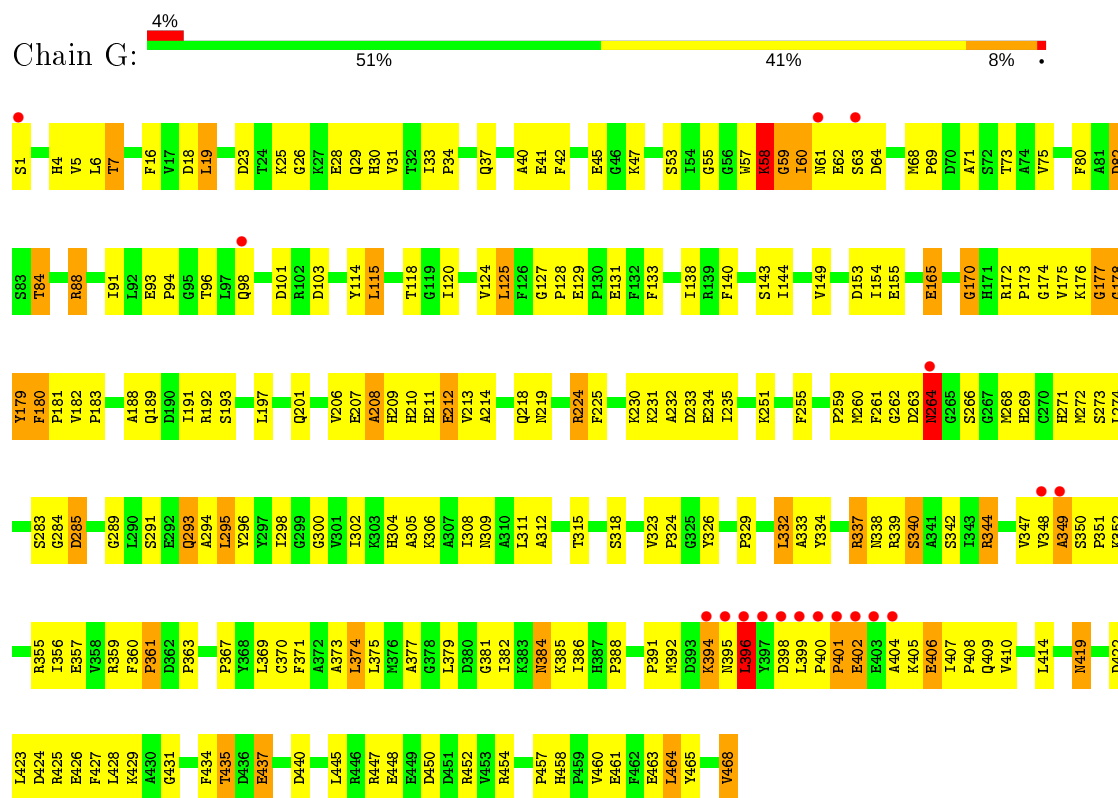


• Molecule 1: GLUTAMINE SYNTHETASE

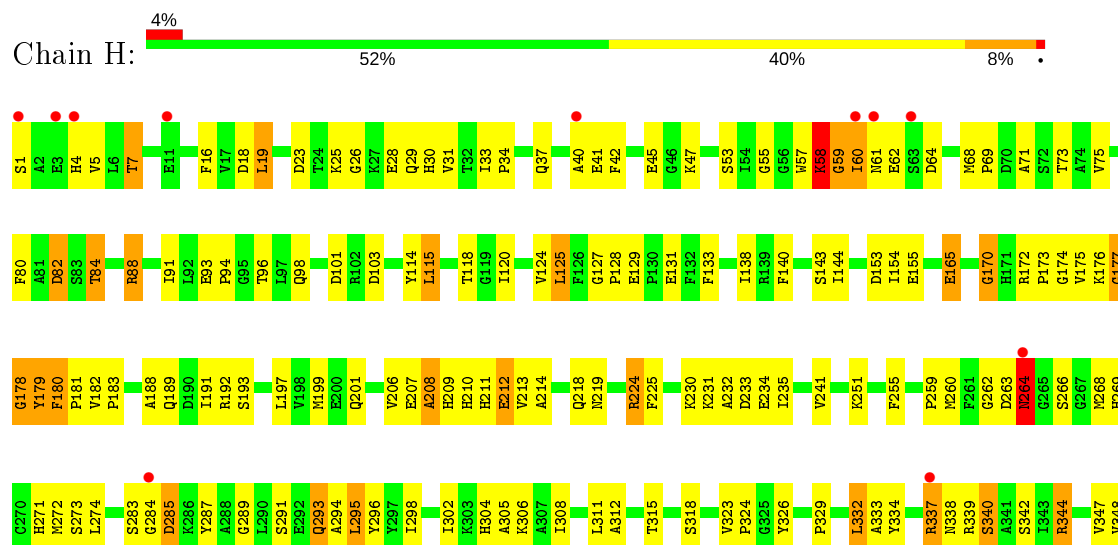


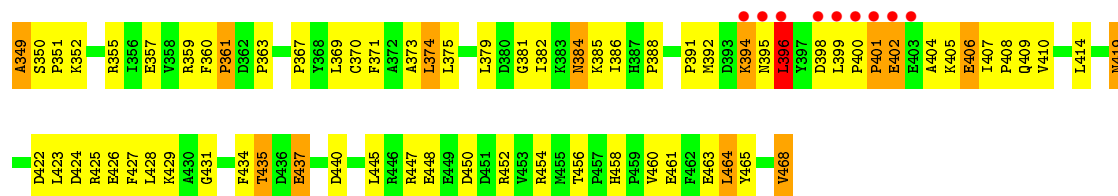


• Molecule 1: GLUTAMINE SYNTHETASE

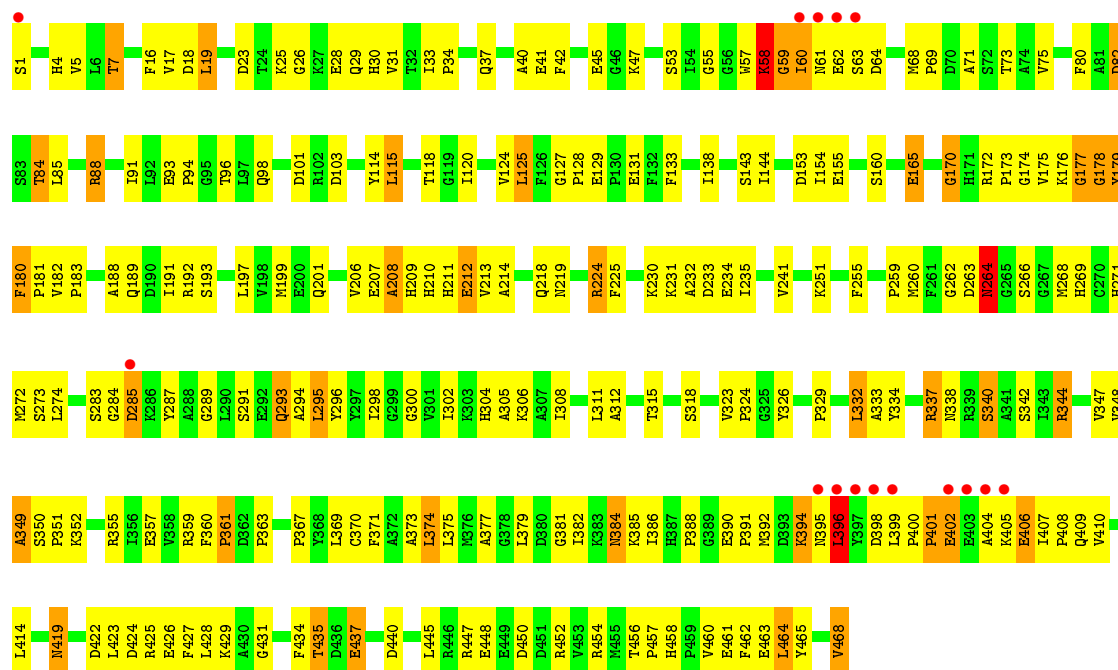


• Molecule 1: GLUTAMINE SYNTHETASE

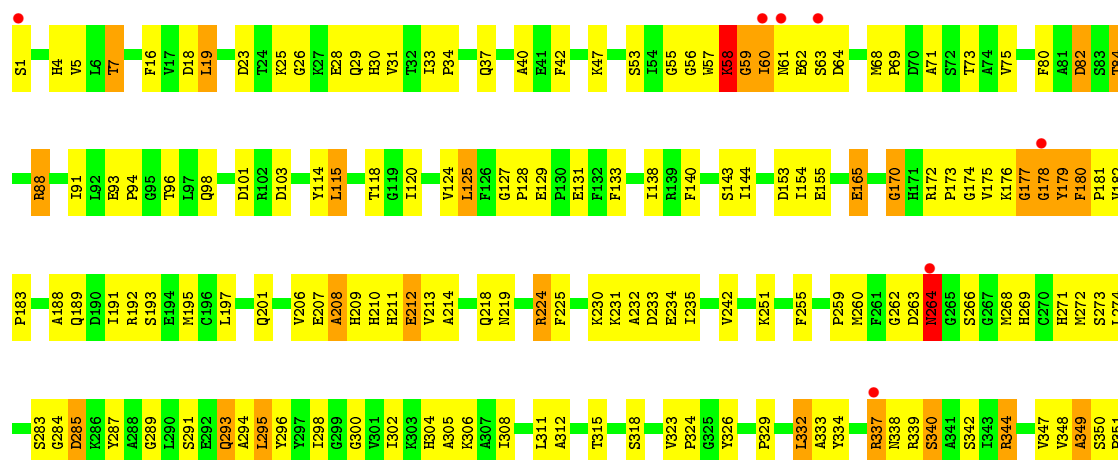


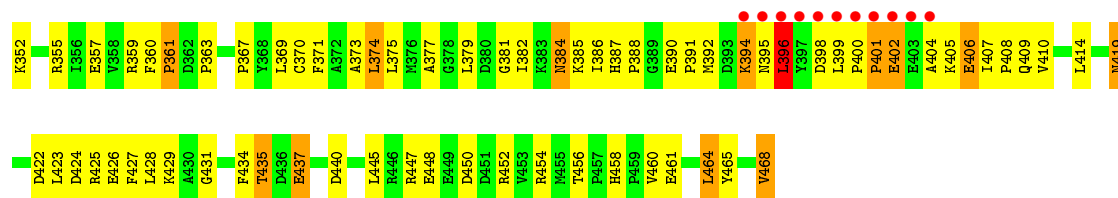


• Molecule 1: GLUTAMINE SYNTHETASE

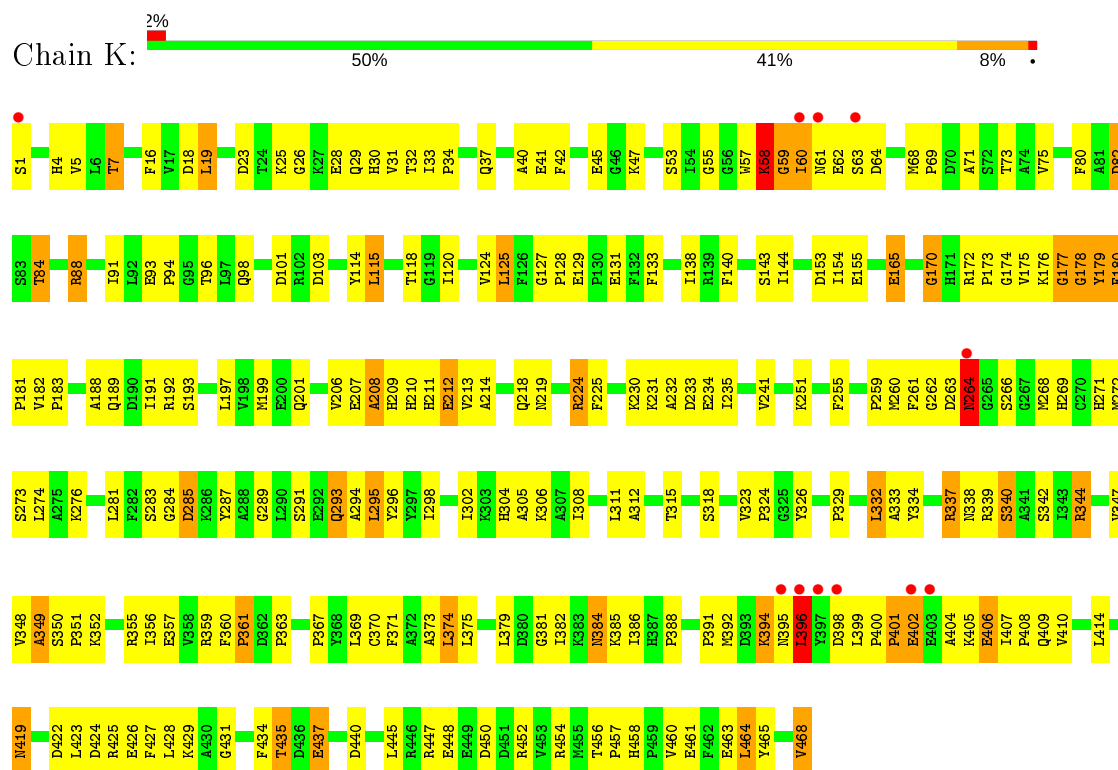


• Molecule 1: GLUTAMINE SYNTHETASE

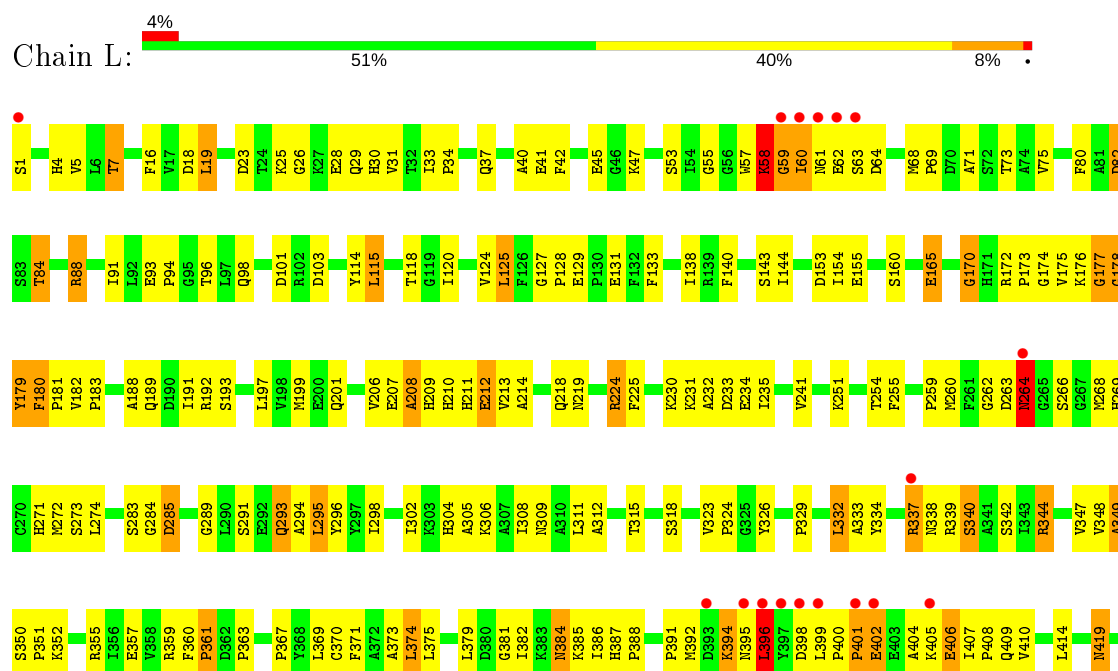




• Molecule 1: GLUTAMINE SYNTHETASE



• Molecule 1: GLUTAMINE SYNTHETASE



D422	L423	D424	R425	E426	F427	L428	K429	A430	G431	F434	T435	D436	E437	D440	L445	R446	R447	E448	E449	D450	T451	R452	V453	R454	M455	T456	P457	H458	P459	V460	E461	L464	Y465	Y466	S467	V468
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	230.60 Å 132.50 Å 195.90 Å 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 2.91 Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.248 , 0.263 0.245 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
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 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	47280	wwPDB-VP
Average B, all atoms (Å 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.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PPQ, MN, ADP

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

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

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

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

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

There are no bond length outliers.

