



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 05:30 am BST

PDB ID : 3TAT  
Title : TYROSINE AMINOTRANSFERASE FROM E. COLI  
Authors : Ko, T.P.; Yang, W.Z.; Wu, S.P.; Tsai, H.; Yuan, H.S.  
Deposited on : 1998-08-12  
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

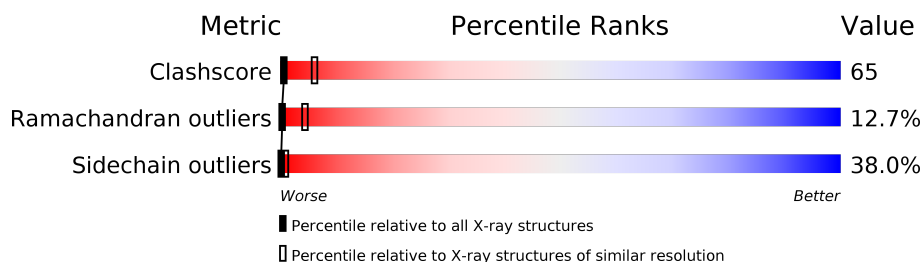
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	397	
1	B	397	
1	C	397	
1	D	397	
1	E	397	
1	F	397	

## 2 Entry composition [i](#)

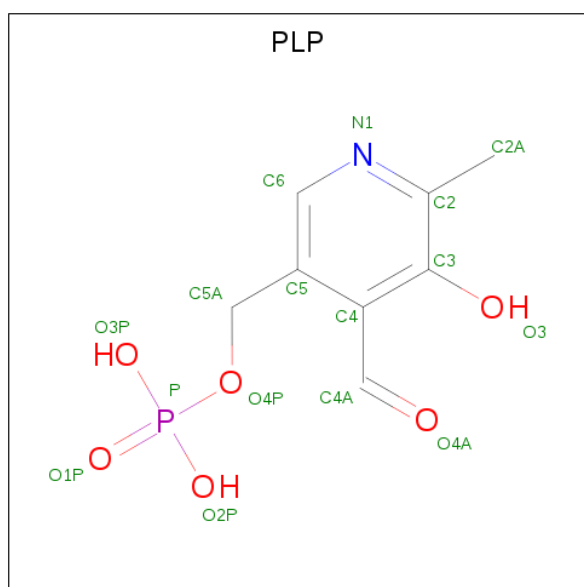
There are 2 unique types of molecules in this entry. The entry contains 18480 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TYROSINE AMINOTRANSFERASE.

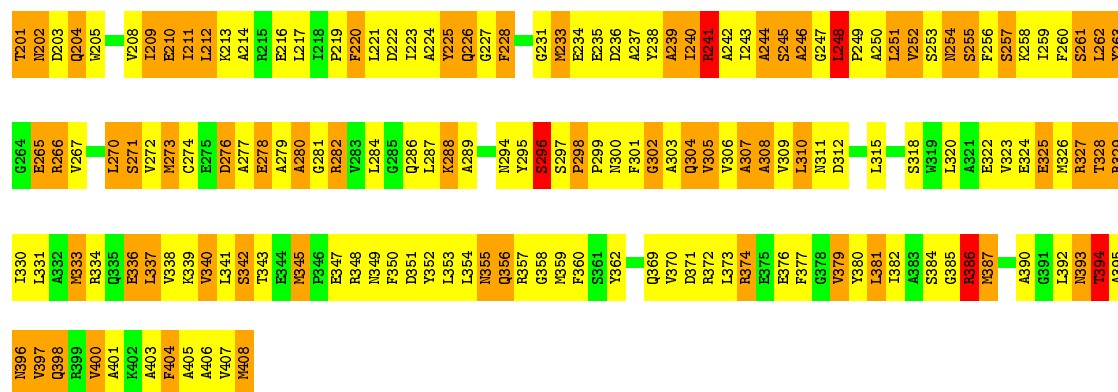
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3065	1950	528	571	16			
1	B	397	Total	C	N	O	S	0	0	0
			3065	1950	528	571	16			
1	C	397	Total	C	N	O	S	0	0	0
			3065	1950	528	571	16			
1	D	397	Total	C	N	O	S	0	0	0
			3065	1950	528	571	16			
1	E	397	Total	C	N	O	S	0	0	0
			3065	1950	528	571	16			
1	F	397	Total	C	N	O	S	0	0	0
			3065	1950	528	571	16			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



