



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:14 pm GMT

PDB ID : 4LNF  
Title : B. subtilis glutamine synthetase structures reveal large active site conformational changes and basis for isoenzyme specific regulation: structure of GS-Q  
Authors : Schumacher, M.A.; Chinnam, N.; Tonthat, N.; Fisher, S.; Wray, L.  
Deposited on : 2013-07-11  
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

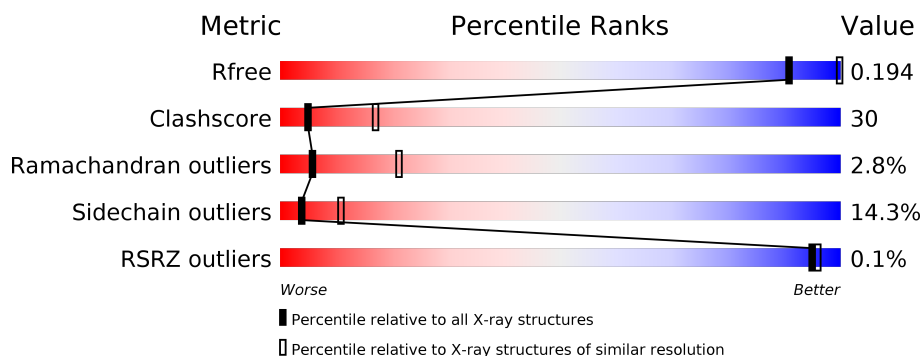
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 Å.

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





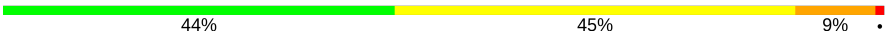

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2289 (2.98-2.90)
Clashscore	112137	2543 (2.98-2.90)
Ramachandran outliers	110173	2475 (2.98-2.90)
Sidechain outliers	110143	2477 (2.98-2.90)
RSRZ outliers	101464	2301 (2.98-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	443	<div> <div>53%</div> <div>39%</div> <div>9%</div> </div>
1	B	443	<div> <div>48%</div> <div>45%</div> <div>7%</div> </div>
1	C	443	<div> <div>48%</div> <div>43%</div> <div>9%</div> </div>
1	D	443	<div> <div>51%</div> <div>40%</div> <div>8%</div> <div>•</div> </div>
1	E	443	<div> <div>54%</div> <div>38%</div> <div>7%</div> <div>•</div> </div>
1	F	443	<div> <div>46%</div> <div>43%</div> <div>9%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	443	
1	H	443	
1	I	443	
1	J	443	
1	K	443	
1	L	443	

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
2	MG	B	501	-	-	-	X
2	MG	C	503	-	-	-	X
2	MG	H	501	-	-	-	X
2	MG	K	501	-	-	-	X
3	GLN	E	501	-	-	-	X
3	GLN	F	503	-	-	-	X
3	GLN	K	503	-	-	-	X
4	PO4	A	504	-	-	X	X
4	PO4	C	504	-	-	X	-
4	PO4	G	504	-	-	X	X
4	PO4	H	504	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 42824 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	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	B	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	C	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	D	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	E	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	F	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	G	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	H	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	I	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	J	441	Total	C	N	O	S	0	0	0
			3521	2250	587	668	16			
1	K	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	L	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

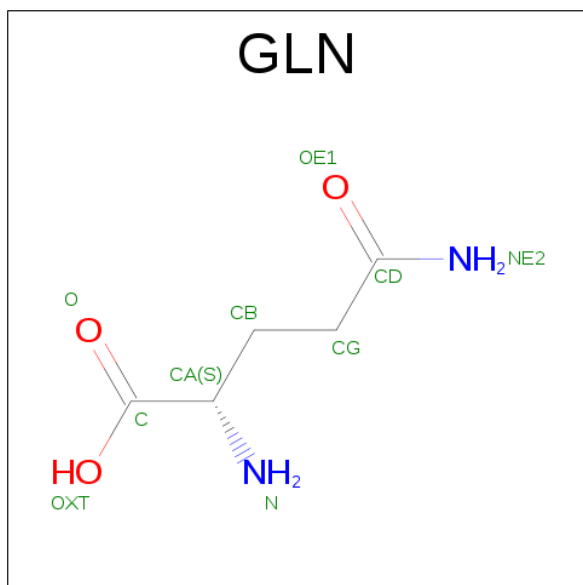
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	3	Total	Mg	0	0
			3	3		
2	J	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	3	Total 3	Mg 3	0	0
2	K	3	Total 3	Mg 3	0	0
2	E	3	Total 3	Mg 3	0	0
2	H	3	Total 3	Mg 3	0	0
2	B	3	Total 3	Mg 3	0	0
2	I	3	Total 3	Mg 3	0	0
2	C	3	Total 3	Mg 3	0	0
2	A	3	Total 3	Mg 3	0	0
2	L	3	Total 3	Mg 3	0	0
2	F	3	Total 3	Mg 3	0	0

- Molecule 3 is GLUTAMINE (three-letter code: GLN) (formula: C<sub>5</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>).



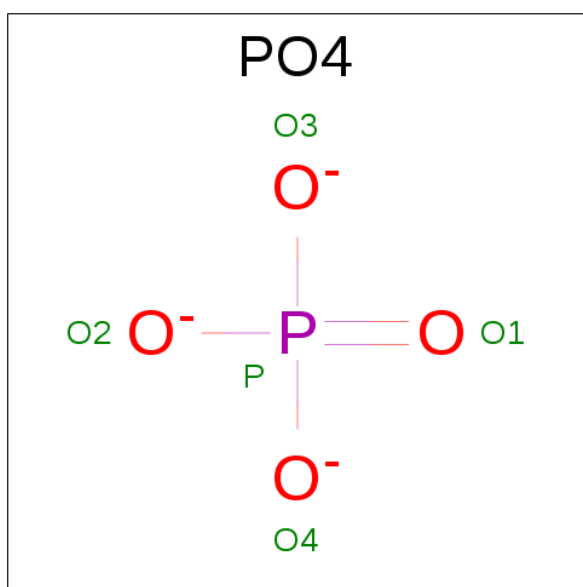
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 9	C 5	N 2	O 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			9	5	2	2		
3	C	1	Total	C	N	O	0	0
			9	5	2	2		
3	D	1	Total	C	N	O	0	0
			9	5	2	2		
3	E	1	Total	C	N	O	0	0
			9	5	2	2		
3	F	1	Total	C	N	O	0	0
			9	5	2	2		
3	G	1	Total	C	N	O	0	0
			9	5	2	2		
3	H	1	Total	C	N	O	0	0
			9	5	2	2		
3	I	1	Total	C	N	O	0	0
			9	5	2	2		
3	J	1	Total	C	N	O	0	0
			9	5	2	2		
3	K	1	Total	C	N	O	0	0
			9	5	2	2		
3	L	1	Total	C	N	O	0	0
			10	5	2	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	G	1	Total O P 5 4 1	0	0
4	H	1	Total O P 5 4 1	0	0

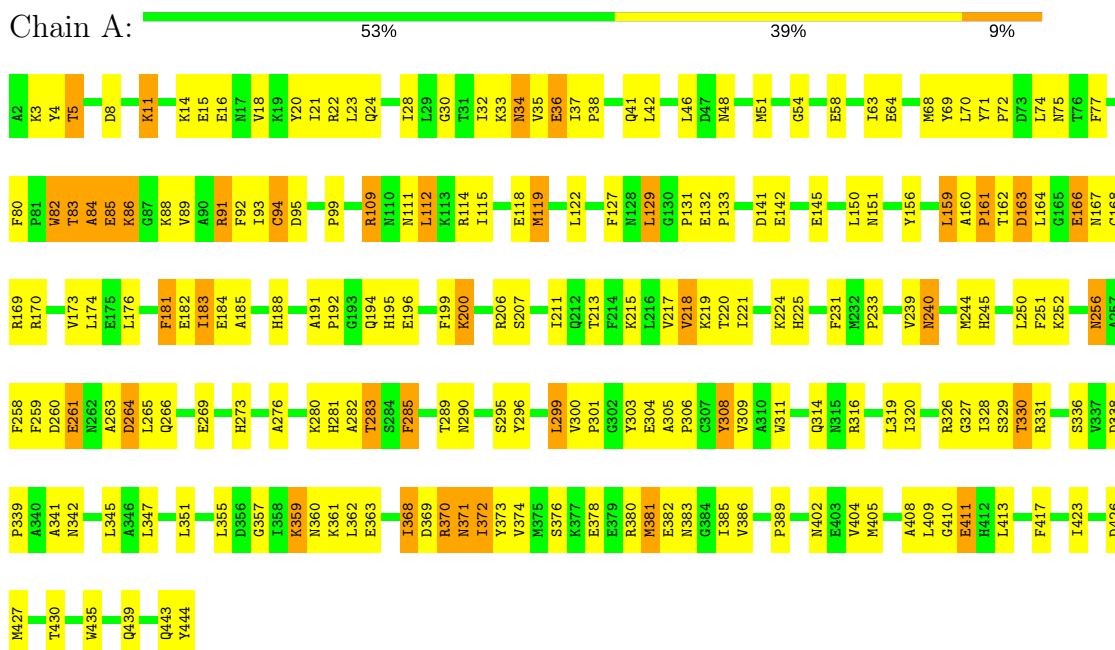
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	16	Total O 16 16	0	0
5	B	20	Total O 20 20	0	0
5	C	18	Total O 18 18	0	0
5	D	29	Total O 29 29	0	0
5	E	18	Total O 18 18	0	0
5	F	19	Total O 19 19	0	0
5	G	14	Total O 14 14	0	0
5	H	21	Total O 21 21	0	0
5	I	21	Total O 21 21	0	0
5	J	27	Total O 27 27	0	0
5	K	27	Total O 27 27	0	0
5	L	23	Total O 23 23	0	0

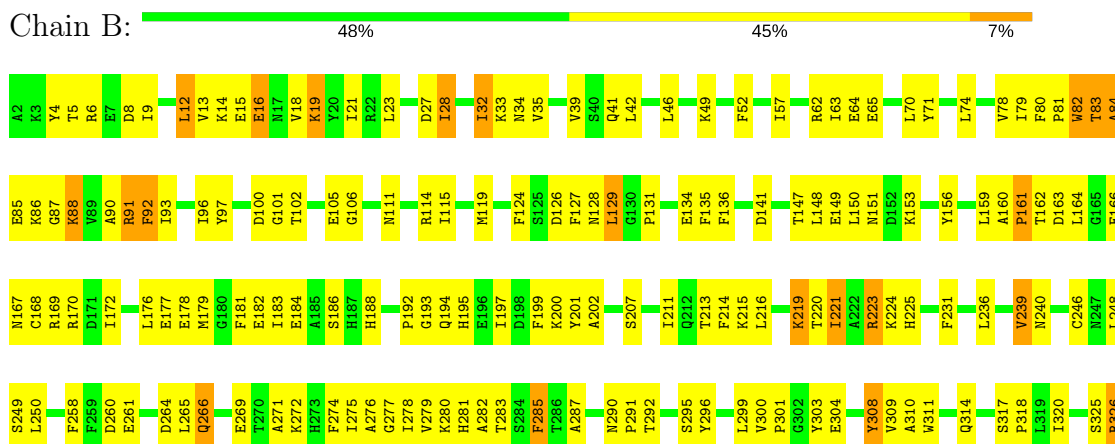
### 3 Residue-property plots

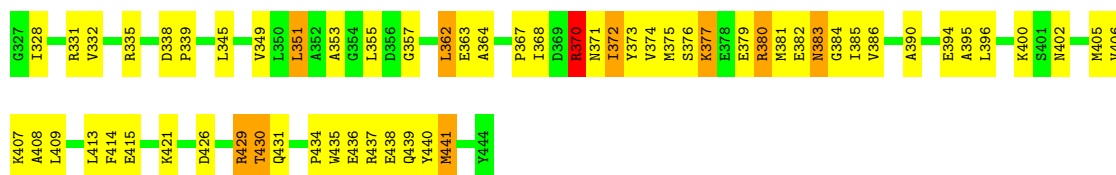
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



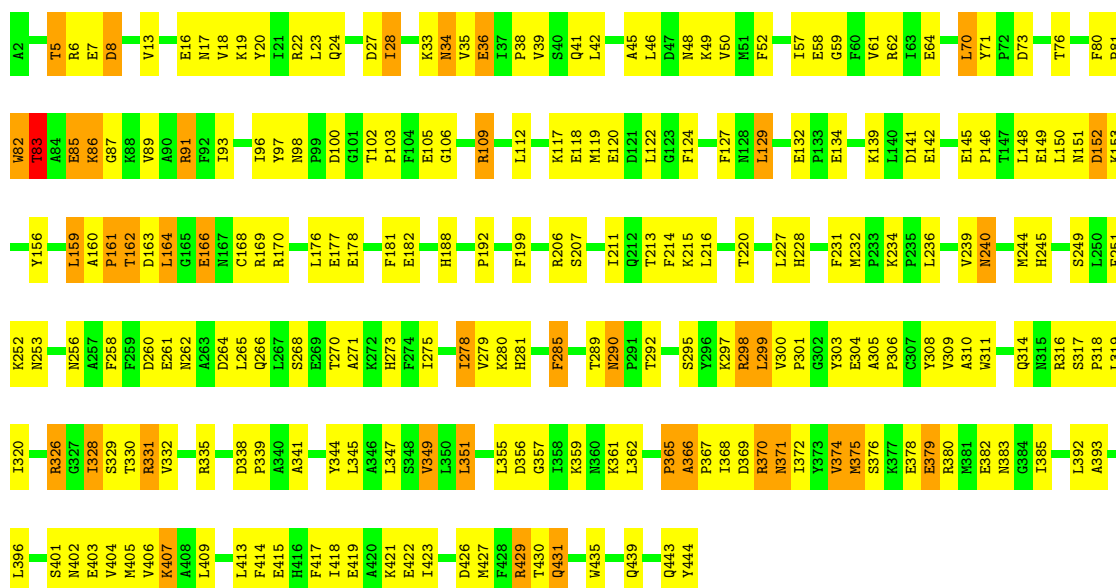
#### • Molecule 1: Glutamine synthetase





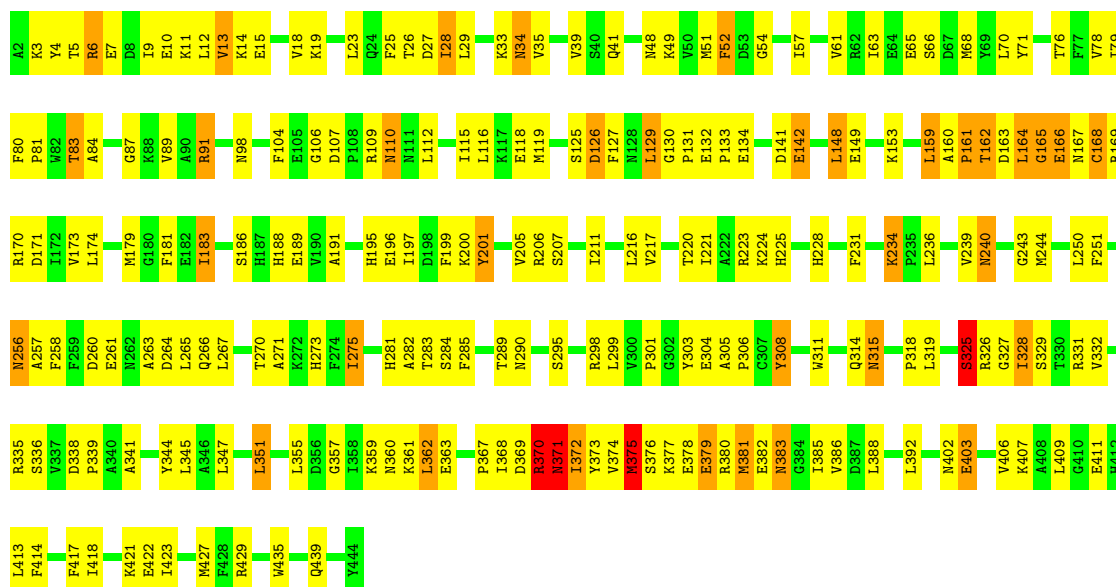
• Molecule 1: Glutamine synthetase

Chain C: 48% 43% 9%



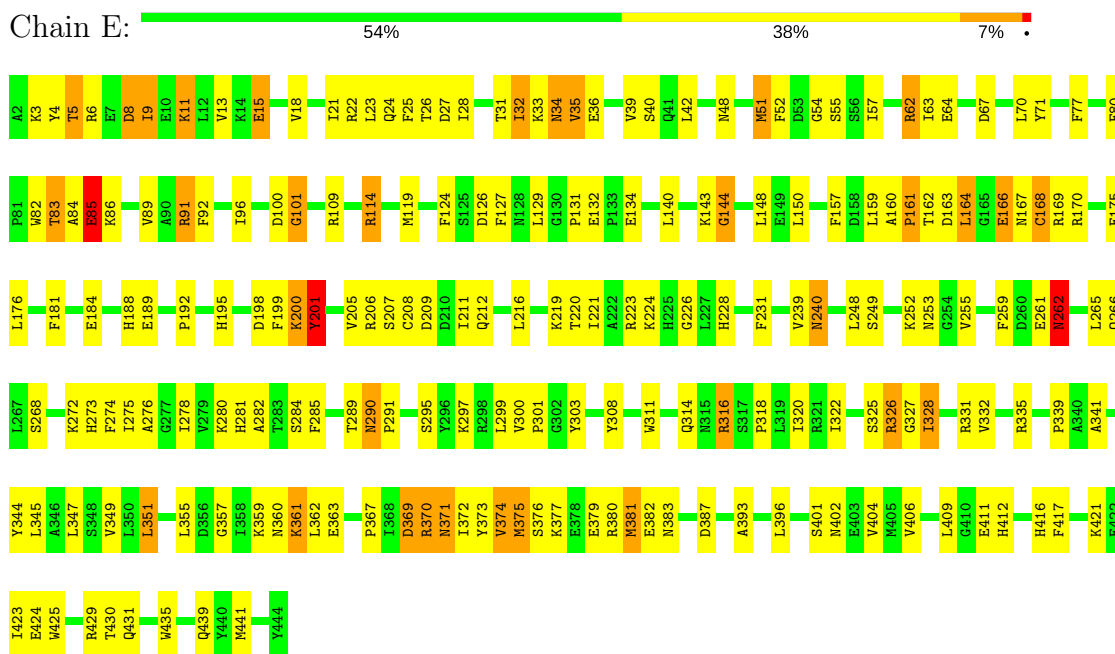
• Molecule 1: Glutamine synthetase

Chain D: 51% 40% 8%



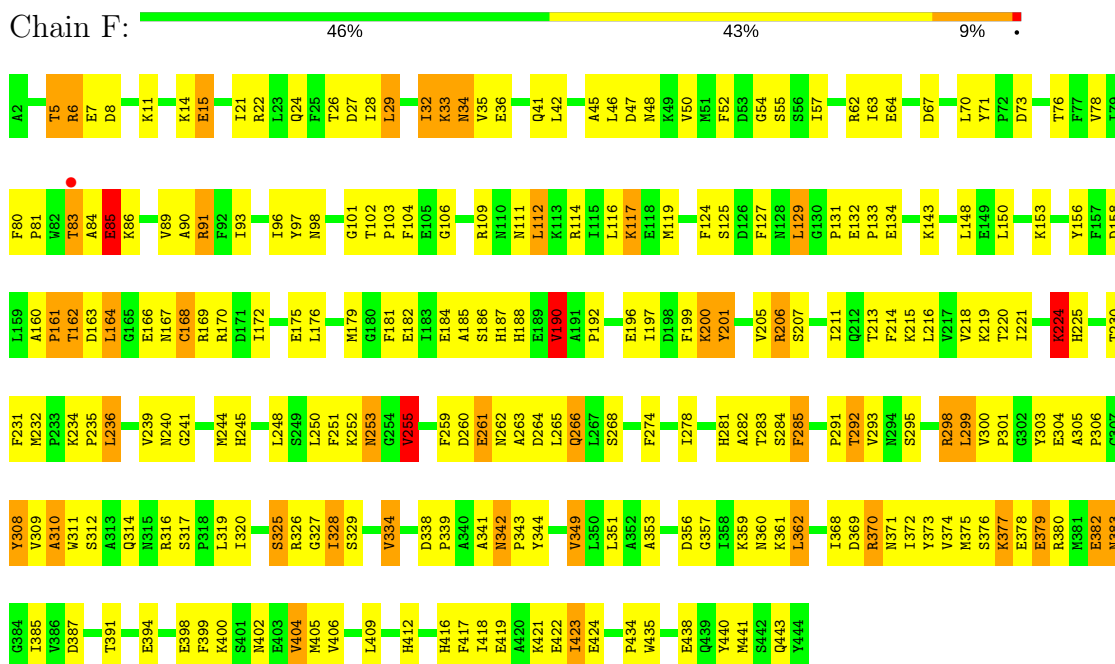
• Molecule 1: Glutamine synthetase

## Chain E:



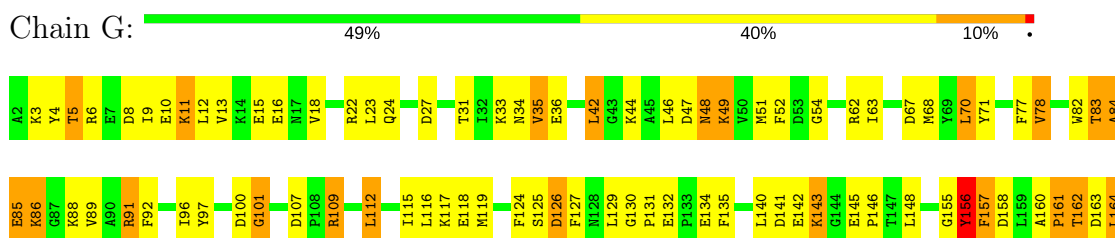
## • Molecule 1: Glutamine synthetase

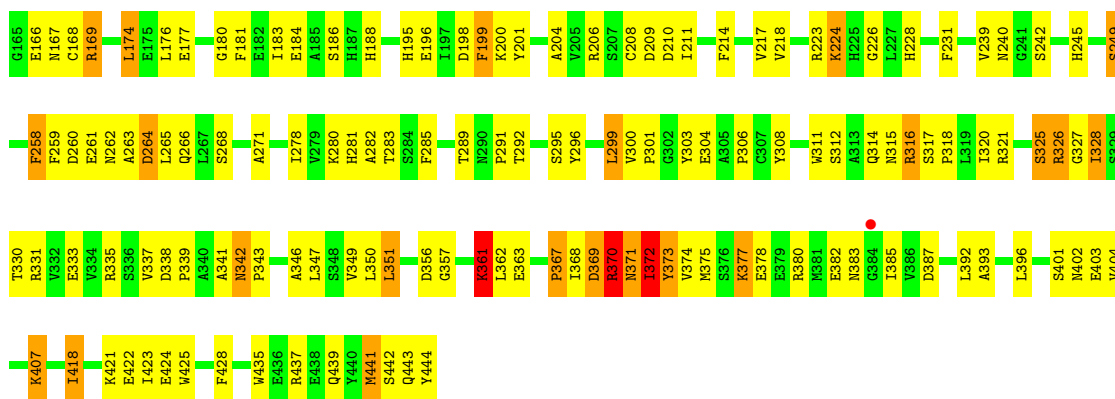
## Chain F:



## • Molecule 1: Glutamine synthetase

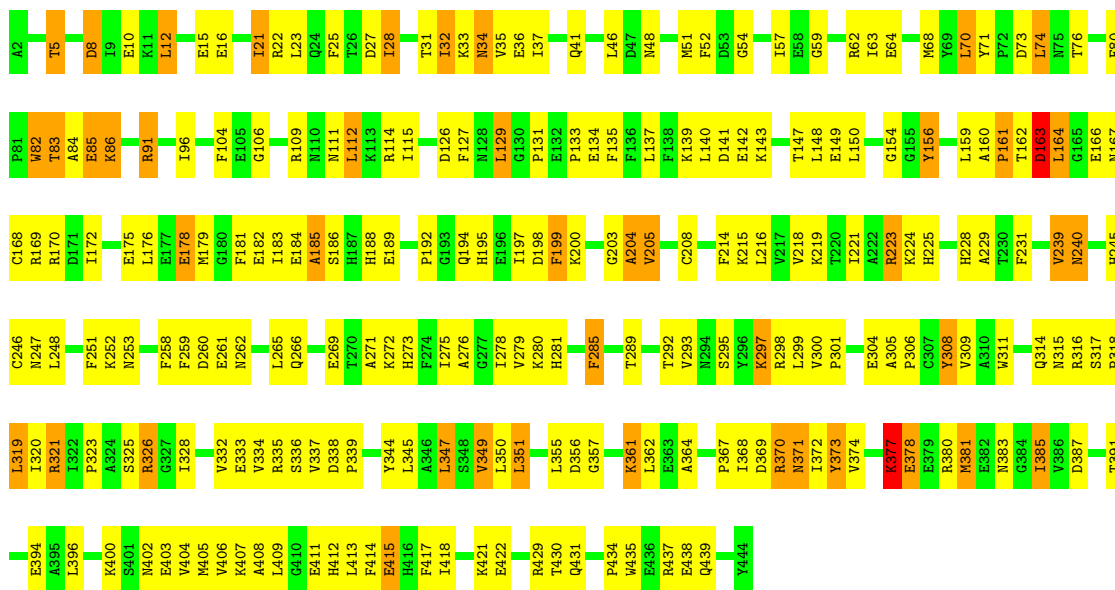
## Chain G:





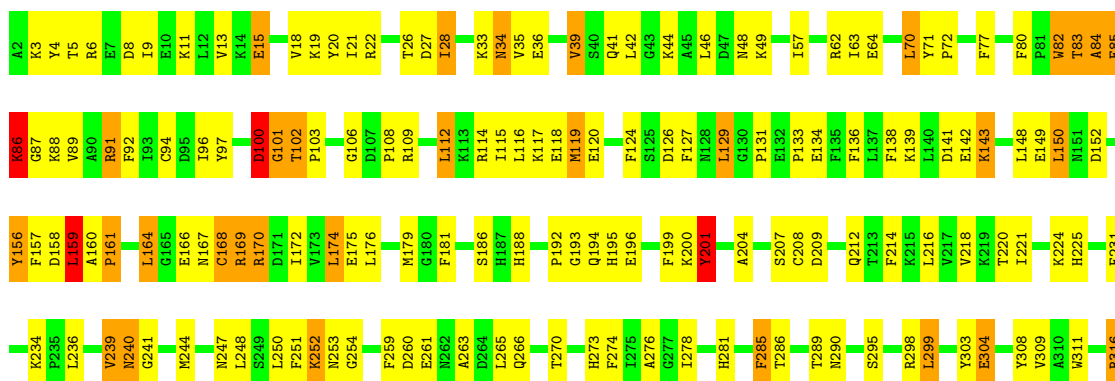
• Molecule 1: Glutamine synthetase

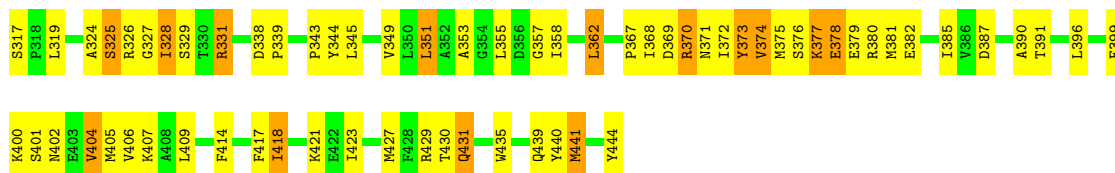
Chain H: 47% 43% 10%



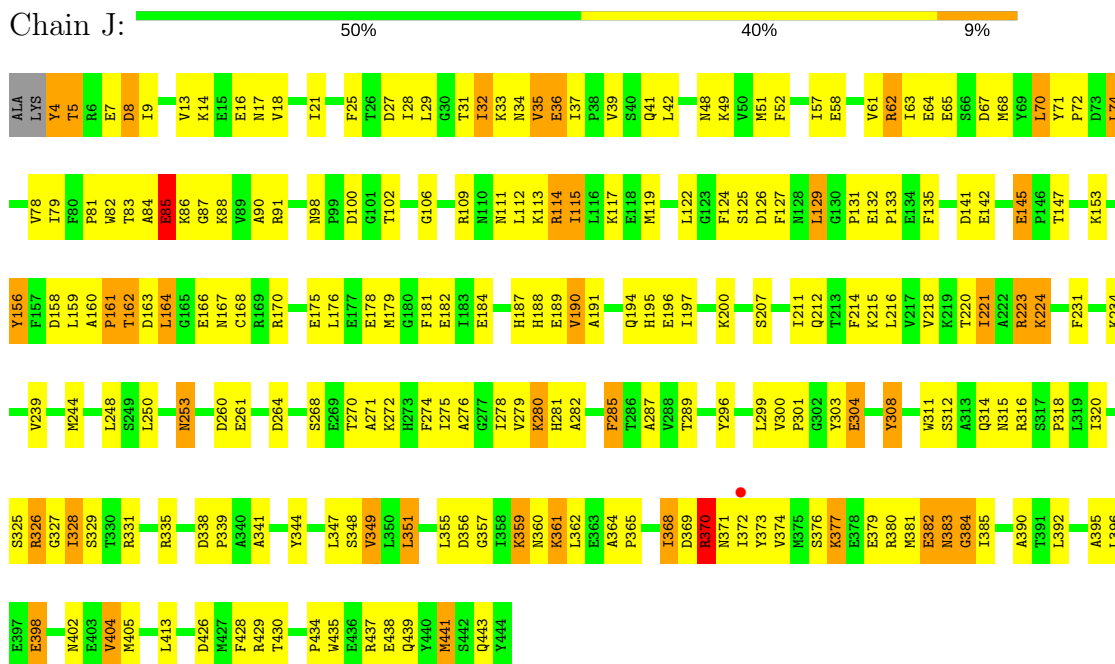
• Molecule 1: Glutamine synthetase

Chain I: 49% 40% 10%

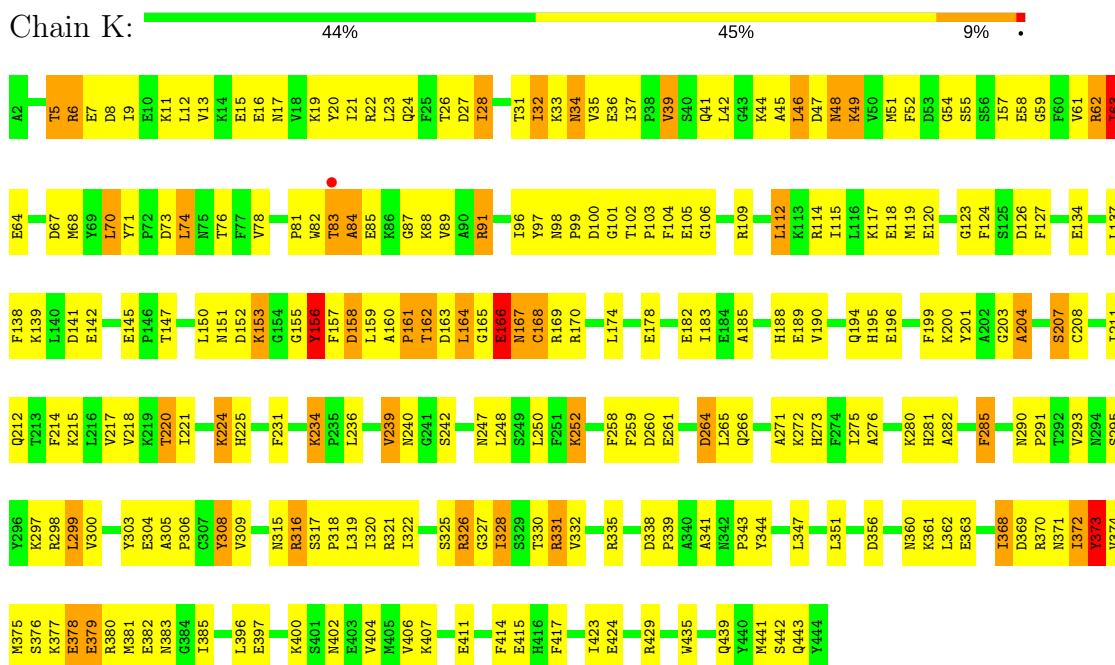




• Molecule 1: Glutamine synthetase

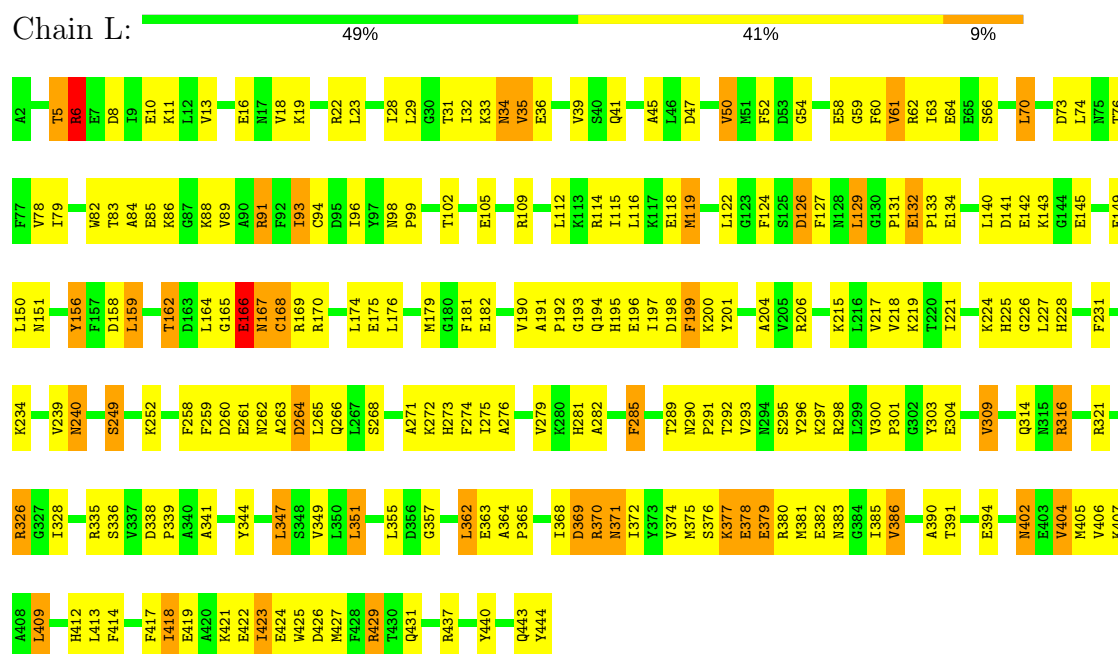


• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase

Chain L:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.00Å 137.50Å 137.70Å 119.80° 90.30° 93.40°	Depositor
Resolution (Å)	119.01 – 2.95 119.01 – 2.95	Depositor EDS
% Data completeness (in resolution range)	96.0 (119.01-2.95) 76.9 (119.01-2.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.194 , 0.259 0.186 , 0.194	Depositor DCC
$R_{free}$ test set	11493 reflections (7.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.2	Xtriage
Anisotropy	0.719	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 17.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.357 for -h,-k-l,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	42824	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG

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	0.43	0/3618	0.56	0/4895
1	B	0.44	0/3618	0.56	0/4895
1	C	0.44	0/3618	0.58	0/4895
1	D	0.45	1/3618 (0.0%)	0.58	0/4895
1	E	0.46	1/3618 (0.0%)	0.58	0/4895
1	F	0.45	0/3618	0.58	0/4895
1	G	0.44	0/3618	0.59	0/4895
1	H	0.43	0/3618	0.57	0/4895
1	I	0.44	0/3618	0.58	0/4895
1	J	0.45	0/3604	0.57	0/4877
1	K	0.46	0/3618	0.59	0/4895
1	L	0.44	0/3618	0.58	0/4895
All	All	0.45	2/43402 (0.0%)	0.58	0/58722

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	189	GLU	CD-OE2	5.29	1.31	1.25
1	E	168	CYS	CB-SG	-5.09	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3535	0	3466	222	0
1	B	3535	0	3466	238	0
1	C	3535	0	3466	210	0
1	D	3535	0	3466	216	0
1	E	3535	0	3466	218	0
1	F	3535	0	3466	251	0
1	G	3535	0	3466	211	0
1	H	3535	0	3466	228	0
1	I	3535	0	3466	232	0
1	J	3521	0	3448	212	0
1	K	3535	0	3466	261	0
1	L	3535	0	3466	207	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
2	K	3	0	0	0	0
2	L	3	0	0	0	0
3	A	9	0	7	0	0
3	B	9	0	7	1	0
3	C	9	0	7	3	0
3	D	9	0	7	1	0
3	E	9	0	7	2	0
3	F	9	0	7	1	0
3	G	9	0	7	0	0
3	H	9	0	7	5	0
3	I	9	0	7	1	0
3	J	9	0	7	1	0
3	K	9	0	7	1	0
3	L	10	0	7	0	0
4	A	5	0	0	3	0
4	C	5	0	0	3	0
4	G	5	0	0	2	0
4	H	5	0	0	1	0
5	A	16	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	20	0	0	1	0
5	C	18	0	0	0	0
5	D	29	0	0	4	0
5	E	18	0	0	2	0
5	F	19	0	0	4	0
5	G	14	0	0	0	0
5	H	21	0	0	2	0
5	I	21	0	0	0	0
5	J	27	0	0	1	0
5	K	27	0	0	2	0
5	L	23	0	0	0	0
All	All	42824	0	41658	2533	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 30.