All (24) bond angle outliers are listed below:

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

There are no chirality outliers.

All (12) planarity outliers are listed below:

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

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

5.2 Too-close contacts [i](#)

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (3738) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:4482:ADP:C1'	3:L:4482:ADP:N9	1.70	1.54
3:C:4473:ADP:N9	3:C:4473:ADP:C1'	1.70	1.53
3:I:4479:ADP:N9	3:I:4479:ADP:C1'	1.70	1.53
3:H:4478:ADP:N9	3:H:4478:ADP:C1'	1.70	1.52
3:B:4472:ADP:C1'	3:B:4472:ADP:N9	1.70	1.52
3:J:4480:ADP:C1'	3:J:4480:ADP:N9	1.70	1.51
3:K:4481:ADP:N9	3:K:4481:ADP:C1'	1.70	1.51
3:A:4471:ADP:C1'	3:A:4471:ADP:N9	1.70	1.50
3:F:4476:ADP:N9	3:F:4476:ADP:C1'	1.70	1.50
3:G:4477:ADP:C1'	3:G:4477:ADP:N9	1.70	1.49
3:D:4474:ADP:C1'	3:D:4474:ADP:N9	1.70	1.49
3:E:4475:ADP:C1'	3:E:4475:ADP:N9	1.70	1.49
1:C:211[B]:HIS:CE1	5:C:6044:HOH:O	1.82	1.27
1:F:211[B]:HIS:CE1	5:F:5906:HOH:O	1.82	1.27
1:K:211[B]:HIS:CE1	5:K:1381:HOH:O	1.85	1.26
1:D:211[B]:HIS:O	1:D:212[B]:GLU:HG2	1.07	1.25
1:J:337:ARG:HG3	1:J:338:ASN:N	1.31	1.25
1:L:211[B]:HIS:CE1	5:L:1534:HOH:O	1.85	1.25
1:H:211[B]:HIS:CE1	5:H:5912:HOH:O	1.91	1.24
1:K:211[B]:HIS:O	1:K:212[B]:GLU:HG2	1.07	1.24
1:D:337:ARG:HG3	1:D:338:ASN:N	1.31	1.24
1:G:211[B]:HIS:O	1:G:212[B]:GLU:HG2	1.07	1.23
1:L:337:ARG:HG3	1:L:338:ASN:N	1.31	1.23
1:A:211[B]:HIS:O	1:A:212[B]:GLU:HG2	1.07	1.23
1:I:211[B]:HIS:O	1:I:212[B]:GLU:HG2	1.07	1.23
1:F:211[B]:HIS:O	1:F:212[B]:GLU:HG2	1.07	1.23
1:E:211[B]:HIS:CE1	5:E:769:HOH:O	1.87	1.22
1:C:211[B]:HIS:O	1:C:212[B]:GLU:HG2	1.07	1.22
1:G:211[B]:HIS:CE1	5:G:6054:HOH:O	1.86	1.22
1:L:211[B]:HIS:O	1:L:212[B]:GLU:HG2	1.07	1.22
1:B:211[B]:HIS:CE1	5:B:6045:HOH:O	1.92	1.22
1:H:211[B]:HIS:O	1:H:212[B]:GLU:HG2	1.07	1.21
1:E:211[B]:HIS:O	1:E:212[B]:GLU:HG2	1.07	1.21
1:A:337:ARG:HG3	1:A:338:ASN:N	1.31	1.20
1:D:211[B]:HIS:CE1	5:D:6046:HOH:O	1.90	1.20
1:B:211[B]:HIS:O	1:B:212[B]:GLU:HG2	1.07	1.20
1:J:211[B]:HIS:O	1:J:212[B]:GLU:HG2	1.07	1.20
1:G:337:ARG:HG3	1:G:338:ASN:N	1.31	1.19
1:B:337:ARG:HG3	1:B:338:ASN:N	1.32	1.19
1:K:337:ARG:HG3	1:K:338:ASN:N	1.32	1.19
1:F:337:ARG:HG3	1:F:338:ASN:N	1.31	1.19
1:I:211[B]:HIS:CE1	5:I:5913:HOH:O	1.93	1.19

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1:SER:OG	1:I:5:VAL:HG23	2.22	0.40
1:I:17:VAL:HA	1:I:85:LEU:O	2.22	0.40
1:J:300:GLY:HA3	1:J:377:ALA:O	2.21	0.40
1:K:179[B]:TYR:HB3	1:K:180[B]:PHE:CD2	2.56	0.40
1:K:271:HIS:HA	1:K:356:ILE:O	2.22	0.40
1:K:423:LEU:O	1:K:425:ARG:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2	10
1	B	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2	10
1	C	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2	10
1	D	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2	10
1	E	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2	10
1	F	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2	10
1	G	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2	10
1	H	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2	10
1	I	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2	10
1	J	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2	10
1	K	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2	10
1	L	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	2	10
All	All	5784/5616 (103%)	4932 (85%)	600 (10%)	252 (4%)	4	10

All (252) Ramachandran outliers are listed below:

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

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

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

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

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

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	395/384 (103%)	350 (89%)	45 (11%)	5	17
1	B	395/384 (103%)	350 (89%)	45 (11%)	5	17
1	C	395/384 (103%)	350 (89%)	45 (11%)	5	17
1	D	395/384 (103%)	350 (89%)	45 (11%)	5	17
1	E	395/384 (103%)	350 (89%)	45 (11%)	5	17
1	F	395/384 (103%)	350 (89%)	45 (11%)	5	17
1	G	395/384 (103%)	350 (89%)	45 (11%)	5	17
1	H	395/384 (103%)	350 (89%)	45 (11%)	5	17
1	I	395/384 (103%)	350 (89%)	45 (11%)	5	17
1	J	395/384 (103%)	350 (89%)	45 (11%)	5	17
1	K	395/384 (103%)	350 (89%)	45 (11%)	5	17
1	L	395/384 (103%)	350 (89%)	45 (11%)	5	17
All	All	4740/4608 (103%)	4200 (89%)	540 (11%)	6	17

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 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	I	4479	2	24,29,29	2.62	8 (33%)	29,45,45	3.38	12 (41%)
3	ADP	K	4481	2	24,29,29	2.62	8 (33%)	29,45,45	3.39	12 (41%)
4	PPQ	E	5904	2	4,10,10	1.27	0	2,14,14	8.53	2 (100%)
4	PPQ	B	5901	2	4,10,10	1.25	0	2,14,14	8.53	2 (100%)
4	PPQ	H	5907	2	4,10,10	1.28	0	2,14,14	8.54	2 (100%)
4	PPQ	C	5902	2	4,10,10	1.25	0	2,14,14	8.52	2 (100%)
4	PPQ	K	5910	2	4,10,10	1.22	0	2,14,14	8.51	2 (100%)
3	ADP	B	4472	2	24,29,29	2.61	8 (33%)	29,45,45	3.38	12 (41%)
4	PPQ	I	5908	2	4,10,10	1.28	0	2,14,14	8.53	2 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PPQ	F	5905	2	4,10,10	1.25	0	2,14,14	8.52	2 (100%)
3	ADP	J	4480	2	24,29,29	2.62	8 (33%)	29,45,45	3.38	12 (41%)
3	ADP	D	4474	2	24,29,29	2.61	8 (33%)	29,45,45	3.38	12 (41%)
4	PPQ	G	5906	2	4,10,10	1.25	0	2,14,14	8.53	2 (100%)
3	ADP	F	4476	2	24,29,29	2.61	8 (33%)	29,45,45	3.38	12 (41%)
3	ADP	A	4471	2	24,29,29	2.62	8 (33%)	29,45,45	3.38	12 (41%)
3	ADP	L	4482	2	24,29,29	2.63	8 (33%)	29,45,45	3.38	12 (41%)
3	ADP	H	4478	2	24,29,29	2.62	8 (33%)	29,45,45	3.38	12 (41%)
4	PPQ	D	5903	2	4,10,10	1.26	0	2,14,14	8.52	2 (100%)
3	ADP	C	4473	2	24,29,29	2.62	8 (33%)	29,45,45	3.38	12 (41%)
4	PPQ	J	5909	2	4,10,10	1.26	0	2,14,14	8.53	2 (100%)
3	ADP	E	4475	2	24,29,29	2.61	8 (33%)	29,45,45	3.38	12 (41%)
4	PPQ	A	5900	2	4,10,10	1.26	0	2,14,14	8.52	2 (100%)
3	ADP	G	4477	2	24,29,29	2.62	8 (33%)	29,45,45	3.38	12 (41%)
4	PPQ	L	5911	2	4,10,10	1.25	0	2,14,14	8.53	2 (100%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	I	4479	2	-	5/12/32/32	0/3/3/3
3	ADP	K	4481	2	-	5/12/32/32	0/3/3/3
4	PPQ	E	5904	2	-	3/6/10/10	-
4	PPQ	B	5901	2	-	3/6/10/10	-
4	PPQ	H	5907	2	-	3/6/10/10	-
4	PPQ	C	5902	2	-	3/6/10/10	-
4	PPQ	K	5910	2	-	3/6/10/10	-
3	ADP	B	4472	2	-	5/12/32/32	0/3/3/3
4	PPQ	I	5908	2	-	3/6/10/10	-
4	PPQ	F	5905	2	-	3/6/10/10	-
3	ADP	J	4480	2	-	5/12/32/32	0/3/3/3
3	ADP	D	4474	2	-	5/12/32/32	0/3/3/3
4	PPQ	G	5906	2	-	3/6/10/10	-
3	ADP	F	4476	2	-	5/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	4471	2	-	5/12/32/32	0/3/3/3
3	ADP	L	4482	2	-	5/12/32/32	0/3/3/3
3	ADP	H	4478	2	-	5/12/32/32	0/3/3/3
4	PPQ	D	5903	2	-	3/6/10/10	-
3	ADP	C	4473	2	-	5/12/32/32	0/3/3/3
4	PPQ	J	5909	2	-	3/6/10/10	-
3	ADP	E	4475	2	-	5/12/32/32	0/3/3/3
4	PPQ	A	5900	2	-	3/6/10/10	-
3	ADP	G	4477	2	-	5/12/32/32	0/3/3/3
4	PPQ	L	5911	2	-	3/6/10/10	-

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	4482	ADP	O4'-C1'	7.46	1.51	1.41
3	K	4481	ADP	O4'-C1'	7.46	1.51	1.41
3	J	4480	ADP	O4'-C1'	7.45	1.51	1.41
3	I	4479	ADP	O4'-C1'	7.44	1.51	1.41
3	G	4477	ADP	O4'-C1'	7.44	1.51	1.41
3	E	4475	ADP	O4'-C1'	7.43	1.51	1.41
3	D	4474	ADP	O4'-C1'	7.42	1.51	1.41
3	A	4471	ADP	O4'-C1'	7.42	1.51	1.41
3	C	4473	ADP	O4'-C1'	7.41	1.51	1.41
3	H	4478	ADP	O4'-C1'	7.40	1.51	1.41
3	F	4476	ADP	O4'-C1'	7.39	1.51	1.41
3	B	4472	ADP	O4'-C1'	7.38	1.51	1.41
3	C	4473	ADP	C4-N3	4.98	1.42	1.35
3	J	4480	ADP	C4-N3	4.97	1.42	1.35
3	G	4477	ADP	C4-N3	4.93	1.42	1.35
3	H	4478	ADP	C4-N3	4.92	1.42	1.35
3	F	4476	ADP	C4-N3	4.92	1.42	1.35
3	L	4482	ADP	C4-N3	4.91	1.42	1.35
3	I	4479	ADP	C4-N3	4.91	1.42	1.35
3	A	4471	ADP	C4-N3	4.91	1.42	1.35
3	E	4475	ADP	C4-N3	4.90	1.42	1.35
3	D	4474	ADP	C4-N3	4.90	1.42	1.35
3	B	4472	ADP	C4-N3	4.87	1.42	1.35
3	K	4481	ADP	C4-N3	4.86	1.42	1.35
3	L	4482	ADP	C2-N3	4.28	1.39	1.32
3	B	4472	ADP	C2-N3	4.28	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	4478	ADP	C2-N3	4.27	1.39	1.32
3	K	4481	ADP	C2-N3	4.27	1.39	1.32
3	A	4471	ADP	C2-N3	4.25	1.39	1.32
3	I	4479	ADP	C2-N3	4.25	1.39	1.32
3	D	4474	ADP	C2-N3	4.25	1.38	1.32
3	E	4475	ADP	C2-N3	4.24	1.38	1.32
3	F	4476	ADP	C2-N3	4.23	1.38	1.32
3	C	4473	ADP	C2-N3	4.23	1.38	1.32
3	J	4480	ADP	C2-N3	4.23	1.38	1.32
3	G	4477	ADP	C2-N3	4.22	1.38	1.32
3	I	4479	ADP	O4'-C4'	4.16	1.54	1.45
3	L	4482	ADP	O4'-C4'	4.16	1.54	1.45
3	E	4475	ADP	O4'-C4'	4.15	1.54	1.45
3	B	4472	ADP	O4'-C4'	4.14	1.54	1.45
3	K	4481	ADP	O4'-C4'	4.14	1.54	1.45
3	A	4471	ADP	O4'-C4'	4.13	1.54	1.45
3	H	4478	ADP	O4'-C4'	4.13	1.54	1.45
3	F	4476	ADP	O4'-C4'	4.13	1.54	1.45
3	G	4477	ADP	O4'-C4'	4.12	1.54	1.45
3	D	4474	ADP	O4'-C4'	4.12	1.54	1.45
3	C	4473	ADP	O4'-C4'	4.10	1.54	1.45
3	J	4480	ADP	O4'-C4'	4.09	1.54	1.45
3	H	4478	ADP	PB-O3B	3.85	1.69	1.54
3	I	4479	ADP	PB-O3B	3.85	1.69	1.54
3	J	4480	ADP	PB-O3B	3.85	1.69	1.54
3	C	4473	ADP	PB-O3B	3.85	1.69	1.54
3	L	4482	ADP	PB-O3B	3.85	1.69	1.54
3	B	4472	ADP	PB-O3B	3.84	1.69	1.54
3	K	4481	ADP	PB-O3B	3.84	1.69	1.54
3	A	4471	ADP	PB-O3B	3.84	1.69	1.54
3	D	4474	ADP	PB-O3B	3.83	1.69	1.54
3	G	4477	ADP	PB-O3B	3.83	1.69	1.54
3	E	4475	ADP	PB-O3B	3.83	1.69	1.54
3	F	4476	ADP	PB-O3B	3.82	1.69	1.54
3	I	4479	ADP	C6-N6	-3.15	1.22	1.34
3	E	4475	ADP	C6-N6	-3.14	1.22	1.34
3	D	4474	ADP	C6-N6	-3.14	1.22	1.34
3	J	4480	ADP	C6-N6	-3.14	1.22	1.34
3	B	4472	ADP	C6-N6	-3.13	1.22	1.34
3	L	4482	ADP	C6-N6	-3.13	1.22	1.34
3	A	4471	ADP	C6-N6	-3.13	1.22	1.34
3	H	4478	ADP	C6-N6	-3.13	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4476	ADP	C6-N6	-3.13	1.22	1.34
3	G	4477	ADP	C6-N6	-3.13	1.22	1.34
3	K	4481	ADP	C6-N6	-3.12	1.22	1.34
3	C	4473	ADP	C6-N6	-3.12	1.22	1.34
3	H	4478	ADP	C3'-C4'	-2.32	1.47	1.53
3	L	4482	ADP	C3'-C4'	-2.31	1.47	1.53
3	J	4480	ADP	C3'-C4'	-2.31	1.47	1.53
3	B	4472	ADP	C3'-C4'	-2.30	1.47	1.53
3	A	4471	ADP	C3'-C4'	-2.30	1.47	1.53
3	G	4477	ADP	C3'-C4'	-2.30	1.47	1.53
3	I	4479	ADP	C3'-C4'	-2.29	1.47	1.53
3	D	4474	ADP	C3'-C4'	-2.29	1.47	1.53
3	F	4476	ADP	C3'-C4'	-2.29	1.47	1.53
3	K	4481	ADP	C3'-C4'	-2.29	1.47	1.53
3	E	4475	ADP	C3'-C4'	-2.28	1.47	1.53
3	C	4473	ADP	C3'-C4'	-2.28	1.47	1.53
3	H	4478	ADP	PB-O1B	2.08	1.57	1.50
3	F	4476	ADP	PB-O1B	2.08	1.57	1.50
3	J	4480	ADP	PB-O1B	2.08	1.57	1.50
3	L	4482	ADP	PB-O1B	2.07	1.57	1.50
3	D	4474	ADP	PB-O1B	2.07	1.57	1.50
3	A	4471	ADP	PB-O1B	2.07	1.57	1.50
3	G	4477	ADP	PB-O1B	2.06	1.57	1.50
3	C	4473	ADP	PB-O1B	2.06	1.57	1.50
3	K	4481	ADP	PB-O1B	2.06	1.57	1.50
3	E	4475	ADP	PB-O1B	2.06	1.57	1.50
3	I	4479	ADP	PB-O1B	2.06	1.57	1.50
3	B	4472	ADP	PB-O1B	2.04	1.57	1.50