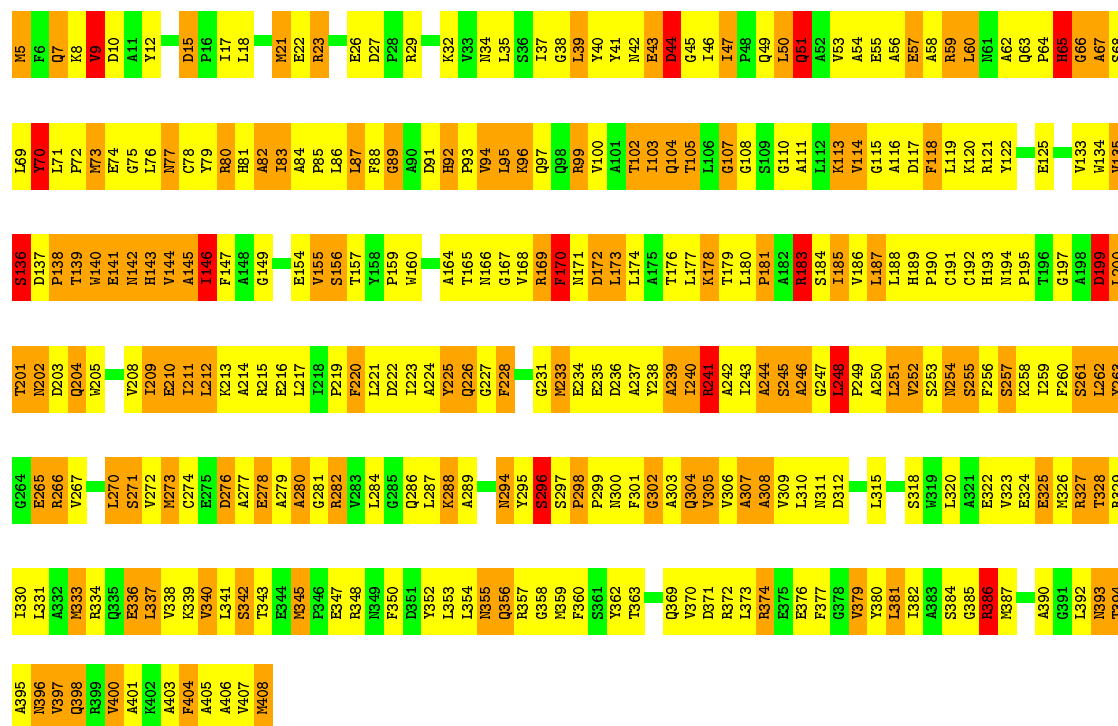
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		





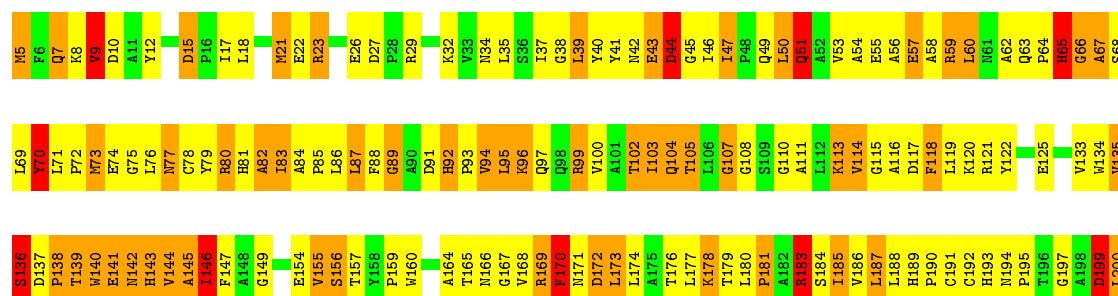
### • Molecule 1: TYROSINE AMINOTRANSFERASE