All (2533) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:160:ALA:HB1	1:K:161:PRO:HD2	1.20	1.10
1:G:84:ALA:HB2	1:G:88:LYS:HD3	1.30	1.10
1:H:357:GLY:HA2	1:H:362:LEU:HD23	1.21	1.09
1:K:316:ARG:HD3	1:K:316:ARG:N	1.66	1.09
1:A:357:GLY:HA2	1:A:362:LEU:HD12	1.11	1.08
1:C:22:ARG:HG2	1:C:34:ASN:HD22	1.17	1.08
1:C:357:GLY:HA2	1:C:362:LEU:HD12	1.35	1.08
1:J:357:GLY:HA2	1:J:362:LEU:HD12	1.25	1.08
1:A:163:ASP:HA	1:A:170:ARG:HH21	1.03	1.08
1:E:160:ALA:HB1	1:E:161:PRO:HD2	1.34	1.07
1:E:22:ARG:HH11	1:E:22:ARG:HG2	1.15	1.06
1:J:328:ILE:HD13	1:J:328:ILE:H	1.18	1.05
1:I:170:ARG:HH11	1:I:170:ARG:HG2	1.20	1.05
1:D:6:ARG:HH11	1:D:6:ARG:HG3	1.21	1.05
1:D:160:ALA:HB1	1:D:161:PRO:HD2	1.35	1.05
1:L:377:LYS:HG2	1:L:378:GLU:H	1.22	1.05
1:A:163:ASP:HB3	1:B:83:THR:HG21	1.37	1.04
1:E:357:GLY:HA2	1:E:362:LEU:HD12	1.38	1.04
1:F:160:ALA:HB1	1:F:161:PRO:HD2	1.36	1.03
1:I:261:GLU:HA	1:I:266:GLN:HG2	1.35	1.03
1:G:164:LEU:HD11	1:L:224:LYS:HD3	1.40	1.03
1:B:325:SER:HB2	1:B:331:ARG:HH22	1.21	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:258:PHE:HB2	1:G:271:ALA:HB2	1.39	1.00
1:J:145:GLU:HA	1:J:145:GLU:OE1	1.61	1.00
1:F:377:LYS:HG2	1:F:378:GLU:N	1.72	1.00
1:H:147:THR:HG22	1:H:149:GLU:H	1.25	0.99
1:D:370:ARG:HB2	1:D:370:ARG:HH11	1.23	0.99
1:H:160:ALA:HB1	1:H:161:PRO:HD2	1.44	0.99
1:H:261:GLU:HA	1:H:266:GLN:HG2	1.42	0.99
1:H:131:PRO:HG2	1:H:199:PHE:HE1	1.24	0.98
1:C:164:LEU:HD11	1:D:224:LYS:HG3	1.42	0.98
1:L:105:GLU:OE2	1:L:412:HIS:HB3	1.62	0.98
1:J:64:GLU:HG2	1:K:316:ARG:HD2	1.46	0.98
1:K:316:ARG:NH2	1:K:370:ARG:HA	1.79	0.98
1:C:13:VAL:HG13	1:C:18:VAL:HB	1.45	0.98
1:E:328:ILE:H	1:E:328:ILE:HD12	1.26	0.97
1:J:371:ASN:HD22	1:J:374:VAL:HG12	1.30	0.96
1:E:84:ALA:O	1:E:85:GLU:HB2	1.66	0.96
1:L:119:MET:HE1	1:L:127:PHE:HB2	1.46	0.96
1:I:83:THR:HG21	1:I:89:VAL:HB	1.45	0.96
1:I:83:THR:O	1:I:85:GLU:HG3	1.67	0.95
1:B:371:ASN:HD22	1:B:374:VAL:HG13	1.32	0.95
1:B:281:HIS:HD2	1:B:402:ASN:HD21	0.96	0.95
1:J:383:ASN:HB2	1:J:385:ILE:HD13	1.49	0.95
1:I:85:GLU:O	1:I:86:LYS:HB3	1.66	0.94
1:H:273:HIS:CD2	1:H:361:LYS:HA	2.03	0.94
1:A:261:GLU:HA	1:A:266:GLN:HG2	1.50	0.94
1:C:371:ASN:HB3	1:C:374:VAL:HG12	1.48	0.93
1:G:164:LEU:HD13	1:L:224:LYS:HB2	1.49	0.93
1:E:85:GLU:HA	1:E:85:GLU:OE2	1.68	0.93
1:I:281:HIS:HD2	1:I:402:ASN:HD21	0.95	0.93
1:A:72:PRO:HA	1:A:94:CYS:HB3	1.51	0.92
1:I:150:LEU:HD13	1:I:192:PRO:HB2	1.50	0.92
1:C:371:ASN:HB3	1:C:374:VAL:CG1	1.99	0.92
1:F:232:MET:HE1	1:L:437:ARG:HA	1.50	0.92
1:H:285:PHE:HB2	1:H:349:VAL:HG11	1.52	0.92
1:H:223:ARG:HH22	1:H:228:HIS:HD2	1.09	0.92
1:H:131:PRO:HG2	1:H:199:PHE:CE1	2.03	0.91
1:A:281:HIS:HD2	1:A:402:ASN:HD21	1.14	0.91
1:D:160:ALA:HB3	1:D:169:ARG:HH12	1.35	0.91
1:F:377:LYS:HG2	1:F:378:GLU:H	1.31	0.91
1:C:22:ARG:HG2	1:C:34:ASN:ND2	1.85	0.91
1:I:160:ALA:HB1	1:I:161:PRO:HD2	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:280:LYS:HD3	1:K:281:HIS:CE1	2.05	0.91
1:K:115:ILE:HG22	1:K:351:LEU:HD12	1.51	0.91
1:A:132:GLU:OE2	4:A:504:PO4:O1	1.89	0.90
1:K:372:ILE:O	1:K:373:TYR:HB2	1.70	0.90
1:C:160:ALA:HB3	1:C:169:ARG:NH2	1.86	0.90
1:F:357:GLY:HA2	1:F:362:LEU:HD22	1.53	0.90
1:I:371:ASN:HB2	1:I:374:VAL:CG2	2.01	0.90
1:B:357:GLY:HA2	1:B:362:LEU:HD23	1.53	0.89
1:E:281:HIS:HD2	1:E:402:ASN:HD21	1.20	0.89
1:F:160:ALA:HB2	1:F:188:HIS:CD2	2.07	0.89
1:H:208:CYS:SG	1:H:347:LEU:HD23	2.12	0.89
1:E:83:THR:HG21	1:E:89:VAL:HB	1.53	0.89
1:I:281:HIS:CD2	1:I:402:ASN:HD21	1.88	0.89
1:J:74:LEU:H	1:J:74:LEU:HD22	1.37	0.89
1:J:368:ILE:HG21	1:J:372:ILE:HD11	1.52	0.88
1:A:163:ASP:HA	1:A:170:ARG:NH2	1.87	0.88
1:E:51:MET:HE3	1:E:67:ASP:HB3	1.56	0.88
1:F:160:ALA:HB3	1:F:169:ARG:NH2	1.87	0.88
1:I:370:ARG:HB2	1:I:371:ASN:OD1	1.73	0.88
1:B:160:ALA:HB3	1:B:169:ARG:HH12	1.38	0.87
1:G:258:PHE:CB	1:G:271:ALA:HB2	2.05	0.87
1:A:163:ASP:HB3	1:B:83:THR:CG2	2.03	0.87
1:D:261:GLU:HA	1:D:266:GLN:HG2	1.55	0.86
1:G:184:GLU:HG2	1:G:200:LYS:HD3	1.54	0.86
1:L:261:GLU:HA	1:L:266:GLN:HE21	1.39	0.86
1:H:273:HIS:HD2	1:H:361:LYS:HA	1.36	0.86
1:K:156:TYR:O	1:K:158:ASP:N	2.06	0.86
1:I:86:LYS:HG3	1:I:86:LYS:O	1.76	0.86
1:J:100:ASP:OD1	1:J:102:THR:HG22	1.76	0.86
1:H:223:ARG:HH22	1:H:228:HIS:CD2	1.93	0.86
1:B:281:HIS:CD2	1:B:402:ASN:HD21	1.89	0.85
1:G:160:ALA:HB1	1:G:161:PRO:HD2	1.54	0.85
1:L:402:ASN:HD21	1:L:404:VAL:HG13	1.41	0.85
1:E:316:ARG:HB2	1:E:370:ARG:HH12	1.39	0.85
1:F:285:PHE:HB2	1:F:349:VAL:CG1	2.07	0.85
1:F:375:MET:HB3	1:F:379:GLU:HB2	1.56	0.85
1:C:160:ALA:HB3	1:C:169:ARG:HH22	1.36	0.85
1:C:380:ARG:HB3	1:C:385:ILE:HB	1.59	0.85
1:H:160:ALA:HB3	1:H:169:ARG:HH12	1.42	0.85
1:I:160:ALA:HB3	1:I:169:ARG:HH12	1.41	0.84
1:D:170:ARG:HH12	1:E:85:GLU:HG2	1.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:231:PHE:HB3	1:J:339:PRO:HB2	1.58	0.84
1:K:100:ASP:OD1	1:K:102:THR:HG22	1.77	0.84
1:L:182:GLU:HG2	1:L:200:LYS:HD2	1.60	0.84
1:B:437:ARG:HD3	1:H:148:LEU:HD21	1.59	0.84
1:K:316:ARG:HH21	1:K:370:ARG:HD2	1.42	0.84
1:I:83:THR:CG2	1:I:89:VAL:HB	2.08	0.83
1:H:285:PHE:HB2	1:H:349:VAL:CG1	2.08	0.83
1:B:357:GLY:HA2	1:B:362:LEU:CD2	2.08	0.83
1:D:129:LEU:HG	1:D:347:LEU:HD11	1.60	0.83
1:F:371:ASN:O	1:F:374:VAL:HG22	1.79	0.83
1:D:325:SER:O	1:D:326:ARG:HD3	1.79	0.83
1:B:115:ILE:HG22	1:B:351:LEU:HD13	1.58	0.83
1:G:316:ARG:HH11	1:G:373:TYR:HB2	1.43	0.83
1:H:231:PHE:HB3	1:H:339:PRO:HB2	1.60	0.83
1:E:164:LEU:HD11	1:F:224:LYS:HG3	1.59	0.83
1:A:261:GLU:H	1:A:261:GLU:CD	1.79	0.83
1:K:22:ARG:HH11	1:K:22:ARG:HG2	1.42	0.83
1:B:371:ASN:O	1:B:374:VAL:HG22	1.79	0.82
1:B:370:ARG:HD3	1:B:371:ASN:N	1.94	0.82
1:E:328:ILE:N	1:E:328:ILE:HD12	1.94	0.82
1:E:314:GLN:HE21	1:F:64:GLU:HB3	1.45	0.82
1:G:370:ARG:H	1:G:370:ARG:HD3	1.44	0.82
1:I:357:GLY:HA2	1:I:362:LEU:HD22	1.62	0.82
1:L:357:GLY:HA2	1:L:362:LEU:HD22	1.61	0.82
1:E:375:MET:HE2	1:E:379:GLU:HB3	1.61	0.82
1:E:164:LEU:HD12	1:F:224:LYS:HB2	1.60	0.81
1:C:375:MET:HG2	1:C:379:GLU:HB3	1.61	0.81
1:A:224:LYS:HB2	1:F:164:LEU:CD1	2.11	0.81
1:H:281:HIS:HD2	1:H:402:ASN:HD21	1.28	0.81
1:L:119:MET:CE	1:L:127:PHE:HB2	2.10	0.81
1:G:78:VAL:HG13	1:G:91:ARG:HG3	1.62	0.81
1:A:63:ILE:HG22	1:A:64:GLU:HG3	1.62	0.81
1:I:377:LYS:HD3	1:I:378:GLU:OE2	1.79	0.81
1:K:20:TYR:OH	1:K:36:GLU:HG3	1.80	0.81
1:H:357:GLY:CA	1:H:362:LEU:HD23	2.08	0.81
1:K:160:ALA:CB	1:K:161:PRO:HD2	2.05	0.81
1:C:278:ILE:HG22	1:C:320:ILE:HD11	1.64	0.80
1:F:338:ASP:HB2	1:F:339:PRO:HD2	1.61	0.80
1:H:35:VAL:HG11	1:H:70:LEU:HD21	1.64	0.80
1:L:63:ILE:HG22	1:L:64:GLU:HG3	1.64	0.80
1:F:342:ASN:HD22	1:F:342:ASN:C	1.85	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:382:GLU:C	1:F:383:ASN:HD22	1.84	0.80
1:K:11:LYS:HE2	1:K:15:GLU:HG2	1.62	0.80
1:D:28:ILE:HG12	1:D:28:ILE:O	1.82	0.80
1:I:63:ILE:O	1:J:316:ARG:HD3	1.80	0.79
1:K:19:LYS:HD2	1:K:87:GLY:HA3	1.64	0.79
1:A:48:ASN:HB3	1:A:71:TYR:CD1	2.18	0.79
1:G:357:GLY:HA2	1:G:362:LEU:HD12	1.63	0.79
1:H:224:LYS:HG3	1:I:164:LEU:HD21	1.63	0.79
1:C:415:GLU:OE1	1:C:415:GLU:HA	1.81	0.79
1:E:176:LEU:O	1:E:181:PHE:HB2	1.82	0.79
1:B:127:PHE:CZ	1:B:248:LEU:HD22	2.17	0.79
1:L:231:PHE:HB3	1:L:339:PRO:HB2	1.65	0.79
1:F:371:ASN:HD22	1:F:374:VAL:HG13	1.48	0.79
1:H:32:ILE:HD11	1:I:159:LEU:HD23	1.64	0.79
1:H:63:ILE:HG22	1:H:64:GLU:HG3	1.62	0.79
1:A:163:ASP:CA	1:A:170:ARG:HH21	1.93	0.79
1:G:54:GLY:HA3	1:G:68:MET:HG3	1.65	0.79
1:A:164:LEU:HD11	1:B:224:LYS:HB2	1.65	0.79
1:G:115:ILE:HG22	1:G:351:LEU:HD13	1.65	0.78
1:K:33:LYS:HA	1:L:158:ASP:HA	1.64	0.78
1:L:423:ILE:O	1:L:427:MET:HG3	1.83	0.78
1:I:240:ASN:HD22	1:I:303:TYR:HD1	1.29	0.78
1:L:316:ARG:HD2	1:L:316:ARG:C	2.03	0.78
1:A:308:TYR:CE1	1:A:372:ILE:HD11	2.18	0.78
1:G:224:LYS:HB2	1:H:164:LEU:HD22	1.65	0.78
1:H:371:ASN:O	1:H:374:VAL:HG22	1.82	0.78
1:H:133:PRO:HD2	1:H:197:ILE:O	1.83	0.78
1:B:21:ILE:HD13	1:B:42:LEU:HD13	1.64	0.78
1:E:328:ILE:H	1:E:328:ILE:CD1	1.97	0.78
1:J:160:ALA:HB1	1:J:161:PRO:HD2	1.64	0.78
1:L:402:ASN:HD22	1:L:402:ASN:C	1.87	0.78
1:B:300:VAL:HG13	1:B:301:PRO:HD2	1.62	0.78
1:C:132:GLU:OE2	4:C:504:PO4:O2	2.00	0.78
1:I:371:ASN:HB2	1:I:374:VAL:HG21	1.63	0.78
1:I:64:GLU:HB3	1:J:314:GLN:NE2	1.99	0.77
1:A:119:MET:CE	1:A:127:PHE:HB2	2.13	0.77
1:C:100:ASP:OD1	1:C:102:THR:HG22	1.84	0.77
1:G:285:PHE:HB2	1:G:349:VAL:HG21	1.65	0.77
1:F:232:MET:HE2	1:L:440:TYR:HB2	1.65	0.77
1:J:98:ASN:HD22	1:J:102:THR:HG23	1.49	0.77
1:K:160:ALA:HB3	1:K:169:ARG:HH12	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:315:ASN:ND2	1:K:370:ARG:H	1.83	0.77
1:I:63:ILE:HG22	1:I:64:GLU:HG3	1.66	0.77
1:G:249:SER:HA	1:G:258:PHE:CZ	2.20	0.77
1:D:315:ASN:C	1:E:64:GLU:HG2	2.05	0.77
1:D:256:ASN:HD22	1:D:258:PHE:H	1.33	0.77
1:E:169:ARG:HH11	1:E:195:HIS:CD2	2.02	0.77
1:C:160:ALA:HB1	1:C:161:PRO:HD2	1.65	0.76
1:G:132:GLU:OE1	4:G:504:PO4:O1	2.02	0.76
1:K:383:ASN:HB2	1:K:385:ILE:HD13	1.64	0.76
1:G:311:TRP:CZ2	1:G:367:PRO:HG3	2.20	0.76
1:C:280:LYS:HD3	1:C:281:HIS:CE1	2.20	0.76
1:E:22:ARG:CG	1:E:22:ARG:HH11	1.98	0.76
1:L:377:LYS:HG2	1:L:378:GLU:N	1.98	0.76
1:D:256:ASN:ND2	1:D:258:PHE:H	1.83	0.76
1:A:41:GLN:HE22	1:F:200:LYS:NZ	1.83	0.76
1:E:357:GLY:HA2	1:E:362:LEU:CD1	2.16	0.76
1:H:28:ILE:HD12	1:H:413:LEU:HD23	1.66	0.76
1:K:51:MET:HE2	1:K:67:ASP:HB3	1.67	0.76
1:D:160:ALA:HB2	1:D:188:HIS:CD2	2.20	0.76
1:K:163:ASP:HA	1:K:170:ARG:HH21	1.49	0.75
1:E:22:ARG:HG2	1:E:22:ARG:NH1	1.94	0.75
1:H:371:ASN:HB3	1:H:374:VAL:HG13	1.66	0.75
1:B:150:LEU:HD13	1:B:192:PRO:HB2	1.66	0.75
1:D:6:ARG:NH1	1:D:6:ARG:HG3	1.97	0.75
1:E:51:MET:CE	1:E:67:ASP:HB3	2.16	0.75
1:J:83:THR:HG22	1:K:163:ASP:HB3	1.69	0.75
1:K:316:ARG:HD3	1:K:316:ARG:H	1.47	0.75
1:E:129:LEU:HD23	1:E:248:LEU:HD23	1.69	0.75
1:E:157:PHE:O	1:F:33:LYS:HB3	1.87	0.75
1:I:20:TYR:HB3	1:I:89:VAL:HG22	1.68	0.75
1:K:11:LYS:HG3	1:K:15:GLU:OE2	1.87	0.75
1:J:115:ILE:HG22	1:J:351:LEU:HD13	1.69	0.74
1:J:223:ARG:CG	1:J:223:ARG:HH11	2.00	0.74
1:K:63:ILE:O	1:L:316:ARG:HD3	1.87	0.74
1:I:169:ARG:HD2	1:I:186:SER:HB2	1.70	0.74
1:B:82:TRP:HE3	1:B:82:TRP:H	1.34	0.74
1:I:261:GLU:HA	1:I:266:GLN:CG	2.16	0.74
1:J:328:ILE:H	1:J:328:ILE:CD1	1.98	0.74
1:C:164:LEU:HD11	1:D:224:LYS:CG	2.15	0.74
1:F:28:ILE:HD11	1:F:417:PHE:HB2	1.70	0.74
1:G:316:ARG:NH1	1:G:373:TYR:HB2	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:281:HIS:HD2	1:I:402:ASN:ND2	1.79	0.74
1:G:338:ASP:HB2	1:G:339:PRO:HD2	1.70	0.74
1:G:6:ARG:O	1:G:10:GLU:HG3	1.88	0.74
1:D:165:GLY:O	5:D:617:HOH:O	2.05	0.74
1:J:328:ILE:HD13	1:J:328:ILE:N	1.99	0.74
1:A:281:HIS:CD2	1:A:402:ASN:HD21	2.04	0.74
1:D:234:LYS:HE3	1:D:239:VAL:O	1.87	0.74
1:I:170:ARG:HG2	1:I:170:ARG:NH1	2.00	0.74
1:K:9:ILE:HD13	1:K:74:LEU:HD12	1.70	0.73
1:A:3:LYS:HB3	1:A:75:ASN:OD1	1.87	0.73
1:J:224:LYS:HB2	1:K:164:LEU:HD21	1.70	0.73
1:F:285:PHE:HB2	1:F:349:VAL:HG11	1.69	0.73
1:F:85:GLU:O	1:F:86:LYS:HB2	1.86	0.73
1:A:30:GLY:HA2	1:A:342:ASN:ND2	2.02	0.73
1:I:6:ARG:HG3	1:I:46:LEU:HD13	1.69	0.73
1:B:377:LYS:O	1:B:381:MET:HG2	1.88	0.73
1:E:208:CYS:SG	1:E:347:LEU:HD12	2.27	0.73
1:H:131:PRO:CG	1:H:199:PHE:HE1	2.01	0.73
1:F:370:ARG:HG2	1:F:371:ASN:N	2.02	0.73
1:H:357:GLY:HA2	1:H:362:LEU:CD2	2.10	0.73
1:H:378:GLU:O	1:H:381:MET:HG3	1.87	0.73
1:D:370:ARG:HB2	1:D:370:ARG:NH1	2.03	0.73
1:K:11:LYS:O	1:K:15:GLU:HG3	1.88	0.73
1:K:315:ASN:HD21	1:K:370:ARG:H	1.37	0.73
1:D:406:VAL:HG22	1:D:414:PHE:CE1	2.24	0.73
1:J:371:ASN:ND2	1:J:374:VAL:H	1.87	0.73
1:J:398:GLU:OE2	5:J:614:HOH:O	2.06	0.73
1:H:300:VAL:HG13	1:H:301:PRO:HD2	1.69	0.72
1:J:63:ILE:HG22	1:K:316:ARG:HD2	1.71	0.72
1:B:223:ARG:HH11	1:B:223:ARG:HG3	1.55	0.72
1:G:403:GLU:O	1:G:407:LYS:HG2	1.87	0.72
1:H:5:THR:HG23	1:H:8:ASP:OD1	1.88	0.72
1:J:9:ILE:O	1:J:13:VAL:HG23	1.90	0.72
1:J:160:ALA:HB2	1:J:188:HIS:CD2	2.25	0.72
1:A:224:LYS:HB2	1:F:164:LEU:HD12	1.71	0.72
1:H:402:ASN:OD1	1:H:404:VAL:HG12	1.88	0.72
1:A:159:LEU:HG	1:B:34:ASN:OD1	1.88	0.72
1:E:160:ALA:CB	1:E:161:PRO:HD2	2.17	0.72
1:C:98:ASN:HD22	1:C:102:THR:HG23	1.55	0.72
1:F:97:TYR:HE2	1:F:103:PRO:HG3	1.54	0.72
1:F:232:MET:CE	1:L:437:ARG:HA	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:GLU:CD	1:A:261:GLU:N	2.42	0.72
1:D:418:ILE:O	1:D:422:GLU:HG3	1.88	0.72
1:E:265:LEU:O	1:E:326:ARG:NH1	2.22	0.72
1:B:4:TYR:HB3	1:B:9:ILE:HD11	1.72	0.72
1:H:214:PHE:O	1:H:218:VAL:HG23	1.88	0.72
1:C:403:GLU:O	1:C:407:LYS:HG3	1.90	0.72
1:E:311:TRP:CZ2	1:E:367:PRO:HG3	2.25	0.72
1:L:316:ARG:O	1:L:316:ARG:HD2	1.89	0.71
1:G:342:ASN:C	1:G:342:ASN:HD22	1.94	0.71
1:G:167:ASN:HD21	1:L:22:ARG:HH22	1.39	0.71
1:A:300:VAL:CG1	1:A:301:PRO:HD2	2.20	0.71
1:C:311:TRP:CZ2	1:C:367:PRO:HD3	2.25	0.71
1:G:155:GLY:O	1:G:156:TYR:O	2.08	0.71
1:J:129:LEU:HD13	1:J:131:PRO:HG3	1.73	0.71
1:B:309:VAL:HG23	1:B:386:VAL:O	1.90	0.71
1:G:82:TRP:CD1	1:G:83:THR:N	2.58	0.71
1:A:162:THR:HG22	1:A:163:ASP:N	2.06	0.71
1:F:419:GLU:O	1:F:423:ILE:HG23	1.90	0.71
1:B:82:TRP:HE1	1:B:220:THR:HG21	1.54	0.71
1:J:4:TYR:CD2	1:J:4:TYR:N	2.58	0.71
1:A:326:ARG:HD3	1:A:330:THR:OG1	1.89	0.71
1:F:376:SER:N	1:F:379:GLU:HG3	2.06	0.71
1:J:260:ASP:HB2	1:J:268:SER:HA	1.73	0.71
1:L:217:VAL:O	1:L:221:ILE:HG12	1.91	0.71
1:C:162:THR:HG21	1:D:220:THR:OG1	1.91	0.70
1:J:224:LYS:CB	1:K:164:LEU:HD21	2.21	0.70
1:K:160:ALA:HB2	1:K:188:HIS:HB2	1.73	0.70
1:B:182:GLU:O	1:B:200:LYS:HG3	1.91	0.70
1:B:281:HIS:HD2	1:B:402:ASN:ND2	1.81	0.70
1:G:156:TYR:O	1:G:158:ASP:N	2.24	0.70
1:G:328:ILE:HD12	1:G:328:ILE:N	2.06	0.70
1:A:359:LYS:HZ3	1:A:359:LYS:HB3	1.56	0.70
1:G:383:ASN:HB2	1:G:385:ILE:HD12	1.73	0.70
1:B:236:LEU:HB2	1:B:239:VAL:CG2	2.22	0.70
1:C:176:LEU:O	1:C:181:PHE:HB2	1.91	0.70
1:K:48:ASN:HB3	1:K:71:TYR:CD1	2.27	0.70
1:G:160:ALA:CB	1:G:188:HIS:CD2	2.74	0.70
1:G:86:LYS:O	1:G:86:LYS:HG3	1.90	0.70
1:J:279:VAL:HG11	1:J:365:PRO:HG2	1.74	0.70
1:E:160:ALA:HB3	1:E:169:ARG:HH12	1.57	0.70
1:K:51:MET:CE	1:K:67:ASP:HB3	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:TRP:CZ2	1:D:367:PRO:HG3	2.27	0.70
1:G:160:ALA:HB2	1:G:188:HIS:CD2	2.26	0.70
1:H:371:ASN:HB3	1:H:374:VAL:CG1	2.21	0.70
1:L:390:ALA:HB3	1:L:394:GLU:OE1	1.91	0.70
1:L:418:ILE:O	1:L:422:GLU:HG3	1.92	0.70
1:B:129:LEU:HD23	1:B:248:LEU:HD23	1.73	0.69
1:E:100:ASP:OD2	1:E:101:GLY:N	2.22	0.69
1:C:22:ARG:CG	1:C:34:ASN:ND2	2.55	0.69
1:C:435:TRP:O	1:C:439:GLN:HG2	1.91	0.69
1:E:28:ILE:HG22	1:E:57:ILE:O	1.92	0.69
1:H:321:ARG:HG2	1:H:335:ARG:HD2	1.73	0.69
1:B:84:ALA:HA	1:B:87:GLY:O	1.93	0.69
1:F:261:GLU:HA	1:F:266:GLN:NE2	2.07	0.69
1:F:259:PHE:CD2	1:F:327:GLY:HA2	2.27	0.69
1:H:223:ARG:NH2	1:H:228:HIS:HD2	1.85	0.69
1:E:316:ARG:HB2	1:E:370:ARG:NH1	2.07	0.69
1:F:28:ILE:HG22	1:F:57:ILE:O	1.91	0.69
1:J:435:TRP:O	1:J:439:GLN:HG2	1.92	0.69
1:J:98:ASN:HB2	1:J:102:THR:O	1.93	0.69
1:A:119:MET:HE1	1:A:127:PHE:HB2	1.74	0.69
1:A:359:LYS:NZ	1:A:359:LYS:HB3	2.08	0.69
1:D:160:ALA:CB	1:D:188:HIS:HD2	2.06	0.69
1:I:380:ARG:HA	1:I:385:ILE:HD12	1.74	0.69
1:E:285:PHE:HB2	1:E:349:VAL:HG11	1.74	0.69
1:F:160:ALA:CB	1:F:188:HIS:CD2	2.76	0.69
1:J:48:ASN:HB3	1:J:71:TYR:CE1	2.28	0.69
1:C:160:ALA:HB2	1:C:188:HIS:CD2	2.27	0.69
1:F:160:ALA:CB	1:F:188:HIS:HD2	2.04	0.69
1:F:368:ILE:HG21	1:F:372:ILE:HD11	1.74	0.69
1:J:4:TYR:HD2	1:J:4:TYR:N	1.89	0.69
1:J:189:GLU:OE1	3:J:503:GLN:OE1	2.11	0.69
1:B:13:VAL:HG13	1:B:18:VAL:HB	1.74	0.69
1:L:191:ALA:HB3	1:L:194:GLN:HE21	1.57	0.69
1:K:63:ILE:HG22	1:K:64:GLU:HG3	1.73	0.69
1:C:281:HIS:HD2	1:C:402:ASN:HD21	1.39	0.68
1:C:83:THR:HG22	1:C:85:GLU:OE2	1.92	0.68
1:E:140:LEU:HD12	1:E:226:GLY:C	2.12	0.68
1:K:375:MET:HG3	1:K:380:ARG:HG3	1.75	0.68
1:E:169:ARG:HH11	1:E:195:HIS:HD2	1.38	0.68
1:K:315:ASN:HB3	1:K:318:PRO:HG3	1.75	0.68
1:B:223:ARG:NH1	1:B:223:ARG:HG3	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:LEU:HB2	1:D:239:VAL:HG22	1.75	0.68
1:F:97:TYR:CE2	1:F:103:PRO:HG3	2.29	0.68
1:G:164:LEU:CD1	1:L:224:LYS:HB2	2.23	0.68
1:B:394:GLU:OE1	5:B:605:HOH:O	2.11	0.68
1:D:159:LEU:HD23	1:E:32:ILE:HD11	1.76	0.68
1:G:377:LYS:HZ2	1:G:380:ARG:HH22	1.41	0.68
1:G:4:TYR:HB3	1:G:9:ILE:CD1	2.24	0.68
1:H:147:THR:HG22	1:H:149:GLU:N	2.03	0.68
1:A:206:ARG:HH11	1:A:206:ARG:HG2	1.59	0.68
1:A:308:TYR:HE1	1:A:372:ILE:HD11	1.57	0.68
1:B:211:ILE:O	1:B:215:LYS:HG3	1.94	0.68
1:G:27:ASP:HB3	1:G:33:LYS:HE3	1.75	0.68
1:K:309:VAL:HA	1:K:319:LEU:HD23	1.76	0.68
1:A:282:ALA:HA	1:A:285:PHE:CZ	2.29	0.68
1:F:148:LEU:HD11	1:L:437:ARG:HD3	1.75	0.68
1:J:224:LYS:CG	1:K:164:LEU:HD21	2.24	0.68
1:B:81:PRO:HD2	1:B:82:TRP:CZ3	2.29	0.67
1:C:199:PHE:HZ	1:C:214:PHE:CD1	2.13	0.67
1:E:160:ALA:O	1:E:161:PRO:O	2.12	0.67
1:E:189:GLU:OE1	3:E:501:GLN:OE1	2.12	0.67
1:K:182:GLU:HB3	1:K:200:LYS:HD2	1.76	0.67
1:A:435:TRP:O	1:A:439:GLN:HG2	1.94	0.67
1:F:24:GLN:NE2	1:F:91:ARG:HH11	1.92	0.67
1:J:85:GLU:O	1:J:86:LYS:HB2	1.93	0.67
1:D:236:LEU:HB2	1:D:239:VAL:CG2	2.25	0.67
1:F:160:ALA:HB3	1:F:169:ARG:HH21	1.59	0.67
1:A:164:LEU:CD1	1:B:224:LYS:HB2	2.25	0.67
1:C:231:PHE:O	1:C:339:PRO:HG2	1.95	0.67
1:E:285:PHE:HB2	1:E:349:VAL:CG1	2.25	0.67
1:F:300:VAL:HG13	1:F:301:PRO:HD2	1.74	0.67
1:A:435:TRP:HB2	5:A:602:HOH:O	1.95	0.67
1:D:131:PRO:HG2	1:D:199:PHE:CD1	2.30	0.67
1:E:160:ALA:HB2	1:E:188:HIS:CD2	2.29	0.67
1:E:314:GLN:NE2	1:F:64:GLU:HB3	2.08	0.67
1:E:48:ASN:HB3	1:E:71:TYR:CD1	2.30	0.67
1:E:5:THR:HG23	1:E:8:ASP:OD1	1.95	0.67
1:G:142:GLU:CD	1:G:142:GLU:H	1.97	0.67
1:L:234:LYS:HD2	1:L:298:ARG:HA	1.76	0.67
1:C:45:ALA:HA	1:C:50:VAL:HG23	1.75	0.67
1:H:280:LYS:HD3	1:H:281:HIS:CE1	2.28	0.67
1:B:96:ILE:HD12	1:B:96:ILE:N	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:HIS:HD2	1:D:402:ASN:HD21	1.41	0.67
1:E:351:LEU:HD22	1:E:355:LEU:HG	1.77	0.67
1:E:316:ARG:CB	1:E:370:ARG:HH12	2.07	0.67
1:J:64:GLU:HG2	1:K:316:ARG:CD	2.22	0.67
1:K:281:HIS:HD2	1:K:402:ASN:HD21	1.41	0.67
1:D:83:THR:HG21	1:D:89:VAL:HB	1.75	0.67
1:H:315:ASN:ND2	1:H:373:TYR:OH	2.27	0.67
1:A:182:GLU:HB3	1:A:200:LYS:HG3	1.76	0.66
1:H:319:LEU:HD12	1:H:336:SER:HB3	1.77	0.66
1:I:150:LEU:CD1	1:I:192:PRO:HB2	2.24	0.66
1:K:13:VAL:HG21	1:K:42:LEU:CD2	2.25	0.66
1:K:308:TYR:CD1	1:K:372:ILE:HG13	2.29	0.66
1:A:83:THR:HG21	1:A:89:VAL:H	1.58	0.66
1:D:134:GLU:OE2	3:D:503:GLN:OE1	2.12	0.66
1:K:127:PHE:CZ	1:K:248:LEU:HD22	2.30	0.66
1:B:151:ASN:OD1	1:B:193:GLY:HA2	1.96	0.66
1:D:19:LYS:HG3	1:D:87:GLY:HA3	1.77	0.66
1:E:371:ASN:HA	1:E:374:VAL:CG2	2.26	0.66
1:A:169:ARG:NH2	1:A:195:HIS:ND1	2.43	0.66
1:F:285:PHE:HB2	1:F:349:VAL:HG13	1.76	0.66
1:I:308:TYR:CD1	1:I:372:ILE:HG22	2.30	0.66
1:J:27:ASP:OD1	1:J:31:THR:HB	1.95	0.66
1:K:298:ARG:NH2	1:K:338:ASP:HB3	2.11	0.66
1:A:264:ASP:OD1	1:A:264:ASP:N	2.29	0.66
1:C:48:ASN:HB3	1:C:71:TYR:CD1	2.31	0.66
1:G:371:ASN:OD1	1:G:371:ASN:N	2.27	0.66
1:I:27:ASP:HB3	1:I:33:LYS:HD2	1.78	0.66
1:L:371:ASN:OD1	1:L:374:VAL:HB	1.96	0.66
1:G:200:LYS:HE2	1:L:41:GLN:OE1	1.95	0.66
1:J:359:LYS:NZ	1:J:359:LYS:HB3	2.10	0.66
1:L:191:ALA:HB3	1:L:194:GLN:NE2	2.10	0.66
1:A:20:TYR:HB3	1:A:89:VAL:HG13	1.78	0.66
1:A:316:ARG:HD3	1:B:63:ILE:O	1.96	0.66
1:B:81:PRO:HD2	1:B:82:TRP:HZ3	1.61	0.66
1:C:236:LEU:HB2	1:C:239:VAL:CG2	2.26	0.66
1:D:260:ASP:O	1:D:266:GLN:HA	1.96	0.66
1:F:22:ARG:HH11	1:F:22:ARG:HG2	1.60	0.66
1:F:57:ILE:HD11	1:F:96:ILE:HG13	1.77	0.66
1:G:308:TYR:OH	1:G:372:ILE:HG23	1.96	0.66
1:J:371:ASN:ND2	1:J:374:VAL:HG12	2.08	0.66
1:K:13:VAL:HG21	1:K:42:LEU:HD21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:83:THR:HA	1:L:85:GLU:OE2	1.96	0.66
1:L:316:ARG:HB2	1:L:370:ARG:HH12	1.59	0.65
1:L:419:GLU:O	1:L:423:ILE:HG23	1.96	0.65
1:H:166:GLU:CD	1:H:166:GLU:O	2.35	0.65
1:I:338:ASP:HB2	1:I:339:PRO:HD2	1.77	0.65
1:B:371:ASN:ND2	1:B:374:VAL:HG13	2.08	0.65
1:A:160:ALA:HB1	1:A:161:PRO:HD2	1.78	0.65
1:C:338:ASP:HB2	1:C:339:PRO:HD2	1.78	0.65
1:D:372:ILE:HG13	1:D:373:TYR:H	1.60	0.65
1:E:381:MET:C	1:E:383:ASN:H	1.98	0.65
1:H:63:ILE:HG22	1:H:64:GLU:CG	2.26	0.65
1:C:371:ASN:O	1:C:374:VAL:HG13	1.97	0.65
1:A:36:GLU:OE2	1:F:169:ARG:NH1	2.30	0.65
1:H:142:GLU:H	1:H:142:GLU:CD	1.99	0.65
1:I:142:GLU:H	1:I:142:GLU:CD	1.98	0.65
1:C:357:GLY:CA	1:C:362:LEU:HD12	2.20	0.65
1:F:176:LEU:O	1:F:181:PHE:HB2	1.97	0.65
1:L:391:THR:OG1	1:L:394:GLU:HG3	1.97	0.65
1:L:70:LEU:HD12	1:L:94:CYS:HB3	1.77	0.65
1:C:443:GLN:HG2	1:C:444:TYR:CE2	2.32	0.65
1:D:11:LYS:O	1:D:15:GLU:HG3	1.97	0.65
1:F:156:TYR:HB2	1:F:190:VAL:HG12	1.79	0.65
1:F:380:ARG:HG2	1:F:385:ILE:HG21	1.79	0.65
1:H:261:GLU:HA	1:H:266:GLN:CG	2.23	0.65
1:L:402:ASN:ND2	1:L:405:MET:H	1.95	0.65
1:J:281:HIS:HD2	1:J:402:ASN:HD21	1.45	0.65
1:B:134:GLU:OE2	3:B:503:GLN:HB2	1.97	0.64
1:B:406:VAL:HG22	1:B:414:PHE:CE1	2.31	0.64
1:F:292:THR:O	1:F:295:SER:HB2	1.96	0.64
1:K:316:ARG:HH22	1:K:370:ARG:HA	1.62	0.64
1:D:170:ARG:NH1	1:E:85:GLU:HG2	2.09	0.64
1:G:67:ASP:O	1:G:68:MET:HG2	1.96	0.64
1:H:304:GLU:HG2	1:H:335:ARG:HH12	1.62	0.64
1:A:159:LEU:HD13	1:B:32:ILE:HD11	1.79	0.64
1:B:338:ASP:HB2	1:B:339:PRO:HD2	1.79	0.64
1:F:383:ASN:HD22	1:F:383:ASN:N	1.95	0.64
1:G:134:GLU:O	1:G:242:SER:HB3	1.98	0.64
1:L:273:HIS:O	1:L:276:ALA:HB3	1.98	0.64
1:B:381:MET:O	1:B:383:ASN:N	2.30	0.64
1:I:240:ASN:ND2	1:I:303:TYR:HD1	1.96	0.64
1:I:404:VAL:HG22	1:I:405:MET:HE2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:441:MET:O	1:J:441:MET:HG3	1.96	0.64
1:J:52:PHE:CE1	1:J:70:LEU:HD13	2.32	0.64
1:A:30:GLY:HA2	1:A:342:ASN:HD22	1.63	0.64
1:G:377:LYS:NZ	1:G:380:ARG:HH22	1.94	0.64
1:H:259:PHE:CZ	1:H:261:GLU:HB3	2.33	0.64
1:K:385:ILE:HD12	1:K:385:ILE:N	2.12	0.64
1:D:206:ARG:HH11	1:D:206:ARG:HG3	1.62	0.64
1:E:131:PRO:HG2	1:E:199:PHE:HD1	1.63	0.64
1:G:23:LEU:HB3	1:G:70:LEU:CD2	2.28	0.64
1:J:32:ILE:HD11	1:J:216:LEU:HD12	1.77	0.64
1:E:205:VAL:HG13	1:E:206:ARG:N	2.13	0.64
1:F:368:ILE:HG21	1:F:372:ILE:CD1	2.27	0.64
1:G:23:LEU:HB3	1:G:70:LEU:HD21	1.80	0.64
1:H:215:LYS:O	1:H:219:LYS:HG3	1.97	0.64
1:H:316:ARG:HB3	1:H:373:TYR:CE1	2.33	0.64
1:L:404:VAL:HG22	1:L:405:MET:HE2	1.79	0.64
1:A:162:THR:CG2	1:A:163:ASP:H	2.11	0.64
1:C:278:ILE:CG2	1:C:320:ILE:HD11	2.28	0.64
1:D:256:ASN:HD22	1:D:257:ALA:N	1.96	0.64
1:D:234:LYS:HG3	1:D:298:ARG:HA	1.80	0.64
1:D:28:ILE:HD11	1:D:417:PHE:HB2	1.79	0.64
1:G:245:HIS:ND1	4:G:504:PO4:O1	2.31	0.64
1:J:175:GLU:HG3	1:J:221:ILE:HD11	1.80	0.64
1:K:160:ALA:HB1	1:K:161:PRO:CD	2.12	0.64
1:B:407:LYS:HB3	1:B:407:LYS:NZ	2.13	0.64
1:E:231:PHE:HB3	1:E:339:PRO:HB2	1.79	0.64
1:H:317:SER:N	1:H:373:TYR:OH	2.31	0.64
1:L:83:THR:HG21	1:L:89:VAL:HB	1.79	0.64
1:D:160:ALA:CB	1:D:161:PRO:HD2	2.17	0.63
1:D:243:GLY:CA	1:D:298:ARG:NH1	2.61	0.63
1:E:316:ARG:H	1:E:370:ARG:NH1	1.96	0.63
1:H:224:LYS:HG3	1:I:164:LEU:CD2	2.28	0.63
1:A:314:GLN:NE2	5:A:614:HOH:O	2.30	0.63
1:C:109:ARG:HD2	1:C:344:TYR:CE2	2.33	0.63
1:L:224:LYS:HG2	1:L:225:HIS:CD2	2.34	0.63
1:L:231:PHE:HB3	1:L:339:PRO:CB	2.27	0.63
1:B:231:PHE:HB3	1:B:339:PRO:HB2	1.78	0.63
1:B:248:LEU:HB2	1:B:332:VAL:HG23	1.79	0.63
1:C:375:MET:HA	1:C:379:GLU:OE1	1.98	0.63
1:I:57:ILE:HD11	1:I:96:ILE:HG12	1.79	0.63
1:B:32:ILE:HD11	1:B:216:LEU:HD22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:PHE:HB3	1:C:339:PRO:HB2	1.81	0.63
1:D:162:THR:HG21	1:E:220:THR:OG1	1.97	0.63
1:F:402:ASN:O	1:F:406:VAL:HG23	1.97	0.63
1:I:236:LEU:HB2	1:I:239:VAL:HG13	1.79	0.63
1:I:231:PHE:HB3	1:I:339:PRO:HB2	1.80	0.63
1:L:303:TYR:O	1:L:304:GLU:HB2	1.98	0.63
1:E:357:GLY:CA	1:E:362:LEU:HD12	2.23	0.63
1:E:372:ILE:HG13	1:E:373:TYR:H	1.64	0.63
1:F:253:ASN:O	1:F:253:ASN:ND2	2.31	0.63
1:F:293:VAL:HB	1:L:440:TYR:OH	1.99	0.63
1:C:24:GLN:NE2	1:C:91:ARG:HH11	1.96	0.63
1:C:151:ASN:O	1:C:152:ASP:HB3	1.99	0.63
1:E:316:ARG:H	1:E:370:ARG:HH12	1.46	0.63
1:I:371:ASN:HB2	1:I:374:VAL:HG22	1.80	0.63
1:I:376:SER:HB2	1:I:377:LYS:NZ	2.13	0.63
1:J:189:GLU:OE2	1:J:190:VAL:HG12	1.99	0.63
1:E:55:SER:O	1:E:62:ARG:HG2	1.99	0.63
1:H:292:THR:O	1:H:295:SER:HB2	1.99	0.63
1:A:281:HIS:HD2	1:A:402:ASN:ND2	1.93	0.63
1:E:164:LEU:CD1	1:F:224:LYS:HG3	2.29	0.63
1:F:160:ALA:O	1:F:161:PRO:O	2.17	0.63
1:G:368:ILE:O	1:G:369:ASP:HB2	1.98	0.63
1:H:35:VAL:HG11	1:H:70:LEU:CD2	2.29	0.63
1:I:166:GLU:O	1:I:168:CYS:N	2.32	0.63
1:A:142:GLU:CD	1:A:142:GLU:H	1.99	0.62
1:D:166:GLU:HG2	1:D:168:CYS:H	1.64	0.62
1:E:201:TYR:O	1:E:201:TYR:CD2	2.52	0.62
1:B:150:LEU:CD1	1:B:192:PRO:HB2	2.29	0.62
1:B:296:TYR:HB3	1:B:390:ALA:O	1.99	0.62
1:F:441:MET:O	1:L:228:HIS:HE1	1.82	0.62
1:I:316:ARG:O	1:I:316:ARG:HD2	2.00	0.62
1:L:300:VAL:HG13	1:L:301:PRO:HD2	1.79	0.62
1:B:32:ILE:O	1:B:32:ILE:HG12	1.99	0.62
1:C:378:GLU:H	1:C:378:GLU:CD	2.02	0.62
1:D:115:ILE:HG22	1:D:351:LEU:HD12	1.82	0.62
1:F:281:HIS:HE1	1:F:356:ASP:OD2	1.82	0.62
1:I:170:ARG:HH11	1:I:170:ARG:CG	2.05	0.62
1:J:160:ALA:HB2	1:J:188:HIS:HD2	1.64	0.62
1:J:300:VAL:HG13	1:J:301:PRO:HD2	1.81	0.62
1:K:261:GLU:HA	1:K:266:GLN:NE2	2.14	0.62
1:A:30:GLY:CA	1:A:342:ASN:HD22	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ASN:C	1:A:34:ASN:ND2	2.52	0.62
1:F:24:GLN:HE21	1:F:91:ARG:HD3	1.64	0.62
1:H:265:LEU:O	1:H:326:ARG:NH1	2.32	0.62
1:I:440:TYR:HD1	1:I:444:TYR:HE2	1.48	0.62
1:L:170:ARG:HG2	1:L:170:ARG:HH11	1.65	0.62
1:G:83:THR:HG21	1:G:89:VAL:HB	1.82	0.62
1:H:380:ARG:O	1:H:385:ILE:HB	2.00	0.62
1:L:406:VAL:HG22	1:L:414:PHE:CE1	2.34	0.62
1:G:16:GLU:OE1	1:G:16:GLU:HA	1.98	0.62
1:K:220:THR:OG1	1:L:162:THR:HG21	1.98	0.62
1:E:77:PHE:HD1	1:E:92:PHE:CZ	2.18	0.62
1:F:132:GLU:OE2	1:F:245:HIS:ND1	2.33	0.62
1:I:80:PHE:CD1	1:I:89:VAL:HG12	2.35	0.62
1:J:359:LYS:NZ	1:J:359:LYS:CB	2.63	0.62
1:J:357:GLY:CA	1:J:362:LEU:HD12	2.16	0.62
1:K:160:ALA:O	1:K:162:THR:N	2.33	0.62
1:L:133:PRO:HD2	1:L:197:ILE:O	1.99	0.62
1:B:300:VAL:CG1	1:B:301:PRO:HD2	2.28	0.61
1:E:150:LEU:HD13	1:E:192:PRO:O	2.01	0.61
1:H:378:GLU:HA	1:H:381:MET:HG2	1.83	0.61
1:L:175:GLU:O	1:L:179:MET:HB2	2.00	0.61
1:A:355:LEU:O	1:A:359:LYS:HG2	1.99	0.61
1:E:23:LEU:HB3	1:E:70:LEU:HD23	1.80	0.61
1:G:312:SER:HB2	1:G:368:ILE:HG13	1.82	0.61
1:H:285:PHE:C	1:H:285:PHE:HD1	2.04	0.61
1:J:132:GLU:HB3	1:J:196:GLU:OE1	2.01	0.61
1:B:57:ILE:HD11	1:B:96:ILE:HG12	1.81	0.61
1:C:355:LEU:O	1:C:359:LYS:HG2	2.00	0.61
1:D:357:GLY:HA2	1:D:362:LEU:HD22	1.82	0.61
1:H:54:GLY:O	1:H:57:ILE:HD12	2.00	0.61
1:I:378:GLU:O	1:I:382:GLU:HB2	2.00	0.61
1:K:370:ARG:HH22	1:K:374:VAL:HG13	1.64	0.61
1:H:139:LYS:O	1:H:147:THR:HB	1.99	0.61
1:H:109:ARG:HG3	1:H:344:TYR:CE2	2.35	0.61
1:K:273:HIS:O	1:K:276:ALA:HB3	2.00	0.61
1:F:435:TRP:CD1	1:L:431:GLN:HG2	2.36	0.61
1:C:370:ARG:O	1:C:371:ASN:HB2	2.00	0.61
1:E:268:SER:O	1:E:272:LYS:HD2	2.00	0.61
1:E:371:ASN:HA	1:E:374:VAL:HG23	1.80	0.61
1:I:308:TYR:CD1	1:I:372:ILE:CG2	2.84	0.61
1:K:9:ILE:CD1	1:K:74:LEU:HD12	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:142:GLU:H	1:L:142:GLU:CD	2.04	0.61
1:A:359:LYS:NZ	1:A:359:LYS:CB	2.62	0.61
1:B:147:THR:HG22	1:B:148:LEU:N	2.15	0.61
1:B:21:ILE:CD1	1:B:42:LEU:HD13	2.30	0.61
1:F:54:GLY:O	1:F:57:ILE:HG13	2.01	0.61
1:G:224:LYS:HB2	1:H:164:LEU:CD2	2.31	0.61
1:I:199:PHE:HZ	1:I:214:PHE:CG	2.17	0.61
1:I:260:ASP:OD2	1:I:263:ALA:HB2	2.01	0.61
1:A:368:ILE:HD11	1:A:385:ILE:HD11	1.83	0.61
1:C:357:GLY:HA2	1:C:362:LEU:CD1	2.22	0.61
1:C:71:TYR:CG	1:C:97:TYR:HD1	2.18	0.61
1:D:163:ASP:HB2	1:E:82:TRP:HE1	1.66	0.61
1:H:351:LEU:HD22	1:H:355:LEU:HG	1.83	0.61
1:H:48:ASN:HB3	1:H:71:TYR:CD1	2.35	0.61
1:C:163:ASP:HB3	1:D:83:THR:HG22	1.83	0.61
1:D:160:ALA:O	1:D:161:PRO:O	2.18	0.61
1:G:249:SER:HA	1:G:258:PHE:CE1	2.36	0.61
1:H:396:LEU:HD22	1:H:418:ILE:HD13	1.82	0.61
1:J:359:LYS:HZ3	1:J:359:LYS:HB3	1.63	0.61
1:E:430:THR:HG22	1:K:300:VAL:HG11	1.82	0.61
1:C:71:TYR:CG	1:C:97:TYR:CD1	2.89	0.61
1:D:160:ALA:CB	1:D:188:HIS:CD2	2.83	0.61
1:D:290:ASN:HB3	1:D:295:SER:HB3	1.83	0.61
1:D:76:THR:O	1:D:78:VAL:HG23	2.01	0.61
1:E:129:LEU:HD13	1:E:131:PRO:HD3	1.81	0.61
1:K:22:ARG:HG2	1:K:22:ARG:NH1	2.14	0.61
1:A:119:MET:HE3	1:A:127:PHE:HB2	1.79	0.61
1:A:264:ASP:O	1:A:265:LEU:HB2	2.01	0.61
1:B:160:ALA:HB2	1:B:188:HIS:CD2	2.36	0.61
1:I:34:ASN:HD22	1:I:34:ASN:C	2.03	0.60
1:J:115:ILE:HG22	1:J:351:LEU:CD1	2.30	0.60
1:K:156:TYR:C	1:K:158:ASP:H	2.04	0.60
1:L:351:LEU:HD22	1:L:355:LEU:HG	1.81	0.60