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	4480	ADP	O4'-C1'-C2'	-10.81	91.13	106.93
3	L	4482	ADP	O4'-C1'-C2'	-10.81	91.13	106.93
3	C	4473	ADP	O4'-C1'-C2'	-10.80	91.14	106.93
3	B	4472	ADP	O4'-C1'-C2'	-10.80	91.15	106.93
3	A	4471	ADP	O4'-C1'-C2'	-10.80	91.15	106.93
3	K	4481	ADP	O4'-C1'-C2'	-10.80	91.15	106.93
3	D	4474	ADP	O4'-C1'-C2'	-10.80	91.15	106.93
3	G	4477	ADP	O4'-C1'-C2'	-10.79	91.15	106.93
3	E	4475	ADP	O4'-C1'-C2'	-10.79	91.16	106.93
3	H	4478	ADP	O4'-C1'-C2'	-10.78	91.17	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	4479	ADP	O4'-C1'-C2'	-10.78	91.17	106.93
3	F	4476	ADP	O4'-C1'-C2'	-10.77	91.19	106.93
4	H	5907	PPQ	PDP-CGP-CBP	9.93	132.71	114.53
4	G	5906	PPQ	PDP-CGP-CBP	9.93	132.71	114.53
4	I	5908	PPQ	PDP-CGP-CBP	9.92	132.70	114.53
4	F	5905	PPQ	PDP-CGP-CBP	9.92	132.70	114.53
4	E	5904	PPQ	PDP-CGP-CBP	9.91	132.68	114.53
4	L	5911	PPQ	PDP-CGP-CBP	9.91	132.67	114.53
4	A	5900	PPQ	PDP-CGP-CBP	9.90	132.67	114.53
4	B	5901	PPQ	PDP-CGP-CBP	9.90	132.66	114.53
4	D	5903	PPQ	PDP-CGP-CBP	9.90	132.66	114.53
4	C	5902	PPQ	PDP-CGP-CBP	9.89	132.65	114.53
4	K	5910	PPQ	PDP-CGP-CBP	9.89	132.63	114.53
4	J	5909	PPQ	PDP-CGP-CBP	9.88	132.63	114.53
3	I	4479	ADP	O5'-C5'-C4'	8.34	137.70	108.99
3	K	4481	ADP	O5'-C5'-C4'	8.34	137.70	108.99
3	L	4482	ADP	O5'-C5'-C4'	8.34	137.70	108.99
3	D	4474	ADP	O5'-C5'-C4'	8.34	137.69	108.99
3	A	4471	ADP	O5'-C5'-C4'	8.33	137.68	108.99
3	E	4475	ADP	O5'-C5'-C4'	8.33	137.68	108.99
3	F	4476	ADP	O5'-C5'-C4'	8.33	137.67	108.99
3	G	4477	ADP	O5'-C5'-C4'	8.33	137.67	108.99
3	H	4478	ADP	O5'-C5'-C4'	8.33	137.66	108.99
3	C	4473	ADP	O5'-C5'-C4'	8.33	137.65	108.99
3	J	4480	ADP	O5'-C5'-C4'	8.33	137.65	108.99
3	B	4472	ADP	O5'-C5'-C4'	8.32	137.63	108.99
4	J	5909	PPQ	CEP-PDP-CGP	6.91	119.81	107.62
4	B	5901	PPQ	CEP-PDP-CGP	6.89	119.78	107.62
4	L	5911	PPQ	CEP-PDP-CGP	6.88	119.76	107.62
4	D	5903	PPQ	CEP-PDP-CGP	6.88	119.75	107.62
4	C	5902	PPQ	CEP-PDP-CGP	6.87	119.75	107.62
4	E	5904	PPQ	CEP-PDP-CGP	6.87	119.75	107.62
4	H	5907	PPQ	CEP-PDP-CGP	6.87	119.75	107.62
4	A	5900	PPQ	CEP-PDP-CGP	6.87	119.75	107.62
4	K	5910	PPQ	CEP-PDP-CGP	6.87	119.74	107.62
4	I	5908	PPQ	CEP-PDP-CGP	6.86	119.73	107.62
4	G	5906	PPQ	CEP-PDP-CGP	6.86	119.73	107.62
4	F	5905	PPQ	CEP-PDP-CGP	6.85	119.70	107.62
3	G	4477	ADP	C1'-N9-C4	5.06	135.53	126.64
3	E	4475	ADP	C1'-N9-C4	5.06	135.53	126.64
3	C	4473	ADP	C1'-N9-C4	5.06	135.53	126.64
3	K	4481	ADP	C1'-N9-C4	5.05	135.52	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4471	ADP	C1'-N9-C4	5.04	135.50	126.64
3	J	4480	ADP	C1'-N9-C4	5.04	135.50	126.64
3	B	4472	ADP	C1'-N9-C4	5.04	135.50	126.64
3	L	4482	ADP	C1'-N9-C4	5.04	135.49	126.64
3	I	4479	ADP	C1'-N9-C4	5.03	135.48	126.64
3	H	4478	ADP	C1'-N9-C4	5.03	135.48	126.64
3	F	4476	ADP	C1'-N9-C4	5.03	135.48	126.64
3	D	4474	ADP	C1'-N9-C4	5.03	135.48	126.64
3	L	4482	ADP	C4-C5-N7	4.81	114.41	109.40
3	K	4481	ADP	C4-C5-N7	4.81	114.41	109.40
3	B	4472	ADP	C4-C5-N7	4.80	114.40	109.40
3	G	4477	ADP	C4-C5-N7	4.79	114.39	109.40
3	A	4471	ADP	C4-C5-N7	4.77	114.37	109.40
3	C	4473	ADP	C4-C5-N7	4.77	114.37	109.40
3	I	4479	ADP	C4-C5-N7	4.76	114.36	109.40
3	J	4480	ADP	C4-C5-N7	4.74	114.34	109.40
3	F	4476	ADP	C4-C5-N7	4.74	114.34	109.40
3	H	4478	ADP	C4-C5-N7	4.74	114.33	109.40
3	D	4474	ADP	C4-C5-N7	4.72	114.32	109.40
3	E	4475	ADP	C4-C5-N7	4.72	114.32	109.40
3	C	4473	ADP	C5'-C4'-C3'	-3.95	100.39	115.18
3	F	4476	ADP	C5'-C4'-C3'	-3.94	100.41	115.18
3	I	4479	ADP	C5'-C4'-C3'	-3.94	100.42	115.18
3	J	4480	ADP	C5'-C4'-C3'	-3.94	100.42	115.18
3	B	4472	ADP	C5'-C4'-C3'	-3.94	100.42	115.18
3	H	4478	ADP	C5'-C4'-C3'	-3.94	100.42	115.18
3	A	4471	ADP	C5'-C4'-C3'	-3.94	100.43	115.18
3	G	4477	ADP	C5'-C4'-C3'	-3.94	100.43	115.18
3	D	4474	ADP	C5'-C4'-C3'	-3.93	100.45	115.18
3	E	4475	ADP	C5'-C4'-C3'	-3.93	100.45	115.18
3	K	4481	ADP	C5'-C4'-C3'	-3.93	100.46	115.18
3	L	4482	ADP	C5'-C4'-C3'	-3.92	100.47	115.18
3	H	4478	ADP	C3'-C2'-C1'	-3.67	95.45	100.98
3	E	4475	ADP	C3'-C2'-C1'	-3.67	95.45	100.98
3	K	4481	ADP	C3'-C2'-C1'	-3.66	95.47	100.98
3	F	4476	ADP	C3'-C2'-C1'	-3.65	95.48	100.98
3	D	4474	ADP	C3'-C2'-C1'	-3.65	95.49	100.98
3	A	4471	ADP	C3'-C2'-C1'	-3.65	95.49	100.98
3	B	4472	ADP	C3'-C2'-C1'	-3.65	95.49	100.98
3	G	4477	ADP	C3'-C2'-C1'	-3.64	95.49	100.98
3	J	4480	ADP	O4'-C4'-C5'	3.64	121.36	109.37
3	B	4472	ADP	O4'-C4'-C5'	3.64	121.35	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	4477	ADP	O4'-C4'-C5'	3.64	121.35	109.37
3	E	4475	ADP	O4'-C4'-C5'	3.64	121.35	109.37
3	J	4480	ADP	C3'-C2'-C1'	-3.64	95.50	100.98
3	F	4476	ADP	O4'-C4'-C5'	3.64	121.34	109.37
3	K	4481	ADP	O4'-C4'-C5'	3.64	121.33	109.37
3	H	4478	ADP	O4'-C4'-C5'	3.64	121.33	109.37
3	D	4474	ADP	O4'-C4'-C5'	3.63	121.33	109.37
3	A	4471	ADP	O4'-C4'-C5'	3.63	121.33	109.37
3	C	4473	ADP	C3'-C2'-C1'	-3.63	95.51	100.98
3	I	4479	ADP	C3'-C2'-C1'	-3.63	95.51	100.98
3	C	4473	ADP	O4'-C4'-C5'	3.63	121.31	109.37
3	L	4482	ADP	O4'-C4'-C5'	3.63	121.31	109.37
3	L	4482	ADP	C3'-C2'-C1'	-3.63	95.52	100.98
3	I	4479	ADP	O4'-C4'-C5'	3.61	121.26	109.37
3	B	4472	ADP	PA-O5'-C5'	3.14	140.12	121.68
3	I	4479	ADP	PA-O5'-C5'	3.14	140.11	121.68
3	K	4481	ADP	PA-O5'-C5'	3.14	140.11	121.68
3	L	4482	ADP	PA-O5'-C5'	3.14	140.10	121.68
3	C	4473	ADP	PA-O5'-C5'	3.14	140.10	121.68
3	D	4474	ADP	PA-O5'-C5'	3.14	140.09	121.68
3	A	4471	ADP	PA-O5'-C5'	3.14	140.08	121.68
3	J	4480	ADP	PA-O5'-C5'	3.14	140.07	121.68
3	G	4477	ADP	PA-O5'-C5'	3.14	140.07	121.68
3	H	4478	ADP	PA-O5'-C5'	3.13	140.06	121.68
3	F	4476	ADP	PA-O5'-C5'	3.13	140.06	121.68
3	E	4475	ADP	PA-O5'-C5'	3.13	140.05	121.68
3	K	4481	ADP	O2B-PB-O3A	3.01	114.71	104.64
3	J	4480	ADP	O2B-PB-O3A	3.00	114.70	104.64
3	C	4473	ADP	O2B-PB-O3A	3.00	114.68	104.64
3	I	4479	ADP	O2B-PB-O3A	2.99	114.68	104.64
3	H	4478	ADP	O2B-PB-O3A	2.99	114.68	104.64
3	F	4476	ADP	O2B-PB-O3A	2.99	114.67	104.64
3	L	4482	ADP	O2B-PB-O3A	2.99	114.66	104.64
3	E	4475	ADP	O2B-PB-O3A	2.99	114.66	104.64
3	A	4471	ADP	O2B-PB-O3A	2.99	114.66	104.64
3	B	4472	ADP	O2B-PB-O3A	2.99	114.65	104.64
3	D	4474	ADP	O2B-PB-O3A	2.98	114.63	104.64
3	G	4477	ADP	O2B-PB-O3A	2.97	114.61	104.64
3	F	4476	ADP	O2'-C2'-C1'	2.58	120.36	110.85
3	I	4479	ADP	O2'-C2'-C1'	2.57	120.33	110.85
3	D	4474	ADP	O2'-C2'-C1'	2.57	120.33	110.85
3	A	4471	ADP	O2'-C2'-C1'	2.56	120.33	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4473	ADP	O2'-C2'-C1'	2.56	120.32	110.85
3	G	4477	ADP	O2'-C2'-C1'	2.56	120.31	110.85
3	H	4478	ADP	O2'-C2'-C1'	2.56	120.31	110.85
3	B	4472	ADP	O2'-C2'-C1'	2.56	120.31	110.85
3	K	4481	ADP	O2'-C2'-C1'	2.56	120.30	110.85
3	E	4475	ADP	O2'-C2'-C1'	2.55	120.29	110.85
3	J	4480	ADP	O2'-C2'-C1'	2.55	120.28	110.85
3	L	4482	ADP	O2'-C2'-C1'	2.55	120.27	110.85
3	J	4480	ADP	O3'-C3'-C2'	2.52	119.97	111.82
3	E	4475	ADP	O3'-C3'-C2'	2.52	119.97	111.82
3	B	4472	ADP	O3'-C3'-C2'	2.52	119.97	111.82
3	H	4478	ADP	O3'-C3'-C2'	2.52	119.97	111.82
3	D	4474	ADP	O3'-C3'-C2'	2.51	119.94	111.82
3	K	4481	ADP	O3'-C3'-C2'	2.51	119.94	111.82
3	L	4482	ADP	O3'-C3'-C2'	2.51	119.94	111.82
3	G	4477	ADP	O3'-C3'-C2'	2.51	119.94	111.82
3	C	4473	ADP	O3'-C3'-C2'	2.51	119.94	111.82
3	A	4471	ADP	O3'-C3'-C2'	2.51	119.94	111.82
3	F	4476	ADP	O3'-C3'-C2'	2.51	119.93	111.82
3	I	4479	ADP	O3'-C3'-C2'	2.50	119.91	111.82
3	H	4478	ADP	O5'-PA-O1A	-2.10	100.86	109.07
3	G	4477	ADP	O5'-PA-O1A	-2.10	100.86	109.07
3	K	4481	ADP	O5'-PA-O1A	-2.10	100.88	109.07
3	E	4475	ADP	O5'-PA-O1A	-2.09	100.88	109.07
3	F	4476	ADP	O5'-PA-O1A	-2.09	100.89	109.07
3	A	4471	ADP	O5'-PA-O1A	-2.09	100.89	109.07
3	L	4482	ADP	O5'-PA-O1A	-2.09	100.89	109.07
3	J	4480	ADP	O5'-PA-O1A	-2.09	100.90	109.07
3	D	4474	ADP	O5'-PA-O1A	-2.09	100.91	109.07
3	C	4473	ADP	O5'-PA-O1A	-2.09	100.92	109.07
3	B	4472	ADP	O5'-PA-O1A	-2.08	100.92	109.07
3	I	4479	ADP	O5'-PA-O1A	-2.08	100.93	109.07