1:A:290:ASN:HB3	1:A:295:SER:HB3	1.81	0.60
1:B:376:SER:HB2	1:B:379:GLU:HG3	1.83	0.60
1:D:26:THR:HG22	1:D:27:ASP:O	2.00	0.60
1:H:435:TRP:O	1:H:439:GLN:HG2	2.01	0.60
1:J:338:ASP:HB2	1:J:339:PRO:CD	2.31	0.60
1:F:232:MET:CE	1:L:440:TYR:HB2	2.32	0.60
1:J:74:LEU:HD22	1:J:74:LEU:N	2.14	0.60
1:L:402:ASN:ND2	1:L:402:ASN:C	2.55	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ASN:HD22	1:A:34:ASN:C	2.05	0.60
1:L:309:VAL:HG23	1:L:386:VAL:O	2.02	0.60
1:A:114:ARG:NH1	1:A:115:ILE:HD11	2.16	0.60
1:D:377:LYS:O	1:D:381:MET:HB2	2.01	0.60
1:H:168:CYS:O	1:H:172:ILE:HG13	2.00	0.60
1:I:325:SER:O	1:I:326:ARG:HD3	2.02	0.60
1:F:160:ALA:HB3	1:F:169:ARG:HH22	1.66	0.60
1:F:24:GLN:NE2	1:F:91:ARG:HD3	2.16	0.60
1:K:54:GLY:HA3	1:K:68:MET:SD	2.42	0.60
1:A:127:PHE:CE2	1:A:351:LEU:HB2	2.37	0.60
1:C:316:ARG:HD3	1:D:63:ILE:O	2.01	0.60
1:I:80:PHE:HD1	1:I:89:VAL:HG12	1.67	0.60
1:D:133:PRO:HG3	1:D:199:PHE:HE1	1.66	0.60
1:D:200:LYS:O	1:D:201:TYR:O	2.20	0.60
1:D:84:ALA:HA	1:D:87:GLY:O	2.02	0.60
1:A:273:HIS:O	1:A:276:ALA:HB3	2.01	0.60
1:C:299:LEU:HD12	1:C:306:PRO:O	2.02	0.60
1:H:23:LEU:HB2	1:H:35:VAL:HG13	1.84	0.60
1:I:371:ASN:O	1:I:375:MET:HG2	2.02	0.60
1:J:74:LEU:CD2	1:J:74:LEU:H	2.12	0.60
1:F:187:HIS:HD2	1:F:188:HIS:O	1.85	0.60
1:I:234:LYS:HE3	1:I:239:VAL:O	2.02	0.60
1:A:162:THR:CG2	1:A:163:ASP:N	2.64	0.59
1:C:300:VAL:HG13	1:C:301:PRO:HD2	1.82	0.59
1:D:264:ASP:O	1:D:265:LEU:HB2	2.02	0.59
1:E:129:LEU:HD23	1:E:248:LEU:CD2	2.31	0.59
1:H:63:ILE:O	1:I:316:ARG:HD3	2.01	0.59
1:K:37:ILE:HD12	1:K:41:GLN:HB2	1.83	0.59
1:A:164:LEU:HD11	1:B:224:LYS:CB	2.31	0.59
1:G:371:ASN:O	1:G:374:VAL:HG13	2.02	0.59
1:G:374:VAL:HG22	1:G:375:MET:N	2.17	0.59
1:K:328:ILE:HG13	1:K:328:ILE:O	2.02	0.59
1:K:83:THR:O	1:K:84:ALA:HB3	2.02	0.59
1:L:300:VAL:CG1	1:L:301:PRO:HD2	2.32	0.59
1:A:207:SER:O	1:A:211:ILE:HG13	2.02	0.59
1:C:160:ALA:CB	1:C:188:HIS:CD2	2.85	0.59
1:D:383:ASN:HB2	1:D:385:ILE:HG12	1.84	0.59
1:F:342:ASN:HD22	1:F:343:PRO:N	2.01	0.59
1:H:12:LEU:O	1:H:16:GLU:HB2	2.02	0.59
1:I:109:ARG:NH1	1:I:209:ASP:OD1	2.35	0.59
1:I:368:ILE:HD13	1:I:370:ARG:NH2	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:129:LEU:CD1	1:J:131:PRO:HG3	2.32	0.59
1:J:370:ARG:HH11	1:J:370:ARG:HG2	1.67	0.59
1:K:363:GLU:OE2	1:K:363:GLU:HA	2.00	0.59
1:K:28:ILE:HD11	1:K:417:PHE:HB2	1.85	0.59
1:C:328:ILE:HD13	1:C:328:ILE:H	1.68	0.59
1:G:96:ILE:HG12	1:G:107:ASP:CG	2.23	0.59
1:G:116:LEU:HD23	1:G:351:LEU:HD11	1.83	0.59
1:D:228:HIS:HE1	1:J:441:MET:O	1.86	0.59
1:L:119:MET:HG2	1:L:124:PHE:HB2	1.84	0.59
1:A:164:LEU:HD11	1:B:224:LYS:CG	2.33	0.59
1:B:83:THR:O	1:B:84:ALA:HB2	2.02	0.59
1:E:224:LYS:O	1:E:224:LYS:HD2	2.01	0.59
1:F:22:ARG:HD2	1:F:80:PHE:HE1	1.67	0.59
1:G:224:LYS:HD2	1:H:164:LEU:HD21	1.84	0.59
1:E:316:ARG:N	1:E:370:ARG:HH12	2.01	0.59
1:B:160:ALA:HB1	1:B:161:PRO:HD2	1.85	0.59
1:E:77:PHE:HB2	1:E:92:PHE:CE2	2.38	0.59
1:F:368:ILE:HG21	1:F:372:ILE:CG1	2.32	0.59
1:G:156:TYR:C	1:G:158:ASP:H	2.04	0.59
1:G:357:GLY:HA2	1:G:362:LEU:CD1	2.30	0.59
1:G:52:PHE:CE1	1:G:70:LEU:HD12	2.38	0.59
1:K:142:GLU:H	1:K:142:GLU:CD	2.04	0.59
1:A:20:TYR:OH	1:A:36:GLU:HG3	2.02	0.59
1:D:275:ILE:HD13	1:D:275:ILE:H	1.68	0.59
1:D:303:TYR:O	1:D:304:GLU:HB2	2.01	0.59
1:E:4:TYR:HB3	1:E:9:ILE:CD1	2.33	0.59
1:H:319:LEU:CD1	1:H:336:SER:HB3	2.32	0.59
1:I:80:PHE:HD2	1:I:179:MET:CE	2.15	0.59
1:L:28:ILE:CD1	1:L:58:GLU:HA	2.33	0.59
1:B:282:ALA:HA	1:B:285:PHE:CZ	2.38	0.59
1:C:141:ASP:OD1	1:C:145:GLU:HB2	2.03	0.59
1:D:131:PRO:HG2	1:D:199:PHE:HD1	1.68	0.59
1:E:311:TRP:CH2	1:E:367:PRO:HG3	2.38	0.59
1:H:272:LYS:HZ2	1:H:364:ALA:HB3	1.67	0.59
1:J:338:ASP:HB2	1:J:339:PRO:HD2	1.85	0.59
1:C:52:PHE:CE1	1:C:70:LEU:HD13	2.38	0.59
1:G:82:TRP:HD1	1:G:83:THR:N	2.01	0.59
1:L:417:PHE:O	1:L:421:LYS:HG2	2.03	0.59
1:B:318:PRO:O	1:B:335:ARG:HD3	2.03	0.58
1:C:134:GLU:OE1	3:C:502:GLN:N	2.37	0.58
1:C:351:LEU:HD22	1:C:355:LEU:HG	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ARG:C	1:C:91:ARG:HD2	2.23	0.58
1:D:224:LYS:HE2	1:D:225:HIS:CE1	2.38	0.58
1:D:243:GLY:HA2	1:D:298:ARG:NH1	2.18	0.58
1:F:440:TYR:OH	1:L:293:VAL:HB	2.03	0.58
1:G:129:LEU:CD1	1:G:347:LEU:HD21	2.33	0.58
1:K:231:PHE:HB3	1:K:339:PRO:HB2	1.83	0.58
1:G:164:LEU:CD1	1:L:224:LYS:HD3	2.26	0.58
1:A:22:ARG:HH22	1:F:167:ASN:HD21	1.50	0.58
1:A:319:LEU:HD12	1:A:336:SER:HB3	1.84	0.58
1:C:365:PRO:O	1:C:366:ALA:HB2	2.01	0.58
1:F:27:ASP:HB3	1:F:33:LYS:HD2	1.85	0.58
1:F:328:ILE:H	1:F:328:ILE:HD12	1.68	0.58
1:F:368:ILE:HG21	1:F:372:ILE:HG13	1.85	0.58
1:F:298:ARG:NH1	3:F:503:GLN:O	2.36	0.58
1:G:281:HIS:HE1	1:G:356:ASP:OD2	1.86	0.58
1:K:17:ASN:HD22	1:K:87:GLY:HA2	1.67	0.58
1:E:163:ASP:HB3	1:F:83:THR:HG22	1.85	0.58
1:I:126:ASP:HB2	1:I:251:PHE:HB2	1.84	0.58
1:I:329:SER:O	1:I:331:ARG:HD2	2.02	0.58
1:K:338:ASP:HB2	1:K:339:PRO:HD2	1.85	0.58
1:L:264:ASP:N	1:L:264:ASP:OD1	2.36	0.58
1:L:261:GLU:HA	1:L:266:GLN:NE2	2.13	0.58
1:A:160:ALA:HB3	1:A:169:ARG:HH12	1.69	0.58
1:E:208:CYS:SG	1:E:347:LEU:CD1	2.91	0.58
1:H:281:HIS:NE2	1:H:404:VAL:HG11	2.18	0.58
1:D:275:ILE:HD13	1:D:275:ILE:N	2.19	0.58
1:D:282:ALA:HA	1:D:285:PHE:CZ	2.39	0.58
1:J:380:ARG:O	1:J:385:ILE:HB	2.03	0.58
1:L:109:ARG:HG3	1:L:344:TYR:CE2	2.38	0.58
1:B:16:GLU:OE2	1:B:16:GLU:HA	2.03	0.58
1:E:252:LYS:O	1:E:253:ASN:HB2	2.03	0.58
1:I:308:TYR:HD1	1:I:372:ILE:CG2	2.17	0.58
1:K:280:LYS:HD2	1:K:362:LEU:HD21	1.84	0.58
1:C:27:ASP:HB3	1:C:33:LYS:HE3	1.86	0.58
1:C:371:ASN:HB3	1:C:374:VAL:HG11	1.85	0.58
1:D:265:LEU:O	1:D:326:ARG:NH1	2.34	0.58
1:E:134:GLU:OE2	3:E:501:GLN:HB2	2.03	0.58
1:J:129:LEU:HB3	1:J:207:SER:OG	2.03	0.58
1:A:289:THR:O	1:A:341:ALA:HB2	2.02	0.58
1:K:27:ASP:OD1	1:K:31:THR:HB	2.04	0.58
1:A:217:VAL:O	1:A:221:ILE:HG12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:ARG:O	1:B:441:MET:HB3	2.04	0.58
1:E:308:TYR:HH	1:E:373:TYR:HD1	1.51	0.58
1:H:285:PHE:C	1:H:285:PHE:CD1	2.77	0.58
1:I:285:PHE:HB2	1:I:349:VAL:HG11	1.86	0.58
1:D:217:VAL:O	1:D:221:ILE:HG12	2.03	0.58
1:E:318:PRO:O	1:E:335:ARG:HD3	2.04	0.58
1:F:252:LYS:O	1:F:255:VAL:HG23	2.04	0.58
1:I:160:ALA:HB2	1:I:188:HIS:HB2	1.86	0.58
1:I:231:PHE:O	1:I:339:PRO:HG2	2.03	0.58
1:J:223:ARG:HG3	1:J:223:ARG:HH11	1.68	0.58
1:A:28:ILE:HD11	1:A:417:PHE:HB2	1.86	0.57
1:C:146:PRO:HG3	1:C:228:HIS:CD2	2.39	0.57
1:G:5:THR:HG23	1:G:8:ASP:CG	2.23	0.57
1:I:19:LYS:HA	1:I:39:VAL:HB	1.85	0.57
1:C:431:GLN:HG2	1:I:435:TRP:CD1	2.39	0.57
1:L:423:ILE:HG13	1:L:424:GLU:N	2.19	0.57
1:A:22:ARG:NH2	1:F:167:ASN:HD21	2.02	0.57
1:B:169:ARG:NH2	1:B:195:HIS:ND1	2.52	0.57
1:C:109:ARG:HG2	1:C:109:ARG:HH21	1.69	0.57
1:G:318:PRO:O	1:G:335:ARG:HD3	2.03	0.57
1:G:5:THR:H	1:G:8:ASP:HB2	1.69	0.57
1:A:160:ALA:O	1:A:161:PRO:O	2.21	0.57
1:A:357:GLY:HA2	1:A:362:LEU:CD1	2.06	0.57
1:B:18:VAL:HG21	1:B:79:ILE:HD12	1.84	0.57
1:C:290:ASN:HB3	1:C:295:SER:HB3	1.87	0.57
1:D:166:GLU:HG2	1:D:168:CYS:N	2.18	0.57
1:D:207:SER:O	1:D:211:ILE:HG13	2.05	0.57
1:E:311:TRP:CB	1:E:320:ILE:HB	2.34	0.57
1:B:23:LEU:HB3	1:B:70:LEU:HD23	1.86	0.57
1:D:28:ILE:HD11	1:D:417:PHE:CA	2.34	0.57
1:J:282:ALA:HA	1:J:285:PHE:CE2	2.40	0.57
1:B:160:ALA:HB1	1:B:161:PRO:CD	2.34	0.57
1:E:13:VAL:HG13	1:E:18:VAL:HB	1.86	0.57
1:G:383:ASN:HB2	1:G:385:ILE:CD1	2.34	0.57
1:H:22:ARG:NH1	1:H:36:GLU:OE1	2.37	0.57
1:I:440:TYR:HD1	1:I:444:TYR:CE2	2.22	0.57
1:J:142:GLU:CD	1:J:142:GLU:H	2.07	0.57
1:J:70:LEU:O	1:J:72:PRO:HD3	2.05	0.57
1:B:325:SER:HB2	1:B:331:ARG:NH2	2.05	0.57
1:B:409:LEU:O	1:B:413:LEU:HD12	2.03	0.57
1:G:377:LYS:HD2	1:G:387:ASP:OD1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:86:LYS:HE2	1:J:178:GLU:OE1	2.05	0.57
1:J:182:GLU:HB3	1:J:200:LYS:HD3	1.86	0.57
1:J:32:ILE:CD1	1:J:216:LEU:HD12	2.34	0.57
1:H:129:LEU:CD1	1:H:347:LEU:HD21	2.34	0.57
1:I:64:GLU:HB3	1:J:314:GLN:HE21	1.68	0.57
1:A:300:VAL:HG12	1:A:301:PRO:HD2	1.86	0.57
1:B:162:THR:HG22	1:B:163:ASP:H	1.68	0.57
1:B:280:LYS:HD3	1:B:281:HIS:CE1	2.40	0.57
1:B:314:GLN:HG3	1:B:314:GLN:O	2.05	0.57
1:B:18:VAL:HG21	1:B:79:ILE:CD1	2.35	0.57
1:C:311:TRP:O	1:C:367:PRO:HA	2.04	0.57
1:E:435:TRP:O	1:E:439:GLN:HG2	2.03	0.57
1:F:380:ARG:HG2	1:F:385:ILE:CG2	2.35	0.57
1:H:385:ILE:N	1:H:385:ILE:HD13	2.19	0.57
1:J:371:ASN:HD21	1:J:373:TYR:HB2	1.69	0.57
1:K:335:ARG:NH2	5:K:607:HOH:O	2.37	0.57
1:B:435:TRP:O	1:B:439:GLN:HG2	2.05	0.57
1:C:414:PHE:O	1:C:418:ILE:HD13	2.04	0.57
1:F:376:SER:H	1:F:379:GLU:HG3	1.68	0.57
1:G:129:LEU:HD11	1:G:347:LEU:HD21	1.86	0.57
1:G:22:ARG:NH1	1:G:36:GLU:HG2	2.19	0.57
1:G:282:ALA:HA	1:G:285:PHE:CE2	2.39	0.57
1:L:182:GLU:HG2	1:L:200:LYS:CD	2.34	0.57
1:J:28:ILE:HG13	1:J:57:ILE:O	2.05	0.57
1:K:212:GLN:HE22	1:K:215:LYS:NZ	2.02	0.57
1:A:162:THR:HG22	1:A:163:ASP:H	1.65	0.56
1:G:378:GLU:OE2	1:G:378:GLU:HA	2.04	0.56
1:K:78:VAL:HG21	1:K:91:ARG:NH2	2.20	0.56
1:A:215:LYS:HG2	1:A:231:PHE:CE2	2.40	0.56
1:A:443:GLN:HE21	1:A:444:TYR:HE2	1.51	0.56
1:H:377:LYS:HA	1:H:380:ARG:NH2	2.20	0.56
1:K:316:ARG:NH2	1:K:370:ARG:HD2	2.17	0.56
1:A:330:THR:HG22	1:A:330:THR:O	2.04	0.56
1:B:311:TRP:CE2	1:B:367:PRO:HB3	2.40	0.56
1:B:311:TRP:CZ2	1:B:367:PRO:HB3	2.39	0.56
1:C:298:ARG:NH1	3:C:502:GLN:O	2.39	0.56
1:E:127:PHE:CD2	1:E:351:LEU:HG	2.40	0.56
1:E:240:ASN:O	5:E:602:HOH:O	2.18	0.56
1:E:84:ALA:O	1:E:85:GLU:CB	2.45	0.56
1:F:160:ALA:HB1	1:F:161:PRO:CD	2.24	0.56
1:F:435:TRP:HB2	5:F:613:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:434:PRO:O	1:F:438:GLU:HG3	2.05	0.56
1:G:285:PHE:HB2	1:G:349:VAL:CG2	2.32	0.56
1:H:34:ASN:HB3	1:I:159:LEU:HD22	1.87	0.56
1:I:11:LYS:O	1:I:15:GLU:HB2	2.05	0.56
1:J:426:ASP:O	1:J:430:THR:HG23	2.05	0.56
1:K:32:ILE:HD11	1:L:159:LEU:HD23	1.88	0.56
1:K:406:VAL:HG22	1:K:414:PHE:CE1	2.40	0.56
1:L:260:ASP:O	1:L:266:GLN:HA	2.05	0.56
1:L:292:THR:O	1:L:295:SER:HB2	2.05	0.56
1:A:309:VAL:HG13	1:A:319:LEU:HD22	1.87	0.56
1:D:383:ASN:C	1:D:385:ILE:H	2.06	0.56
1:I:345:LEU:HD22	1:I:409:LEU:CD2	2.35	0.56
1:B:164:LEU:HD12	1:C:220:THR:HG22	1.86	0.56
1:C:234:LYS:HE3	1:C:239:VAL:O	2.05	0.56
1:F:377:LYS:CG	1:F:378:GLU:N	2.57	0.56
1:G:125:SER:C	1:G:126:ASP:OD2	2.43	0.56
1:I:399:PHE:HZ	1:I:409:LEU:HD12	1.70	0.56
1:K:104:PHE:CZ	1:K:106:GLY:HA3	2.40	0.56
1:K:371:ASN:O	1:K:374:VAL:HG22	2.05	0.56
1:A:338:ASP:HB2	1:A:339:PRO:HD2	1.88	0.56
1:C:213:THR:O	1:C:216:LEU:HB3	2.06	0.56
1:C:329:SER:O	1:C:331:ARG:HD3	2.06	0.56
1:E:300:VAL:HG13	1:E:301:PRO:HD2	1.88	0.56
1:G:374:VAL:CG2	1:G:375:MET:N	2.67	0.56
1:K:236:LEU:HB2	1:K:239:VAL:HG23	1.88	0.56
1:G:162:THR:HG22	1:G:163:ASP:H	1.70	0.56
1:G:42:LEU:HD12	1:G:42:LEU:O	2.05	0.56
1:I:417:PHE:O	1:I:421:LYS:HG2	2.05	0.56
1:K:208:CYS:SG	1:K:343:PRO:HB2	2.45	0.56
1:K:370:ARG:NH2	1:K:374:VAL:HG22	2.19	0.56
1:A:160:ALA:HB2	1:A:188:HIS:CD2	2.41	0.56
1:B:381:MET:C	1:B:383:ASN:H	2.09	0.56
1:F:206:ARG:O	1:F:206:ARG:HD3	2.06	0.56
1:C:349:VAL:HG22	1:C:405:MET:SD	2.45	0.56
1:K:281:HIS:HE1	1:K:356:ASP:OD1	1.88	0.56
1:A:95:ASP:OD1	1:A:109:ARG:HD2	2.05	0.56
1:B:80:PHE:HB3	1:B:82:TRP:CZ3	2.41	0.56
1:E:160:ALA:CB	1:E:169:ARG:HH12	2.19	0.56
1:F:383:ASN:ND2	1:F:383:ASN:N	2.52	0.56
1:I:285:PHE:HB2	1:I:349:VAL:CG1	2.36	0.56
1:J:325:SER:O	1:J:326:ARG:HD3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:155:GLY:O	1:K:156:TYR:O	2.24	0.56
1:K:250:LEU:HB2	1:K:258:PHE:CE2	2.41	0.56
1:K:37:ILE:CD1	1:K:45:ALA:HB2	2.35	0.56
1:L:166:GLU:HG3	1:L:167:ASN:H	1.71	0.56
1:A:405:MET:O	1:A:408:ALA:HB3	2.06	0.56
1:C:164:LEU:HD11	1:D:224:LYS:CB	2.36	0.56
1:D:363:GLU:HA	1:D:363:GLU:OE1	2.04	0.56
1:E:3:LYS:HE2	1:E:4:TYR:CE1	2.41	0.56
1:H:378:GLU:HA	1:H:381:MET:CG	2.36	0.56
3:H:503:GLN:N	5:H:601:HOH:O	2.38	0.56
1:J:106:GLY:O	1:J:413:LEU:HD21	2.06	0.56
1:B:129:LEU:HD21	1:B:246:CYS:HB3	1.87	0.55
1:D:107:ASP:HB3	1:D:110:ASN:HB2	1.87	0.55
1:D:385:ILE:HD13	1:D:385:ILE:N	2.21	0.55
1:G:78:VAL:HG13	1:G:91:ARG:CG	2.35	0.55
1:H:16:GLU:HA	1:H:16:GLU:OE1	2.06	0.55
1:J:160:ALA:CB	1:J:188:HIS:HD2	2.18	0.55
1:J:223:ARG:HG3	1:J:223:ARG:NH1	2.21	0.55
1:K:152:ASP:O	1:K:153:LYS:HE3	2.06	0.55
1:L:176:LEU:O	1:L:181:PHE:HB2	2.06	0.55
1:L:19:LYS:HA	1:L:39:VAL:HB	1.87	0.55
1:C:97:TYR:CD2	1:C:103:PRO:HA	2.41	0.55
1:D:275:ILE:N	1:D:275:ILE:CD1	2.69	0.55
1:E:169:ARG:NH1	1:E:195:HIS:HD2	2.03	0.55
1:E:402:ASN:O	1:E:406:VAL:HG23	2.06	0.55
1:E:164:LEU:CD1	1:F:224:LYS:HB2	2.34	0.55
1:H:112:LEU:HD11	1:H:204:ALA:HB1	1.88	0.55
1:H:166:GLU:CG	1:H:166:GLU:O	2.54	0.55
1:H:189:GLU:OE1	3:H:503:GLN:OE1	2.23	0.55
1:K:82:TRP:HZ3	1:K:221:ILE:HD11	1.72	0.55
1:L:105:GLU:OE2	1:L:412:HIS:CB	2.46	0.55
1:A:376:SER:O	1:A:380:ARG:N	2.37	0.55
1:A:132:GLU:CD	4:A:504:PO4:O1	2.45	0.55
1:H:115:ILE:HG22	1:H:351:LEU:HD13	1.87	0.55
1:K:370:ARG:NH2	1:K:374:VAL:HG13	2.22	0.55
1:A:260:ASP:O	1:A:263:ALA:HB3	2.06	0.55
1:B:79:ILE:HD13	1:B:90:ALA:HB2	1.87	0.55
1:D:318:PRO:O	1:D:335:ARG:HD2	2.06	0.55
1:E:22:ARG:CG	1:E:22:ARG:NH1	2.63	0.55
1:F:156:TYR:CG	1:F:190:VAL:HG13	2.42	0.55
1:G:160:ALA:CB	1:G:188:HIS:HD2	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:LYS:HB2	1:J:164:LEU:CD2	2.36	0.55
1:K:44:LYS:O	1:K:46:LEU:O	2.24	0.55
1:A:119:MET:HE1	1:A:127:PHE:N	2.21	0.55
1:A:338:ASP:OD2	1:A:338:ASP:C	2.45	0.55
1:D:169:ARG:NH2	1:D:195:HIS:ND1	2.55	0.55
1:D:6:ARG:O	1:D:10:GLU:HG3	2.06	0.55
1:K:21:ILE:HD13	1:K:39:VAL:HA	1.89	0.55
1:L:150:LEU:HD13	1:L:192:PRO:O	2.06	0.55
1:K:5:THR:HG23	1:K:8:ASP:OD2	2.06	0.55
1:E:163:ASP:CB	1:F:83:THR:HG22	2.37	0.55
1:E:4:TYR:HB3	1:E:9:ILE:HD11	1.87	0.55
1:G:82:TRP:HH2	1:G:217:VAL:HG22	1.71	0.55
1:K:291:PRO:HG3	1:K:341:ALA:HA	1.89	0.55
1:K:381:MET:C	1:K:383:ASN:H	2.10	0.55
1:L:96:ILE:N	1:L:96:ILE:HD12	2.22	0.55
1:B:277:GLY:HA3	1:B:353:ALA:O	2.06	0.55
1:H:175:GLU:O	1:H:179:MET:HG3	2.06	0.55
1:K:380:ARG:O	1:K:385:ILE:HB	2.06	0.55
1:L:112:LEU:HD21	1:L:204:ALA:HB1	1.87	0.55
1:L:52:PHE:CD1	1:L:70:LEU:HD22	2.41	0.55
1:E:11:LYS:O	1:E:15:GLU:HG3	2.07	0.55
1:G:132:GLU:HB3	1:G:196:GLU:OE1	2.06	0.55
1:G:13:VAL:HG21	1:G:42:LEU:CD2	2.37	0.55
1:G:300:VAL:HG13	1:G:301:PRO:HD2	1.88	0.55
1:H:104:PHE:CZ	1:H:106:GLY:HA3	2.41	0.55
1:H:260:ASP:O	1:H:266:GLN:HA	2.07	0.55
1:J:48:ASN:HB3	1:J:71:TYR:CD1	2.42	0.55
1:J:58:GLU:O	1:J:61:VAL:HG22	2.07	0.55
1:C:316:ARG:O	1:C:316:ARG:HD2	2.07	0.55
1:E:311:TRP:HB2	1:E:320:ILE:HB	1.89	0.55
1:E:77:PHE:CD1	1:E:92:PHE:CZ	2.95	0.55
1:L:224:LYS:HG3	1:L:224:LYS:O	2.06	0.55
1:A:296:TYR:N	1:A:296:TYR:CD1	2.71	0.54
1:E:201:TYR:C	1:E:201:TYR:CD2	2.79	0.54
1:F:11:LYS:O	1:F:15:GLU:HG3	2.07	0.54
1:F:231:PHE:HB3	1:F:339:PRO:HB2	1.89	0.54
1:I:304:GLU:O	1:I:317:SER:HB2	2.07	0.54
1:I:435:TRP:O	1:I:439:GLN:HG2	2.06	0.54
1:C:232:MET:HE2	1:I:441:MET:HA	1.88	0.54
1:L:265:LEU:O	1:L:326:ARG:NH1	2.40	0.54
1:E:370:ARG:HD2	1:F:64:GLU:OE2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:377:LYS:HD2	1:I:377:LYS:N	2.22	0.54
1:J:191:ALA:H	1:J:194:GLN:NE2	2.05	0.54
1:E:82:TRP:CD1	1:E:83:THR:N	2.74	0.54
1:F:168:CYS:O	1:F:172:ILE:HG12	2.08	0.54
1:F:265:LEU:O	1:F:326:ARG:NH1	2.41	0.54
1:F:338:ASP:HB2	1:F:339:PRO:CD	2.34	0.54
1:H:309:VAL:HG13	1:H:319:LEU:CD2	2.38	0.54
1:I:77:PHE:HB2	1:I:92:PHE:CE2	2.42	0.54
1:K:11:LYS:HE2	1:K:15:GLU:CG	2.35	0.54
1:L:70:LEU:HD12	1:L:94:CYS:CB	2.37	0.54
1:B:160:ALA:HB2	1:B:188:HIS:HB2	1.90	0.54
1:C:82:TRP:O	1:C:83:THR:OG1	2.20	0.54
1:G:129:LEU:HD23	1:G:130:GLY:N	2.22	0.54
1:I:114:ARG:O	1:I:117:LYS:HB3	2.08	0.54
1:I:80:PHE:CZ	1:I:91:ARG:HB3	2.43	0.54
1:J:129:LEU:HD23	1:J:248:LEU:HD23	1.89	0.54
1:C:160:ALA:O	1:C:161:PRO:O	2.25	0.54
1:D:250:LEU:C	1:D:251:PHE:HD1	2.10	0.54
1:G:208:CYS:SG	1:G:347:LEU:HD23	2.48	0.54
1:H:5:THR:HG23	1:H:8:ASP:CG	2.28	0.54
1:I:5:THR:HG22	1:I:8:ASP:OD2	2.07	0.54
1:J:287:ALA:HB2	1:J:395:ALA:HB1	1.89	0.54
1:A:191:ALA:H	1:A:194:GLN:NE2	2.06	0.54
1:C:345:LEU:HD22	1:C:409:LEU:HD22	1.89	0.54
1:E:160:ALA:CB	1:E:188:HIS:CD2	2.90	0.54
1:F:259:PHE:CE2	1:F:327:GLY:HA2	2.41	0.54
1:G:418:ILE:O	1:G:422:GLU:HG3	2.08	0.54
1:H:223:ARG:NH2	1:H:228:HIS:CD2	2.66	0.54
1:A:141:ASP:OD1	1:A:145:GLU:HB2	2.08	0.54
1:A:72:PRO:CA	1:A:94:CYS:HB3	2.31	0.54
1:B:207:SER:O	1:B:211:ILE:HG13	2.08	0.54
1:B:224:LYS:HG2	1:B:224:LYS:O	2.06	0.54
1:E:162:THR:HG21	1:F:220:THR:OG1	2.08	0.54
1:I:100:ASP:HB2	1:I:102:THR:HG23	1.90	0.54
1:J:98:ASN:ND2	1:J:102:THR:HG23	2.21	0.54
1:A:359:LYS:HG3	1:A:360:ASN:HD22	1.72	0.54
1:F:5:THR:HG23	1:F:8:ASP:OD2	2.07	0.54
1:H:308:TYR:CE1	1:H:372:ILE:HG13	2.42	0.54
1:F:24:GLN:HG3	1:F:93:ILE:HD13	1.89	0.54
1:F:48:ASN:HB3	1:F:71:TYR:CE1	2.42	0.54
1:G:85:GLU:O	1:G:86:LYS:CB	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:224:LYS:HE2	1:H:225:HIS:CD2	2.42	0.54
1:K:298:ARG:O	1:K:298:ARG:HG3	2.08	0.54
1:A:328:ILE:HD12	1:A:329:SER:N	2.23	0.54
1:A:357:GLY:CA	1:A:362:LEU:HD12	2.07	0.54
1:B:78:VAL:HG11	1:B:179:MET:CE	2.38	0.54
1:C:370:ARG:NH1	1:C:375:MET:HE3	2.23	0.54
1:E:80:PHE:HB2	1:E:83:THR:CG2	2.38	0.54
1:F:342:ASN:ND2	1:F:342:ASN:C	2.57	0.54
1:H:160:ALA:HB2	1:H:188:HIS:HB2	1.90	0.54
1:L:380:ARG:HG2	1:L:385:ILE:CG2	2.38	0.54
1:A:260:ASP:O	1:A:266:GLN:HA	2.08	0.53
1:B:129:LEU:O	1:B:201:TYR:HA	2.08	0.53
1:B:261:GLU:HA	1:B:266:GLN:HG2	1.91	0.53
1:I:377:LYS:H	1:I:377:LYS:CD	2.19	0.53
1:K:236:LEU:HB2	1:K:239:VAL:CG2	2.38	0.53
1:L:23:LEU:HB2	1:L:35:VAL:HG22	1.90	0.53
1:C:316:ARG:CD	1:D:63:ILE:O	2.55	0.53
1:F:104:PHE:CZ	1:F:106:GLY:HA3	2.43	0.53
1:F:117:LYS:NZ	1:F:117:LYS:HB2	2.24	0.53
1:I:131:PRO:HD2	1:I:199:PHE:HB2	1.89	0.53
1:B:18:VAL:CG2	1:B:79:ILE:HD12	2.39	0.53
1:D:260:ASP:OD1	1:D:263:ALA:HB2	2.08	0.53
1:F:153:LYS:HA	1:F:192:PRO:HB3	1.90	0.53
1:H:21:ILE:HD11	1:H:37:ILE:HD11	1.89	0.53
1:I:316:ARG:HD2	1:I:316:ARG:C	2.29	0.53
1:I:220:THR:HG23	1:J:162:THR:HB	1.91	0.53
1:A:300:VAL:HG13	1:A:301:PRO:HD2	1.89	0.53
1:A:426:ASP:O	1:A:430:THR:HG23	2.08	0.53
1:B:96:ILE:CD1	1:B:96:ILE:N	2.71	0.53
3:C:502:GLN:NE2	4:C:504:PO4:O3	2.41	0.53
1:D:13:VAL:HG12	1:D:14:LYS:N	2.24	0.53
1:D:243:GLY:HA3	1:D:298:ARG:NH1	2.23	0.53
1:H:418:ILE:O	1:H:422:GLU:HG3	2.09	0.53
1:I:239:VAL:CG2	1:I:240:ASN:N	2.70	0.53
1:J:17:ASN:ND2	1:J:87:GLY:HA2	2.23	0.53
1:J:187:HIS:HD2	1:J:188:HIS:O	1.91	0.53
1:J:21:ILE:HD12	1:J:39:VAL:HA	1.91	0.53
1:J:325:SER:HB2	1:J:331:ARG:HH11	1.72	0.53
1:C:264:ASP:O	1:C:265:LEU:HB2	2.09	0.53
1:D:319:LEU:CD1	1:D:336:SER:HB3	2.37	0.53
1:D:54:GLY:HA3	1:D:68:MET:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:PHE:CE1	1:F:70:LEU:HD13	2.43	0.53
1:I:311:TRP:CZ2	1:I:367:PRO:HD3	2.43	0.53
1:J:384:GLY:C	1:J:385:ILE:HD12	2.29	0.53
1:B:265:LEU:O	1:B:326:ARG:NH1	2.42	0.53
1:C:19:LYS:HB2	1:C:87:GLY:HA3	1.89	0.53
1:E:308:TYR:CE1	1:E:372:ILE:HB	2.44	0.53
1:F:11:LYS:HG2	1:F:15:GLU:OE1	2.09	0.53
1:F:283:THR:O	1:F:398:GLU:HG2	2.08	0.53
1:H:160:ALA:HB2	1:H:188:HIS:CD2	2.43	0.53
1:K:138:PHE:CE2	1:K:150:LEU:HD23	2.44	0.53
1:K:160:ALA:HB3	1:K:169:ARG:NH1	2.21	0.53
1:A:83:THR:O	1:A:85:GLU:HG3	2.09	0.53
1:C:426:ASP:O	1:C:430:THR:HG23	2.09	0.53
1:E:96:ILE:N	1:E:96:ILE:HD12	2.24	0.53
1:G:169:ARG:HG3	1:G:195:HIS:ND1	2.23	0.53
1:G:299:LEU:HD12	1:G:306:PRO:O	2.08	0.53
1:G:23:LEU:HB2	1:G:35:VAL:O	2.09	0.53
1:H:275:ILE:O	1:H:279:VAL:HG23	2.08	0.53
1:H:411:GLU:O	1:H:415:GLU:HB2	2.09	0.53
1:H:434:PRO:O	1:H:438:GLU:HG3	2.09	0.53
1:A:91:ARG:NH2	1:A:213:THR:OG1	2.42	0.53
1:A:239:VAL:HG12	1:A:240:ASN:N	2.23	0.53
1:D:54:GLY:HA3	1:D:68:MET:SD	2.48	0.53
1:E:281:HIS:HD2	1:E:402:ASN:ND2	1.98	0.53
1:E:372:ILE:HG13	1:E:373:TYR:N	2.23	0.53
1:F:160:ALA:CB	1:F:161:PRO:HD2	2.20	0.53
1:G:372:ILE:HG22	1:G:373:TYR:N	2.24	0.53
1:I:119:MET:HG3	1:I:124:PHE:HB2	1.90	0.53
1:J:176:LEU:O	1:J:181:PHE:HB2	2.08	0.53
1:J:224:LYS:HB2	1:K:164:LEU:CD2	2.39	0.53
1:J:18:VAL:HA	1:J:88:LYS:HB2	1.91	0.53
1:E:228:HIS:HE1	1:K:441:MET:O	1.91	0.53
1:A:259:PHE:CZ	1:A:261:GLU:HG3	2.43	0.53
1:D:166:GLU:HG2	1:D:167:ASN:N	2.23	0.53
1:H:437:ARG:NH1	5:H:614:HOH:O	2.41	0.53
1:I:70:LEU:O	1:I:72:PRO:HD3	2.09	0.53
1:K:115:ILE:HA	1:K:118:GLU:HG3	1.91	0.53
1:K:411:GLU:O	1:K:415:GLU:HG2	2.09	0.53
1:L:199:PHE:CD1	1:L:199:PHE:N	2.74	0.53
1:B:176:LEU:O	1:B:181:PHE:HB2	2.08	0.53
1:B:308:TYR:CE2	1:B:380:ARG:NH1	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:ARG:HD2	1:E:91:ARG:C	2.30	0.53
1:I:28:ILE:HD11	1:I:417:PHE:HB2	1.91	0.53
1:K:370:ARG:HE	1:K:370:ARG:C	2.13	0.53
1:A:164:LEU:HD11	1:B:224:LYS:HG3	1.89	0.52
1:B:183:ILE:N	1:B:183:ILE:HD12	2.23	0.52
1:D:205:VAL:HG23	1:D:206:ARG:N	2.24	0.52
1:D:338:ASP:HB2	1:D:339:PRO:HD2	1.91	0.52
1:F:83:THR:HG21	1:F:89:VAL:HB	1.91	0.52
1:I:351:LEU:HD22	1:I:355:LEU:HG	1.90	0.52
1:B:8:ASP:O	1:B:12:LEU:HD12	2.09	0.52
1:C:426:ASP:HA	1:C:429:ARG:HG2	1.92	0.52
1:B:223:ARG:CG	1:B:223:ARG:HH11	2.19	0.52
1:D:160:ALA:HB1	1:D:161:PRO:CD	2.25	0.52
1:D:301:PRO:HA	1:D:373:TYR:HE2	1.74	0.52
1:E:259:PHE:CD1	1:E:327:GLY:HA2	2.44	0.52
1:E:27:ASP:OD1	1:E:31:THR:HB	2.08	0.52
1:G:96:ILE:HD13	1:G:96:ILE:N	2.24	0.52
1:H:417:PHE:O	1:H:421:LYS:HG2	2.10	0.52
1:J:398:GLU:OE2	1:J:398:GLU:HA	2.09	0.52
1:B:357:GLY:HA2	1:B:362:LEU:HD22	1.90	0.52
1:D:186:SER:OG	1:E:36:GLU:HG3	2.09	0.52
1:G:392:LEU:O	1:G:392:LEU:HD12	2.09	0.52
1:J:316:ARG:O	1:J:316:ARG:HD2	2.09	0.52
1:K:264:ASP:O	1:K:265:LEU:HB2	2.10	0.52
1:L:285:PHE:CD1	1:L:285:PHE:C	2.83	0.52
1:A:345:LEU:HD21	1:A:413:LEU:HD13	1.91	0.52
1:A:22:ARG:HD3	1:A:34:ASN:OD1	2.09	0.52
1:B:160:ALA:HB2	1:B:188:HIS:HD2	1.74	0.52
1:D:370:ARG:O	1:D:371:ASN:HB2	2.09	0.52
1:D:369:ASP:OD2	1:D:371:ASN:HB3	2.08	0.52
1:F:232:MET:HE1	1:L:437:ARG:CA	2.33	0.52
1:F:34:ASN:ND2	1:F:34:ASN:C	2.63	0.52
1:G:160:ALA:O	1:G:161:PRO:O	2.27	0.52
1:G:259:PHE:CE1	1:G:327:GLY:HA2	2.44	0.52
1:K:52:PHE:CZ	1:K:54:GLY:HA2	2.44	0.52
1:L:28:ILE:HD12	1:L:58:GLU:HA	1.91	0.52
1:C:162:THR:HG22	1:C:163:ASP:H	1.72	0.52
1:C:252:LYS:O	1:C:253:ASN:HB2	2.09	0.52
1:D:206:ARG:NH1	1:D:206:ARG:HG3	2.25	0.52
1:F:325:SER:O	1:F:326:ARG:HD3	2.09	0.52
1:H:25:PHE:CZ	1:H:52:PHE:CE2	2.98	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:28:ILE:HD12	1:J:29:LEU:HG	1.91	0.52
1:J:357:GLY:HA2	1:J:362:LEU:CD1	2.18	0.52
1:K:85:GLU:CD	1:K:85:GLU:N	2.63	0.52
1:L:281:HIS:HD2	1:L:402:ASN:OD1	1.93	0.52
1:A:41:GLN:HE22	1:F:200:LYS:HZ1	1.54	0.52
1:B:106:GLY:O	1:B:413:LEU:HD21	2.09	0.52
1:A:163:ASP:CB	1:B:83:THR:HG21	2.25	0.52
1:C:444:TYR:OXT	1:I:231:PHE:N	2.40	0.52
1:G:109:ARG:NH1	1:G:209:ASP:OD1	2.41	0.52
1:G:308:TYR:CE1	1:G:372:ILE:HD12	2.45	0.52
1:J:13:VAL:HG13	1:J:18:VAL:HB	1.92	0.52
1:K:316:ARG:NH2	1:K:370:ARG:CZ	2.72	0.52
1:K:5:THR:O	1:K:8:ASP:N	2.42	0.52
1:B:371:ASN:HB3	1:B:374:VAL:HG13	1.91	0.52
1:G:119:MET:HG2	1:G:124:PHE:HB2	1.91	0.52
1:G:346:ALA:O	1:G:350:LEU:HG	2.09	0.52
1:J:67:ASP:O	1:J:68:MET:HG3	2.09	0.52
1:K:119:MET:HG2	1:K:124:PHE:HB2	1.90	0.52
1:L:215:LYS:O	1:L:219:LYS:HG2	2.10	0.52
1:A:290:ASN:ND2	1:A:299:LEU:HD21	2.24	0.52
1:A:378:GLU:H	1:A:378:GLU:CD	2.14	0.52
1:F:131:PRO:C	1:F:133:PRO:HD3	2.31	0.52
1:F:260:ASP:O	1:F:266:GLN:HA	2.10	0.52
1:I:13:VAL:HG13	1:I:18:VAL:HB	1.91	0.52
1:K:315:ASN:HD21	1:K:370:ARG:N	2.07	0.52
1:K:16:GLU:HB3	1:K:88:LYS:NZ	2.25	0.52
1:E:169:ARG:HE	1:E:195:HIS:HD2	1.58	0.52
1:E:35:VAL:HG13	1:E:70:LEU:HD21	1.90	0.52
1:H:319:LEU:HG	1:H:319:LEU:O	2.10	0.52
1:H:317:SER:OG	1:H:373:TYR:HE2	1.93	0.52
1:H:54:GLY:HA3	1:H:68:MET:CE	2.40	0.52
1:I:377:LYS:HD2	1:I:377:LYS:H	1.75	0.52
1:K:78:VAL:HG21	1:K:91:ARG:HH21	1.75	0.52
1:A:77:PHE:HB2	1:A:92:PHE:CE2	2.45	0.51
1:C:61:VAL:HG11	1:C:419:GLU:HG2	1.91	0.51
1:F:368:ILE:HG22	1:F:369:ASP:N	2.25	0.51
1:H:147:THR:CG2	1:H:148:LEU:N	2.73	0.51
1:H:372:ILE:O	1:H:380:ARG:HD3	2.11	0.51
1:H:396:LEU:O	1:H:400:LYS:HG2	2.10	0.51
1:K:123:GLY:O	1:K:252:LYS:HD3	2.10	0.51
1:K:258:PHE:HA	1:K:271:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:377:LYS:CG	1:L:378:GLU:N	2.71	0.51
1:C:260:ASP:HB2	1:C:268:SER:HB3	1.92	0.51
1:G:231:PHE:O	1:G:339:PRO:HG2	2.10	0.51
1:G:47:ASP:O	1:G:49:LYS:HG2	2.10	0.51
1:H:169:ARG:NH2	1:H:195:HIS:ND1	2.58	0.51
1:I:100:ASP:OD1	1:I:100:ASP:N	2.32	0.51
1:I:170:ARG:HG3	1:I:174:LEU:HD22	1.91	0.51
1:J:349:VAL:HG22	1:J:405:MET:SD	2.50	0.51
1:K:317:SER:HA	1:K:335:ARG:NH1	2.25	0.51
1:L:134:GLU:HG2	1:L:196:GLU:HB2	1.92	0.51
1:L:141:ASP:OD1	1:L:145:GLU:HB2	2.11	0.51
1:L:165:GLY:O	1:L:167:ASN:N	2.43	0.51
1:B:160:ALA:O	1:B:161:PRO:O	2.28	0.51
1:B:52:PHE:CE1	1:B:70:LEU:HD13	2.45	0.51
1:C:244:MET:HG2	1:C:244:MET:O	2.11	0.51
1:E:160:ALA:CB	1:E:188:HIS:HD2	2.24	0.51
1:E:280:LYS:HD3	1:E:281:HIS:CE1	2.44	0.51
1:G:206:ARG:NH1	1:G:210:ASP:OD1	2.44	0.51
1:I:274:PHE:O	1:I:278:ILE:HG12	2.10	0.51
1:K:76:THR:O	1:K:78:VAL:HG23	2.11	0.51
1:L:114:ARG:NH2	1:L:407:LYS:O	2.43	0.51
1:B:141:ASP:C	1:B:141:ASP:OD2	2.49	0.51
1:B:167:ASN:HD22	1:B:170:ARG:NH1	2.08	0.51
1:F:199:PHE:HZ	1:F:214:PHE:CD1	2.28	0.51
1:I:261:GLU:N	1:I:261:GLU:OE1	2.37	0.51
1:J:285:PHE:C	1:J:285:PHE:CD1	2.83	0.51
1:B:147:THR:HG22	1:B:148:LEU:H	1.75	0.51
1:C:281:HIS:CD2	1:C:402:ASN:HD21	2.26	0.51
1:D:23:LEU:HD13	1:D:70:LEU:HD23	1.92	0.51
1:E:175:GLU:OE1	1:F:86:LYS:HE2	2.10	0.51
1:E:259:PHE:CZ	1:E:261:GLU:HB2	2.46	0.51
1:E:48:ASN:HB3	1:E:71:TYR:CE1	2.44	0.51
1:G:6:ARG:HD2	1:G:46:LEU:HD13	1.92	0.51
1:H:147:THR:HG22	1:H:148:LEU:N	2.24	0.51
1:H:338:ASP:C	1:H:338:ASP:OD2	2.49	0.51
1:A:370:ARG:O	1:A:371:ASN:HB3	2.11	0.51
1:D:13:VAL:HG22	1:D:18:VAL:HB	1.93	0.51
1:E:21:ILE:HD13	1:E:39:VAL:HA	1.93	0.51
1:F:78:VAL:HG11	1:F:179:MET:HE3	1.91	0.51
1:J:383:ASN:N	1:J:383:ASN:OD1	2.43	0.51
1:K:134:GLU:OE2	3:K:503:GLN:NE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:224:LYS:HD2	1:K:225:HIS:CD2	2.46	0.51
1:K:282:ALA:HA	1:K:285:PHE:CZ	2.46	0.51
1:F:150:LEU:HD22	1:F:192:PRO:O	2.11	0.51
1:F:264:ASP:O	1:F:265:LEU:HB2	2.11	0.51
1:F:328:ILE:H	1:F:328:ILE:CD1	2.22	0.51
1:I:176:LEU:O	1:I:181:PHE:HB2	2.11	0.51
1:I:239:VAL:HG23	1:I:240:ASN:N	2.26	0.51
1:J:231:PHE:HB3	1:J:339:PRO:CB	2.37	0.51
1:K:161:PRO:O	1:K:162:THR:HG23	2.10	0.51
1:K:260:ASP:O	1:K:266:GLN:HA	2.10	0.51
1:L:29:LEU:C	1:L:31:THR:H	2.12	0.51
1:A:372:ILE:C	1:A:372:ILE:HD12	2.31	0.51
1:A:41:GLN:HE22	1:F:200:LYS:HZ2	1.54	0.51
1:B:119:MET:HG2	1:B:124:PHE:HB2	1.92	0.51
1:D:141:ASP:HB2	1:D:142:GLU:OE2	2.11	0.51
1:E:208:CYS:HB2	1:E:344:TYR:CE2	2.45	0.51
1:D:159:LEU:HD22	1:E:34:ASN:HB3	1.93	0.51
1:H:51:MET:HE1	1:I:324:ALA:HB3	1.92	0.51
1:I:112:LEU:HD11	1:I:204:ALA:HB1	1.93	0.51
1:C:232:MET:HE1	1:I:441:MET:HB2	1.93	0.51
1:K:82:TRP:CZ3	1:K:221:ILE:HD11	2.46	0.51
1:L:151:ASN:OD1	1:L:193:GLY:HA2	2.10	0.51
1:A:111:ASN:OD1	1:A:114:ARG:HD3	2.11	0.51
1:A:206:ARG:NH1	1:A:206:ARG:HG2	2.26	0.51
1:B:197:ILE:HD12	1:B:214:PHE:HE1	1.76	0.51
1:E:381:MET:O	1:E:383:ASN:N	2.43	0.51
1:H:27:ASP:HB3	1:H:33:LYS:HE3	1.92	0.51
1:J:28:ILE:HD12	1:J:29:LEU:N	2.26	0.51
1:K:435:TRP:O	1:K:439:GLN:HG2	2.11	0.51
1:B:345:LEU:HD22	1:B:409:LEU:HD22	1.92	0.51
1:F:201:TYR:CD1	1:F:201:TYR:C	2.84	0.51
1:F:32:ILE:HD11	1:F:216:LEU:HD22	1.92	0.51
1:F:261:GLU:HA	1:F:266:GLN:HE21	1.75	0.51
1:F:371:ASN:ND2	1:F:373:TYR:HB2	2.26	0.51
1:G:435:TRP:O	1:G:439:GLN:HG2	2.11	0.51
1:G:48:ASN:HB3	1:G:71:TYR:CD1	2.46	0.51
1:K:165:GLY:O	1:K:167:ASN:N	2.44	0.51
1:K:316:ARG:HH21	1:K:370:ARG:CD	2.19	0.51
1:L:426:ASP:O	1:L:429:ARG:HG2	2.11	0.51
1:B:164:LEU:HD11	1:C:82:TRP:CD1	2.46	0.50
1:C:48:ASN:HB3	1:C:71:TYR:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:THR:O	5:F:601:HOH:O	2.18	0.50
1:F:6:ARG:HG3	1:F:46:LEU:HD13	1.93	0.50
1:G:140:LEU:HD12	1:G:226:GLY:HA2	1.93	0.50
1:J:129:LEU:HD12	1:J:207:SER:OG	2.11	0.50
1:J:280:LYS:HG2	1:J:281:HIS:CE1	2.47	0.50
1:J:376:SER:OG	1:J:379:GLU:HG3	2.11	0.50
1:K:141:ASP:OD2	1:K:141:ASP:C	2.50	0.50
1:K:46:LEU:O	1:K:47:ASP:HB2	2.12	0.50
1:L:260:ASP:OD1	1:L:263:ALA:HB2	2.11	0.50
1:L:59:GLY:O	1:L:62:ARG:HB2	2.11	0.50
1:B:370:ARG:HB2	1:B:370:ARG:HH11	1.76	0.50
1:C:106:GLY:O	1:C:413:LEU:HD21	2.10	0.50
1:D:256:ASN:HD21	1:D:258:PHE:HB2	1.76	0.50
1:E:163:ASP:HA	1:E:170:ARG:HH21	1.75	0.50
1:I:259:PHE:CD2	1:I:327:GLY:HA2	2.46	0.50