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	4479	ADP	C5'-O5'-PA-O1A
3	I	4479	ADP	C5'-O5'-PA-O2A
3	K	4481	ADP	C5'-O5'-PA-O1A
3	K	4481	ADP	C5'-O5'-PA-O2A
4	A	5900	PPQ	CBP-CGP-PDP-CEP

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Mol	Chain	Res	Type	Atoms
4	A	5900	PPQ	CBP-CGP-PDP-OEA
4	A	5900	PPQ	CBP-CGP-PDP-OEB
4	E	5904	PPQ	CBP-CGP-PDP-CEP
4	E	5904	PPQ	CBP-CGP-PDP-OEA
4	E	5904	PPQ	CBP-CGP-PDP-OEB
4	B	5901	PPQ	CBP-CGP-PDP-CEP
4	B	5901	PPQ	CBP-CGP-PDP-OEA
4	B	5901	PPQ	CBP-CGP-PDP-OEB
3	L	4482	ADP	C5'-O5'-PA-O1A
3	L	4482	ADP	C5'-O5'-PA-O2A
4	H	5907	PPQ	CBP-CGP-PDP-CEP
4	H	5907	PPQ	CBP-CGP-PDP-OEA
4	H	5907	PPQ	CBP-CGP-PDP-OEB
4	C	5902	PPQ	CBP-CGP-PDP-CEP
4	C	5902	PPQ	CBP-CGP-PDP-OEA
4	C	5902	PPQ	CBP-CGP-PDP-OEB
4	K	5910	PPQ	CBP-CGP-PDP-CEP
4	K	5910	PPQ	CBP-CGP-PDP-OEA
4	K	5910	PPQ	CBP-CGP-PDP-OEB
3	B	4472	ADP	C5'-O5'-PA-O1A
3	B	4472	ADP	C5'-O5'-PA-O2A
4	I	5908	PPQ	CBP-CGP-PDP-CEP
4	I	5908	PPQ	CBP-CGP-PDP-OEA
4	I	5908	PPQ	CBP-CGP-PDP-OEB
4	F	5905	PPQ	CBP-CGP-PDP-CEP
4	F	5905	PPQ	CBP-CGP-PDP-OEA
4	F	5905	PPQ	CBP-CGP-PDP-OEB
3	J	4480	ADP	C5'-O5'-PA-O1A
3	J	4480	ADP	C5'-O5'-PA-O2A
3	D	4474	ADP	C5'-O5'-PA-O1A
3	D	4474	ADP	C5'-O5'-PA-O2A
4	G	5906	PPQ	CBP-CGP-PDP-CEP
4	G	5906	PPQ	CBP-CGP-PDP-OEA
4	G	5906	PPQ	CBP-CGP-PDP-OEB
3	A	4471	ADP	C5'-O5'-PA-O1A
3	A	4471	ADP	C5'-O5'-PA-O2A
3	H	4478	ADP	C5'-O5'-PA-O1A
3	H	4478	ADP	C5'-O5'-PA-O2A
3	F	4476	ADP	C5'-O5'-PA-O1A
3	F	4476	ADP	C5'-O5'-PA-O2A
4	D	5903	PPQ	CBP-CGP-PDP-CEP
4	D	5903	PPQ	CBP-CGP-PDP-OEA

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Mol	Chain	Res	Type	Atoms
4	D	5903	PPQ	CBP-CGP-PDP-OEB
4	J	5909	PPQ	CBP-CGP-PDP-CEP
4	J	5909	PPQ	CBP-CGP-PDP-OEA
4	J	5909	PPQ	CBP-CGP-PDP-OEB
3	E	4475	ADP	C5'-O5'-PA-O1A
3	E	4475	ADP	C5'-O5'-PA-O2A
3	C	4473	ADP	C5'-O5'-PA-O1A
3	C	4473	ADP	C5'-O5'-PA-O2A
3	G	4477	ADP	C5'-O5'-PA-O1A
3	G	4477	ADP	C5'-O5'-PA-O2A
4	L	5911	PPQ	CBP-CGP-PDP-CEP
4	L	5911	PPQ	CBP-CGP-PDP-OEA
4	L	5911	PPQ	CBP-CGP-PDP-OEB
3	I	4479	ADP	C4'-C5'-O5'-PA
3	K	4481	ADP	C4'-C5'-O5'-PA
3	L	4482	ADP	C4'-C5'-O5'-PA
3	B	4472	ADP	C4'-C5'-O5'-PA
3	J	4480	ADP	C4'-C5'-O5'-PA
3	D	4474	ADP	C4'-C5'-O5'-PA
3	A	4471	ADP	C4'-C5'-O5'-PA
3	H	4478	ADP	C4'-C5'-O5'-PA
3	F	4476	ADP	C4'-C5'-O5'-PA
3	E	4475	ADP	C4'-C5'-O5'-PA
3	C	4473	ADP	C4'-C5'-O5'-PA
3	G	4477	ADP	C4'-C5'-O5'-PA
3	I	4479	ADP	PA-O3A-PB-O3B
3	K	4481	ADP	PA-O3A-PB-O3B
3	L	4482	ADP	PA-O3A-PB-O3B
3	B	4472	ADP	PA-O3A-PB-O3B
3	J	4480	ADP	PA-O3A-PB-O3B
3	D	4474	ADP	PA-O3A-PB-O3B
3	A	4471	ADP	PA-O3A-PB-O3B
3	H	4478	ADP	PA-O3A-PB-O3B
3	F	4476	ADP	PA-O3A-PB-O3B
3	E	4475	ADP	PA-O3A-PB-O3B
3	C	4473	ADP	PA-O3A-PB-O3B
3	G	4477	ADP	PA-O3A-PB-O3B
3	I	4479	ADP	C5'-O5'-PA-O3A
3	K	4481	ADP	C5'-O5'-PA-O3A
3	L	4482	ADP	C5'-O5'-PA-O3A
3	B	4472	ADP	C5'-O5'-PA-O3A
3	J	4480	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
3	D	4474	ADP	C5'-O5'-PA-O3A
3	A	4471	ADP	C5'-O5'-PA-O3A
3	H	4478	ADP	C5'-O5'-PA-O3A
3	F	4476	ADP	C5'-O5'-PA-O3A
3	E	4475	ADP	C5'-O5'-PA-O3A
3	C	4473	ADP	C5'-O5'-PA-O3A
3	G	4477	ADP	C5'-O5'-PA-O3A

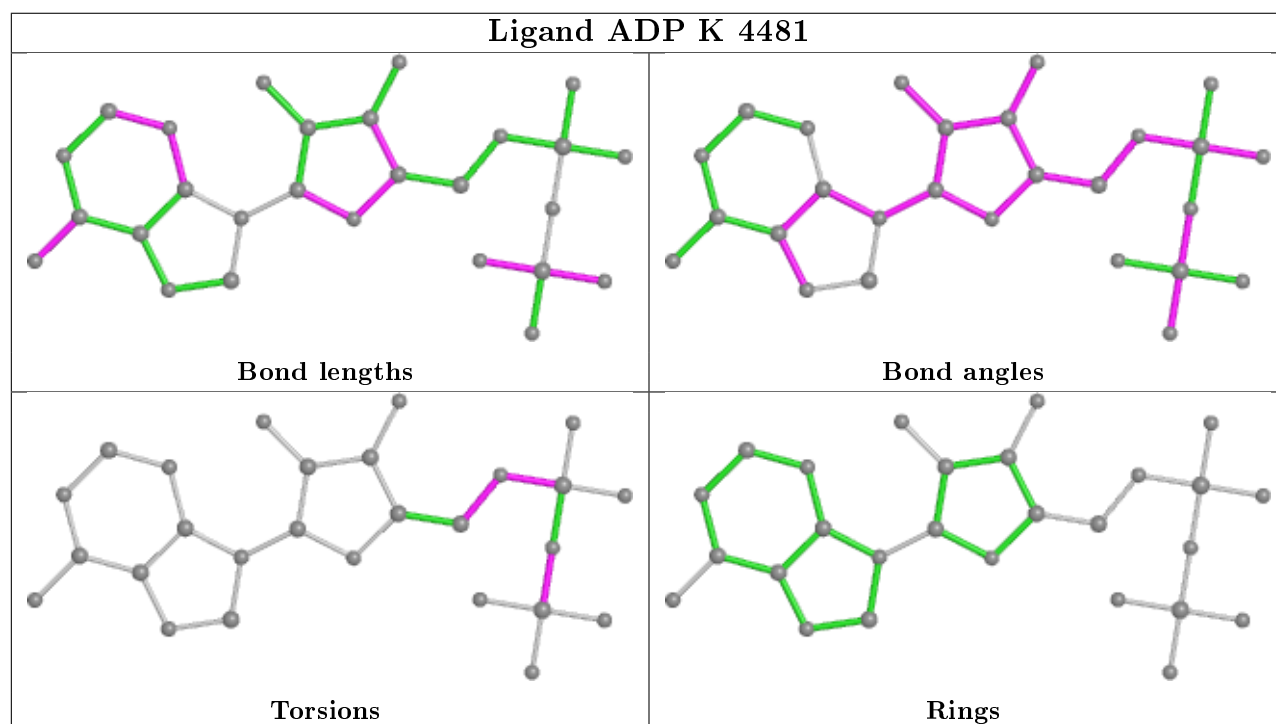
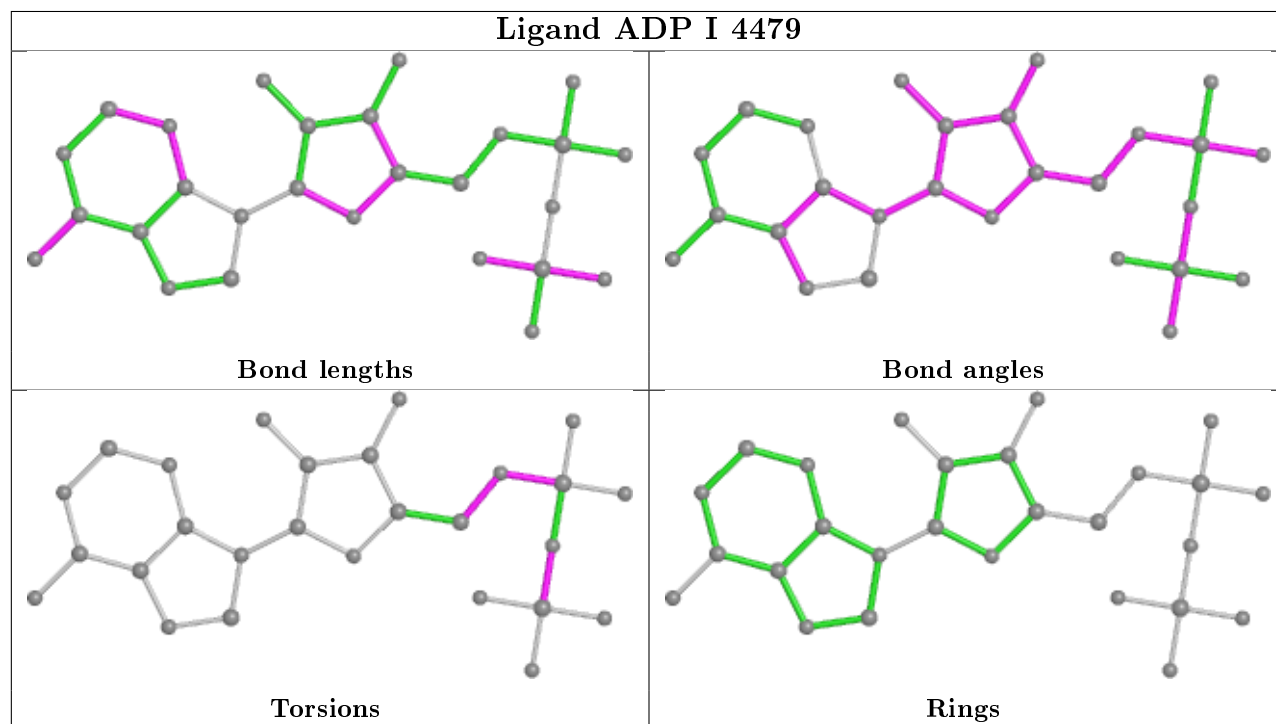
There are no ring outliers.

24 monomers are involved in 172 short contacts:

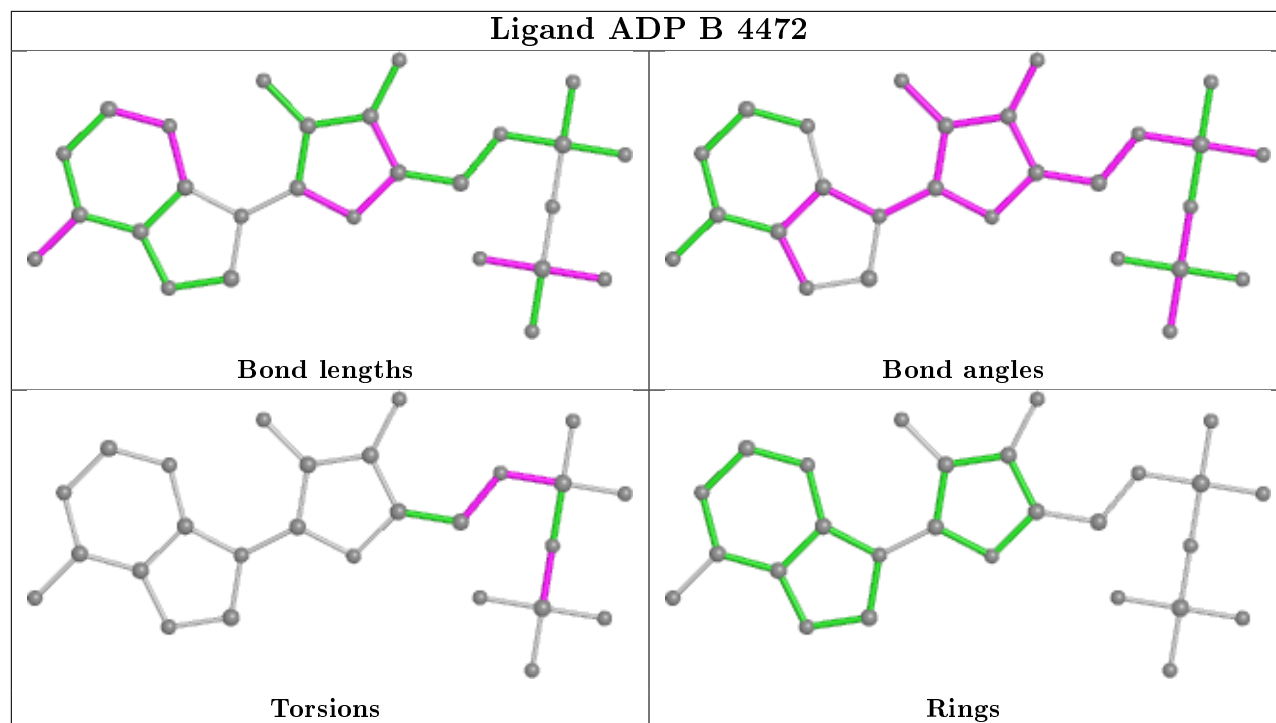
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	4479	ADP	8	0
3	K	4481	ADP	8	0
4	E	5904	PPQ	6	0
4	B	5901	PPQ	7	0
4	H	5907	PPQ	7	0
4	C	5902	PPQ	6	0
4	K	5910	PPQ	5	0
3	B	4472	ADP	8	0
4	I	5908	PPQ	6	0
4	F	5905	PPQ	7	0
3	J	4480	ADP	8	0
3	D	4474	ADP	8	0
4	G	5906	PPQ	6	0
3	F	4476	ADP	8	0
3	A	4471	ADP	8	0
3	L	4482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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

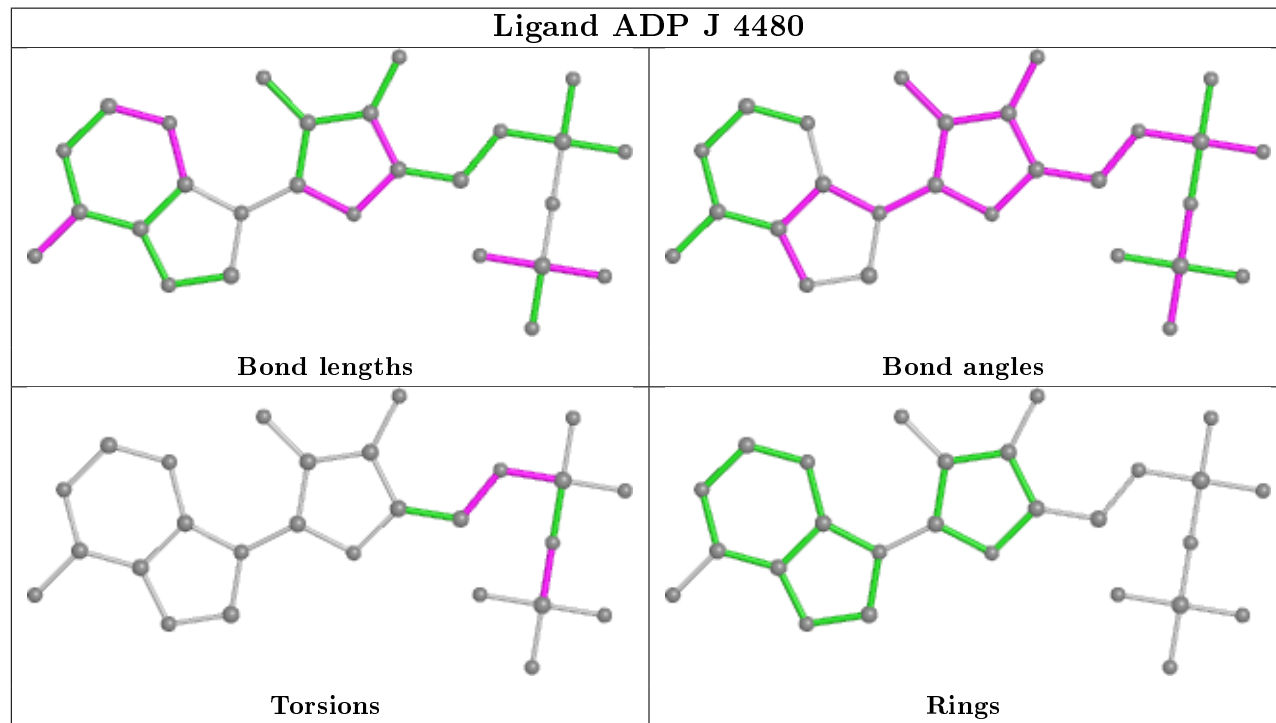
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