1:I:48:ASN:HB3	1:I:71:TYR:CD1	2.47	0.50
1:I:33:LYS:NZ	1:J:158:ASP:OD1	2.45	0.50
1:K:48:ASN:OD1	1:K:48:ASN:N	2.40	0.50
1:C:417:PHE:O	1:C:421:LYS:HG2	2.11	0.50
1:C:57:ILE:HD11	1:C:96:ILE:HG12	1.94	0.50
1:E:114:ARG:HD3	5:E:612:HOH:O	2.12	0.50
1:G:278:ILE:CG2	1:G:320:ILE:HD11	2.41	0.50
1:K:308:TYR:HD1	1:K:372:ILE:CD1	2.23	0.50
1:K:83:THR:HG21	1:K:89:VAL:HB	1.92	0.50
1:L:285:PHE:C	1:L:285:PHE:HD1	2.15	0.50
1:B:160:ALA:HB3	1:B:169:ARG:NH1	2.19	0.50
1:C:251:PHE:CD1	1:C:256:ASN:HA	2.47	0.50
1:D:289:THR:O	1:D:341:ALA:HB2	2.11	0.50
1:H:308:TYR:CD2	1:H:387:ASP:OD1	2.65	0.50
1:I:160:ALA:HB2	1:I:188:HIS:CD2	2.46	0.50
1:J:278:ILE:HG22	1:J:320:ILE:HD11	1.92	0.50
1:K:48:ASN:HB3	1:K:71:TYR:CE1	2.46	0.50
1:K:62:ARG:HD2	1:L:156:TYR:HD2	1.76	0.50
1:A:69:TYR:CE1	1:A:99:PRO:HA	2.46	0.50
1:I:127:PHE:CD2	1:I:351:LEU:HG	2.46	0.50
1:I:134:GLU:OE2	3:I:503:GLN:HB2	2.10	0.50
1:J:303:TYR:O	1:J:304:GLU:HB2	2.12	0.50
1:J:381:MET:O	1:J:383:ASN:O	2.29	0.50
1:A:30:GLY:N	1:A:342:ASN:HD22	2.09	0.50
1:B:163:ASP:HA	1:B:170:ARG:HH12	1.77	0.50
1:D:109:ARG:HG3	1:D:344:TYR:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:ALA:HB1	1:D:188:HIS:HD2	1.73	0.50
1:E:13:VAL:HG21	1:E:42:LEU:CD2	2.42	0.50
1:F:308:TYR:HB3	1:F:387:ASP:HA	1.94	0.50
1:G:11:LYS:NZ	1:G:11:LYS:HB3	2.26	0.50
1:H:160:ALA:O	1:H:161:PRO:O	2.30	0.50
1:J:119:MET:HG2	1:J:124:PHE:HB2	1.94	0.50
1:J:160:ALA:O	1:J:161:PRO:C	2.50	0.50
1:K:259:PHE:CD2	1:K:327:GLY:HA2	2.47	0.50
1:K:46:LEU:C	1:K:48:ASN:H	2.14	0.50
1:A:191:ALA:H	1:A:194:GLN:HE21	1.60	0.50
1:A:311:TRP:CB	1:A:320:ILE:HB	2.42	0.50
1:B:308:TYR:CD1	1:B:372:ILE:CG2	2.94	0.50
1:C:318:PRO:O	1:C:335:ARG:HD3	2.12	0.50
1:E:281:HIS:CD2	1:E:402:ASN:HD21	2.12	0.50
1:D:171:ASP:OD2	1:E:85:GLU:HG3	2.12	0.50
1:F:309:VAL:O	1:F:310:ALA:HB2	2.12	0.50
1:G:141:ASP:OD1	1:G:145:GLU:HB2	2.11	0.50
1:G:281:HIS:HD2	1:G:402:ASN:HD21	1.59	0.50
1:G:311:TRP:CH2	1:G:367:PRO:HG3	2.46	0.50
1:H:289:THR:HB	1:H:337:VAL:HG13	1.94	0.50
1:H:35:VAL:CG1	1:H:70:LEU:HD21	2.40	0.50
1:I:112:LEU:HD22	1:I:116:LEU:HG	1.93	0.50
1:J:100:ASP:OD1	1:J:100:ASP:C	2.49	0.50
1:K:397:GLU:HA	1:K:397:GLU:OE1	2.11	0.50
1:L:140:LEU:HD12	1:L:226:GLY:HA2	1.93	0.50
1:L:224:LYS:HG2	1:L:225:HIS:HD2	1.75	0.50
1:L:34:ASN:C	1:L:34:ASN:ND2	2.65	0.50
1:D:231:PHE:HB3	1:D:339:PRO:HB2	1.94	0.50
1:H:362:LEU:HD22	1:H:362:LEU:N	2.26	0.50
1:I:152:ASP:CG	1:I:188:HIS:HE2	2.14	0.50
1:J:377:LYS:O	1:J:381:MET:HG2	2.12	0.50
1:K:321:ARG:HG2	1:K:322:ILE:N	2.26	0.50
1:L:404:VAL:HG22	1:L:405:MET:CE	2.42	0.50
1:B:160:ALA:CB	1:B:188:HIS:HD2	2.25	0.50
1:B:381:MET:C	1:B:383:ASN:N	2.66	0.50
1:C:5:THR:O	1:C:8:ASP:N	2.44	0.50
1:D:282:ALA:HA	1:D:285:PHE:CE2	2.47	0.50
1:D:372:ILE:O	1:D:380:ARG:HD3	2.12	0.50
1:E:131:PRO:HG2	1:E:199:PHE:CD1	2.45	0.50
1:E:184:GLU:CD	1:E:200:LYS:HG3	2.32	0.50
1:J:160:ALA:O	1:J:161:PRO:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:370:ARG:NH1	1:J:370:ARG:HG2	2.27	0.50
1:K:259:PHE:CG	1:K:327:GLY:HA2	2.47	0.50
1:L:304:GLU:O	1:L:335:ARG:NH2	2.42	0.50
1:A:220:THR:HG23	1:F:162:THR:HB	1.94	0.49
1:A:5:THR:H	1:A:8:ASP:HB2	1.77	0.49
1:B:407:LYS:HB3	1:B:407:LYS:HZ2	1.77	0.49
1:C:392:LEU:O	1:C:396:LEU:HG	2.12	0.49
1:C:6:ARG:HD2	1:C:46:LEU:HD13	1.93	0.49
1:F:368:ILE:HG13	1:F:372:ILE:HD11	1.94	0.49
1:G:183:ILE:HA	1:G:199:PHE:HA	1.92	0.49
1:G:71:TYR:CG	1:G:97:TYR:CD1	3.00	0.49
1:B:28:ILE:HD12	1:B:413:LEU:HD22	1.93	0.49
1:C:59:GLY:O	1:C:62:ARG:HG3	2.11	0.49
1:E:13:VAL:HG21	1:E:42:LEU:HD21	1.93	0.49
1:F:22:ARG:NH1	1:F:22:ARG:HG2	2.27	0.49
1:G:85:GLU:N	1:G:85:GLU:CD	2.64	0.49
1:K:317:SER:N	1:K:318:PRO:HD3	2.27	0.49
1:D:13:VAL:CG1	1:D:14:LYS:N	2.75	0.49
1:C:162:THR:HG23	1:D:216:LEU:HD11	1.94	0.49
1:I:152:ASP:OD1	1:I:193:GLY:HA2	2.12	0.49
1:I:380:ARG:O	1:I:385:ILE:HB	2.12	0.49
1:I:5:THR:HG22	1:I:8:ASP:CG	2.32	0.49
1:C:376:SER:O	1:C:379:GLU:HB2	2.12	0.49
1:B:164:LEU:HD21	1:C:82:TRP:HB3	1.95	0.49
1:D:380:ARG:O	1:D:385:ILE:HB	2.12	0.49
1:E:3:LYS:HG2	1:E:4:TYR:N	2.27	0.49
1:E:52:PHE:CE1	1:E:70:LEU:CD1	2.95	0.49
1:H:129:LEU:HD21	1:H:246:CYS:HB3	1.94	0.49
1:H:48:ASN:HB3	1:H:71:TYR:CE1	2.47	0.49
1:I:380:ARG:C	1:I:382:GLU:H	2.15	0.49
1:K:115:ILE:CG2	1:K:351:LEU:HD12	2.31	0.49
1:K:48:ASN:ND2	1:K:71:TYR:CD2	2.80	0.49
1:C:142:GLU:H	1:C:142:GLU:CD	2.16	0.49
1:F:131:PRO:O	1:F:133:PRO:HD3	2.12	0.49
1:H:406:VAL:HG13	1:H:414:PHE:CD1	2.47	0.49
1:K:319:LEU:HG	1:K:320:ILE:HG13	1.95	0.49
1:L:116:LEU:O	1:L:119:MET:HB3	2.12	0.49
1:A:282:ALA:HA	1:A:285:PHE:CE2	2.47	0.49
1:B:12:LEU:O	1:B:16:GLU:HB2	2.12	0.49
1:B:351:LEU:HD22	1:B:355:LEU:HG	1.95	0.49
1:A:200:LYS:NZ	1:B:41:GLN:OE1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LYS:HD2	1:C:149:GLU:HB3	1.95	0.49
1:D:223:ARG:NH2	5:D:614:HOH:O	2.45	0.49
1:F:215:LYS:O	1:F:219:LYS:HD3	2.11	0.49
1:H:273:HIS:O	1:H:276:ALA:HB3	2.13	0.49
1:I:152:ASP:OD2	1:I:188:HIS:NE2	2.39	0.49
1:I:376:SER:OG	1:I:379:GLU:HG3	2.12	0.49
1:I:3:LYS:HE2	1:I:4:TYR:CE1	2.47	0.49
1:J:122:LEU:HD21	1:J:359:LYS:HZ1	1.78	0.49
1:K:377:LYS:O	1:K:381:MET:HB2	2.12	0.49
1:C:309:VAL:HG13	1:C:319:LEU:CD2	2.43	0.49
1:F:232:MET:SD	1:F:235:PRO:HA	2.52	0.49
1:F:27:ASP:OD2	1:F:27:ASP:C	2.50	0.49
1:F:418:ILE:O	1:F:422:GLU:HG3	2.13	0.49
1:H:176:LEU:O	1:H:181:PHE:HB2	2.11	0.49
1:H:391:THR:OG1	1:H:394:GLU:HG3	2.13	0.49
1:I:4:TYR:HB3	1:I:9:ILE:HD11	1.95	0.49
1:L:443:GLN:NE2	1:L:444:TYR:CE2	2.81	0.49
1:B:276:ALA:HB2	1:B:364:ALA:HA	1.94	0.49
1:F:125:SER:N	1:F:251:PHE:O	2.45	0.49
1:G:83:THR:O	1:G:85:GLU:HG3	2.13	0.49
1:H:106:GLY:O	1:H:413:LEU:HD21	2.12	0.49
1:I:224:LYS:HB2	1:J:164:LEU:HD21	1.95	0.49
1:L:275:ILE:O	1:L:279:VAL:HG23	2.12	0.49
1:A:250:LEU:C	1:A:251:PHE:HD1	2.16	0.49
1:A:34:ASN:O	1:A:34:ASN:ND2	2.41	0.49
1:A:3:LYS:HE2	1:A:4:TYR:CE1	2.48	0.49
1:B:162:THR:HB	1:C:220:THR:HG23	1.95	0.49
1:F:325:SER:HB2	1:F:329:SER:HB3	1.95	0.49
1:G:292:THR:O	1:G:295:SER:HB2	2.13	0.49
1:G:325:SER:HB2	1:G:331:ARG:HH22	1.78	0.49
1:J:383:ASN:O	1:J:385:ILE:N	2.37	0.49
1:K:368:ILE:HG12	1:K:372:ILE:HG22	1.94	0.49
1:A:308:TYR:CE1	1:A:372:ILE:CD1	2.94	0.49
1:B:82:TRP:O	1:B:83:THR:HG23	2.13	0.49
1:C:24:GLN:HG3	1:C:93:ILE:HG12	1.94	0.49
1:E:289:THR:O	1:E:341:ALA:HB2	2.13	0.49
1:G:261:GLU:O	1:G:266:GLN:NE2	2.46	0.49
1:G:291:PRO:HG3	1:G:341:ALA:HA	1.94	0.49
1:B:431:GLN:O	1:H:297:LYS:NZ	2.46	0.49
1:I:106:GLY:O	1:I:108:PRO:HD3	2.13	0.49
1:K:380:ARG:HG2	1:K:385:ILE:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLU:HA	1:A:16:GLU:OE2	2.12	0.48
1:A:86:LYS:HZ1	1:F:175:GLU:CD	2.16	0.48
1:B:287:ALA:HB2	1:B:395:ALA:O	2.12	0.48
1:E:129:LEU:CD1	1:E:131:PRO:HD3	2.44	0.48
1:F:156:TYR:CD1	1:F:190:VAL:HG13	2.48	0.48
1:F:182:GLU:O	1:F:200:LYS:HG3	2.13	0.48
1:J:35:VAL:HG13	1:J:70:LEU:HD21	1.95	0.48
1:J:383:ASN:HB2	1:J:385:ILE:CD1	2.33	0.48
1:K:139:LYS:O	1:K:147:THR:HG23	2.13	0.48
1:L:119:MET:HE1	1:L:127:PHE:CB	2.31	0.48
1:A:250:LEU:O	1:A:251:PHE:HD1	1.95	0.48
1:A:37:ILE:HD12	1:A:38:PRO:O	2.13	0.48
1:B:166:GLU:HG2	1:B:168:CYS:H	1.79	0.48
1:B:23:LEU:HB3	1:B:70:LEU:CD2	2.42	0.48
1:D:200:LYS:O	1:D:201:TYR:C	2.52	0.48
1:E:207:SER:O	1:E:211:ILE:HG13	2.13	0.48
1:F:57:ILE:HD12	1:F:104:PHE:CE2	2.47	0.48
1:G:249:SER:HA	1:G:258:PHE:HZ	1.74	0.48
1:H:134:GLU:OE2	3:H:503:GLN:OE1	2.29	0.48
1:I:34:ASN:ND2	1:I:34:ASN:C	2.65	0.48
1:I:396:LEU:O	1:I:400:LYS:HG3	2.13	0.48
1:C:300:VAL:HG21	1:I:430:THR:HG22	1.94	0.48
1:I:96:ILE:N	1:I:96:ILE:HD12	2.28	0.48
1:J:78:VAL:HG12	1:J:79:ILE:N	2.28	0.48
1:K:248:LEU:N	1:K:332:VAL:O	2.42	0.48
1:L:159:LEU:C	1:L:159:LEU:HD12	2.33	0.48
1:L:170:ARG:HG2	1:L:170:ARG:NH1	2.28	0.48
1:C:234:LYS:HD3	1:C:298:ARG:HA	1.95	0.48
1:C:338:ASP:OD2	1:C:338:ASP:C	2.52	0.48
1:D:132:GLU:HB3	1:D:196:GLU:OE1	2.13	0.48
1:F:274:PHE:O	1:F:278:ILE:HG12	2.14	0.48
1:G:370:ARG:H	1:G:370:ARG:CD	2.19	0.48
1:H:129:LEU:HD11	1:H:347:LEU:HD21	1.95	0.48
1:J:369:ASP:CG	1:J:370:ARG:H	2.16	0.48
1:K:371:ASN:HB3	1:K:375:MET:CE	2.42	0.48
1:K:46:LEU:HB3	5:K:614:HOH:O	2.13	0.48
1:L:129:LEU:O	1:L:201:TYR:HA	2.13	0.48
1:L:268:SER:O	1:L:271:ALA:HB3	2.13	0.48
1:A:115:ILE:HA	1:A:118:GLU:HG3	1.96	0.48
1:D:351:LEU:O	1:D:355:LEU:HG	2.13	0.48
1:D:374:VAL:HG22	1:D:375:MET:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:SER:O	1:D:380:ARG:HG3	2.14	0.48
1:D:28:ILE:HD11	1:D:417:PHE:CB	2.41	0.48
1:E:240:ASN:HD22	1:E:303:TYR:HD1	1.61	0.48
1:E:345:LEU:HD22	1:E:409:LEU:CD2	2.43	0.48
1:F:371:ASN:HD21	1:F:373:TYR:HB2	1.78	0.48
1:I:208:CYS:HB3	1:I:344:TYR:CE2	2.47	0.48
1:I:270:THR:HG23	1:I:358:ILE:HD13	1.96	0.48
1:I:368:ILE:HB	1:I:372:ILE:HD11	1.95	0.48
1:I:44:LYS:HE2	1:J:184:GLU:OE2	2.14	0.48
1:K:152:ASP:C	1:K:153:LYS:HE3	2.34	0.48
1:K:27:ASP:CG	1:K:31:THR:HB	2.34	0.48
1:K:240:ASN:ND2	1:K:303:TYR:HD2	2.10	0.48
1:K:78:VAL:HG23	1:K:91:ARG:HE	1.76	0.48
1:A:122:LEU:HD21	1:A:359:LYS:HZ3	1.77	0.48
1:B:127:PHE:HZ	1:B:248:LEU:HD22	1.72	0.48
1:E:131:PRO:HD2	1:E:199:PHE:HB2	1.95	0.48
1:F:133:PRO:HD2	1:F:197:ILE:O	2.13	0.48
1:F:260:ASP:HB2	1:F:268:SER:HB3	1.96	0.48
1:H:141:ASP:OD2	1:H:143:LYS:N	2.47	0.48
1:K:19:LYS:HA	1:K:39:VAL:HB	1.95	0.48
1:K:46:LEU:C	1:K:48:ASN:N	2.66	0.48
1:L:249:SER:HA	1:L:258:PHE:CE1	2.48	0.48
1:A:54:GLY:HA3	1:A:68:MET:SD	2.53	0.48
1:C:118:GLU:O	1:C:122:LEU:HD23	2.13	0.48
1:C:371:ASN:CB	1:C:374:VAL:HG12	2.31	0.48
1:D:170:ARG:HG3	1:D:174:LEU:HD11	1.96	0.48
1:F:129:LEU:HD22	1:F:131:PRO:HD3	1.95	0.48
1:G:129:LEU:C	1:G:129:LEU:HD23	2.33	0.48
1:H:127:PHE:CZ	1:H:248:LEU:HD22	2.47	0.48
1:I:48:ASN:HB3	1:I:71:TYR:CE1	2.47	0.48
1:J:86:LYS:HE3	1:K:178:GLU:OE1	2.12	0.48
1:K:309:VAL:HA	1:K:319:LEU:CD2	2.40	0.48
1:A:258:PHE:HB2	1:A:330:THR:HG22	1.95	0.48
1:D:372:ILE:HG13	1:D:373:TYR:N	2.27	0.48
1:F:308:TYR:CE1	1:F:372:ILE:HG21	2.48	0.48
1:J:162:THR:HG22	1:J:163:ASP:H	1.79	0.48
1:K:402:ASN:O	1:K:406:VAL:HG23	2.14	0.48
1:E:431:GLN:HG2	1:K:435:TRP:CD1	2.49	0.48
1:L:129:LEU:HD12	1:L:347:LEU:HD11	1.94	0.48
1:B:310:ALA:HB1	1:B:368:ILE:HG12	1.95	0.48
1:B:429:ARG:HD3	1:B:430:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:TYR:O	1:D:33:LYS:NZ	2.37	0.48
1:D:129:LEU:HD13	1:D:131:PRO:HD3	1.96	0.48
1:F:244:MET:HE2	1:F:339:PRO:HA	1.95	0.48
1:F:45:ALA:HA	1:F:50:VAL:HG23	1.96	0.48
1:F:24:GLN:HE22	1:F:91:ARG:HH11	1.61	0.48
1:I:160:ALA:O	1:I:161:PRO:O	2.32	0.48
1:J:271:ALA:O	1:J:275:ILE:HG13	2.14	0.48
1:K:32:ILE:HG13	1:K:32:ILE:O	2.12	0.48
1:K:247:ASN:HB3	1:K:331:ARG:HG3	1.95	0.48
1:L:368:ILE:HG21	1:L:372:ILE:HG23	1.96	0.48
1:A:129:LEU:HD13	1:A:131:PRO:HG3	1.94	0.48
1:A:221:ILE:O	1:A:224:LYS:HB3	2.14	0.48
1:C:24:GLN:NE2	1:C:91:ARG:NH1	2.60	0.48
1:I:316:ARG:HB3	1:I:373:TYR:CE1	2.49	0.48
1:C:23:LEU:HD12	1:C:35:VAL:HG22	1.95	0.48
1:D:160:ALA:HB2	1:D:188:HIS:HB2	1.95	0.48
1:D:380:ARG:HB3	1:D:385:ILE:HG21	1.96	0.48
1:D:403:GLU:O	1:D:407:LYS:HG3	2.14	0.48
1:F:52:PHE:CE2	1:F:54:GLY:HA2	2.49	0.48
1:I:390:ALA:C	1:I:391:THR:HG23	2.34	0.48
1:J:281:HIS:HE1	1:J:356:ASP:OD1	1.96	0.48
1:L:169:ARG:NH2	1:L:195:HIS:ND1	2.58	0.48
1:B:100:ASP:OD1	1:B:101:GLY:N	2.47	0.47
1:B:314:GLN:NE2	1:C:64:GLU:HB2	2.29	0.47
1:D:315:ASN:O	1:E:64:GLU:HG2	2.14	0.47
1:E:83:THR:CG2	1:E:89:VAL:HB	2.35	0.47
1:G:342:ASN:HD22	1:G:343:PRO:N	2.12	0.47
1:H:351:LEU:CD2	1:H:355:LEU:HG	2.44	0.47
1:H:80:PHE:CZ	1:H:91:ARG:HB3	2.49	0.47
1:I:84:ALA:HB2	1:I:88:LYS:HG2	1.96	0.47
1:J:109:ARG:HG3	1:J:344:TYR:CE2	2.49	0.47
1:K:166:GLU:O	1:K:168:CYS:N	2.47	0.47
1:K:285:PHE:CD1	1:K:285:PHE:C	2.87	0.47
1:B:32:ILE:CD1	1:B:216:LEU:HD22	2.43	0.47
1:D:360:ASN:O	1:D:361:LYS:C	2.51	0.47
1:F:55:SER:O	1:F:62:ARG:HG3	2.14	0.47
1:H:48:ASN:OD1	1:H:48:ASN:N	2.47	0.47
1:I:247:ASN:HB3	1:I:331:ARG:HG3	1.96	0.47
1:K:109:ARG:HG3	1:K:344:TYR:CE2	2.49	0.47
1:K:370:ARG:C	1:K:370:ARG:NE	2.67	0.47
1:K:385:ILE:CD1	1:K:385:ILE:N	2.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ARG:NH1	1:A:36:GLU:OE1	2.47	0.47
1:B:82:TRP:O	1:B:82:TRP:CG	2.67	0.47
1:D:273:HIS:CE1	1:D:361:LYS:HA	2.49	0.47
1:D:338:ASP:OD2	1:D:338:ASP:C	2.53	0.47
1:F:250:LEU:HA	1:F:250:LEU:HD23	1.72	0.47
1:G:5:THR:HG23	1:G:8:ASP:OD1	2.14	0.47
1:G:86:LYS:HD2	1:H:178:GLU:OE1	2.15	0.47
1:I:326:ARG:HD3	1:I:326:ARG:HA	1.53	0.47
1:J:371:ASN:HD22	1:J:374:VAL:CG1	2.14	0.47
1:K:119:MET:CE	1:K:120:GLU:HG3	2.44	0.47
1:L:381:MET:O	1:L:383:ASN:N	2.47	0.47
1:L:425:TRP:CZ3	1:L:429:ARG:HD2	2.49	0.47
1:A:259:PHE:CE2	1:A:261:GLU:HG3	2.50	0.47
1:A:360:ASN:O	1:A:361:LYS:C	2.52	0.47
1:B:178:GLU:OE2	1:C:86:LYS:HG3	2.15	0.47
1:C:365:PRO:O	1:C:366:ALA:CB	2.63	0.47
1:C:379:GLU:O	1:C:382:GLU:HB3	2.15	0.47
1:D:78:VAL:HG11	1:D:179:MET:HE3	1.97	0.47
1:D:243:GLY:CA	1:D:298:ARG:HH12	2.27	0.47
1:E:376:SER:H	1:E:379:GLU:HB2	1.79	0.47
1:H:163:ASP:OD1	1:H:170:ARG:NE	2.48	0.47
1:H:184:GLU:O	1:H:185:ALA:HB2	2.13	0.47
1:H:82:TRP:HE1	1:H:221:ILE:HD11	1.80	0.47
1:J:141:ASP:HB3	1:J:147:THR:HG22	1.95	0.47
1:K:290:ASN:HB3	1:K:295:SER:HB3	1.96	0.47
1:D:173:VAL:HG22	1:D:183:ILE:HD13	1.94	0.47
1:J:163:ASP:HA	1:J:170:ARG:NH1	2.29	0.47
1:J:17:ASN:HD21	1:J:87:GLY:HA2	1.79	0.47
1:J:28:ILE:CD1	1:J:29:LEU:HG	2.44	0.47
1:B:182:GLU:HB3	1:B:200:LYS:HE2	1.96	0.47
1:B:271:ALA:O	1:B:275:ILE:HD12	2.15	0.47
1:D:170:ARG:O	1:D:174:LEU:HD12	2.15	0.47
1:F:303:TYR:CD2	1:F:303:TYR:N	2.83	0.47
1:F:309:VAL:HG13	1:F:319:LEU:HD23	1.96	0.47
1:H:162:THR:C	1:H:164:LEU:H	2.18	0.47
1:K:100:ASP:C	1:K:100:ASP:OD1	2.51	0.47
1:K:199:PHE:HZ	1:K:214:PHE:CG	2.32	0.47
1:K:378:GLU:N	1:K:378:GLU:CD	2.68	0.47
1:A:319:LEU:CD1	1:A:336:SER:HB3	2.45	0.47
1:B:136:PHE:CE2	1:B:194:GLN:HB2	2.49	0.47
1:B:224:LYS:HE2	1:B:225:HIS:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ILE:HD11	1:C:413:LEU:HD23	1.95	0.47
1:F:111:ASN:O	1:F:114:ARG:HB3	2.15	0.47
1:F:156:TYR:HB2	1:F:190:VAL:CG1	2.42	0.47
1:I:170:ARG:NH1	1:I:170:ARG:CG	2.70	0.47
1:I:224:LYS:HE3	1:I:225:HIS:NE2	2.28	0.47
1:I:35:VAL:CG1	1:I:70:LEU:HD21	2.45	0.47
1:J:312:SER:OG	1:J:315:ASN:HB2	2.14	0.47
1:J:360:ASN:O	1:J:361:LYS:C	2.52	0.47
1:J:371:ASN:HD22	1:J:374:VAL:H	1.60	0.47
1:K:194:GLN:C	1:K:195:HIS:CD2	2.88	0.47
1:L:201:TYR:C	1:L:201:TYR:CD1	2.87	0.47
1:B:23:LEU:HD13	1:B:70:LEU:HD23	1.97	0.47
1:D:377:LYS:O	1:D:381:MET:N	2.32	0.47
1:E:160:ALA:HB1	1:E:161:PRO:CD	2.25	0.47
1:E:26:THR:OG1	1:E:212:GLN:NE2	2.48	0.47
1:G:312:SER:O	1:G:321:ARG:HA	2.15	0.47
1:G:320:ILE:HA	1:G:333:GLU:O	2.15	0.47
1:I:97:TYR:CE2	1:I:103:PRO:HG3	2.50	0.47
1:I:22:ARG:NH1	1:I:36:GLU:OE1	2.48	0.47
1:I:404:VAL:HG22	1:I:405:MET:CE	2.44	0.47
1:J:127:PHE:CD2	1:J:351:LEU:HG	2.48	0.47
1:J:385:ILE:HD12	1:J:385:ILE:N	2.30	0.47
1:A:184:GLU:O	1:A:185:ALA:HB2	2.15	0.47
1:A:347:LEU:HD13	1:A:347:LEU:HA	1.80	0.47
1:D:148:LEU:N	1:D:148:LEU:HD23	2.30	0.47
1:D:164:LEU:O	1:D:165:GLY:O	2.33	0.47
1:E:396:LEU:HA	1:E:396:LEU:HD23	1.78	0.47
1:F:241:GLY:HA3	1:F:298:ARG:HG2	1.96	0.47
1:G:71:TYR:CD1	1:G:97:TYR:CD1	3.03	0.47
1:H:129:LEU:HD12	1:H:347:LEU:HD21	1.97	0.47
1:I:402:ASN:OD1	1:I:402:ASN:C	2.54	0.47
1:L:28:ILE:HD11	1:L:58:GLU:HA	1.97	0.47
1:A:184:GLU:OE1	1:A:200:LYS:HE3	2.15	0.47
1:A:314:GLN:HG3	1:A:314:GLN:O	2.15	0.47
1:B:164:LEU:HB2	1:C:220:THR:HG22	1.95	0.47
1:C:153:LYS:HA	1:C:192:PRO:HB3	1.96	0.47
1:I:241:GLY:HA3	1:I:298:ARG:HG3	1.97	0.47
1:J:223:ARG:HG2	1:J:223:ARG:HH11	1.76	0.47
1:J:281:HIS:CD2	1:J:402:ASN:HD21	2.30	0.47
1:K:378:GLU:HB2	1:K:379:GLU:OE1	2.15	0.47
1:K:383:ASN:C	1:K:385:ILE:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:165:GLY:O	1:L:166:GLU:C	2.53	0.47
1:L:260:ASP:OD2	1:L:260:ASP:C	2.53	0.47
1:L:70:LEU:HA	1:L:70:LEU:HD13	1.60	0.47
1:A:245:HIS:ND1	4:A:504:PO4:O1	2.48	0.47
1:B:115:ILE:CG2	1:B:351:LEU:HD13	2.38	0.47
1:C:289:THR:O	1:C:341:ALA:HB2	2.15	0.47
1:C:159:LEU:HD22	1:D:34:ASN:CB	2.44	0.47
1:D:359:LYS:CB	1:D:359:LYS:NZ	2.78	0.47
1:E:129:LEU:HD12	1:E:207:SER:HB3	1.96	0.47
1:H:28:ILE:HD12	1:H:413:LEU:CD2	2.40	0.47
1:K:234:LYS:HE2	1:K:298:ARG:HA	1.97	0.47
1:L:73:ASP:C	1:L:73:ASP:OD1	2.54	0.47
1:A:82:TRP:O	1:A:83:THR:C	2.54	0.46
1:D:256:ASN:HD22	1:D:256:ASN:C	2.18	0.46
1:E:129:LEU:C	1:E:129:LEU:HD13	2.34	0.46
1:E:109:ARG:NH1	1:E:209:ASP:OD1	2.43	0.46
1:E:393:ALA:HB2	1:E:425:TRP:CE2	2.50	0.46
1:F:164:LEU:HA	1:F:164:LEU:HD23	1.81	0.46
1:H:59:GLY:O	1:H:62:ARG:HG3	2.14	0.46
1:I:91:ARG:C	1:I:91:ARG:HD2	2.35	0.46
1:J:109:ARG:O	1:J:113:LYS:HG3	2.15	0.46
1:K:217:VAL:O	1:K:221:ILE:HG12	2.15	0.46
1:K:22:ARG:HH11	1:K:22:ARG:CG	2.20	0.46
1:L:11:LYS:HE2	1:L:11:LYS:HB3	1.44	0.46
1:A:176:LEU:O	1:A:181:PHE:HB2	2.15	0.46
1:B:176:LEU:HD11	1:B:214:PHE:HD1	1.80	0.46
1:B:396:LEU:O	1:B:400:LYS:HG3	2.14	0.46
1:C:127:PHE:CD2	1:C:351:LEU:HG	2.50	0.46
1:C:370:ARG:HH21	1:C:374:VAL:CG2	2.28	0.46
1:E:119:MET:HG2	1:E:124:PHE:HB2	1.95	0.46
1:H:10:GLU:HA	1:H:10:GLU:OE1	2.14	0.46
1:H:251:PHE:N	1:H:251:PHE:HD1	2.13	0.46
1:H:258:PHE:HA	1:H:271:ALA:HB2	1.98	0.46
1:I:353:ALA:HB2	1:I:405:MET:HE3	1.98	0.46
1:B:186:SER:O	1:C:36:GLU:HG2	2.15	0.46
1:D:133:PRO:HD2	1:D:197:ILE:O	2.15	0.46
1:E:322:ILE:HD11	1:E:332:VAL:HG22	1.97	0.46
1:E:371:ASN:HA	1:E:374:VAL:HG21	1.95	0.46
1:G:371:ASN:C	1:G:374:VAL:HG13	2.35	0.46
1:H:135:PHE:HB3	1:H:231:PHE:CE1	2.51	0.46
1:J:282:ALA:HA	1:J:285:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:376:SER:O	1:K:379:GLU:HG2	2.15	0.46
1:K:381:MET:C	1:K:383:ASN:N	2.69	0.46
1:L:5:THR:O	1:L:6:ARG:C	2.53	0.46
1:B:276:ALA:HB2	1:B:364:ALA:CA	2.46	0.46
1:B:85:GLU:O	1:B:86:LYS:CB	2.63	0.46
1:C:310:ALA:HB1	1:C:368:ILE:HG12	1.98	0.46
1:C:36:GLU:H	1:C:36:GLU:HG2	1.55	0.46
1:E:132:GLU:HG2	1:E:198:ASP:OD1	2.16	0.46
1:F:224:LYS:HD2	1:F:225:HIS:CD2	2.50	0.46
1:F:48:ASN:HB3	1:F:71:TYR:CD1	2.49	0.46
1:G:375:MET:HG3	1:G:380:ARG:HG3	1.96	0.46
1:H:383:ASN:C	1:H:385:ILE:H	2.18	0.46
1:H:46:LEU:HD22	1:H:74:LEU:HD11	1.97	0.46
1:I:127:PHE:CZ	1:I:248:LEU:HD22	2.51	0.46
1:I:250:LEU:C	1:I:251:PHE:HD1	2.17	0.46
1:J:326:ARG:HA	1:J:326:ARG:HD3	1.38	0.46
1:J:402:ASN:OD1	1:J:404:VAL:HG13	2.16	0.46
1:K:308:TYR:CE1	1:K:372:ILE:HG13	2.51	0.46
1:K:326:ARG:HD2	1:K:330:THR:HG23	1.97	0.46
1:L:351:LEU:CD2	1:L:355:LEU:HG	2.46	0.46
1:A:48:ASN:HB3	1:A:71:TYR:CE1	2.50	0.46
1:D:376:SER:H	1:D:379:GLU:HB2	1.80	0.46
1:E:290:ASN:HB3	1:E:295:SER:HB3	1.97	0.46
1:E:32:ILE:HD11	1:E:216:LEU:HD12	1.97	0.46
1:E:393:ALA:HB2	1:E:425:TRP:CD2	2.51	0.46
1:E:167:ASN:HD21	1:F:22:ARG:NH2	2.14	0.46
1:F:299:LEU:HD12	1:F:306:PRO:O	2.16	0.46
1:G:51:MET:HE3	1:G:67:ASP:HB3	1.97	0.46
1:H:182:GLU:O	1:H:200:LYS:HG2	2.15	0.46
1:J:163:ASP:HA	1:J:170:ARG:HH12	1.79	0.46
1:J:211:ILE:O	1:J:215:LYS:HG3	2.16	0.46
1:K:97:TYR:HD2	1:K:101:GLY:O	1.97	0.46
1:L:33:LYS:O	1:L:34:ASN:HB3	2.14	0.46
1:A:14:LYS:HE2	1:A:14:LYS:HB2	1.81	0.46
1:A:423:ILE:O	1:A:427:MET:HG3	2.15	0.46
1:C:326:ARG:HD3	1:C:326:ARG:HA	1.72	0.46
1:G:77:PHE:CD1	1:G:92:PHE:CZ	3.03	0.46
1:I:169:ARG:NH2	1:I:195:HIS:ND1	2.63	0.46
1:I:212:GLN:OE1	1:I:343:PRO:HG3	2.16	0.46
1:J:308:TYR:CZ	1:J:372:ILE:HB	2.51	0.46
1:A:290:ASN:HD22	1:A:299:LEU:HD21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:GLU:O	1:C:383:ASN:ND2	2.48	0.46
1:C:414:PHE:CE1	1:C:418:ILE:HD11	2.50	0.46
1:C:20:TYR:HB3	1:C:89:VAL:HG22	1.98	0.46
1:E:164:LEU:HB2	1:F:220:THR:CG2	2.46	0.46
1:E:326:ARG:HD3	1:E:326:ARG:HA	1.49	0.46
1:E:308:TYR:OH	1:E:373:TYR:HD1	1.98	0.46
1:E:381:MET:C	1:E:383:ASN:N	2.66	0.46
1:F:14:LYS:NZ	1:F:14:LYS:HB2	2.30	0.46
1:H:251:PHE:N	1:H:251:PHE:CD1	2.84	0.46
1:B:430:THR:HG22	1:H:300:VAL:HG21	1.97	0.46
1:H:278:ILE:CG2	1:H:320:ILE:HD11	2.46	0.46
1:J:318:PRO:O	1:J:335:ARG:HD3	2.15	0.46
1:A:34:ASN:ND2	1:A:36:GLU:OE1	2.45	0.46
1:D:345:LEU:HD22	1:D:409:LEU:HD22	1.98	0.46
1:E:239:VAL:HG23	1:E:240:ASN:N	2.30	0.46
1:E:325:SER:HB2	1:E:331:ARG:HH22	1.80	0.46
1:F:172:ILE:CD1	1:F:218:VAL:HA	2.46	0.46
1:H:308:TYR:HD2	1:H:387:ASP:OD1	1.97	0.46
1:J:61:VAL:O	1:J:62:ARG:C	2.55	0.46
1:L:417:PHE:HD2	1:L:418:ILE:HD13	1.80	0.46
1:D:106:GLY:O	1:D:413:LEU:HD21	2.16	0.46
1:E:27:ASP:CG	1:E:31:THR:HB	2.36	0.46
1:B:435:TRP:CD1	1:H:431:GLN:HG2	2.50	0.46
1:J:145:GLU:CA	1:J:145:GLU:OE1	2.44	0.46
1:J:37:ILE:HG22	1:K:185:ALA:HB2	1.98	0.46
1:K:73:ASP:CG	1:K:76:THR:HG23	2.36	0.46
1:L:6:ARG:NH1	1:L:10:GLU:OE2	2.43	0.46
1:L:126:ASP:N	1:L:126:ASP:OD2	2.49	0.46
1:L:383:ASN:O	1:L:385:ILE:HD12	2.16	0.46
1:A:111:ASN:O	1:A:115:ILE:HG12	2.16	0.46
1:A:83:THR:OG1	1:A:84:ALA:N	2.49	0.46
1:D:116:LEU:O	1:D:119:MET:HG2	2.15	0.46
1:D:380:ARG:HB3	1:D:385:ILE:CG2	2.45	0.46
1:E:205:VAL:HG13	1:E:206:ARG:H	1.82	0.46
1:E:80:PHE:HB2	1:E:83:THR:HG21	1.99	0.46
1:F:211:ILE:O	1:F:214:PHE:HB3	2.15	0.46
1:F:285:PHE:CB	1:F:349:VAL:HG13	2.46	0.46
1:J:179:MET:HE3	1:J:179:MET:HB3	1.78	0.46
1:L:296:TYR:N	1:L:296:TYR:CD1	2.84	0.46
1:L:52:PHE:CE2	1:L:54:GLY:HA2	2.51	0.46
1:A:20:TYR:O	1:A:21:ILE:HD13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:LEU:HB2	1:B:239:VAL:HG23	1.99	0.45
1:B:275:ILE:O	1:B:279:VAL:HG23	2.16	0.45
1:B:371:ASN:HB3	1:B:374:VAL:CG1	2.46	0.45
1:C:129:LEU:HB3	1:C:207:SER:OG	2.15	0.45
1:C:211:ILE:O	1:C:215:LYS:HG3	2.16	0.45
1:C:290:ASN:N	1:C:290:ASN:ND2	2.64	0.45
1:C:35:VAL:HG13	1:C:70:LEU:HD21	1.98	0.45
1:C:378:GLU:CD	1:C:378:GLU:N	2.68	0.45
1:C:97:TYR:CD2	1:C:103:PRO:CA	2.99	0.45
1:D:3:LYS:HE2	1:D:4:TYR:CE1	2.51	0.45
1:I:82:TRP:O	1:I:83:THR:C	2.54	0.45
1:J:224:LYS:HG3	1:K:164:LEU:HD21	1.97	0.45
1:K:370:ARG:O	1:K:371:ASN:ND2	2.49	0.45
1:B:85:GLU:O	1:B:85:GLU:HG3	2.17	0.45
1:D:383:ASN:OD1	1:D:383:ASN:N	2.47	0.45
1:F:391:THR:OG1	1:F:394:GLU:HG3	2.17	0.45
1:H:370:ARG:HD2	1:H:371:ASN:H	1.81	0.45
1:K:19:LYS:HD2	1:K:87:GLY:CA	2.40	0.45
1:A:300:VAL:HG12	1:A:301:PRO:CD	2.47	0.45
1:B:215:LYS:O	1:B:219:LYS:HB2	2.17	0.45
1:C:298:ARG:NH1	1:C:305:ALA:HB2	2.30	0.45
1:D:315:ASN:HD21	1:D:372:ILE:HG12	1.82	0.45
1:E:273:HIS:O	1:E:276:ALA:HB3	2.16	0.45
1:F:304:GLU:O	1:F:317:SER:HB2	2.15	0.45
1:G:361:LYS:HB3	1:G:361:LYS:HE2	1.71	0.45
1:I:80:PHE:HA	1:I:179:MET:HE2	1.96	0.45
1:K:26:THR:HG22	1:K:27:ASP:O	2.16	0.45
1:K:282:ALA:HA	1:K:285:PHE:CE1	2.50	0.45
1:L:6:ARG:NH2	1:L:47:ASP:OD1	2.48	0.45
1:B:303:TYR:O	1:B:304:GLU:HB2	2.16	0.45
1:B:326:ARG:HA	1:B:326:ARG:HD3	1.49	0.45
1:B:426:ASP:OD1	1:B:429:ARG:HD2	2.16	0.45
1:B:42:LEU:O	1:B:46:LEU:HG	2.16	0.45
1:C:160:ALA:HB2	1:C:188:HIS:CG	2.51	0.45
1:C:199:PHE:CZ	1:C:214:PHE:CD1	2.99	0.45
1:B:156:TYR:HD2	1:C:62:ARG:HD2	1.81	0.45
1:D:243:GLY:HA2	1:D:298:ARG:HH12	1.81	0.45
1:D:5:THR:O	1:D:6:ARG:C	2.55	0.45
1:E:32:ILE:CD1	1:E:216:LEU:HD12	2.46	0.45
1:E:266:GLN:OE1	1:E:326:ARG:HG3	2.16	0.45
1:F:248:LEU:HD11	1:F:334:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:308:TYR:CZ	1:G:372:ILE:HD12	2.52	0.45
1:G:62:ARG:HD2	1:H:156:TYR:HD2	1.81	0.45
1:H:298:ARG:NH1	3:H:503:GLN:O	2.49	0.45
1:J:81:PRO:HG2	1:J:82:TRP:H	1.81	0.45
1:J:220:THR:HG22	1:K:164:LEU:HD13	1.98	0.45
1:K:234:LYS:HE3	1:K:297:LYS:O	2.16	0.45
1:L:381:MET:C	1:L:383:ASN:H	2.20	0.45
1:A:150:LEU:HD13	1:A:192:PRO:O	2.16	0.45
1:F:6:ARG:NH1	1:F:47:ASP:OD1	2.50	0.45
1:G:342:ASN:C	1:G:342:ASN:ND2	2.63	0.45
1:G:82:TRP:CG	1:H:164:LEU:HD12	2.51	0.45
1:K:22:ARG:NH1	1:K:22:ARG:CG	2.80	0.45
1:B:170:ARG:HG3	1:C:20:TYR:CE2	2.52	0.45
1:B:27:ASP:OD1	1:B:33:LYS:HE3	2.17	0.45
1:B:434:PRO:HA	1:B:437:ARG:NH1	2.31	0.45
1:B:5:THR:O	1:B:6:ARG:C	2.55	0.45
1:C:109:ARG:NH2	1:C:109:ARG:HG2	2.30	0.45
1:D:142:GLU:CD	1:D:142:GLU:H	2.19	0.45
1:F:34:ASN:HD22	1:F:34:ASN:C	2.20	0.45
1:G:143:LYS:HE2	1:G:143:LYS:HB2	1.66	0.45
1:G:184:GLU:CG	1:G:200:LYS:HD3	2.36	0.45
1:G:314:GLN:O	1:G:369:ASP:OD2	2.34	0.45
1:H:54:GLY:HA3	1:H:68:MET:HE3	1.98	0.45
1:I:156:TYR:O	1:I:158:ASP:N	2.50	0.45
1:I:224:LYS:CB	1:J:164:LEU:HD21	2.46	0.45
1:I:396:LEU:HD11	1:I:421:LYS:HB3	1.99	0.45
1:J:81:PRO:HG2	1:J:82:TRP:CE3	2.52	0.45
1:K:207:SER:O	1:K:211:ILE:HG13	2.16	0.45
1:K:396:LEU:O	1:K:400:LYS:HD3	2.16	0.45
1:L:115:ILE:O	1:L:118:GLU:HB3	2.17	0.45
1:L:279:VAL:HG11	1:L:365:PRO:HG3	1.99	0.45
1:L:374:VAL:O	1:L:376:SER:N	2.49	0.45
1:C:393:ALA:O	1:C:396:LEU:N	2.49	0.45
1:D:327:GLY:C	1:D:329:SER:H	2.19	0.45
1:E:205:VAL:CG1	1:E:206:ARG:N	2.79	0.45
1:F:167:ASN:HB3	1:F:170:ARG:NH2	2.31	0.45
1:F:291:PRO:HG3	1:F:341:ALA:HA	1.99	0.45
1:F:21:ILE:HG12	1:F:42:LEU:HD13	1.99	0.45
1:H:21:ILE:HD11	1:H:23:LEU:HD21	1.99	0.45
1:I:252:LYS:HB3	1:I:252:LYS:HZ2	1.80	0.45
1:J:368:ILE:HD12	1:J:368:ILE:HA	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:285:PHE:HD1	1:K:285:PHE:C	2.20	0.45
1:L:347:LEU:HD23	1:L:347:LEU:HA	1.48	0.45
1:L:76:THR:HB	1:L:93:ILE:HG13	1.99	0.45
1:B:376:SER:O	1:B:380:ARG:HB2	2.16	0.45
1:D:271:ALA:O	1:D:275:ILE:HD13	2.17	0.45
1:F:116:LEU:O	1:F:119:MET:HB3	2.17	0.45
1:G:239:VAL:HG23	1:G:240:ASN:N	2.32	0.45
1:H:86:LYS:HB2	1:H:86:LYS:NZ	2.32	0.45
1:I:273:HIS:O	1:I:276:ALA:HB3	2.16	0.45
1:J:115:ILE:N	1:J:115:ILE:CD1	2.80	0.45
1:B:405:MET:O	1:B:408:ALA:HB3	2.17	0.45
1:C:407:LYS:NZ	1:C:407:LYS:HB3	2.32	0.45
1:D:381:MET:C	1:D:383:ASN:H	2.20	0.45
1:D:68:MET:CE	1:D:104:PHE:HB2	2.47	0.45
1:E:80:PHE:HB2	1:E:83:THR:HG23	1.99	0.45
1:F:252:LYS:O	1:F:253:ASN:OD1	2.35	0.45
1:F:281:HIS:O	1:F:284:SER:N	2.48	0.45
1:H:203:GLY:O	1:H:204:ALA:C	2.55	0.45
1:H:204:ALA:O	1:H:205:VAL:C	2.55	0.45
1:H:304:GLU:HG2	1:H:335:ARG:NH1	2.28	0.45
1:I:129:LEU:O	1:I:201:TYR:HA	2.17	0.45
1:I:295:SER:O	1:I:299:LEU:HD22	2.17	0.45
1:J:260:ASP:HB2	1:J:268:SER:CA	2.46	0.45
1:J:36:GLU:HG2	1:J:36:GLU:H	1.63	0.45
1:K:368:ILE:HG12	1:K:372:ILE:CG2	2.47	0.45
1:B:88:LYS:HE2	1:B:88:LYS:HB2	1.60	0.45
1:B:5:THR:O	1:B:8:ASP:N	2.50	0.45
1:C:402:ASN:O	1:C:406:VAL:HG23	2.17	0.45
1:D:54:GLY:O	1:D:57:ILE:HD13	2.17	0.45
1:E:272:LYS:HA	1:E:275:ILE:HD12	1.99	0.45
1:G:115:ILE:O	1:G:118:GLU:HB2	2.17	0.45
1:G:264:ASP:O	1:G:265:LEU:HB2	2.17	0.45
1:G:402:ASN:O	1:G:403:GLU:C	2.55	0.45
1:I:124:PHE:HD2	1:I:252:LYS:HG3	1.82	0.45
1:I:239:VAL:HG23	1:I:240:ASN:H	1.81	0.45
1:K:16:GLU:HB3	1:K:88:LYS:HZ2	1.82	0.45
1:L:402:ASN:ND2	1:L:404:VAL:H	2.15	0.45
1:C:311:TRP:CB	1:C:320:ILE:HB	2.47	0.44
1:D:265:LEU:O	1:D:267:LEU:HD22	2.17	0.44
1:E:261:GLU:O	1:E:262:ASN:CG	2.54	0.44
1:E:431:GLN:O	1:K:297:LYS:NZ	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:303:TYR:O	1:G:304:GLU:HB2	2.16	0.44
1:G:326:ARG:HD3	1:G:330:THR:OG1	2.16	0.44
1:H:154:GLY:C	1:H:188:HIS:CE1	2.90	0.44
1:H:28:ILE:CD1	1:H:413:LEU:HD23	2.43	0.44
1:I:224:LYS:HB2	1:J:164:LEU:HD22	1.99	0.44
1:J:62:ARG:HD2	1:K:156:TYR:CD1	2.53	0.44
1:L:114:ARG:NH2	1:L:115:ILE:HD11	2.33	0.44
1:L:370:ARG:HD2	1:L:370:ARG:HA	1.78	0.44
1:A:22:ARG:NH1	1:A:36:GLU:CD	2.71	0.44
1:A:405:MET:CE	1:A:405:MET:HA	2.46	0.44
1:A:435:TRP:CE3	1:G:428:PHE:HD1	2.36	0.44
1:B:351:LEU:CD2	1:B:355:LEU:HG	2.47	0.44
1:C:163:ASP:HA	1:C:170:ARG:NH1	2.32	0.44
1:D:39:VAL:O	1:D:39:VAL:HG22	2.17	0.44
1:F:73:ASP:CG	1:F:76:THR:HG23	2.37	0.44
1:H:137:LEU:HD23	1:H:229:ALA:HA	1.99	0.44
1:H:316:ARG:O	1:H:316:ARG:HD2	2.17	0.44
1:I:252:LYS:O	1:I:253:ASN:HB2	2.17	0.44
1:I:26:THR:HG22	1:I:27:ASP:O	2.18	0.44
1:I:35:VAL:HG11	1:I:70:LEU:CD2	2.46	0.44
1:A:280:LYS:HD3	1:A:281:HIS:CE1	2.53	0.44
1:A:283:THR:HG22	1:A:389:PRO:HD3	1.99	0.44
1:B:177:GLU:HG3	1:C:38:PRO:HB3	1.99	0.44
1:B:261:GLU:HA	1:B:266:GLN:CG	2.47	0.44
1:A:159:LEU:CD1	1:B:32:ILE:HD11	2.47	0.44
1:D:25:PHE:CD2	1:D:25:PHE:N	2.84	0.44
1:D:308:TYR:CE1	1:D:373:TYR:CE1	3.05	0.44
1:E:285:PHE:HB2	1:E:349:VAL:HG13	1.99	0.44
1:E:316:ARG:HD3	1:F:63:ILE:O	2.17	0.44
1:E:369:ASP:O	1:E:370:ARG:HB2	2.17	0.44
1:F:326:ARG:HD3	1:F:326:ARG:HA	1.62	0.44
1:H:308:TYR:HD1	1:H:372:ILE:HD12	1.83	0.44
1:I:83:THR:O	1:I:84:ALA:C	2.55	0.44
1:J:359:LYS:HZ2	1:J:359:LYS:CB	2.29	0.44
1:J:371:ASN:ND2	1:J:373:TYR:HB2	2.32	0.44
1:A:224:LYS:NZ	1:A:225:HIS:CE1	2.85	0.44
1:A:327:GLY:O	1:A:330:THR:HB	2.18	0.44
1:C:96:ILE:HD12	1:C:96:ILE:N	2.32	0.44
1:E:22:ARG:HH12	1:E:36:GLU:CD	2.21	0.44
1:F:305:ALA:HA	1:F:306:PRO:HD3	1.72	0.44
1:L:58:GLU:O	1:L:61:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:78:VAL:HG13	1:L:91:ARG:HE	1.81	0.44