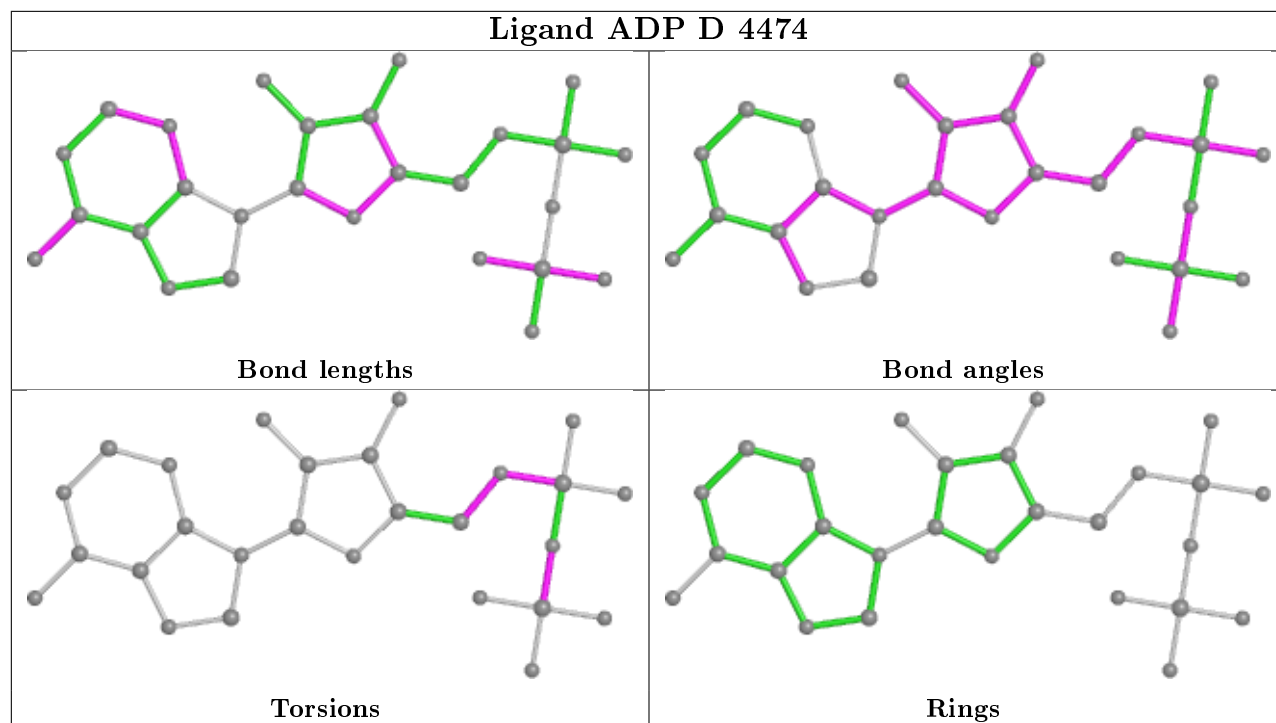
Ligand ADP B 4472



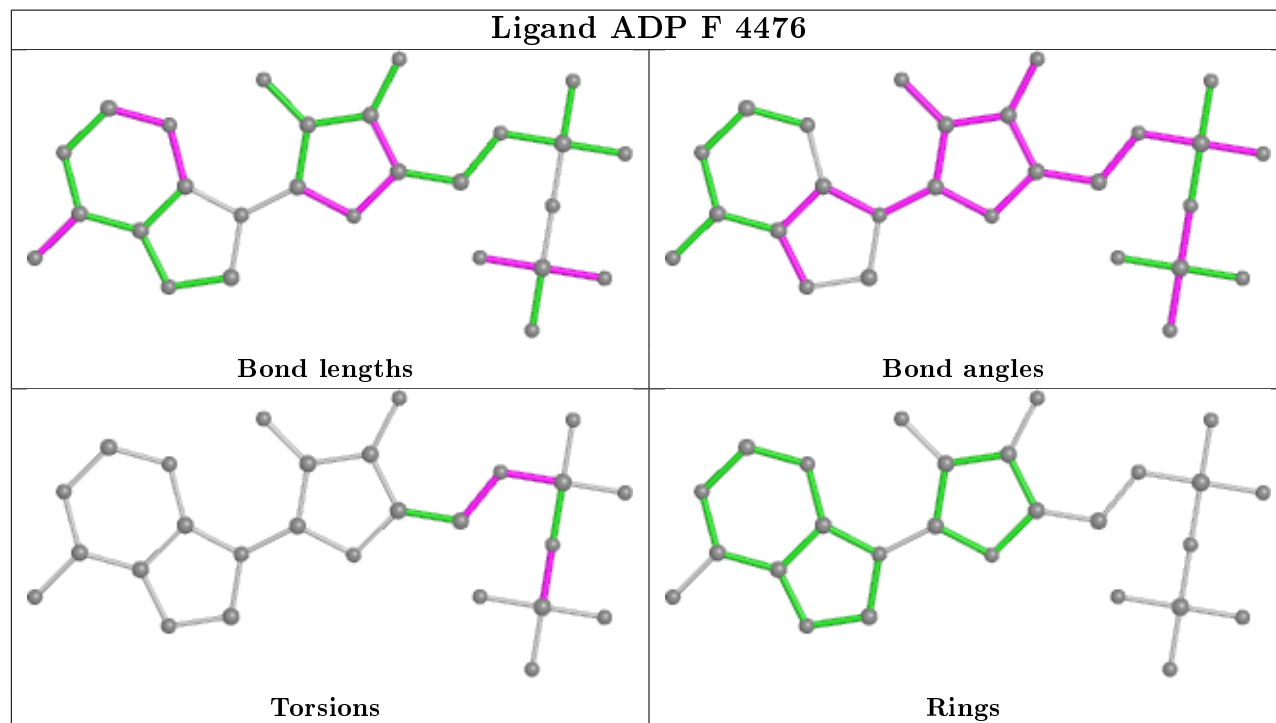
Ligand ADP J 4480



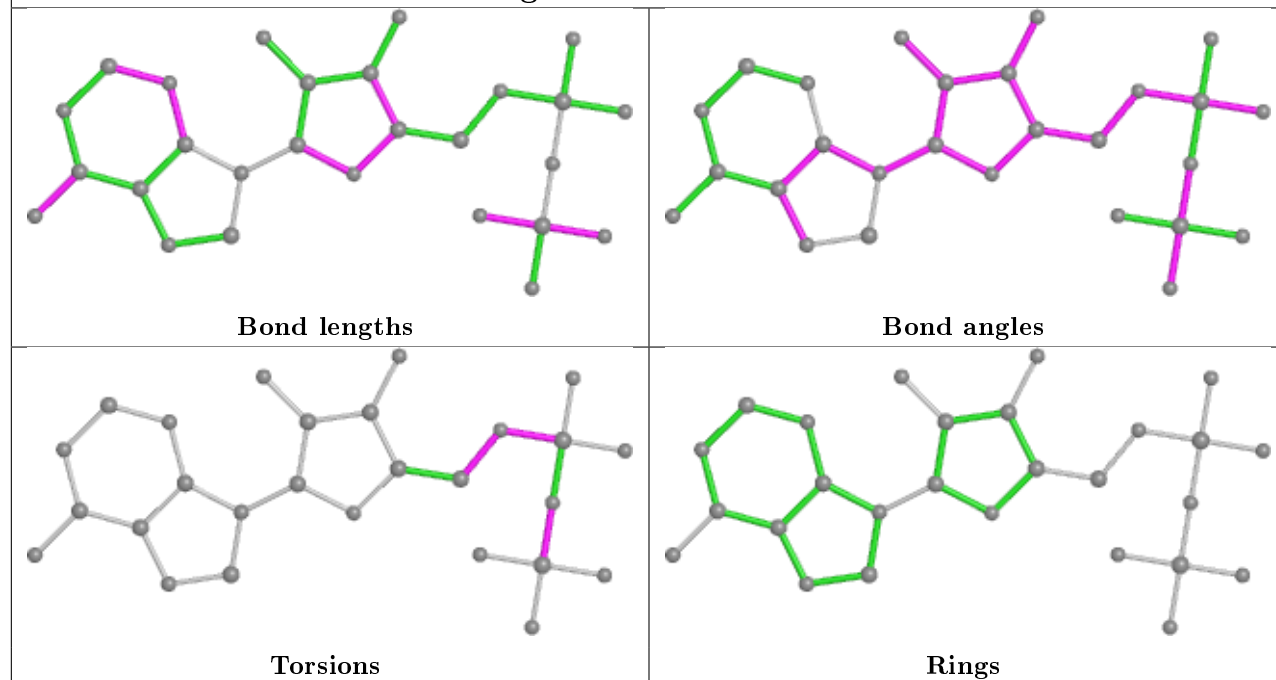
Ligand ADP D 4474



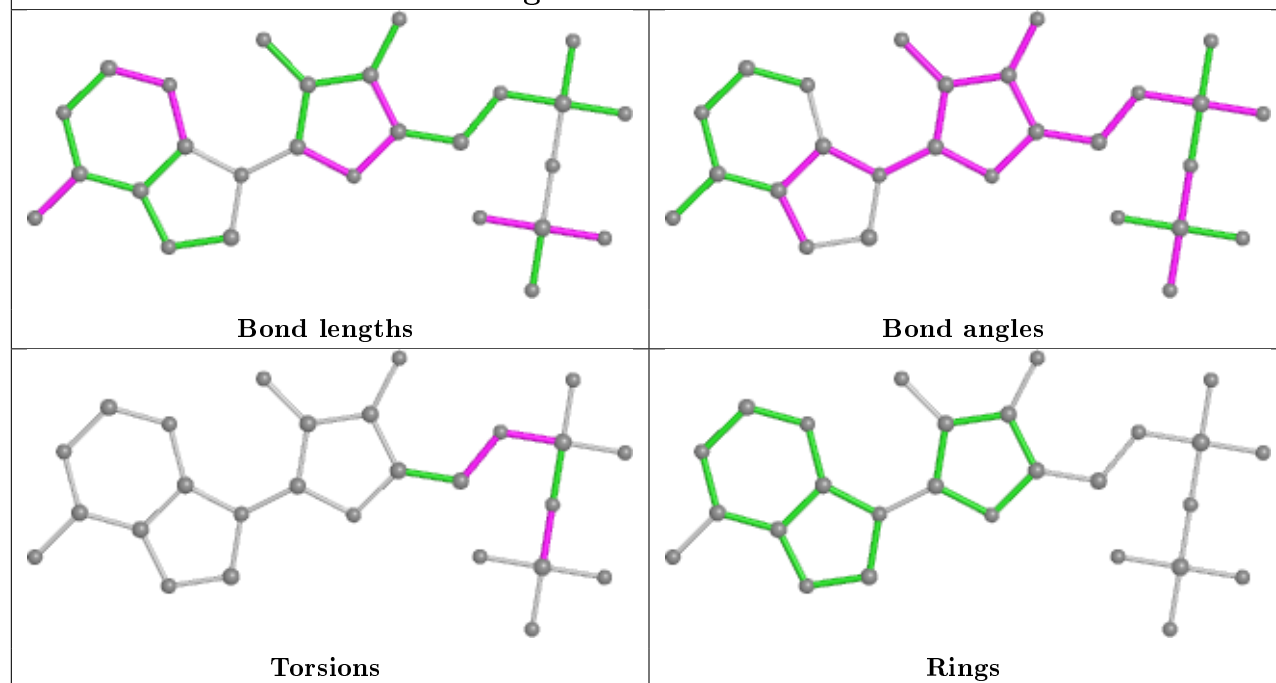
Ligand ADP F 4476



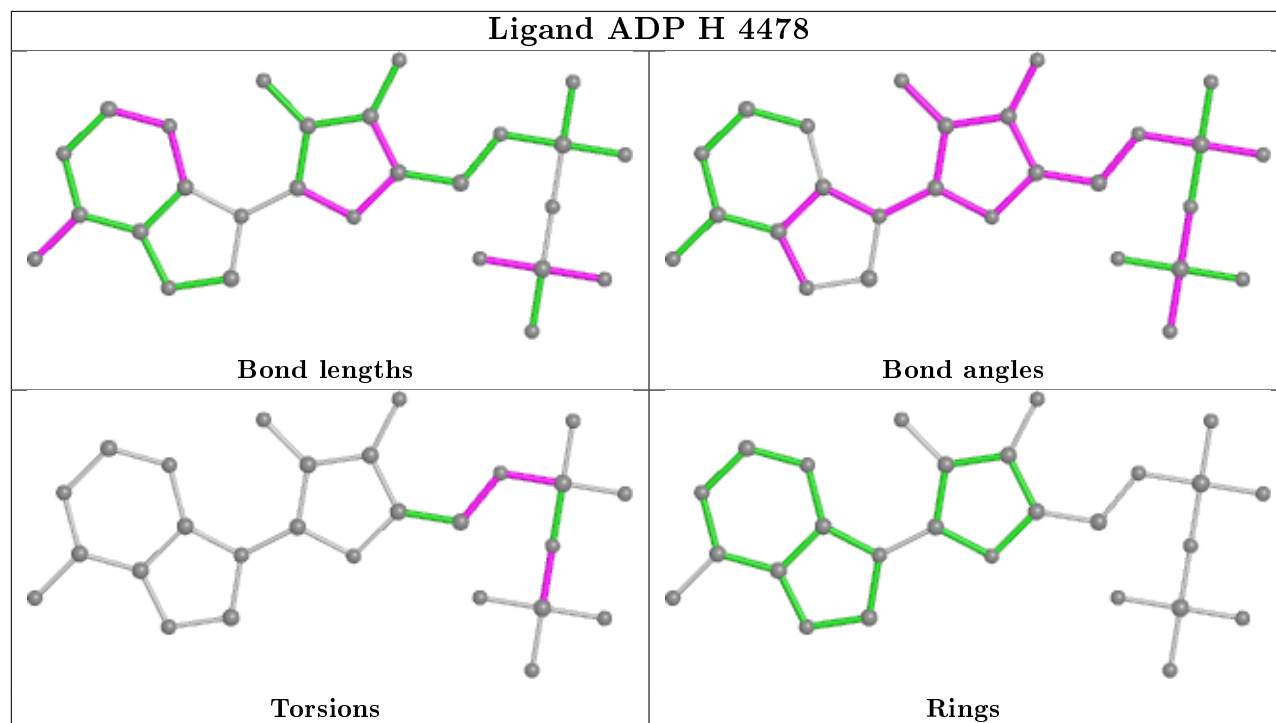
Ligand ADP A 4471



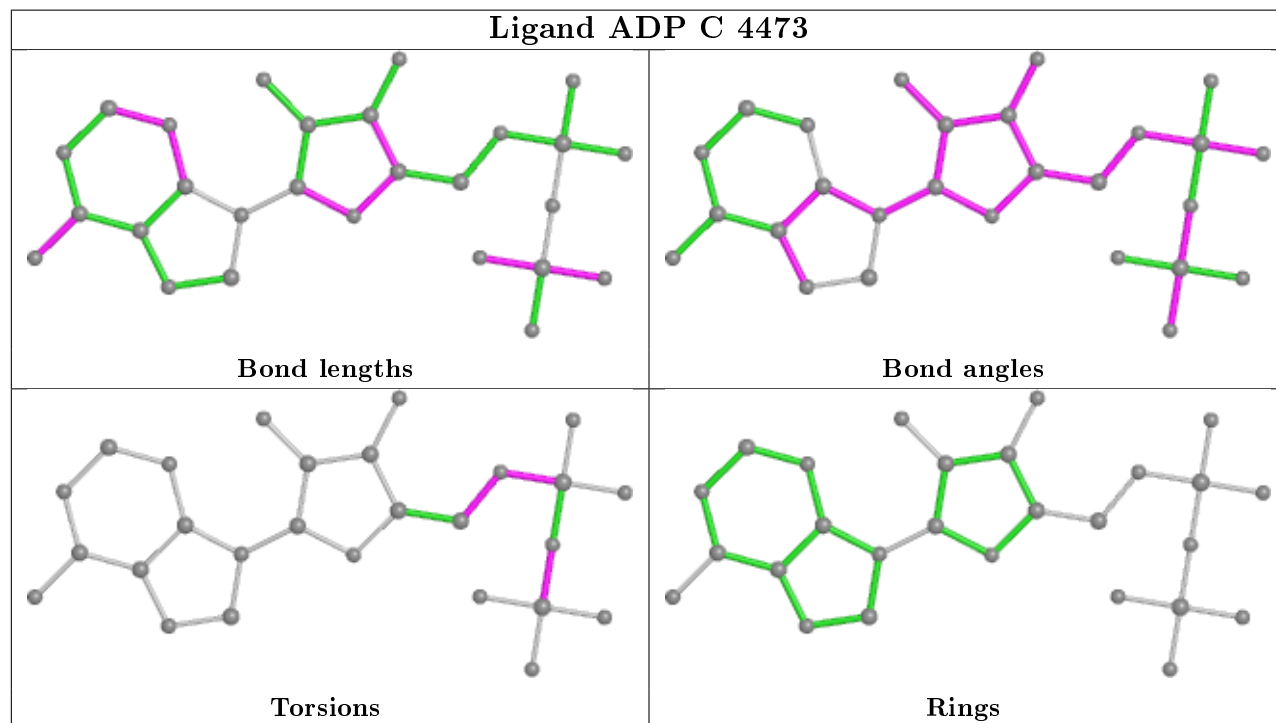
Ligand ADP L 4482

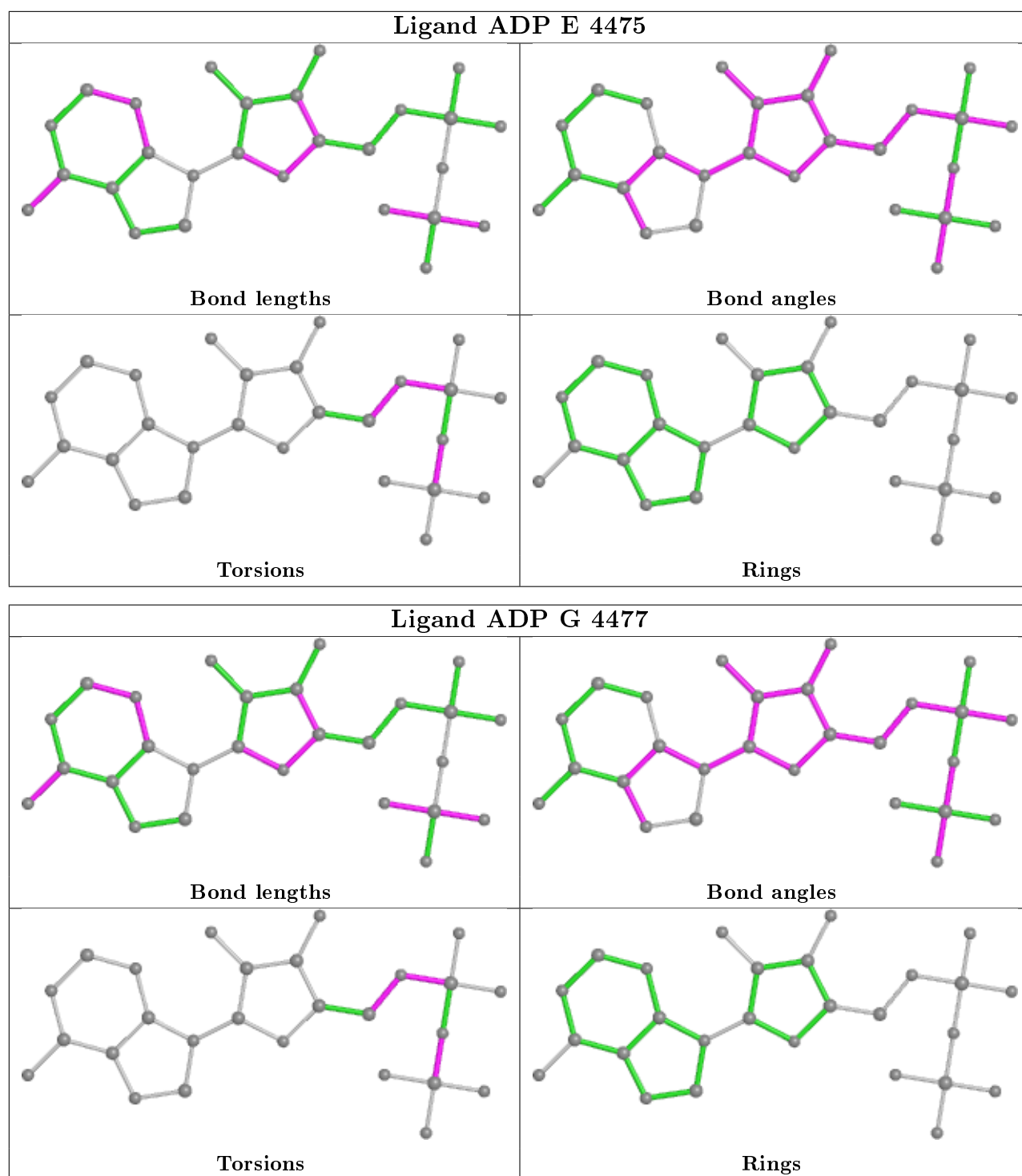


Ligand ADP H 4478



Ligand ADP C 4473





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%)	0.10	30 (6%)	19	15	20, 47, 80, 100	94 (20%)
1	B	468/468 (100%)	-0.16	18 (3%)	40	36	20, 47, 80, 100	94 (20%)
1	C	468/468 (100%)	-0.19	20 (4%)	35	31	20, 47, 80, 100	94 (20%)
1	D	468/468 (100%)	-0.29	21 (4%)	33	29	20, 47, 80, 100	94 (20%)
1	E	468/468 (100%)	-0.22	16 (3%)	45	40	20, 47, 80, 100	94 (20%)
1	F	468/468 (100%)	-0.16	24 (5%)	28	24	20, 47, 80, 100	94 (20%)
1	G	468/468 (100%)	-0.30	18 (3%)	40	36	20, 47, 80, 100	94 (20%)
1	H	468/468 (100%)	-0.25	20 (4%)	35	31	20, 47, 80, 100	94 (20%)
1	I	468/468 (100%)	-0.36	15 (3%)	47	43	20, 47, 80, 100	94 (20%)
1	J	468/468 (100%)	-0.26	18 (3%)	40	36	20, 47, 80, 100	94 (20%)
1	K	468/468 (100%)	-0.35	11 (2%)	59	56	20, 47, 80, 100	94 (20%)
1	L	468/468 (100%)	-0.30	17 (3%)	42	37	20, 47, 80, 100	94 (20%)
All	All	5616/5616 (100%)	-0.23	228 (4%)	37	32	20, 47, 81, 100	1128 (20%)

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	396	LEU	10.3
1	F	396	LEU	8.7
1	L	396	LEU	7.7
1	D	395	ASN	7.4
1	J	60	ILE	7.3
1	I	63	SER	7.0
1	A	404	ALA	6.9
1	J	398	ASP	6.8
1	J	396	LEU	6.4
1	C	396	LEU	6.3
1	H	337	ARG	6.2

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Mol	Chain	Res	Type	RSRZ
1	C	63	SER	5.8
1	F	398	ASP	5.7
1	E	63	SER	5.6
1	K	395	ASN	5.6
1	C	395	ASN	5.5
1	L	397	TYR	5.5
1	F	401	PRO	5.5
1	B	404	ALA	5.4
1	A	395	ASN	5.4
1	F	63	SER	5.4
1	C	398	ASP	5.2
1	G	401	PRO	5.2
1	E	395	ASN	5.1
1	J	403	GLU	5.0
1	D	398	ASP	5.0
1	H	60	ILE	5.0
1	F	404	ALA	4.9
1	A	399	LEU	4.9
1	C	61	ASN	4.9
1	J	399	LEU	4.9
1	G	398	ASP	4.9
1	B	399	LEU	4.9
1	A	277	ASN	4.9
1	A	60	ILE	4.8
1	G	63	SER	4.8
1	K	63	SER	4.8
1	H	402	GLU	4.7
1	L	395	ASN	4.5
1	J	402	GLU	4.5
1	F	402	GLU	4.5
1	H	401	PRO	4.4
1	L	402	GLU	4.4
1	A	285	ASP	4.3
1	K	398	ASP	4.3
1	F	395	ASN	4.3
1	A	400	PRO	4.2
1	G	395	ASN	4.2
1	A	396	LEU	4.2
1	H	398	ASP	4.2
1	D	394	LYS	4.2
1	K	397	TYR	4.1
1	D	60	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	G	397	TYR	4.0
1	F	400	PRO	4.0
1	K	1	SER	4.0
1	E	1	SER	4.0
1	E	398	ASP	4.0
1	L	398	ASP	4.0
1	C	394	LYS	3.9
1	A	398	ASP	3.9
1	J	337	ARG	3.9
1	D	400	PRO	3.9
1	A	403	GLU	3.9
1	J	397	TYR	3.9
1	A	402	GLU	3.9
1	I	61	ASN	3.8
1	K	402	GLU	3.8
1	D	399	LEU	3.8
1	D	396	LEU	3.8
1	H	264[A]	ASN	3.8
1	C	402	GLU	3.8
1	G	396	LEU	3.7
1	H	396	LEU	3.7
1	G	404	ALA	3.7
1	D	401	PRO	3.7
1	K	60	ILE	3.6
1	B	1	SER	3.6
1	F	1	SER	3.6
1	D	404	ALA	3.6
1	G	402	GLU	3.6
1	F	264[A]	ASN	3.5
1	L	401	PRO	3.5
1	B	400	PRO	3.5
1	I	398	ASP	3.5
1	F	62	GLU	3.5
1	F	349	ALA	3.5
1	H	61	ASN	3.4
1	K	403	GLU	3.4
1	L	61	ASN	3.4
1	A	62	GLU	3.4
1	A	63	SER	3.4
1	L	63	SER	3.4
1	B	395	ASN	3.4
1	E	283	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	I	1	SER	3.4
1	B	337	ARG	3.3
1	E	61	ASN	3.3
1	E	396	LEU	3.3
1	G	399	LEU	3.3
1	A	351	PRO	3.2
1	A	401	PRO	3.2
1	G	264[A]	ASN	3.2
1	L	264[A]	ASN	3.2
1	A	378	GLY	3.2
1	C	59	GLY	3.2
1	C	397	TYR	3.2
1	G	403	GLU	3.2
1	L	62	GLU	3.2
1	A	348	VAL	3.2
1	H	395	ASN	3.2
1	D	402	GLU	3.2
1	E	404	ALA	3.1
1	J	401	PRO	3.1
1	D	337	ARG	3.1
1	A	3	GLU	3.1
1	F	394	LYS	3.1
1	B	398	ASP	3.1
1	L	1	SER	3.1
1	F	397	TYR	3.1
1	H	400	PRO	3.1
1	J	395	ASN	3.1
1	I	60	ILE	3.0
1	C	264[A]	ASN	3.0
1	G	349	ALA	3.0
1	H	1	SER	2.9
1	H	4	HIS	2.9
1	A	116	ARG	2.9
1	I	402	GLU	2.9
1	C	404	ALA	2.9
1	F	61	ASN	2.9
1	G	98	GLN	2.9
1	C	60	ILE	2.9
1	A	394	LYS	2.8
1	F	348	VAL	2.8
1	H	63	SER	2.8
1	D	63	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	399	LEU	2.8
1	I	404	ALA	2.8
1	E	337	ARG	2.8
1	I	62	GLU	2.8
1	F	60	ILE	2.7
1	C	1	SER	2.7
1	I	285	ASP	2.7
1	B	98	GLN	2.7
1	J	63	SER	2.7
1	B	63	SER	2.7
1	A	58	LYS	2.7
1	K	61	ASN	2.7
1	B	55	GLY	2.7
1	I	397	TYR	2.7
1	A	397	TYR	2.7
1	C	3	GLU	2.7
1	J	178[A]	GLY	2.6
1	B	61	ASN	2.6
1	F	59	GLY	2.6
1	G	400	PRO	2.6
1	E	394	LYS	2.6
1	L	399	LEU	2.6
1	A	286	LYS	2.6
1	B	60	ILE	2.6
1	E	393	ASP	2.6
1	C	62	GLU	2.5
1	D	278	GLY	2.5
1	A	278	GLY	2.5
1	D	264[A]	ASN	2.5
1	C	337	ARG	2.5
1	G	61	ASN	2.5
1	F	284	GLY	2.5
1	L	60	ILE	2.5
1	A	337	ARG	2.5
1	F	406	GLU	2.5
1	E	278	GLY	2.5
1	D	94	PRO	2.5
1	D	1	SER	2.5
1	B	352	LYS	2.5
1	L	337	ARG	2.4
1	F	56	GLY	2.4
1	B	401	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	264[A]	ASN	2.4
1	A	273	SER	2.4
1	H	11	GLU	2.4
1	D	397	TYR	2.4
1	I	395	ASN	2.4
1	G	394	LYS	2.4
1	E	60	ILE	2.4
1	D	98	GLN	2.3
1	C	7	THR	2.3
1	I	405	LYS	2.3
1	L	405	LYS	2.3
1	H	403	GLU	2.3
1	J	400	PRO	2.3
1	L	393	ASP	2.3
1	G	1	SER	2.3
1	H	3	GLU	2.3
1	E	12	HIS	2.3
1	I	403	GLU	2.3
1	J	394	LYS	2.2
1	G	348	VAL	2.2
1	D	403	GLU	2.2
1	E	7	THR	2.2
1	J	404	ALA	2.2
1	D	62	GLU	2.2
1	H	284	GLY	2.2
1	B	387	HIS	2.2
1	C	401	PRO	2.2
1	H	394	LYS	2.2
1	B	264[A]	ASN	2.1
1	L	59	GLY	2.1
1	J	61	ASN	2.1
1	B	394	LYS	2.1
1	F	405	LYS	2.1
1	F	390	GLU	2.1
1	F	399	LEU	2.1
1	K	264[A]	ASN	2.1
1	H	399	LEU	2.1
1	I	396	LEU	2.1
1	B	58	LYS	2.1
1	A	324	PRO	2.1
1	A	4	HIS	2.1
1	J	1	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	40	ALA	2.0
1	E	406	GLU	2.0
1	J	264[A]	ASN	2.0
1	C	349	ALA	2.0
1	C	393	ASP	2.0
1	A	279	THR	2.0
1	D	7	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADP	L	4482	27/27	0.73	0.42	42,80,100,100	27
3	ADP	C	4473	27/27	0.76	0.36	42,80,100,100	27
3	ADP	I	4479	27/27	0.78	0.36	42,80,100,100	27
3	ADP	K	4481	27/27	0.78	0.35	42,80,100,100	27
3	ADP	E	4475	27/27	0.79	0.39	42,80,100,100	27
3	ADP	H	4478	27/27	0.81	0.32	42,80,100,100	27
3	ADP	B	4472	27/27	0.82	0.31	42,80,100,100	27
3	ADP	F	4476	27/27	0.82	0.41	42,80,100,100	27
3	ADP	J	4480	27/27	0.84	0.30	42,80,100,100	27
3	ADP	A	4471	27/27	0.84	0.35	42,80,100,100	27
3	ADP	G	4477	27/27	0.84	0.28	42,80,100,100	27
3	ADP	D	4474	27/27	0.88	0.34	42,80,100,100	27
2	MN	H	470	1/1	0.91	0.07	43,43,43,43	0
4	PPQ	B	5901	11/11	0.91	0.20	16,36,70,83	11
4	PPQ	F	5905	11/11	0.92	0.20	16,36,70,83	11
2	MN	C	469	1/1	0.92	0.07	41,41,41,41	0

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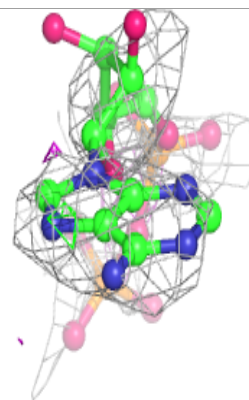
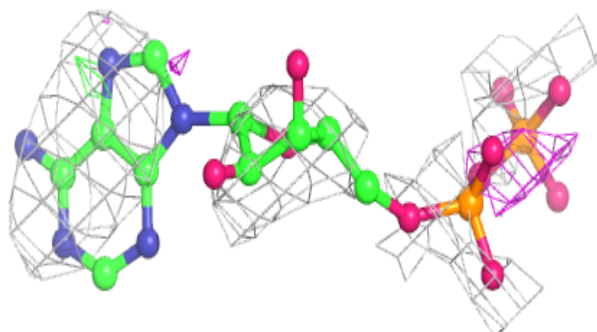
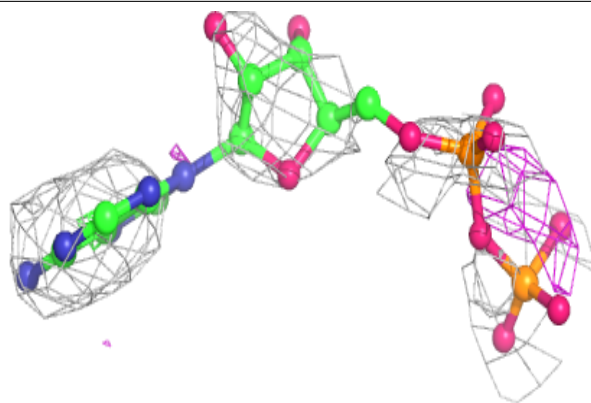
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	G	469	1/1	0.92	0.08	41,41,41,41	0
4	PPQ	H	5907	11/11	0.93	0.20	16,36,70,83	11
2	MN	D	469	1/1	0.93	0.07	41,41,41,41	0
4	PPQ	I	5908	11/11	0.93	0.22	16,36,70,83	11
4	PPQ	G	5906	11/11	0.93	0.17	16,36,70,83	11
4	PPQ	D	5903	11/11	0.93	0.19	16,36,70,83	11
4	PPQ	C	5902	11/11	0.94	0.16	16,36,70,83	11
4	PPQ	K	5910	11/11	0.94	0.17	16,36,70,83	11
4	PPQ	E	5904	11/11	0.94	0.15	16,36,70,83	11
4	PPQ	A	5900	11/11	0.95	0.16	16,36,70,83	11
4	PPQ	J	5909	11/11	0.95	0.19	16,36,70,83	11
2	MN	E	469	1/1	0.95	0.04	41,41,41,41	0
4	PPQ	L	5911	11/11	0.95	0.21	16,36,70,83	11
2	MN	H	469	1/1	0.96	0.10	41,41,41,41	0
2	MN	A	469	1/1	0.97	0.06	41,41,41,41	0
2	MN	F	469	1/1	0.97	0.06	41,41,41,41	0
2	MN	A	470	1/1	0.97	0.03	43,43,43,43	0
2	MN	E	470	1/1	0.97	0.06	43,43,43,43	0
2	MN	K	469	1/1	0.97	0.11	41,41,41,41	0
2	MN	F	470	1/1	0.98	0.06	43,43,43,43	0
2	MN	D	470	1/1	0.98	0.08	43,43,43,43	0
2	MN	L	470	1/1	0.98	0.05	43,43,43,43	0
2	MN	L	469	1/1	0.98	0.11	41,41,41,41	0
2	MN	C	470	1/1	0.98	0.03	43,43,43,43	0
2	MN	B	470	1/1	0.98	0.05	43,43,43,43	0
2	MN	B	469	1/1	0.98	0.04	41,41,41,41	0
2	MN	K	470	1/1	0.98	0.04	43,43,43,43	0
2	MN	I	470	1/1	0.99	0.04	43,43,43,43	0
2	MN	J	470	1/1	0.99	0.02	43,43,43,43	0
2	MN	I	469	1/1	0.99	0.06	41,41,41,41	0
2	MN	J	469	1/1	0.99	0.07	41,41,41,41	0
2	MN	G	470	1/1	0.99	0.04	43,43,43,43	0

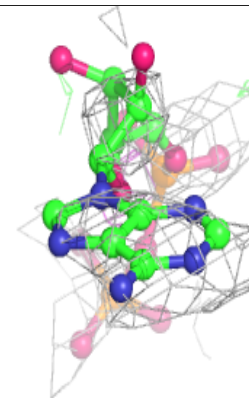
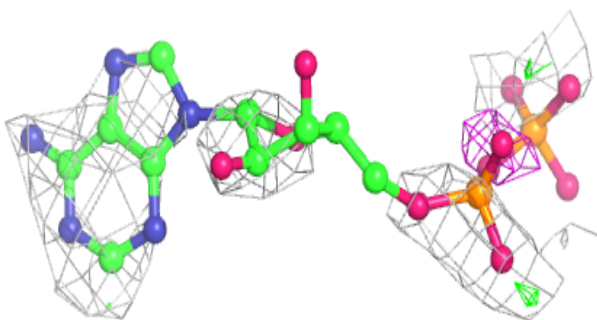
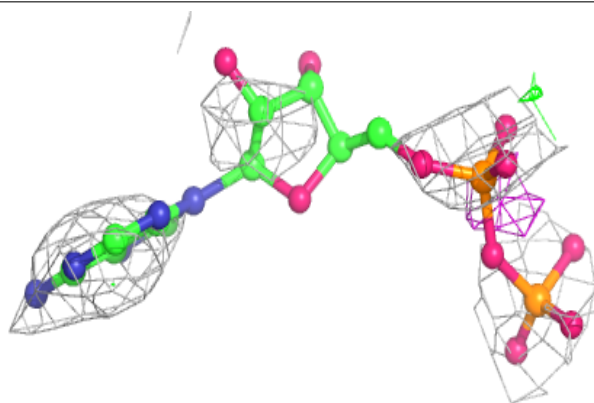
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP L 4482:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

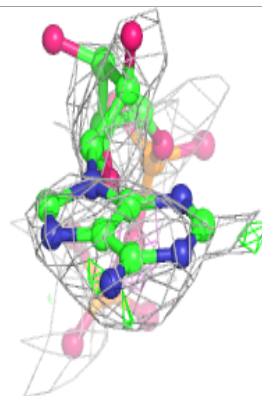
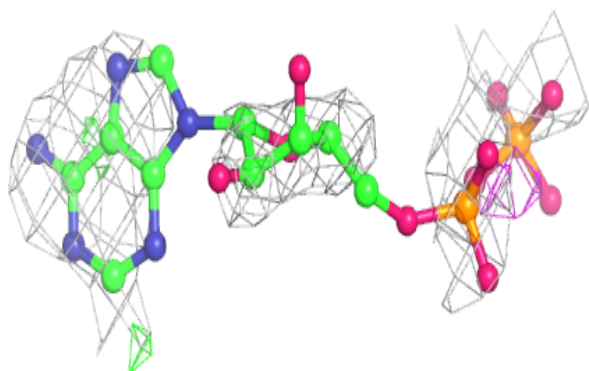
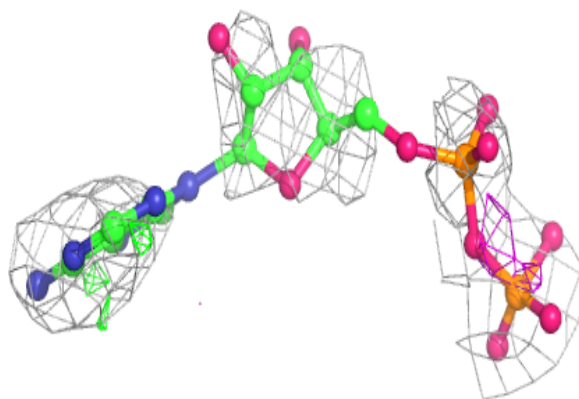
**Electron density around ADP C 4473:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

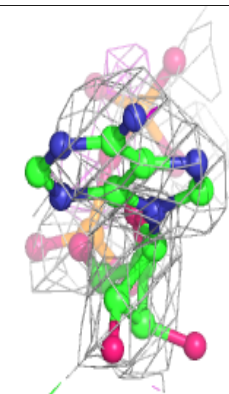
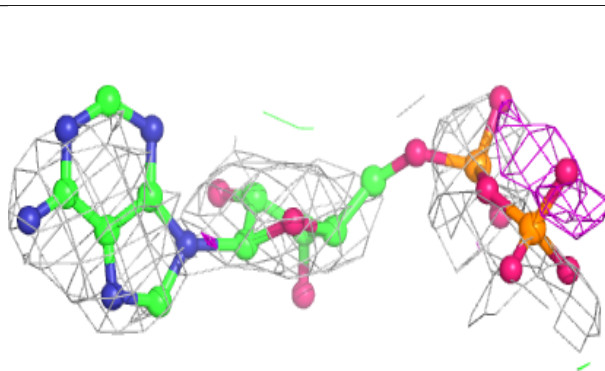
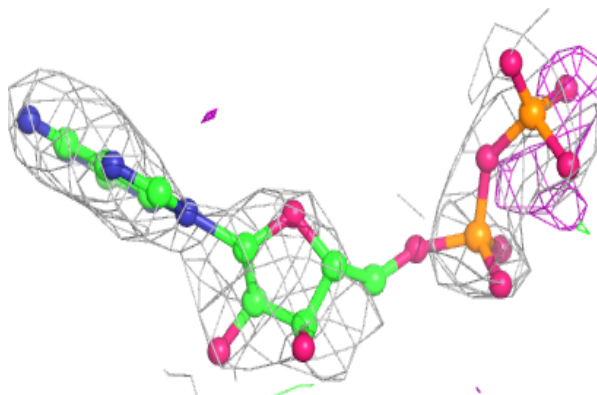


Electron density around ADP I 4479:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