1:A:23:LEU:HD13	1:A:70:LEU:HD23	1.99	0.44
1:B:128:ASN:HA	1:B:202:ALA:O	2.18	0.44
1:B:85:GLU:O	1:B:86:LYS:HB2	2.18	0.44
1:C:163:ASP:HA	1:C:170:ARG:HH12	1.82	0.44
1:C:177:GLU:HG2	5:D:624:HOH:O	2.16	0.44
1:E:259:PHE:CE1	1:E:327:GLY:HA2	2.53	0.44
1:F:148:LEU:HD12	1:F:236:LEU:HD23	2.00	0.44
1:H:96:ILE:HD13	1:H:96:ILE:N	2.32	0.44
1:I:286:THR:HA	1:I:289:THR:OG1	2.18	0.44
1:I:20:TYR:OH	1:I:36:GLU:HG3	2.17	0.44
1:I:390:ALA:O	1:I:391:THR:CG2	2.64	0.44
1:J:13:VAL:HG21	1:J:42:LEU:HD21	1.99	0.44
1:K:49:LYS:HA	1:K:49:LYS:HD3	1.75	0.44
1:L:326:ARG:HA	1:L:326:ARG:HD3	1.67	0.44
1:L:423:ILE:HG13	1:L:424:GLU:H	1.83	0.44
1:A:372:ILE:HG13	1:A:373:TYR:N	2.32	0.44
1:C:258:PHE:HA	1:C:271:ALA:HB2	1.99	0.44
1:C:80:PHE:HA	1:C:81:PRO:HD3	1.67	0.44
1:C:162:THR:HB	1:D:220:THR:HG23	1.99	0.44
1:D:372:ILE:HD12	1:D:373:TYR:CE1	2.52	0.44
1:D:402:ASN:C	1:D:402:ASN:OD1	2.56	0.44
1:E:274:PHE:O	1:E:278:ILE:HG12	2.17	0.44
1:E:314:GLN:NE2	1:F:64:GLU:CB	2.80	0.44
1:F:112:LEU:HA	1:F:112:LEU:HD23	1.70	0.44
1:F:71:TYR:CG	1:F:97:TYR:CD1	3.05	0.44
1:F:5:THR:O	1:F:7:GLU:N	2.51	0.44
1:G:328:ILE:HD12	1:G:328:ILE:H	1.82	0.44
1:G:374:VAL:HG22	1:G:375:MET:H	1.81	0.44
1:H:134:GLU:OE2	3:H:503:GLN:HB2	2.18	0.44
1:I:63:ILE:HD13	1:I:63:ILE:HA	1.79	0.44
1:I:48:ASN:OD1	1:I:72:PRO:HD2	2.17	0.44
1:K:293:VAL:HG23	1:K:424:GLU:HG2	1.99	0.44
1:L:132:GLU:HB3	1:L:198:ASP:OD1	2.18	0.44
1:A:402:ASN:C	1:A:402:ASN:OD1	2.56	0.44
1:C:285:PHE:CD1	1:C:285:PHE:C	2.90	0.44
1:C:314:GLN:HE22	1:D:66:SER:HB2	1.82	0.44
1:E:282:ALA:HA	1:E:285:PHE:CZ	2.52	0.44
1:E:23:LEU:CB	1:E:70:LEU:HD23	2.47	0.44
1:F:175:GLU:HA	1:F:175:GLU:OE1	2.17	0.44
1:F:109:ARG:HD2	1:F:344:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:80:PHE:HA	1:F:81:PRO:HD3	1.77	0.44
1:G:169:ARG:NH2	1:G:195:HIS:ND1	2.65	0.44
1:I:240:ASN:ND2	1:I:303:TYR:CD1	2.83	0.44
1:I:265:LEU:O	1:I:326:ARG:NH1	2.51	0.44
1:I:380:ARG:HB3	1:I:385:ILE:HB	2.00	0.44
1:J:250:LEU:HD23	1:J:250:LEU:HA	1.86	0.44
1:K:236:LEU:CB	1:K:239:VAL:HG23	2.47	0.44
1:K:242:SER:O	1:K:339:PRO:HD2	2.17	0.44
1:L:272:LYS:O	1:L:364:ALA:HB2	2.17	0.44
1:C:151:ASN:ND2	1:C:166:GLU:OE2	2.51	0.44
1:C:418:ILE:HD12	1:C:418:ILE:N	2.32	0.44
1:G:201:TYR:CD1	1:G:201:TYR:C	2.91	0.44
1:G:82:TRP:CH2	1:G:217:VAL:HG22	2.53	0.44
1:G:78:VAL:CG1	1:G:91:ARG:NE	2.80	0.44
1:I:166:GLU:OE2	1:I:166:GLU:O	2.36	0.44
1:J:5:THR:HG23	1:J:8:ASP:CG	2.37	0.44
1:K:214:PHE:O	1:K:218:VAL:HG23	2.17	0.44
1:K:316:ARG:HH21	1:K:370:ARG:HA	1.75	0.44
1:C:102:THR:OG1	1:C:103:PRO:HD2	2.17	0.44
1:D:6:ARG:NH1	1:D:6:ARG:CG	2.72	0.44
1:E:25:PHE:HE2	1:E:35:VAL:HG12	1.82	0.44
1:G:338:ASP:OD2	1:G:338:ASP:C	2.56	0.44
1:J:435:TRP:CH2	1:J:439:GLN:HG3	2.53	0.44
1:K:220:THR:HG23	1:L:162:THR:HB	1.99	0.44
1:K:308:TYR:CE2	1:K:380:ARG:NH1	2.86	0.44
1:K:360:ASN:O	1:K:361:LYS:C	2.56	0.44
1:L:234:LYS:HD3	1:L:297:LYS:O	2.17	0.44
1:L:84:ALA:HB2	1:L:88:LYS:HD3	1.99	0.44
1:B:78:VAL:HG11	1:B:179:MET:HE2	2.00	0.43
1:C:443:GLN:O	1:C:443:GLN:HG3	2.18	0.43
1:D:68:MET:HE2	1:D:104:PHE:HB2	1.99	0.43
1:D:78:VAL:HG12	1:D:79:ILE:N	2.33	0.43
1:D:98:ASN:HD21	1:D:104:PHE:HA	1.83	0.43
1:E:32:ILE:HD11	1:E:216:LEU:CD1	2.48	0.43
1:E:261:GLU:O	1:E:262:ASN:CB	2.66	0.43
1:E:54:GLY:O	1:E:57:ILE:HD12	2.18	0.43
1:F:162:THR:C	1:F:164:LEU:H	2.21	0.43
1:F:84:ALA:O	1:F:85:GLU:O	2.35	0.43
1:G:259:PHE:CD1	1:G:327:GLY:HA2	2.53	0.43
1:H:111:ASN:OD1	1:H:114:ARG:NH1	2.50	0.43
1:G:44:LYS:HE2	1:H:184:GLU:OE1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:281:HIS:HE1	1:H:356:ASP:OD2	2.00	0.43
1:H:316:ARG:HB3	1:H:373:TYR:CZ	2.53	0.43
1:H:405:MET:O	1:H:408:ALA:HB3	2.18	0.43
1:I:134:GLU:HG2	1:I:196:GLU:OE1	2.18	0.43
1:I:141:ASP:HB2	1:I:142:GLU:OE1	2.17	0.43
1:I:440:TYR:CD1	1:I:444:TYR:HE2	2.32	0.43
1:K:203:GLY:O	1:K:204:ALA:C	2.57	0.43
1:K:212:GLN:HE22	1:K:215:LYS:HZ1	1.66	0.43
1:L:289:THR:OG1	1:L:290:ASN:ND2	2.51	0.43
1:L:5:THR:HG23	1:L:8:ASP:CG	2.39	0.43
1:A:309:VAL:HG13	1:A:319:LEU:CD2	2.46	0.43
1:C:71:TYR:CD2	1:C:97:TYR:CD1	3.06	0.43
1:D:25:PHE:CZ	1:D:52:PHE:CE2	3.06	0.43
1:A:64:GLU:HG2	1:F:316:ARG:HA	2.00	0.43
1:F:402:ASN:OD1	1:F:404:VAL:HG13	2.18	0.43
1:G:86:LYS:O	1:G:86:LYS:CG	2.63	0.43
1:H:403:GLU:O	1:H:403:GLU:OE2	2.35	0.43
1:I:367:PRO:O	1:I:370:ARG:NH1	2.50	0.43
1:K:189:GLU:OE2	1:K:190:VAL:HG23	2.18	0.43
1:K:84:ALA:N	1:K:85:GLU:OE2	2.52	0.43
1:L:380:ARG:HG2	1:L:385:ILE:HG21	1.99	0.43
1:L:96:ILE:N	1:L:96:ILE:CD1	2.81	0.43
1:A:220:THR:OG1	1:F:162:THR:HG21	2.19	0.43
1:A:443:GLN:HG2	1:A:444:TYR:CD2	2.53	0.43
1:B:311:TRP:HB3	1:B:320:ILE:HB	2.00	0.43
1:F:148:LEU:HD11	1:L:437:ARG:CD	2.45	0.43
1:G:377:LYS:HD3	1:G:380:ARG:CZ	2.49	0.43
1:H:86:LYS:HE2	1:I:175:GLU:OE1	2.19	0.43
1:I:136:PHE:CE2	1:I:194:GLN:HB2	2.53	0.43
1:J:214:PHE:CZ	1:J:218:VAL:HG21	2.53	0.43
1:J:369:ASP:CG	1:J:370:ARG:N	2.71	0.43
1:K:5:THR:O	1:K:7:GLU:N	2.51	0.43
1:K:64:GLU:HB3	1:L:314:GLN:HE21	1.83	0.43
1:G:157:PHE:C	1:L:33:LYS:HD2	2.38	0.43
1:C:176:LEU:HD22	1:C:181:PHE:CE1	2.53	0.43
1:C:304:GLU:O	1:C:317:SER:HB2	2.17	0.43
1:E:412:HIS:CE1	1:E:416:HIS:CE1	3.06	0.43
1:F:357:GLY:HA2	1:F:362:LEU:CD2	2.37	0.43
1:F:359:LYS:HG3	1:F:360:ASN:ND2	2.33	0.43
1:F:417:PHE:O	1:F:421:LYS:HG2	2.17	0.43
1:H:21:ILE:HG12	1:H:37:ILE:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:396:LEU:HD11	1:H:421:LYS:HB3	2.00	0.43
1:I:308:TYR:HD1	1:I:372:ILE:HG21	1.84	0.43
1:J:133:PRO:HD2	1:J:197:ILE:O	2.18	0.43
1:K:59:GLY:O	1:K:62:ARG:HG3	2.18	0.43
1:L:377:LYS:O	1:L:381:MET:HG2	2.17	0.43
1:A:122:LEU:HD12	1:A:355:LEU:HD13	2.01	0.43
1:B:167:ASN:HD21	1:C:22:ARG:HH22	1.66	0.43
1:D:383:ASN:C	1:D:385:ILE:N	2.72	0.43
1:F:221:ILE:O	1:F:224:LYS:HB3	2.19	0.43
1:F:371:ASN:OD1	1:F:373:TYR:HB2	2.19	0.43
1:F:402:ASN:C	1:F:402:ASN:OD1	2.57	0.43
1:H:305:ALA:HA	1:H:306:PRO:HD3	1.80	0.43
1:I:285:PHE:CD1	1:I:285:PHE:C	2.92	0.43
1:J:160:ALA:HB2	1:J:188:HIS:HB2	1.99	0.43
1:K:23:LEU:HB3	1:K:70:LEU:HD22	2.01	0.43
1:K:371:ASN:HB3	1:K:375:MET:HE1	2.00	0.43
1:A:162:THR:C	1:A:164:LEU:H	2.21	0.43
1:B:166:GLU:HG2	1:B:168:CYS:N	2.32	0.43
1:B:135:PHE:CZ	1:B:195:HIS:HB2	2.53	0.43
1:D:370:ARG:CB	1:D:370:ARG:HH11	2.12	0.43
1:F:281:HIS:O	1:F:282:ALA:C	2.56	0.43
1:K:305:ALA:HA	1:K:306:PRO:HD3	1.74	0.43
1:K:98:ASN:HB3	1:K:99:PRO:HD2	2.00	0.43
1:A:345:LEU:HD22	1:A:409:LEU:HD22	2.01	0.43
1:C:85:GLU:O	1:C:86:LYS:HB2	2.18	0.43
1:D:371:ASN:HD21	1:D:374:VAL:HG22	1.84	0.43
1:F:213:THR:O	1:F:216:LEU:HB3	2.19	0.43
1:F:197:ILE:HD12	1:F:214:PHE:CE1	2.54	0.43
1:G:308:TYR:CD2	1:G:380:ARG:NH1	2.87	0.43
1:G:82:TRP:O	1:G:83:THR:C	2.57	0.43
1:H:269:GLU:HA	1:H:269:GLU:OE2	2.19	0.43
1:J:289:THR:O	1:J:341:ALA:HB2	2.19	0.43
1:K:134:GLU:HG2	1:K:196:GLU:HB2	2.01	0.43
1:L:218:VAL:O	1:L:219:LYS:C	2.56	0.43
1:A:11:LYS:HE2	1:A:15:GLU:OE1	2.19	0.43
1:E:85:GLU:OE2	1:E:85:GLU:CA	2.52	0.43
1:G:296:TYR:N	1:G:296:TYR:CD1	2.86	0.43
1:G:396:LEU:HD11	1:G:421:LYS:HB3	2.00	0.43
1:H:239:VAL:HG23	1:H:240:ASN:N	2.34	0.43
1:H:280:LYS:HD3	1:H:281:HIS:NE2	2.33	0.43
1:H:326:ARG:HD3	1:H:326:ARG:HA	1.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:368:ILE:HD13	1:H:368:ILE:N	2.33	0.43
1:H:380:ARG:HD2	1:H:385:ILE:HG21	2.01	0.43
1:H:396:LEU:HD22	1:H:418:ILE:CD1	2.48	0.43
1:H:73:ASP:OD1	1:H:73:ASP:C	2.57	0.43
1:I:380:ARG:NH1	1:I:387:ASP:OD1	2.52	0.43
1:K:112:LEU:HD23	1:K:112:LEU:HA	1.72	0.43
1:K:372:ILE:HG12	1:K:372:ILE:O	2.18	0.43
1:L:409:LEU:HD12	1:L:413:LEU:HB3	2.00	0.43
1:A:231:PHE:O	1:A:339:PRO:HG2	2.18	0.43
1:A:80:PHE:HB3	1:A:82:TRP:CE3	2.54	0.43
1:D:191:ALA:HB2	1:D:240:ASN:HB2	2.00	0.43
1:D:48:ASN:HB3	1:D:71:TYR:CE1	2.53	0.43
1:I:317:SER:O	1:I:373:TYR:OH	2.36	0.43
1:I:402:ASN:O	1:I:406:VAL:HG23	2.19	0.43
1:I:82:TRP:HB2	1:I:83:THR:H	1.48	0.43
1:I:62:ARG:NE	1:J:156:TYR:CE2	2.87	0.43
1:K:83:THR:O	1:K:84:ALA:CB	2.65	0.43
1:G:167:ASN:ND2	1:L:22:ARG:HH22	2.11	0.43
1:D:347:LEU:HD23	1:D:347:LEU:HA	1.66	0.43
1:E:127:PHE:CE2	1:E:351:LEU:HG	2.53	0.43
1:F:409:LEU:HA	1:F:409:LEU:HD23	1.61	0.43
1:G:48:ASN:N	1:G:48:ASN:OD1	2.52	0.43
1:H:281:HIS:CE1	1:H:356:ASP:OD2	2.71	0.43
1:H:63:ILE:HD13	1:H:63:ILE:HA	1.77	0.43
1:H:73:ASP:O	1:H:76:THR:OG1	2.33	0.43
1:J:338:ASP:CB	1:J:339:PRO:CD	2.96	0.43
1:K:28:ILE:HD11	1:K:417:PHE:CB	2.49	0.43
1:K:33:LYS:O	1:K:34:ASN:HB3	2.19	0.43
1:K:37:ILE:HD12	1:K:41:GLN:CB	2.47	0.43
1:K:62:ARG:HD2	1:L:156:TYR:CD2	2.54	0.43
1:K:57:ILE:HD11	1:K:96:ILE:HG13	2.00	0.43
1:A:265:LEU:O	1:A:326:ARG:NH1	2.51	0.42
1:C:369:ASP:O	1:C:370:ARG:C	2.56	0.42
1:D:308:TYR:HE1	1:D:373:TYR:CD1	2.37	0.42
1:F:310:ALA:HB1	1:F:368:ILE:HG12	2.01	0.42
1:G:317:SER:N	1:G:318:PRO:CD	2.81	0.42
1:G:421:LYS:HA	1:G:421:LYS:HD3	1.81	0.42
1:H:150:LEU:HD13	1:H:192:PRO:O	2.18	0.42
1:I:85:GLU:O	1:I:86:LYS:CB	2.48	0.42
1:J:191:ALA:H	1:J:194:GLN:HE21	1.67	0.42
1:J:370:ARG:HB3	1:J:371:ASN:H	1.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:291:PRO:HG3	1:L:341:ALA:HA	2.00	0.42
1:A:251:PHE:CD1	1:A:256:ASN:HA	2.54	0.42
1:C:5:THR:O	1:C:6:ARG:C	2.57	0.42
1:C:73:ASP:CG	1:C:76:THR:HG23	2.39	0.42
1:D:375:MET:HB2	1:D:379:GLU:HB3	2.00	0.42
1:D:7:GLU:CD	1:D:7:GLU:H	2.22	0.42
1:E:297:LYS:HD3	1:E:297:LYS:HA	1.81	0.42
1:E:396:LEU:HD11	1:E:421:LYS:HB3	2.01	0.42
1:F:300:VAL:CG1	1:F:301:PRO:HD2	2.47	0.42
1:F:423:ILE:HG13	1:F:424:GLU:N	2.33	0.42
1:H:221:ILE:O	1:H:224:LYS:HB3	2.20	0.42
1:H:345:LEU:HD22	1:H:409:LEU:HD22	2.01	0.42
1:I:124:PHE:HB3	1:I:250:LEU:HD22	2.00	0.42
1:I:376:SER:HB2	1:I:377:LYS:HZ3	1.83	0.42
1:J:437:ARG:O	1:J:441:MET:HB3	2.19	0.42
1:K:27:ASP:C	1:K:27:ASP:OD2	2.58	0.42
1:C:109:ARG:HD2	1:C:344:TYR:CZ	2.53	0.42
1:C:71:TYR:CD1	1:C:97:TYR:HD1	2.37	0.42
1:D:374:VAL:CG2	1:D:375:MET:N	2.82	0.42
1:D:381:MET:C	1:D:383:ASN:N	2.72	0.42
1:F:201:TYR:C	1:F:201:TYR:HD1	2.23	0.42
1:G:12:LEU:HA	1:G:12:LEU:HD23	1.66	0.42
1:G:131:PRO:HG2	1:G:199:PHE:HE1	1.83	0.42
1:G:258:PHE:HB3	1:G:271:ALA:HB2	1.96	0.42
1:G:85:GLU:O	1:G:86:LYS:HB2	2.19	0.42
1:H:311:TRP:CZ2	1:H:367:PRO:HD3	2.55	0.42
1:H:385:ILE:CD1	1:H:385:ILE:N	2.81	0.42
1:H:83:THR:C	1:H:85:GLU:OE2	2.58	0.42
1:K:42:LEU:O	1:K:45:ALA:HB3	2.19	0.42
1:L:16:GLU:HG2	1:L:79:ILE:HD13	2.01	0.42
1:A:305:ALA:HA	1:A:306:PRO:HD3	1.91	0.42
1:A:46:LEU:C	1:A:48:ASN:H	2.23	0.42
1:B:162:THR:CG2	1:C:216:LEU:HD11	2.49	0.42
1:B:183:ILE:N	1:B:183:ILE:CD1	2.82	0.42
1:B:28:ILE:O	1:B:28:ILE:HG13	2.18	0.42
1:B:291:PRO:HB2	1:B:421:LYS:NZ	2.34	0.42
1:B:426:ASP:HA	1:B:429:ARG:HG3	2.01	0.42
1:B:436:GLU:OE2	1:H:297:LYS:HD3	2.20	0.42
1:C:275:ILE:O	1:C:279:VAL:HG23	2.20	0.42
1:C:371:ASN:ND2	5:D:621:HOH:O	2.45	0.42
1:D:169:ARG:HD2	1:D:186:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:LEU:O	1:D:201:TYR:HA	2.20	0.42
1:F:285:PHE:CD1	1:F:285:PHE:C	2.93	0.42
1:F:29:LEU:HD21	1:F:421:LYS:NZ	2.33	0.42
1:G:258:PHE:HA	1:G:268:SER:OG	2.19	0.42
1:H:167:ASN:HB3	1:H:170:ARG:NH2	2.34	0.42
1:H:245:HIS:CE1	4:H:504:PO4:O3	2.73	0.42
1:H:308:TYR:CD1	1:H:372:ILE:HG13	2.54	0.42
1:K:183:ILE:N	1:K:183:ILE:HD13	2.35	0.42
1:K:299:LEU:HD12	1:K:299:LEU:HA	1.93	0.42
1:K:5:THR:O	1:K:6:ARG:C	2.58	0.42
1:L:168:CYS:SG	1:L:227:LEU:HD12	2.60	0.42
1:A:371:ASN:OD1	1:A:371:ASN:O	2.37	0.42
1:A:70:LEU:HG	1:A:94:CYS:SG	2.60	0.42
1:C:153:LYS:HG2	1:C:153:LYS:H	1.63	0.42
1:C:374:VAL:HG22	1:C:375:MET:N	2.34	0.42
1:D:129:LEU:HD22	1:D:130:GLY:N	2.34	0.42
1:G:328:ILE:H	1:G:328:ILE:CD1	2.33	0.42
1:A:231:PHE:HB2	1:G:444:TYR:OXT	2.20	0.42
1:J:351:LEU:HD22	1:J:355:LEU:HG	2.00	0.42
1:K:380:ARG:CG	1:K:385:ILE:HG21	2.49	0.42
1:L:239:VAL:HG23	1:L:240:ASN:N	2.34	0.42
1:L:376:SER:O	1:L:377:LYS:C	2.58	0.42
1:A:119:MET:HB2	1:A:355:LEU:HD11	2.02	0.42
1:A:164:LEU:HB3	1:B:220:THR:HG23	2.02	0.42
1:A:24:GLN:HB3	1:A:93:ILE:HA	2.01	0.42
1:B:129:LEU:HD13	1:B:131:PRO:HD3	2.01	0.42
1:B:163:ASP:HA	1:B:170:ARG:NH1	2.34	0.42
1:B:213:THR:O	1:B:216:LEU:HB3	2.18	0.42
1:B:236:LEU:HD12	1:B:239:VAL:HG21	2.02	0.42
1:C:240:ASN:ND2	1:C:303:TYR:HD1	2.17	0.42
1:D:12:LEU:HD23	1:D:12:LEU:HA	1.84	0.42
1:D:80:PHE:CZ	1:D:91:ARG:HB3	2.54	0.42
1:F:399:PHE:HZ	1:F:409:LEU:HD12	1.84	0.42
1:I:119:MET:HG2	1:I:120:GLU:N	2.33	0.42
1:I:224:LYS:HE3	1:I:225:HIS:CD2	2.55	0.42
1:J:370:ARG:HA	1:J:370:ARG:HD3	1.72	0.42
1:K:97:TYR:CE2	1:K:103:PRO:HG3	2.55	0.42
1:C:251:PHE:HE1	1:C:256:ASN:ND2	2.18	0.42
1:A:33:LYS:HE2	1:F:158:ASP:OD2	2.19	0.42
1:F:234:LYS:HE3	1:F:239:VAL:O	2.19	0.42
1:F:412:HIS:CE1	1:F:416:HIS:CE1	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:SER:O	1:L:36:GLU:HG2	2.19	0.42
1:G:260:ASP:CG	1:G:263:ALA:HB2	2.39	0.42
1:G:338:ASP:HB2	1:G:339:PRO:CD	2.45	0.42
1:G:368:ILE:O	1:G:369:ASP:CB	2.67	0.42
1:H:176:LEU:HD22	1:H:181:PHE:CD1	2.54	0.42
1:J:141:ASP:OD2	1:J:141:ASP:C	2.58	0.42
1:J:311:TRP:HB3	1:J:320:ILE:HB	2.01	0.42
1:J:380:ARG:HG2	1:J:385:ILE:HG21	2.00	0.42
1:K:316:ARG:NH2	1:K:370:ARG:NH1	2.68	0.42
1:B:162:THR:HG22	1:B:163:ASP:N	2.34	0.42
1:B:199:PHE:HZ	1:B:214:PHE:CD1	2.37	0.42
1:B:258:PHE:HZ	1:B:274:PHE:CD1	2.38	0.42
1:C:17:ASN:ND2	1:C:87:GLY:HA2	2.35	0.42
1:D:160:ALA:CB	1:D:161:PRO:CD	2.94	0.42
1:D:423:ILE:O	1:D:427:MET:HG3	2.19	0.42
1:E:21:ILE:N	1:E:21:ILE:HD12	2.34	0.42
1:E:25:PHE:N	1:E:25:PHE:CD2	2.88	0.42
1:F:282:ALA:HA	1:F:285:PHE:CE2	2.54	0.42
1:G:315:ASN:CG	1:G:316:ARG:H	2.23	0.42
1:G:82:TRP:CD1	1:H:164:LEU:HD12	2.54	0.42
1:K:27:ASP:HB3	1:K:33:LYS:HE3	2.01	0.42
1:L:116:LEU:HD23	1:L:116:LEU:HA	1.85	0.42
1:L:381:MET:C	1:L:383:ASN:N	2.73	0.42
1:L:60:PHE:HE1	1:L:423:ILE:HG12	1.85	0.42
1:B:260:ASP:C	1:B:260:ASP:OD1	2.59	0.42
1:B:379:GLU:O	1:B:383:ASN:ND2	2.53	0.42
1:D:435:TRP:CH2	1:J:428:PHE:HB2	2.55	0.42
1:D:98:ASN:ND2	1:D:104:PHE:HA	2.34	0.42
1:F:89:VAL:HG12	1:F:90:ALA:N	2.35	0.42
1:F:98:ASN:HB2	1:F:102:THR:HG23	2.02	0.42
1:G:377:LYS:NZ	1:G:380:ARG:NH2	2.65	0.42
1:I:274:PHE:C	1:I:274:PHE:CD2	2.93	0.42
1:J:25:PHE:CE1	1:J:33:LYS:HB2	2.55	0.42
1:J:285:PHE:HB2	1:J:349:VAL:CG1	2.50	0.42
1:J:300:VAL:HG13	1:J:301:PRO:CD	2.50	0.42
1:K:261:GLU:HA	1:K:266:GLN:HE21	1.82	0.42
1:L:105:GLU:C	1:L:105:GLU:CD	2.78	0.42
1:L:418:ILE:HD13	1:L:418:ILE:N	2.34	0.42
1:A:413:LEU:HD23	1:A:413:LEU:HA	1.78	0.42
1:B:115:ILE:N	1:B:115:ILE:HD12	2.35	0.42
1:D:305:ALA:HA	1:D:306:PRO:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:TRP:CB	1:F:320:ILE:HB	2.50	0.42
1:I:138:PHE:CE2	1:I:150:LEU:HD23	2.55	0.42
1:I:160:ALA:O	1:I:161:PRO:C	2.57	0.42
1:I:28:ILE:HD13	1:I:28:ILE:O	2.19	0.42
1:L:260:ASP:CG	1:L:263:ALA:HB2	2.41	0.42
1:L:369:ASP:CG	1:L:370:ARG:H	2.23	0.42
1:L:421:LYS:HD3	1:L:421:LYS:HA	1.86	0.42
1:B:14:LYS:HB2	1:B:14:LYS:HE3	1.70	0.41
1:B:186:SER:OG	1:C:36:GLU:HG3	2.20	0.41
1:B:91:ARG:C	1:B:91:ARG:HD2	2.39	0.41
1:C:58:GLU:O	1:C:61:VAL:HG22	2.20	0.41
1:F:184:GLU:O	1:F:185:ALA:HB2	2.20	0.41
1:F:231:PHE:HA	5:F:601:HOH:O	2.20	0.41
1:F:372:ILE:CG2	1:F:380:ARG:HD2	2.50	0.41
1:G:112:LEU:HD11	1:G:204:ALA:HB1	2.02	0.41
1:G:13:VAL:HG21	1:G:42:LEU:HD21	2.02	0.41
1:G:36:GLU:OE1	1:H:186:SER:OG	2.35	0.41
1:H:252:LYS:O	1:H:253:ASN:HB2	2.20	0.41
1:B:440:TYR:OH	1:H:293:VAL:HB	2.19	0.41
1:H:245:HIS:CD2	1:H:335:ARG:HA	2.55	0.41
1:H:403:GLU:HG3	1:H:407:LYS:HE3	2.01	0.41
1:H:104:PHE:HZ	1:H:412:HIS:CE1	2.37	0.41
1:I:160:ALA:HB1	1:I:161:PRO:CD	2.39	0.41
1:J:274:PHE:CE2	1:J:278:ILE:CD1	3.03	0.41
1:J:28:ILE:HD12	1:J:29:LEU:H	1.85	0.41
1:J:16:GLU:O	1:J:88:LYS:HG3	2.20	0.41
1:J:62:ARG:HD2	1:K:156:TYR:HD1	1.84	0.41
1:K:370:ARG:NH2	1:K:371:ASN:O	2.53	0.41
1:K:114:ARG:NH2	1:K:407:LYS:O	2.43	0.41
1:L:182:GLU:CG	1:L:200:LYS:HD2	2.41	0.41
1:L:274:PHE:CD2	1:L:274:PHE:C	2.92	0.41
1:L:379:GLU:O	1:L:383:ASN:OD1	2.38	0.41
1:L:418:ILE:HD12	1:L:418:ILE:HA	1.84	0.41
1:L:98:ASN:HB3	1:L:99:PRO:HD2	2.02	0.41
1:B:215:LYS:O	1:B:219:LYS:HD3	2.21	0.41
1:B:380:ARG:HG3	1:B:385:ILE:HB	2.02	0.41
1:B:83:THR:O	1:B:84:ALA:CB	2.67	0.41
1:D:127:PHE:CD2	1:D:351:LEU:HG	2.55	0.41
1:D:435:TRP:O	1:D:439:GLN:HG2	2.20	0.41
1:E:51:MET:HE1	1:E:67:ASP:HB3	2.01	0.41
1:F:116:LEU:HA	1:F:116:LEU:HD23	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:382:GLU:C	1:F:383:ASN:ND2	2.63	0.41
1:H:34:ASN:ND2	1:H:34:ASN:C	2.74	0.41
1:H:70:LEU:C	1:H:71:TYR:HD1	2.23	0.41
1:I:328:ILE:H	1:I:328:ILE:HG13	1.40	0.41
1:J:27:ASP:CG	1:J:31:THR:HB	2.41	0.41
1:J:392:LEU:O	1:J:396:LEU:HG	2.20	0.41
1:A:162:THR:O	1:A:164:LEU:N	2.54	0.41
1:A:328:ILE:H	1:A:328:ILE:HG13	1.61	0.41
1:C:46:LEU:HD23	1:C:46:LEU:HA	1.88	0.41
1:D:281:HIS:CD2	1:D:402:ASN:HD21	2.30	0.41
1:F:133:PRO:HG2	1:F:199:PHE:HE1	1.84	0.41
1:G:214:PHE:CZ	1:G:218:VAL:HG21	2.55	0.41
1:I:201:TYR:C	1:I:201:TYR:CD2	2.94	0.41
1:J:327:GLY:C	1:J:329:SER:N	2.74	0.41
1:J:78:VAL:CG1	1:J:79:ILE:N	2.83	0.41
1:K:145:GLU:OE2	1:K:145:GLU:HA	2.20	0.41
1:K:272:LYS:HA	1:K:275:ILE:HD12	2.02	0.41
1:K:304:GLU:O	1:K:335:ARG:NH1	2.53	0.41
1:A:119:MET:HE1	1:A:127:PHE:CB	2.48	0.41
1:A:303:TYR:O	1:A:304:GLU:HB2	2.21	0.41
1:A:381:MET:C	1:A:383:ASN:N	2.74	0.41
1:B:184:GLU:OE2	1:B:200:LYS:HD2	2.19	0.41
1:B:129:LEU:CD2	1:B:248:LEU:HD23	2.46	0.41
1:B:381:MET:O	1:B:384:GLY:N	2.35	0.41
1:D:314:GLN:NE2	1:E:64:GLU:HB3	2.35	0.41
1:E:25:PHE:CE1	1:E:33:LYS:HB2	2.55	0.41
1:G:100:ASP:CG	1:G:101:GLY:H	2.23	0.41
1:G:145:GLU:HA	1:G:146:PRO:HD3	1.91	0.41
1:G:289:THR:HB	1:G:337:VAL:HG22	2.01	0.41
1:H:141:ASP:C	1:H:141:ASP:OD2	2.59	0.41
1:H:350:LEU:HA	1:H:350:LEU:HD23	1.92	0.41
1:I:380:ARG:C	1:I:385:ILE:HB	2.41	0.41
1:K:45:ALA:C	1:K:46:LEU:O	2.58	0.41
1:L:115:ILE:HG22	1:L:351:LEU:HD13	2.02	0.41
1:A:368:ILE:HA	1:A:368:ILE:HD12	1.60	0.41
1:B:129:LEU:CD1	1:B:131:PRO:HD3	2.50	0.41
1:B:258:PHE:HA	1:B:271:ALA:HB2	2.03	0.41
1:B:309:VAL:CG2	1:B:386:VAL:HG13	2.51	0.41
1:B:372:ILE:HA	1:B:372:ILE:HD12	1.76	0.41
1:B:91:ARG:HD2	1:B:92:PHE:N	2.35	0.41
1:C:97:TYR:CE2	1:C:103:PRO:HB3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:MET:HG2	1:C:124:PHE:HB2	2.01	0.41
1:C:369:ASP:CG	1:C:370:ARG:H	2.23	0.41
1:C:418:ILE:O	1:C:422:GLU:HG3	2.20	0.41
1:C:82:TRP:C	1:C:83:THR:OG1	2.57	0.41
1:D:244:MET:O	1:D:244:MET:HG2	2.20	0.41
1:H:160:ALA:CB	1:H:161:PRO:HD2	2.24	0.41
1:I:139:LYS:HD3	1:I:149:GLU:CD	2.41	0.41
1:I:124:PHE:CB	1:I:250:LEU:HD22	2.50	0.41
1:J:135:PHE:CZ	1:J:195:HIS:HB2	2.56	0.41
1:L:402:ASN:ND2	1:L:404:VAL:N	2.69	0.41
1:A:261:GLU:C	1:A:263:ALA:H	2.23	0.41
1:B:71:TYR:CD1	1:B:97:TYR:CD1	3.08	0.41
1:C:281:HIS:CE1	1:C:356:ASP:OD2	2.73	0.41
1:C:273:HIS:CE1	1:C:361:LYS:HA	2.56	0.41
1:D:27:ASP:C	1:D:29:LEU:H	2.22	0.41
1:E:11:LYS:O	1:E:15:GLU:CG	2.68	0.41
1:E:164:LEU:HD23	1:E:164:LEU:HA	1.82	0.41
1:F:186:SER:O	1:F:187:HIS:HB3	2.21	0.41
1:F:265:LEU:HD23	1:F:265:LEU:HA	1.85	0.41
1:G:174:LEU:HD12	1:G:174:LEU:HA	1.70	0.41
1:G:176:LEU:O	1:G:181:PHE:HB2	2.20	0.41
1:G:258:PHE:CB	1:G:271:ALA:CB	2.90	0.41
1:G:393:ALA:HB2	1:G:425:TRP:CE2	2.55	0.41
1:H:135:PHE:CZ	1:H:195:HIS:HB2	2.55	0.41
1:H:370:ARG:HD2	1:H:371:ASN:O	2.20	0.41
1:H:85:GLU:N	1:H:85:GLU:CD	2.74	0.41
1:I:175:GLU:HG3	1:I:221:ILE:HD11	2.02	0.41
1:K:120:GLU:HA	1:K:124:PHE:O	2.20	0.41
1:K:363:GLU:OE2	1:K:363:GLU:CA	2.69	0.41
1:L:368:ILE:HG21	1:L:372:ILE:CG2	2.51	0.41
1:A:119:MET:HA	1:A:355:LEU:HD11	2.03	0.41
1:B:290:ASN:HB3	1:B:295:SER:HB3	2.03	0.41
1:A:370:ARG:HD2	1:B:64:GLU:OE2	2.21	0.41
1:E:274:PHE:CE2	1:E:278:ILE:HD11	2.55	0.41
1:F:26:THR:HG22	1:F:27:ASP:O	2.19	0.41
1:G:48:ASN:ND2	1:G:71:TYR:CD2	2.89	0.41
1:H:23:LEU:HD11	1:H:37:ILE:HD13	2.01	0.41
1:I:21:ILE:HG12	1:I:42:LEU:HD13	2.02	0.41
1:K:58:GLU:O	1:K:61:VAL:HG22	2.20	0.41
1:L:166:GLU:HG3	1:L:167:ASN:N	2.34	0.41
1:L:225:HIS:O	1:L:227:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:281:HIS:O	1:L:282:ALA:C	2.59	0.41
1:B:111:ASN:OD1	1:B:114:ARG:NH1	2.54	0.41
1:B:250:LEU:HA	1:B:250:LEU:HD23	1.92	0.41
1:B:274:PHE:CE2	1:B:278:ILE:HD11	2.56	0.41
1:B:291:PRO:HB2	1:B:421:LYS:HZ1	1.86	0.41
1:C:7:GLU:CD	1:C:7:GLU:H	2.24	0.41
1:D:388:LEU:HA	1:D:388:LEU:HD23	1.93	0.41
1:F:97:TYR:CD2	1:F:103:PRO:HA	2.56	0.41
1:F:443:GLN:NE2	5:F:606:HOH:O	2.34	0.41
1:G:265:LEU:O	1:G:326:ARG:NH1	2.53	0.41
1:G:443:GLN:HB3	1:G:444:TYR:CD2	2.55	0.41
1:G:51:MET:CE	1:G:67:ASP:HB3	2.51	0.41
1:H:140:LEU:HD23	1:H:140:LEU:HA	1.81	0.41
1:I:168:CYS:O	1:I:169:ARG:C	2.59	0.41
1:I:351:LEU:O	1:I:355:LEU:HG	2.20	0.41
1:I:414:PHE:O	1:I:418:ILE:HG13	2.21	0.41
1:J:111:ASN:OD1	1:J:114:ARG:NH1	2.54	0.41
1:J:272:LYS:HB3	1:J:272:LYS:HE2	1.77	0.41
1:K:5:THR:HG23	1:K:8:ASP:CG	2.41	0.41
1:K:55:SER:O	1:K:62:ARG:HG2	2.20	0.41
1:A:22:ARG:HH12	1:A:36:GLU:CD	2.24	0.41
1:A:251:PHE:CE1	1:A:256:ASN:HA	2.56	0.41
1:A:369:ASP:O	1:A:371:ASN:N	2.54	0.41
1:A:91:ARG:O	1:A:91:ARG:HG3	2.20	0.41
1:B:172:ILE:HG13	1:B:221:ILE:HG21	2.02	0.41
1:B:278:ILE:HG23	1:B:285:PHE:CZ	2.56	0.41
1:B:317:SER:OG	1:B:373:TYR:CZ	2.72	0.41
1:C:326:ARG:HA	1:C:330:THR:OG1	2.20	0.41
1:B:164:LEU:CD2	1:C:82:TRP:HB3	2.50	0.41
1:D:91:ARG:C	1:D:91:ARG:HD2	2.41	0.41
1:E:28:ILE:HD11	1:E:417:PHE:HB2	2.02	0.41
1:F:197:ILE:HD12	1:F:214:PHE:HE1	1.86	0.41
1:G:23:LEU:HD13	1:G:70:LEU:HD23	2.03	0.41
1:H:247:ASN:OD1	1:H:333:GLU:HB2	2.21	0.41
1:I:115:ILE:O	1:I:118:GLU:HB2	2.21	0.41
1:I:172:ILE:O	1:I:176:LEU:HG	2.20	0.41
1:I:289:THR:OG1	1:I:290:ASN:ND2	2.54	0.41
1:I:351:LEU:HD22	1:I:351:LEU:O	2.21	0.41
1:C:435:TRP:CD1	1:I:431:GLN:HG2	2.56	0.41
1:J:285:PHE:C	1:J:285:PHE:HD1	2.23	0.41
1:L:13:VAL:HG13	1:L:18:VAL:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:PRO:CA	1:A:244:MET:HG3	2.51	0.41
1:A:160:ALA:CB	1:A:188:HIS:CD2	3.03	0.41
1:A:405:MET:HE2	1:A:405:MET:HA	2.03	0.41
1:A:410:GLY:O	1:A:411:GLU:C	2.58	0.41
1:A:83:THR:HA	1:A:85:GLU:OE2	2.21	0.41
1:D:205:VAL:HG23	1:D:206:ARG:H	1.83	0.41
1:D:329:SER:O	1:D:331:ARG:NH2	2.46	0.41
1:E:169:ARG:NE	1:E:195:HIS:HD2	2.19	0.41
1:E:34:ASN:ND2	1:E:34:ASN:C	2.74	0.41
1:E:91:ARG:HD2	1:E:92:PHE:N	2.35	0.41
1:F:168:CYS:O	1:F:172:ILE:CG1	2.68	0.41
1:F:231:PHE:O	1:F:339:PRO:HG2	2.21	0.41
1:F:375:MET:HA	1:F:379:GLU:HG3	2.03	0.41
1:G:146:PRO:HG3	1:G:228:HIS:CD2	2.56	0.41
1:G:127:PHE:HE2	1:G:347:LEU:HD12	1.86	0.41
1:G:91:ARG:HD2	1:G:91:ARG:C	2.41	0.41
1:H:27:ASP:OD2	1:H:31:THR:N	2.53	0.41
1:H:245:HIS:HA	1:H:334:VAL:O	2.21	0.41
1:I:141:ASP:OD2	1:I:143:LYS:N	2.54	0.41
1:J:296:TYR:HB3	1:J:390:ALA:O	2.21	0.41
1:J:79:ILE:HG12	1:J:90:ALA:HB2	2.02	0.41
1:K:316:ARG:HH22	1:K:370:ARG:CZ	2.33	0.41
1:K:8:ASP:O	1:K:12:LEU:HB2	2.21	0.41
1:L:129:LEU:HD22	1:L:131:PRO:HD3	2.02	0.41
1:L:166:GLU:O	1:L:167:ASN:C	2.58	0.41
1:A:252:LYS:NZ	1:A:252:LYS:HB2	2.36	0.41
1:B:52:PHE:CE1	1:B:70:LEU:CD1	3.03	0.41
1:D:160:ALA:HB2	1:D:188:HIS:CG	2.53	0.41
1:E:316:ARG:N	1:E:370:ARG:NH1	2.64	0.41
1:F:127:PHE:CZ	1:F:248:LEU:HD22	2.56	0.41
1:G:88:LYS:HZ3	1:G:88:LYS:HG3	1.72	0.41
1:H:421:LYS:HA	1:H:421:LYS:HD3	1.75	0.41
1:I:100:ASP:HB2	1:I:101:GLY:H	1.72	0.41
1:I:133:PRO:CA	1:I:244:MET:HG3	2.50	0.41
1:I:309:VAL:HG13	1:I:319:LEU:HD22	2.03	0.41
1:I:33:LYS:HE3	1:J:156:TYR:O	2.21	0.41
1:K:316:ARG:NH2	1:K:370:ARG:CD	2.82	0.41
1:K:37:ILE:HD11	1:K:45:ALA:HB2	2.03	0.41
1:L:119:MET:HA	1:L:355:LEU:CD1	2.51	0.41
1:L:380:ARG:O	1:L:385:ILE:HB	2.21	0.41
1:A:112:LEU:HD23	1:A:112:LEU:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:GLU:HB3	1:A:196:GLU:OE2	2.20	0.40
1:A:218:VAL:O	1:A:219:LYS:C	2.60	0.40
1:C:16:GLU:OE2	1:C:16:GLU:HA	2.21	0.40
1:D:115:ILE:CG2	1:D:351:LEU:HD12	2.49	0.40
1:D:383:ASN:O	1:D:385:ILE:N	2.54	0.40
1:D:392:LEU:O	1:D:392:LEU:HD12	2.21	0.40
1:D:417:PHE:O	1:D:421:LYS:HG2	2.21	0.40
1:D:54:GLY:HA3	1:D:68:MET:CG	2.50	0.40
1:E:160:ALA:CB	1:E:161:PRO:CD	2.94	0.40
1:F:124:PHE:CD2	1:F:252:LYS:HG3	2.56	0.40
1:F:374:VAL:HG23	1:F:375:MET:N	2.36	0.40
1:F:421:LYS:HD3	1:F:421:LYS:HA	1.82	0.40
1:G:9:ILE:HG22	1:G:10:GLU:N	2.35	0.40
1:G:27:ASP:OD2	1:G:31:THR:N	2.53	0.40
1:G:423:ILE:O	1:G:424:GLU:C	2.59	0.40
1:G:67:ASP:C	1:G:68:MET:HG2	2.41	0.40
1:H:318:PRO:O	1:H:335:ARG:HD3	2.21	0.40
1:J:351:LEU:O	1:J:355:LEU:HG	2.21	0.40
1:B:162:THR:C	1:B:164:LEU:H	2.24	0.40
1:B:285:PHE:C	1:B:285:PHE:CD1	2.95	0.40
1:B:434:PRO:O	1:B:438:GLU:HG3	2.21	0.40
1:C:227:LEU:HA	1:C:227:LEU:HD23	1.82	0.40
1:D:115:ILE:HA	1:D:118:GLU:HG3	2.03	0.40
1:F:281:HIS:CD2	1:F:402:ASN:HD21	2.40	0.40
1:F:281:HIS:CE1	1:F:356:ASP:OD2	2.69	0.40
1:G:326:ARG:HA	1:G:326:ARG:HD3	1.54	0.40
1:H:189:GLU:HB3	1:H:194:GLN:NE2	2.36	0.40
1:H:402:ASN:OD1	1:H:402:ASN:C	2.59	0.40
1:I:85:GLU:OE2	1:I:87:GLY:O	2.39	0.40
1:J:244:MET:O	1:J:244:MET:HG2	2.22	0.40
1:J:434:PRO:O	1:J:438:GLU:HG3	2.20	0.40
1:K:73:ASP:OD1	1:K:76:THR:HG23	2.21	0.40
1:L:259:PHE:CD1	1:L:260:ASP:N	2.88	0.40
1:B:81:PRO:HG2	1:B:82:TRP:HE3	1.86	0.40
1:C:39:VAL:C	1:C:41:GLN:H	2.23	0.40
1:C:245:HIS:ND1	4:C:504:PO4:O2	2.54	0.40
1:D:160:ALA:HB3	1:D:169:ARG:NH1	2.18	0.40
1:E:316:ARG:C	1:E:316:ARG:HD2	2.40	0.40
1:E:380:ARG:NH1	1:E:387:ASP:OD2	2.54	0.40
1:E:85:GLU:HB3	1:E:86:LYS:H	1.74	0.40
1:F:260:ASP:CG	1:F:263:ALA:HB2	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:338:ASP:OD2	1:I:338:ASP:C	2.59	0.40
1:I:423:ILE:O	1:I:427:MET:HG3	2.22	0.40
1:J:122:LEU:HD21	1:J:359:LYS:NZ	2.36	0.40
1:J:125:SER:HB2	1:J:253:ASN:N	2.36	0.40
1:L:119:MET:HB2	1:L:355:LEU:HD11	2.03	0.40
1:L:338:ASP:HB2	1:L:339:PRO:CD	2.51	0.40
1:L:409:LEU:HA	1:L:409:LEU:HD22	1.88	0.40
1:A:173:VAL:HG13	1:A:183:ILE:HD12	2.04	0.40
1:A:42:LEU:HD12	1:A:42:LEU:O	2.21	0.40
1:B:272:LYS:HE2	1:B:272:LYS:HB2	1.93	0.40
1:B:309:VAL:HG21	1:B:386:VAL:HG13	2.03	0.40
1:C:24:GLN:O	1:C:93:ILE:HA	2.22	0.40
1:D:125:SER:C	1:D:126:ASP:OD1	2.59	0.40
1:D:163:ASP:HA	1:D:167:ASN:HD22	1.87	0.40
1:D:351:LEU:HA	1:D:351:LEU:HD23	1.91	0.40
1:D:371:ASN:ND2	1:D:374:VAL:HG22	2.36	0.40
1:E:169:ARG:HE	1:E:195:HIS:CD2	2.36	0.40
1:F:134:GLU:OE2	1:F:196:GLU:OE2	2.39	0.40
1:G:135:PHE:N	1:G:135:PHE:CD1	2.90	0.40
1:G:42:LEU:HD12	1:G:46:LEU:HG	2.02	0.40
1:I:124:PHE:CD2	1:I:252:LYS:HG3	2.56	0.40
1:J:276:ALA:HB2	1:J:364:ALA:HA	2.02	0.40
1:K:160:ALA:CB	1:K:169:ARG:HH22	2.34	0.40
1:L:298:ARG:O	1:L:298:ARG:HG3	2.21	0.40
1:A:239:VAL:CG1	1:A:240:ASN:N	2.84	0.40
1:A:258:PHE:CB	1:A:330:THR:CG2	2.99	0.40
1:A:258:PHE:HB3	1:A:330:THR:CG2	2.51	0.40
1:B:100:ASP:OD1	1:B:102:THR:HG23	2.22	0.40
1:B:19:LYS:HA	1:B:39:VAL:HB	2.03	0.40
1:B:278:ILE:HG23	1:B:285:PHE:HZ	1.87	0.40
1:C:42:LEU:HD12	1:C:42:LEU:HA	1.92	0.40
1:D:80:PHE:HA	1:D:81:PRO:HD3	1.79	0.40
1:E:140:LEU:HD22	1:E:144:GLY:O	2.22	0.40
1:E:282:ALA:HA	1:E:285:PHE:CE2	2.57	0.40
1:E:360:ASN:O	1:E:361:LYS:C	2.60	0.40
1:E:377:LYS:HA	1:E:380:ARG:NH1	2.36	0.40
1:E:423:ILE:O	1:E:424:GLU:C	2.58	0.40
1:A:224:LYS:HD2	1:F:164:LEU:HD11	2.03	0.40
1:F:353:ALA:N	1:F:405:MET:HE1	2.37	0.40
1:G:181:PHE:HD2	1:G:199:PHE:CD2	2.39	0.40
1:G:437:ARG:O	1:G:441:MET:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:183:ILE:HA	1:H:199:PHE:HB3	2.03	0.40
1:I:374:VAL:CG2	1:I:375:MET:N	2.84	0.40
1:C:232:MET:CE	1:I:441:MET:HA	2.49	0.40
1:I:80:PHE:HD2	1:I:179:MET:HE1	1.86	0.40
1:K:137:LEU:HD23	1:K:137:LEU:HA	1.81	0.40
1:K:161:PRO:O	1:K:162:THR:CB	2.69	0.40
1:K:347:LEU:HD13	1:K:347:LEU:HA	1.97	0.40
1:K:373:TYR:HD2	1:K:373:TYR:HA	1.71	0.40
1:L:409:LEU:CD1	1:L:413:LEU:HB3	2.51	0.40
1:L:45:ALA:HA	1:L:50:VAL:HG22	2.03	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	441/443 (100%)	383 (87%)	46 (10%)	12 (3%)	6	22
1	B	441/443 (100%)	390 (88%)	46 (10%)	5 (1%)	17	47
1	C	441/443 (100%)	392 (89%)	38 (9%)	11 (2%)	6	24
1	D	441/443 (100%)	391 (89%)	38 (9%)	12 (3%)	6	22
1	E	441/443 (100%)	385 (87%)	42 (10%)	14 (3%)	5	17
1	F	441/443 (100%)	385 (87%)	44 (10%)	12 (3%)	6	22
1	G	441/443 (100%)	372 (84%)	52 (12%)	17 (4%)	3	13
1	H	441/443 (100%)	395 (90%)	33 (8%)	13 (3%)	5	20
1	I	441/443 (100%)	385 (87%)	40 (9%)	16 (4%)	4	15
1	J	439/443 (99%)	392 (89%)	36 (8%)	11 (2%)	6	24
1	K	441/443 (100%)	381 (86%)	43 (10%)	17 (4%)	3	13
1	L	441/443 (100%)	382 (87%)	50 (11%)	9 (2%)	9	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5290/5316 (100%)	4633 (88%)	508 (10%)	149 (3%)	6	21

All (149) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	THR
1	A	161	PRO
1	A	166	GLU
1	A	371	ASN
1	A	411	GLU
1	B	84	ALA
1	B	161	PRO
1	C	83	THR
1	C	86	LYS
1	C	161	PRO
1	C	366	ALA
1	C	370	ARG
1	D	83	THR
1	D	161	PRO
1	D	165	GLY
1	D	201	TYR
1	D	315	ASN
1	E	83	THR
1	E	85	GLU
1	E	143	LYS
1	E	161	PRO
1	E	262	ASN
1	F	85	GLU
1	F	161	PRO
1	G	83	THR
1	G	86	LYS
1	G	156	TYR
1	G	161	PRO
1	G	166	GLU
1	G	369	ASP
1	G	370	ARG
1	H	82	TRP
1	H	161	PRO
1	H	204	ALA
1	H	370	ARG
1	I	84	ALA
1	I	86	LYS

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Mol	Chain	Res	Type
1	I	157	PHE
1	I	161	PRO
1	I	167	ASN
1	J	62	ARG
1	J	85	GLU
1	J	161	PRO
1	J	370	ARG
1	K	6	ARG
1	K	83	THR
1	K	156	TYR
1	K	157	PHE
1	K	161	PRO
1	L	82	TRP
1	L	166	GLU
1	L	375	MET
1	A	218	VAL
1	A	370	ARG
1	B	370	ARG
1	B	375	MET
1	B	382	GLU
1	C	166	GLU
1	D	328	ILE
1	D	370	ARG
1	D	371	ASN
1	E	201	TYR
1	E	370	ARG
1	E	382	GLU
1	E	411	GLU
1	F	6	ARG
1	F	166	GLU
1	F	190	VAL
1	F	261	GLU
1	G	84	ALA
1	G	157	PHE
1	G	224	LYS
1	H	86	LYS
1	H	377	LYS
1	I	83	THR
1	I	100	ASP
1	J	261	GLU
1	K	46	LEU
1	K	166	GLU