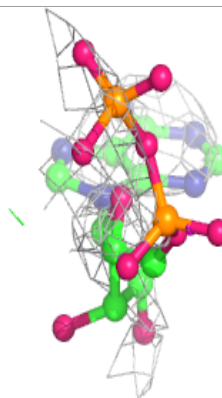
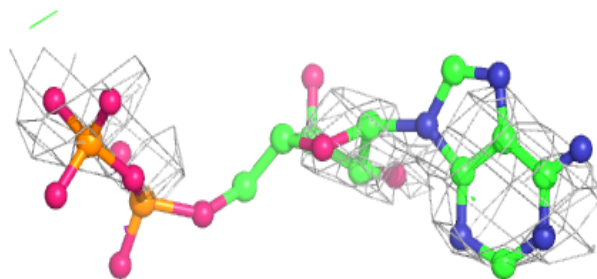
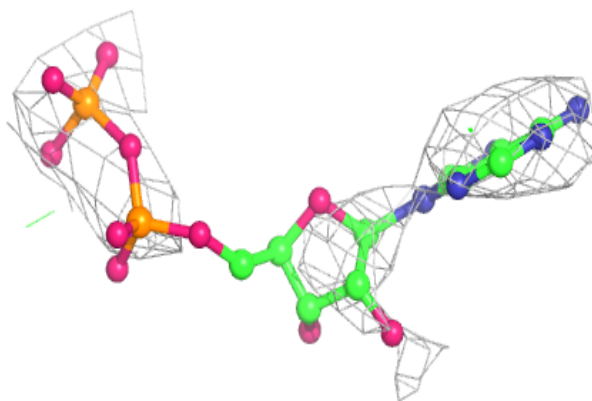
**Electron density around ADP K 4481:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

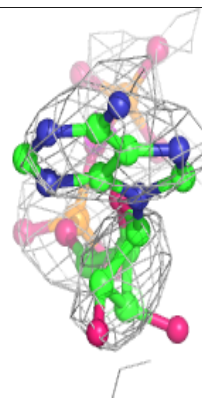
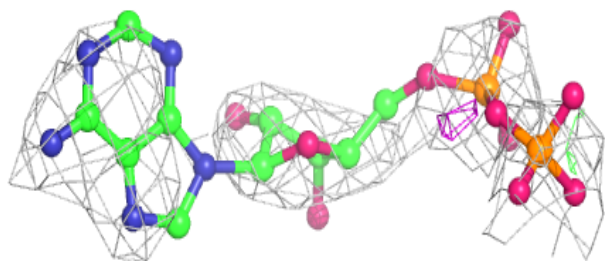
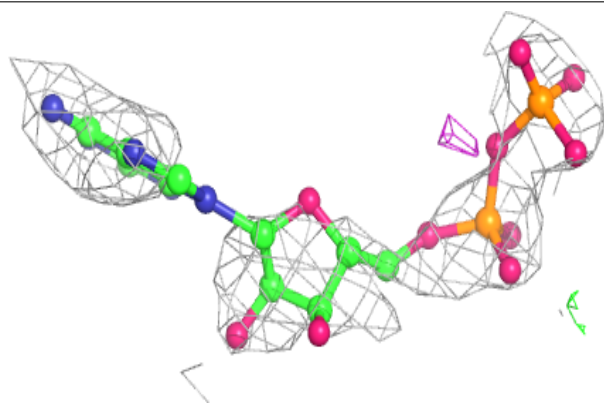


Electron density around ADP E 4475:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

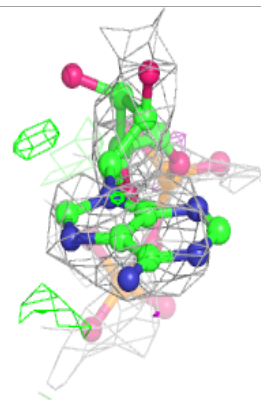
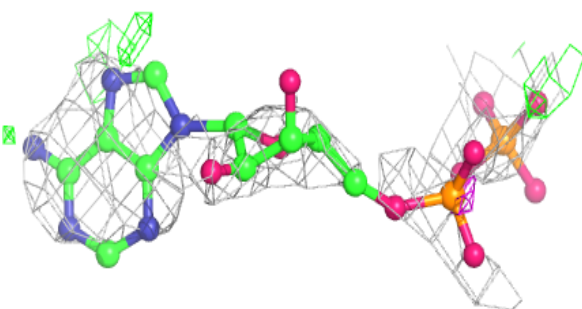
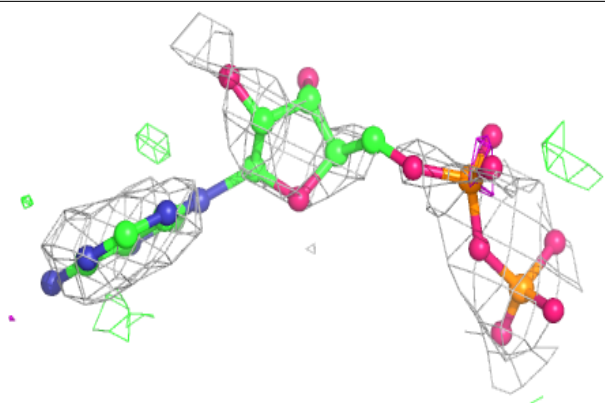
**Electron density around ADP H 4478:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

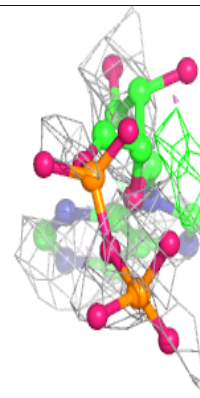
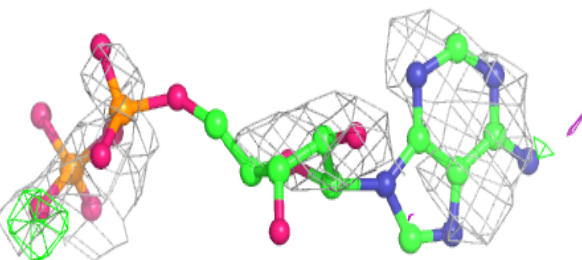
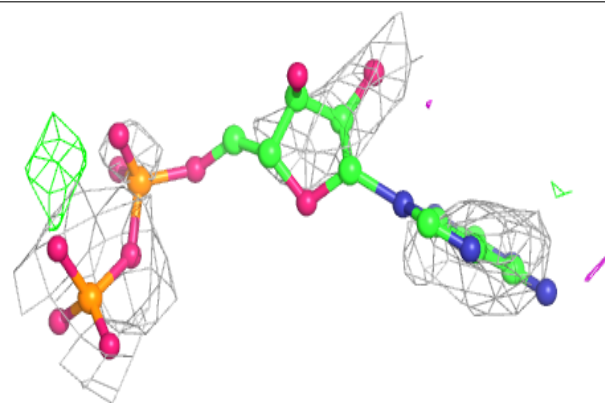


Electron density around ADP B 4472:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

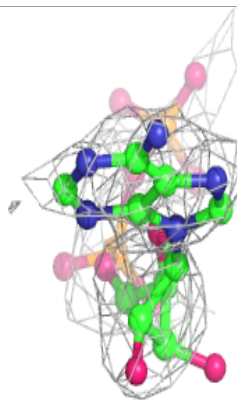
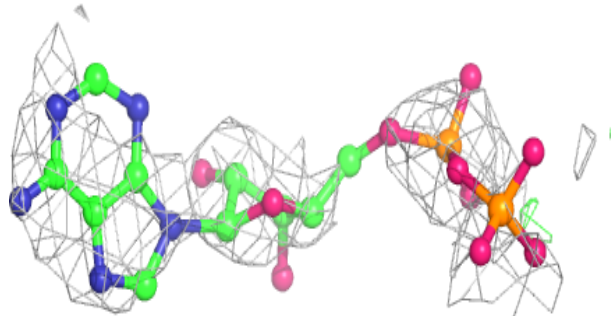
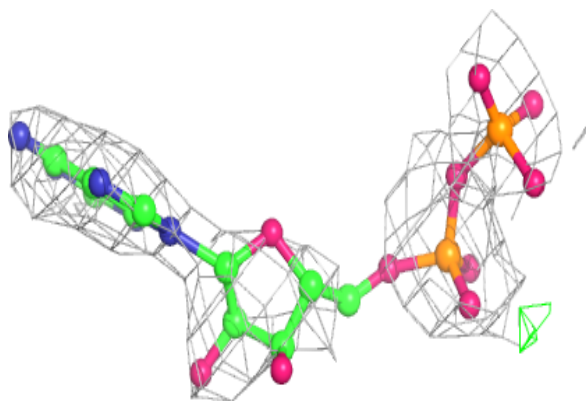
**Electron density around ADP F 4476:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

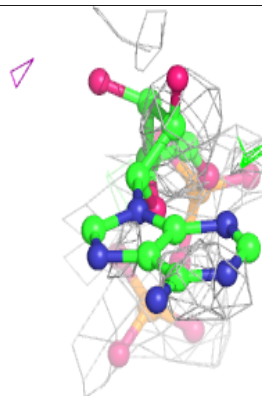
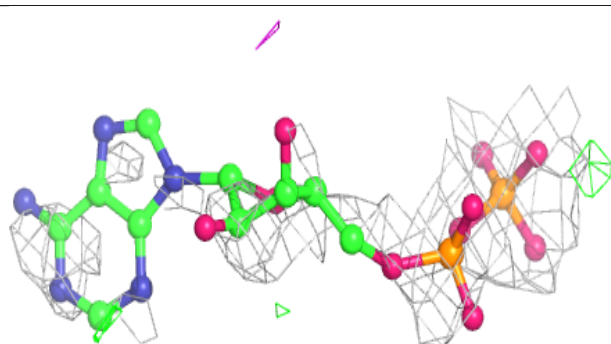
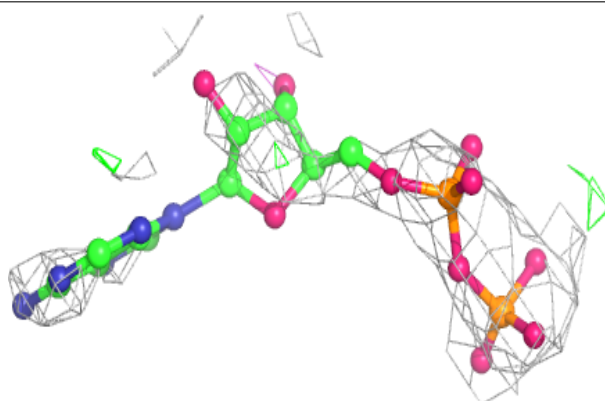


Electron density around ADP J 4480:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

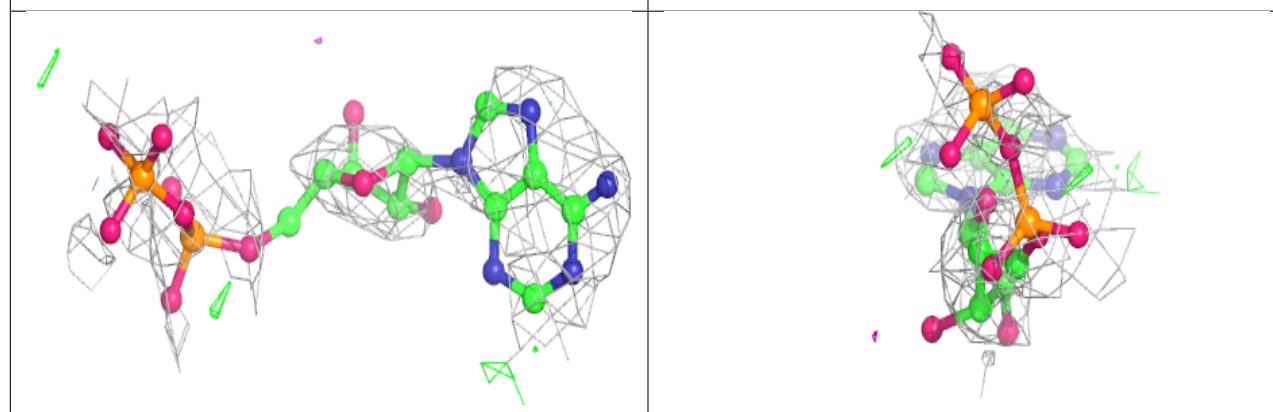
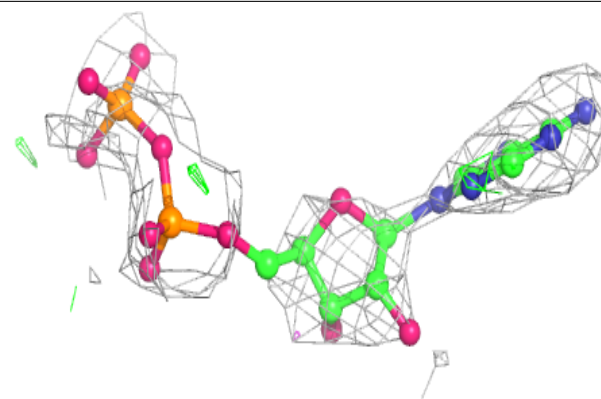
**Electron density around ADP A 4471:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

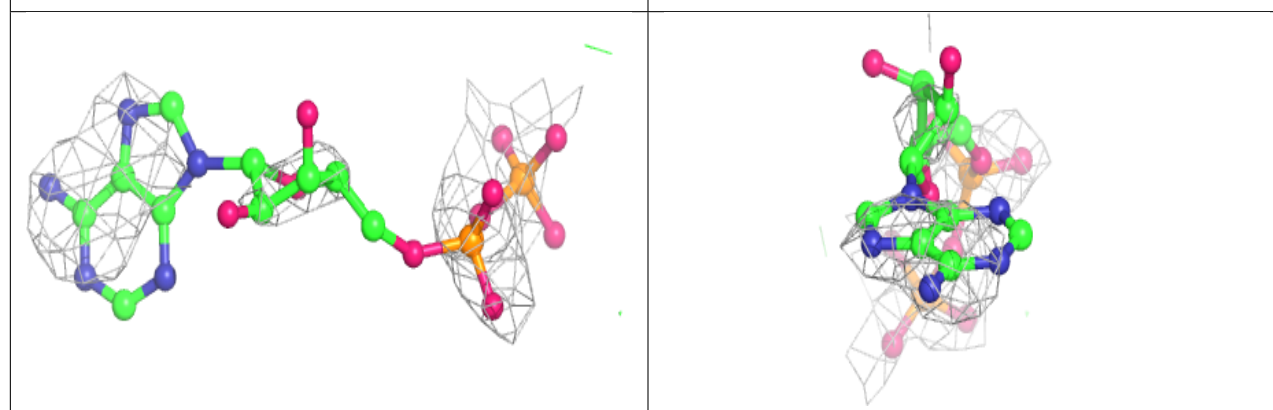
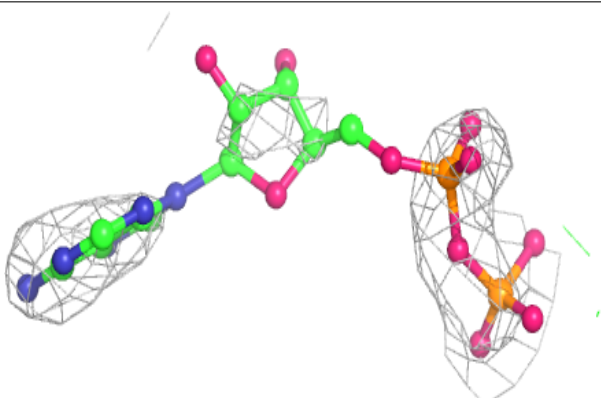


Electron density around ADP G 4477:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP D 4474:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

There are no such residues in this entry.