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Mol	Chain	Res	Type
1	K	167	ASN
1	K	373	TYR
1	L	6	ARG
1	L	369	ASP
1	L	371	ASN
1	L	382	GLU
1	A	84	ALA
1	A	163	ASP
1	A	256	ASN
1	C	365	PRO
1	C	371	ASN
1	D	375	MET
1	E	62	ARG
1	E	166	GLU
1	F	83	THR
1	F	163	ASP
1	F	310	ALA
1	G	3	LYS
1	G	367	PRO
1	H	83	THR
1	I	82	TRP
1	I	159	LEU
1	I	201	TYR
1	I	254	GLY
1	I	325	SER
1	J	166	GLU
1	J	361	LYS
1	J	382	GLU
1	K	62	ARG
1	K	84	ALA
1	K	158	ASP
1	K	162	THR
1	K	204	ALA
1	K	382	GLU
1	A	382	GLU
1	C	379	GLU
1	D	325	SER
1	E	144	GLY
1	F	224	LYS
1	F	255	VAL
1	G	101	GLY
1	G	180	GLY

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Mol	Chain	Res	Type
1	H	84	ALA
1	H	163	ASP
1	H	185	ALA
1	H	262	ASN
1	I	381	MET
1	J	84	ALA
1	J	304	GLU
1	C	261	GLU
1	G	325	SER
1	G	361	LYS
1	H	361	LYS
1	I	101	GLY
1	C	152	ASP
1	G	372	ILE
1	I	304	GLU
1	L	167	ASN
1	D	61	VAL
1	E	101	GLY
1	F	101	GLY
1	L	190	VAL
1	A	233	PRO
1	H	323	PRO
1	K	81	PRO
1	D	372	ILE
1	I	218	VAL
1	K	63	ILE
1	E	291	PRO
1	J	384	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	382/382 (100%)	333 (87%)	49 (13%)	5	15
1	B	382/382 (100%)	330 (86%)	52 (14%)	4	12
1	C	382/382 (100%)	326 (85%)	56 (15%)	3	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	382/382 (100%)	328 (86%)	54 (14%)	4	11
1	E	382/382 (100%)	332 (87%)	50 (13%)	5	14
1	F	382/382 (100%)	327 (86%)	55 (14%)	4	10
1	G	382/382 (100%)	324 (85%)	58 (15%)	3	9
1	H	382/382 (100%)	330 (86%)	52 (14%)	4	12
1	I	382/382 (100%)	329 (86%)	53 (14%)	4	12
1	J	381/382 (100%)	319 (84%)	62 (16%)	3	7
1	K	382/382 (100%)	330 (86%)	52 (14%)	4	12
1	L	382/382 (100%)	324 (85%)	58 (15%)	3	9
All	All	4583/4584 (100%)	3932 (86%)	651 (14%)	4	11

All (651) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	11	LYS
1	A	18	VAL
1	A	32	ILE
1	A	34	ASN
1	A	35	VAL
1	A	36	GLU
1	A	51	MET
1	A	58	GLU
1	A	74	LEU
1	A	82	TRP
1	A	85	GLU
1	A	86	LYS
1	A	88	LYS
1	A	91	ARG
1	A	94	CYS
1	A	109	ARG
1	A	112	LEU
1	A	119	MET
1	A	129	LEU
1	A	151	ASN
1	A	156	TYR
1	A	159	LEU
1	A	166	GLU
1	A	167	ASN

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Mol	Chain	Res	Type
1	A	168	CYS
1	A	174	LEU
1	A	181	PHE
1	A	183	ILE
1	A	199	PHE
1	A	200	LYS
1	A	240	ASN
1	A	261	GLU
1	A	264	ASP
1	A	269	GLU
1	A	283	THR
1	A	285	PHE
1	A	299	LEU
1	A	308	TYR
1	A	330	THR
1	A	331	ARG
1	A	359	LYS
1	A	363	GLU
1	A	368	ILE
1	A	372	ILE
1	A	374	VAL
1	A	381	MET
1	A	386	VAL
1	A	404	VAL
1	B	12	LEU
1	B	15	GLU
1	B	16	GLU
1	B	19	LYS
1	B	28	ILE
1	B	32	ILE
1	B	35	VAL
1	B	49	LYS
1	B	62	ARG
1	B	65	GLU
1	B	74	LEU
1	B	82	TRP
1	B	83	THR
1	B	88	LYS
1	B	91	ARG
1	B	92	PHE
1	B	93	ILE
1	B	105	GLU

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Mol	Chain	Res	Type
1	B	126	ASP
1	B	129	LEU
1	B	149	GLU
1	B	153	LYS
1	B	159	LEU
1	B	219	LYS
1	B	221	ILE
1	B	223	ARG
1	B	239	VAL
1	B	240	ASN
1	B	249	SER
1	B	264	ASP
1	B	266	GLN
1	B	269	GLU
1	B	283	THR
1	B	285	PHE
1	B	292	THR
1	B	299	LEU
1	B	308	TYR
1	B	326	ARG
1	B	328	ILE
1	B	349	VAL
1	B	351	LEU
1	B	362	LEU
1	B	363	GLU
1	B	370	ARG
1	B	372	ILE
1	B	377	LYS
1	B	380	ARG
1	B	383	ASN
1	B	415	GLU
1	B	429	ARG
1	B	430	THR
1	B	441	MET
1	C	5	THR
1	C	8	ASP
1	C	28	ILE
1	C	34	ASN
1	C	36	GLU
1	C	49	LYS
1	C	70	LEU
1	C	82	TRP

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Mol	Chain	Res	Type
1	C	83	THR
1	C	85	GLU
1	C	91	ARG
1	C	105	GLU
1	C	109	ARG
1	C	112	LEU
1	C	117	LYS
1	C	120	GLU
1	C	129	LEU
1	C	148	LEU
1	C	150	LEU
1	C	159	LEU
1	C	162	THR
1	C	164	LEU
1	C	168	CYS
1	C	178	GLU
1	C	182	GLU
1	C	206	ARG
1	C	240	ASN
1	C	249	SER
1	C	262	ASN
1	C	266	GLN
1	C	270	THR
1	C	278	ILE
1	C	285	PHE
1	C	290	ASN
1	C	292	THR
1	C	297	LYS
1	C	298	ARG
1	C	299	LEU
1	C	308	TYR
1	C	326	ARG
1	C	328	ILE
1	C	331	ARG
1	C	332	VAL
1	C	347	LEU
1	C	349	VAL
1	C	351	LEU
1	C	372	ILE
1	C	374	VAL
1	C	375	MET
1	C	401	SER

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Mol	Chain	Res	Type
1	C	404	VAL
1	C	407	LYS
1	C	423	ILE
1	C	427	MET
1	C	429	ARG
1	C	431	GLN
1	D	6	ARG
1	D	9	ILE
1	D	13	VAL
1	D	28	ILE
1	D	34	ASN
1	D	35	VAL
1	D	41	GLN
1	D	49	LYS
1	D	51	MET
1	D	52	PHE
1	D	65	GLU
1	D	91	ARG
1	D	110	ASN
1	D	112	LEU
1	D	126	ASP
1	D	129	LEU
1	D	142	GLU
1	D	148	LEU
1	D	149	GLU
1	D	153	LYS
1	D	159	LEU
1	D	162	THR
1	D	164	LEU
1	D	166	GLU
1	D	168	CYS
1	D	181	PHE
1	D	183	ILE
1	D	234	LYS
1	D	240	ASN
1	D	256	ASN
1	D	270	THR
1	D	275	ILE
1	D	283	THR
1	D	284	SER
1	D	299	LEU
1	D	308	TYR

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Mol	Chain	Res	Type
1	D	325	SER
1	D	328	ILE
1	D	332	VAL
1	D	351	LEU
1	D	362	LEU
1	D	368	ILE
1	D	370	ARG
1	D	371	ASN
1	D	375	MET
1	D	378	GLU
1	D	379	GLU
1	D	381	MET
1	D	382	GLU
1	D	383	ASN
1	D	386	VAL
1	D	403	GLU
1	D	411	GLU
1	D	429	ARG
1	E	5	THR
1	E	6	ARG
1	E	8	ASP
1	E	9	ILE
1	E	11	LYS
1	E	15	GLU
1	E	24	GLN
1	E	32	ILE
1	E	34	ASN
1	E	35	VAL
1	E	40	SER
1	E	51	MET
1	E	63	ILE
1	E	85	GLU
1	E	91	ARG
1	E	114	ARG
1	E	126	ASP
1	E	148	LEU
1	E	159	LEU
1	E	164	LEU
1	E	166	GLU
1	E	168	CYS
1	E	200	LYS
1	E	201	TYR

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Mol	Chain	Res	Type
1	E	219	LYS
1	E	221	ILE
1	E	223	ARG
1	E	240	ASN
1	E	249	SER
1	E	255	VAL
1	E	262	ASN
1	E	284	SER
1	E	290	ASN
1	E	299	LEU
1	E	316	ARG
1	E	326	ARG
1	E	328	ILE
1	E	351	LEU
1	E	359	LYS
1	E	361	LYS
1	E	363	GLU
1	E	369	ASP
1	E	371	ASN
1	E	374	VAL
1	E	375	MET
1	E	381	MET
1	E	401	SER
1	E	404	VAL
1	E	429	ARG
1	E	441	MET
1	F	5	THR
1	F	15	GLU
1	F	29	LEU
1	F	32	ILE
1	F	33	LYS
1	F	34	ASN
1	F	35	VAL
1	F	36	GLU
1	F	41	GLN
1	F	67	ASP
1	F	85	GLU
1	F	91	ARG
1	F	112	LEU
1	F	117	LYS
1	F	129	LEU
1	F	143	LYS

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Mol	Chain	Res	Type
1	F	162	THR
1	F	164	LEU
1	F	168	CYS
1	F	190	VAL
1	F	200	LYS
1	F	201	TYR
1	F	205	VAL
1	F	206	ARG
1	F	207	SER
1	F	224	LYS
1	F	236	LEU
1	F	240	ASN
1	F	253	ASN
1	F	255	VAL
1	F	262	ASN
1	F	266	GLN
1	F	285	PHE
1	F	292	THR
1	F	298	ARG
1	F	299	LEU
1	F	308	TYR
1	F	312	SER
1	F	314	GLN
1	F	325	SER
1	F	328	ILE
1	F	334	VAL
1	F	342	ASN
1	F	349	VAL
1	F	351	LEU
1	F	361	LYS
1	F	362	LEU
1	F	370	ARG
1	F	377	LYS
1	F	379	GLU
1	F	382	GLU
1	F	383	ASN
1	F	400	LYS
1	F	404	VAL
1	F	423	ILE
1	G	5	THR
1	G	11	LYS
1	G	15	GLU

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Mol	Chain	Res	Type
1	G	18	VAL
1	G	24	GLN
1	G	34	ASN
1	G	35	VAL
1	G	42	LEU
1	G	48	ASN
1	G	49	LYS
1	G	63	ILE
1	G	70	LEU
1	G	78	VAL
1	G	85	GLU
1	G	91	ARG
1	G	109	ARG
1	G	112	LEU
1	G	117	LYS
1	G	126	ASP
1	G	143	LYS
1	G	148	LEU
1	G	156	TYR
1	G	162	THR
1	G	164	LEU
1	G	168	CYS
1	G	169	ARG
1	G	174	LEU
1	G	177	GLU
1	G	198	ASP
1	G	199	PHE
1	G	211	ILE
1	G	223	ARG
1	G	249	SER
1	G	258	PHE
1	G	262	ASN
1	G	264	ASP
1	G	280	LYS
1	G	283	THR
1	G	299	LEU
1	G	316	ARG
1	G	326	ARG
1	G	328	ILE
1	G	342	ASN
1	G	351	LEU
1	G	361	LYS

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Mol	Chain	Res	Type
1	G	363	GLU
1	G	370	ARG
1	G	371	ASN
1	G	372	ILE
1	G	373	TYR
1	G	377	LYS
1	G	382	GLU
1	G	401	SER
1	G	404	VAL
1	G	407	LYS
1	G	418	ILE
1	G	441	MET
1	G	442	SER
1	H	5	THR
1	H	8	ASP
1	H	12	LEU
1	H	15	GLU
1	H	21	ILE
1	H	28	ILE
1	H	32	ILE
1	H	34	ASN
1	H	41	GLN
1	H	70	LEU
1	H	74	LEU
1	H	85	GLU
1	H	91	ARG
1	H	112	LEU
1	H	126	ASP
1	H	129	LEU
1	H	156	TYR
1	H	159	LEU
1	H	163	ASP
1	H	164	LEU
1	H	178	GLU
1	H	198	ASP
1	H	199	PHE
1	H	205	VAL
1	H	216	LEU
1	H	223	ARG
1	H	239	VAL
1	H	240	ASN
1	H	285	PHE

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Mol	Chain	Res	Type
1	H	297	LYS
1	H	299	LEU
1	H	308	TYR
1	H	314	GLN
1	H	319	LEU
1	H	321	ARG
1	H	325	SER
1	H	326	ARG
1	H	328	ILE
1	H	332	VAL
1	H	347	LEU
1	H	349	VAL
1	H	351	LEU
1	H	369	ASP
1	H	371	ASN
1	H	373	TYR
1	H	377	LYS
1	H	378	GLU
1	H	381	MET
1	H	385	ILE
1	H	415	GLU
1	H	429	ARG
1	H	430	THR
1	I	15	GLU
1	I	28	ILE
1	I	34	ASN
1	I	39	VAL
1	I	41	GLN
1	I	49	LYS
1	I	70	LEU
1	I	85	GLU
1	I	86	LYS
1	I	91	ARG
1	I	94	CYS
1	I	100	ASP
1	I	102	THR
1	I	112	LEU
1	I	119	MET
1	I	129	LEU
1	I	143	LYS
1	I	148	LEU
1	I	150	LEU

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Mol	Chain	Res	Type
1	I	156	TYR
1	I	159	LEU
1	I	164	LEU
1	I	168	CYS
1	I	169	ARG
1	I	170	ARG
1	I	174	LEU
1	I	200	LYS
1	I	201	TYR
1	I	207	SER
1	I	216	LEU
1	I	239	VAL
1	I	240	ASN
1	I	252	LYS
1	I	285	PHE
1	I	299	LEU
1	I	316	ARG
1	I	328	ILE
1	I	331	ARG
1	I	351	LEU
1	I	362	LEU
1	I	369	ASP
1	I	370	ARG
1	I	373	TYR
1	I	374	VAL
1	I	377	LYS
1	I	378	GLU
1	I	401	SER
1	I	404	VAL
1	I	407	LYS
1	I	418	ILE
1	I	429	ARG
1	I	431	GLN
1	I	441	MET
1	J	4	TYR
1	J	5	THR
1	J	7	GLU
1	J	8	ASP
1	J	14	LYS
1	J	32	ILE
1	J	34	ASN
1	J	35	VAL

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Mol	Chain	Res	Type
1	J	36	GLU
1	J	41	GLN
1	J	49	LYS
1	J	51	MET
1	J	65	GLU
1	J	70	LEU
1	J	74	LEU
1	J	85	GLU
1	J	91	ARG
1	J	112	LEU
1	J	114	ARG
1	J	115	ILE
1	J	117	LYS
1	J	126	ASP
1	J	129	LEU
1	J	145	GLU
1	J	153	LYS
1	J	156	TYR
1	J	159	LEU
1	J	162	THR
1	J	164	LEU
1	J	167	ASN
1	J	168	CYS
1	J	190	VAL
1	J	212	GLN
1	J	221	ILE
1	J	223	ARG
1	J	224	LYS
1	J	234	LYS
1	J	239	VAL
1	J	253	ASN
1	J	264	ASP
1	J	270	THR
1	J	280	LYS
1	J	285	PHE
1	J	299	LEU
1	J	308	TYR
1	J	326	ARG
1	J	328	ILE
1	J	347	LEU
1	J	348	SER
1	J	349	VAL

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Mol	Chain	Res	Type
1	J	351	LEU
1	J	359	LYS
1	J	368	ILE
1	J	370	ARG
1	J	377	LYS
1	J	382	GLU
1	J	383	ASN
1	J	398	GLU
1	J	404	VAL
1	J	429	ARG
1	J	441	MET
1	J	443	GLN
1	K	5	THR
1	K	24	GLN
1	K	28	ILE
1	K	32	ILE
1	K	34	ASN
1	K	35	VAL
1	K	39	VAL
1	K	48	ASN
1	K	49	LYS
1	K	63	ILE
1	K	70	LEU
1	K	74	LEU
1	K	91	ARG
1	K	105	GLU
1	K	112	LEU
1	K	117	LYS
1	K	126	ASP
1	K	151	ASN
1	K	153	LYS
1	K	156	TYR
1	K	159	LEU
1	K	164	LEU
1	K	166	GLU
1	K	168	CYS
1	K	174	LEU
1	K	201	TYR
1	K	207	SER
1	K	220	THR
1	K	224	LYS
1	K	234	LYS

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Mol	Chain	Res	Type
1	K	239	VAL
1	K	252	LYS
1	K	264	ASP
1	K	285	PHE
1	K	299	LEU
1	K	308	TYR
1	K	316	ARG
1	K	325	SER
1	K	326	ARG
1	K	328	ILE
1	K	331	ARG
1	K	368	ILE
1	K	369	ASP
1	K	372	ILE
1	K	373	TYR
1	K	378	GLU
1	K	379	GLU
1	K	404	VAL
1	K	423	ILE
1	K	429	ARG
1	K	442	SER
1	K	443	GLN
1	L	5	THR
1	L	6	ARG
1	L	32	ILE
1	L	34	ASN
1	L	35	VAL
1	L	50	VAL
1	L	61	VAL
1	L	66	SER
1	L	70	LEU
1	L	74	LEU
1	L	86	LYS
1	L	91	ARG
1	L	93	ILE
1	L	102	THR
1	L	119	MET
1	L	122	LEU
1	L	126	ASP
1	L	129	LEU
1	L	132	GLU
1	L	143	LYS

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Mol	Chain	Res	Type
1	L	149	GLU
1	L	156	TYR
1	L	159	LEU
1	L	162	THR
1	L	164	LEU
1	L	166	GLU
1	L	168	CYS
1	L	174	LEU
1	L	199	PHE
1	L	206	ARG
1	L	240	ASN
1	L	249	SER
1	L	252	LYS
1	L	262	ASN
1	L	264	ASP
1	L	285	PHE
1	L	309	VAL
1	L	316	ARG
1	L	321	ARG
1	L	326	ARG
1	L	328	ILE
1	L	336	SER
1	L	347	LEU
1	L	349	VAL
1	L	351	LEU
1	L	362	LEU
1	L	363	GLU
1	L	370	ARG
1	L	377	LYS
1	L	378	GLU
1	L	379	GLU
1	L	386	VAL
1	L	402	ASN
1	L	404	VAL
1	L	409	LEU
1	L	418	ILE
1	L	423	ILE
1	L	429	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (146) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	98	ASN
1	A	194	GLN
1	A	225	HIS
1	A	281	HIS
1	A	314	GLN
1	A	342	ASN
1	A	360	ASN
1	A	371	ASN
1	A	383	ASN
1	A	431	GLN
1	B	17	ASN
1	B	128	ASN
1	B	167	ASN
1	B	194	GLN
1	B	240	ASN
1	B	245	HIS
1	B	281	HIS
1	B	290	ASN
1	B	371	ASN
1	B	383	ASN
1	C	17	ASN
1	C	24	GLN
1	C	34	ASN
1	C	98	ASN
1	C	128	ASN
1	C	151	ASN
1	C	194	GLN
1	C	225	HIS
1	C	228	HIS
1	C	240	ASN
1	C	281	HIS
1	C	290	ASN
1	C	360	ASN
1	C	443	GLN
1	D	34	ASN
1	D	98	ASN
1	D	110	ASN
1	D	167	ASN
1	D	194	GLN
1	D	228	HIS
1	D	256	ASN
1	D	281	HIS

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Mol	Chain	Res	Type
1	D	290	ASN
1	D	314	GLN
1	D	371	ASN
1	E	111	ASN
1	E	167	ASN
1	E	195	HIS
1	E	212	GLN
1	E	225	HIS
1	E	228	HIS
1	E	240	ASN
1	E	262	ASN
1	E	281	HIS
1	E	290	ASN
1	E	314	GLN
1	E	412	HIS
1	F	24	GLN
1	F	41	GLN
1	F	167	ASN
1	F	187	HIS
1	F	225	HIS
1	F	247	ASN
1	F	266	GLN
1	F	281	HIS
1	F	290	ASN
1	F	314	GLN
1	F	342	ASN
1	F	360	ASN
1	F	371	ASN
1	F	383	ASN
1	F	412	HIS
1	G	128	ASN
1	G	167	ASN
1	G	187	HIS
1	G	194	GLN
1	G	225	HIS
1	G	228	HIS
1	G	240	ASN
1	G	281	HIS
1	G	342	ASN
1	G	383	ASN
1	G	443	GLN
1	H	110	ASN

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Mol	Chain	Res	Type
1	H	128	ASN
1	H	187	HIS
1	H	194	GLN
1	H	225	HIS
1	H	228	HIS
1	H	266	GLN
1	H	281	HIS
1	H	290	ASN
1	H	314	GLN
1	H	315	ASN
1	I	41	GLN
1	I	110	ASN
1	I	128	ASN
1	I	151	ASN
1	I	167	ASN
1	I	194	GLN
1	I	240	ASN
1	I	245	HIS
1	I	281	HIS
1	I	290	ASN
1	I	443	GLN
1	J	17	ASN
1	J	34	ASN
1	J	98	ASN
1	J	110	ASN
1	J	187	HIS
1	J	194	GLN
1	J	225	HIS
1	J	228	HIS
1	J	245	HIS
1	J	281	HIS
1	J	290	ASN
1	J	371	ASN
1	J	412	HIS
1	K	17	ASN
1	K	128	ASN
1	K	194	GLN
1	K	212	GLN
1	K	225	HIS
1	K	240	ASN
1	K	247	ASN
1	K	266	GLN

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Mol	Chain	Res	Type
1	K	281	HIS
1	K	290	ASN
1	K	314	GLN
1	K	315	ASN
1	K	371	ASN
1	L	24	GLN
1	L	110	ASN
1	L	128	ASN
1	L	187	HIS
1	L	194	GLN
1	L	225	HIS
1	L	228	HIS
1	L	240	ASN
1	L	253	ASN
1	L	266	GLN
1	L	281	HIS
1	L	290	ASN
1	L	383	ASN
1	L	402	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 52 ligands modelled in this entry, 36 are monoatomic - leaving 16 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	GLN	A	503	2	8,8,9	0.71	0	6,9,11	0.91	0
4	PO4	A	504	2	4,4,4	0.66	0	6,6,6	0.81	0
3	GLN	B	503	2	8,8,9	1.17	1 (12%)	6,9,11	0.99	0
3	GLN	C	502	2	8,8,9	0.99	1 (12%)	6,9,11	0.75	0
4	PO4	C	504	2	4,4,4	0.78	0	6,6,6	0.54	0
3	GLN	D	503	2	8,8,9	1.33	1 (12%)	6,9,11	0.66	0
3	GLN	E	501	2	8,8,9	1.13	1 (12%)	6,9,11	0.86	0
3	GLN	F	503	-	8,8,9	1.14	1 (12%)	6,9,11	0.71	0
3	GLN	G	503	2	8,8,9	0.70	0	6,9,11	0.93	1 (16%)
4	PO4	G	504	2	4,4,4	0.68	0	6,6,6	0.62	0
3	GLN	H	503	2	8,8,9	0.83	0	6,9,11	0.91	0
4	PO4	H	504	2	4,4,4	0.76	0	6,6,6	0.59	0
3	GLN	I	503	-	8,8,9	1.19	1 (12%)	6,9,11	0.55	0
3	GLN	J	503	2	8,8,9	1.04	1 (12%)	6,9,11	0.70	0
3	GLN	K	503	-	8,8,9	0.82	1 (12%)	6,9,11	1.05	1 (16%)
3	GLN	L	503	2	4,9,9	0.29	0	5,11,11	0.56	0

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	GLN	A	503	2	-	0/5/7/9	0/0/0/0
4	PO4	A	504	2	-	0/0/0/0	0/0/0/0
3	GLN	B	503	2	-	0/5/7/9	0/0/0/0
3	GLN	C	502	2	-	0/5/7/9	0/0/0/0
4	PO4	C	504	2	-	0/0/0/0	0/0/0/0
3	GLN	D	503	2	-	0/5/7/9	0/0/0/0
3	GLN	E	501	2	-	0/5/7/9	0/0/0/0
3	GLN	F	503	-	-	0/5/7/9	0/0/0/0
3	GLN	G	503	2	-	0/5/7/9	0/0/0/0
4	PO4	G	504	2	-	0/0/0/0	0/0/0/0
3	GLN	H	503	2	-	0/5/7/9	0/0/0/0
4	PO4	H	504	2	-	0/0/0/0	0/0/0/0
3	GLN	I	503	-	-	0/5/7/9	0/0/0/0
3	GLN	J	503	2	-	0/5/7/9	0/0/0/0
3	GLN	K	503	-	-	0/5/7/9	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLN	L	503	2	-	0/5/9/9	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	503	GLN	CA-C	2.01	1.52	1.50
3	E	501	GLN	CA-C	2.29	1.53	1.50
3	C	502	GLN	CA-C	2.48	1.53	1.50
3	B	503	GLN	CA-C	2.63	1.53	1.50
3	J	503	GLN	CA-C	2.66	1.53	1.50
3	I	503	GLN	CA-C	2.91	1.54	1.50
3	F	503	GLN	CA-C	3.01	1.54	1.50
3	D	503	GLN	CA-C	3.58	1.54	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	503	GLN	O-C-CA	-2.47	118.19	125.02
3	G	503	GLN	O-C-CA	-2.24	118.85	125.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	PO4	3	0
3	B	503	GLN	1	0
3	C	502	GLN	3	0
4	C	504	PO4	3	0
3	D	503	GLN	1	0
3	E	501	GLN	2	0
3	F	503	GLN	1	0
4	G	504	PO4	2	0
3	H	503	GLN	5	0
4	H	504	PO4	1	0
3	I	503	GLN	1	0
3	J	503	GLN	1	0
3	K	503	GLN	1	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	443/443 (100%)	-0.62	0 100 100	24, 38, 70, 96	0
1	B	443/443 (100%)	-0.64	0 100 100	24, 37, 71, 98	0
1	C	443/443 (100%)	-0.66	0 100 100	20, 36, 65, 98	0
1	D	443/443 (100%)	-0.66	0 100 100	22, 34, 68, 92	0
1	E	443/443 (100%)	-0.61	0 100 100	21, 35, 69, 99	0
1	F	443/443 (100%)	-0.59	1 (0%) 94 95	20, 36, 70, 102	0
1	G	443/443 (100%)	-0.63	1 (0%) 94 95	24, 37, 68, 100	0
1	H	443/443 (100%)	-0.60	0 100 100	24, 36, 68, 104	0
1	I	443/443 (100%)	-0.63	0 100 100	20, 35, 67, 97	0
1	J	441/443 (99%)	-0.63	1 (0%) 94 95	21, 34, 67, 98	0
1	K	443/443 (100%)	-0.61	1 (0%) 94 95	22, 36, 70, 106	0
1	L	443/443 (100%)	-0.66	0 100 100	23, 36, 68, 101	0
All	All	5314/5316 (99%)	-0.63	4 (0%) 95 96	20, 36, 70, 106	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	384	GLY	3.2
1	K	83	THR	3.1
1	F	83	THR	3.0
1	J	372	ILE	2.7

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	PO4	G	504	5/5	0.77	0.38	25.58	81,82,94,97	0
4	PO4	H	504	5/5	0.75	0.35	11.18	91,92,112,116	0
4	PO4	A	504	5/5	0.85	0.25	7.31	80,81,89,94	0
3	GLN	F	503	9/10	0.94	0.20	3.84	29,32,35,36	0
2	MG	B	501	1/1	0.96	0.16	3.72	24,24,24,24	0
3	GLN	E	501	9/10	0.92	0.17	3.60	22,26,33,36	0
2	MG	H	501	1/1	0.92	0.20	3.52	32,32,32,32	0
2	MG	C	503	1/1	0.93	0.19	3.20	33,33,33,33	0
2	MG	K	501	1/1	0.88	0.19	2.89	19,19,19,19	0
3	GLN	K	503	9/10	0.87	0.19	2.41	26,33,39,40	0
3	GLN	B	503	9/10	0.97	0.15	1.67	28,34,37,38	0
3	GLN	I	503	9/10	0.94	0.15	1.40	26,29,34,35	0
3	GLN	J	503	9/10	0.88	0.17	1.13	25,32,37,41	0
3	GLN	G	503	9/10	0.93	0.16	0.95	35,39,44,45	0
3	GLN	H	503	9/10	0.94	0.15	0.83	32,37,47,47	0
2	MG	L	501	1/1	0.89	0.16	0.66	22,22,22,22	0
2	MG	B	502	1/1	0.94	0.14	0.45	29,29,29,29	0
3	GLN	L	503	10/10	0.96	0.15	0.40	31,33,41,44	0
2	MG	I	501	1/1	0.91	0.12	-0.04	19,19,19,19	0
3	GLN	D	503	9/10	0.96	0.14	-0.08	23,29,33,35	0
3	GLN	A	503	9/10	0.96	0.14	-0.15	37,41,50,57	0
2	MG	K	502	1/1	0.98	0.13	-0.29	30,30,30,30	0
3	GLN	C	502	9/10	0.94	0.12	-0.70	31,34,37,39	0
2	MG	J	501	1/1	0.98	0.12	-1.48	28,28,28,28	0
4	PO4	C	504	5/5	0.93	0.11	-1.53	35,44,67,68	0
2	MG	F	501	1/1	0.96	0.11	-1.63	34,34,34,34	0
2	MG	L	502	1/1	0.98	0.08	-3.21	26,26,26,26	0
2	MG	E	503	1/1	0.91	0.09	-3.56	25,25,25,25	0
2	MG	H	502	1/1	0.94	0.06	-4.05	50,50,50,50	0
2	MG	F	502	1/1	0.90	0.09	-4.35	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	502	1/1	0.97	0.08	-4.79	45,45,45,45	0
2	MG	I	504	1/1	0.88	0.12	-	28,28,28,28	0
2	MG	G	502	1/1	0.96	0.18	-	35,35,35,35	0
2	MG	H	505	1/1	0.97	0.14	-	21,21,21,21	0
2	MG	K	504	1/1	0.96	0.07	-	21,21,21,21	0
2	MG	L	504	1/1	0.96	0.12	-	28,28,28,28	0
2	MG	B	504	1/1	0.88	0.14	-	39,39,39,39	0
2	MG	E	502	1/1	0.96	0.12	-	28,28,28,28	0
2	MG	A	505	1/1	0.92	0.12	-	31,31,31,31	0
2	MG	C	505	1/1	0.91	0.15	-	32,32,32,32	0
2	MG	E	504	1/1	0.92	0.10	-	30,30,30,30	0
2	MG	I	502	1/1	0.97	0.13	-	28,28,28,28	0
2	MG	D	502	1/1	0.95	0.19	-	35,35,35,35	0
2	MG	A	501	1/1	0.94	0.12	-	31,31,31,31	0
2	MG	G	505	1/1	0.97	0.14	-	31,31,31,31	0
2	MG	F	504	1/1	0.91	0.14	-	25,25,25,25	0
2	MG	J	504	1/1	0.93	0.12	-	21,21,21,21	0
2	MG	G	501	1/1	0.94	0.07	-	45,45,45,45	0
2	MG	J	502	1/1	0.90	0.16	-	23,23,23,23	0
2	MG	D	501	1/1	0.96	0.17	-	23,23,23,23	0
2	MG	D	504	1/1	0.98	0.04	-	20,20,20,20	0
2	MG	C	501	1/1	0.97	0.07	-	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.