Chain C: 20% 47% 29%

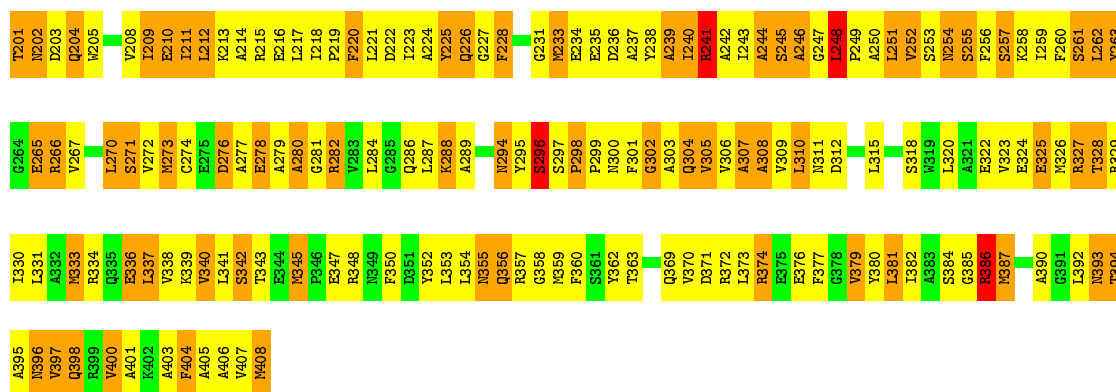


### • Molecule 1: TYROSINE AMINOTRANSFERASE

Chain D: 21% 46% 30%









## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.58Å 126.58Å 156.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.50	Depositor
% Data completeness (in resolution range)	88.5 (30.00-3.50)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.213 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18480	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

## 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: PLP

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	0.38	0/3130	0.59	0/4248
1	B	0.38	0/3130	0.59	0/4248
1	C	0.38	0/3130	0.59	0/4248
1	D	0.38	0/3130	0.59	0/4248
1	E	0.38	0/3130	0.59	0/4248
1	F	0.38	0/3130	0.59	0/4248
All	All	0.38	0/18780	0.59	0/25488

There are no bond length outliers.

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	3065	0	3034	408	0
1	B	3065	0	3034	407	9
1	C	3065	0	3034	410	1
1	D	3065	0	3034	405	0
1	E	3065	0	3034	414	8
1	F	3065	0	3034	413	0
2	A	15	0	7	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	7	1	0
2	C	15	0	7	1	0
2	D	15	0	7	1	0
2	E	15	0	7	1	0
2	F	15	0	7	1	0
All	All	18480	0	18246	2397	9

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 65.

All (2397) 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:C:274:CYS:SG	1:D:5:MET:HE1	1.90	1.10
1:D:248:LEU:HB3	1:D:249:PRO:HD3	1.40	1.02
1:C:248:LEU:HB3	1:C:249:PRO:HD3	1.40	1.02
1:B:248:LEU:HB3	1:B:249:PRO:HD3	1.40	1.02
1:E:248:LEU:HB3	1:E:249:PRO:HD3	1.40	1.01
1:F:186:VAL:HG12	1:F:188:LEU:HD11	1.45	0.99
1:D:186:VAL:HG12	1:D:188:LEU:HD11	1.45	0.98
1:F:248:LEU:HB3	1:F:249:PRO:HD3	1.40	0.98
1:C:186:VAL:HG12	1:C:188:LEU:HD11	1.45	0.98
1:B:186:VAL:HG12	1:B:188:LEU:HD11	1.45	0.98
1:A:248:LEU:HB3	1:A:249:PRO:HD3	1.40	0.98
1:A:186:VAL:HG12	1:A:188:LEU:HD11	1.45	0.98
1:E:373:LEU:HD11	1:E:407:VAL:HG21	1.47	0.97
1:E:89:GLY:H	1:E:241:ARG:HH21	1.07	0.97
1:F:373:LEU:HD11	1:F:407:VAL:HG21	1.47	0.97
1:A:373:LEU:HD11	1:A:407:VAL:HG21	1.47	0.96
1:D:89:GLY:H	1:D:241:ARG:HH21	1.07	0.95
1:E:186:VAL:HG12	1:E:188:LEU:HD11	1.45	0.95
1:B:373:LEU:HD11	1:B:407:VAL:HG21	1.47	0.95
1:C:373:LEU:HD11	1:C:407:VAL:HG21	1.47	0.95
1:D:373:LEU:HD11	1:D:407:VAL:HG21	1.47	0.94
1:C:89:GLY:H	1:C:241:ARG:HH21	1.07	0.94
1:E:183:ARG:HA	1:E:217:LEU:HA	1.49	0.94
1:C:274:CYS:SG	1:D:5:MET:CE	2.57	0.93
1:D:183:ARG:HA	1:D:217:LEU:HA	1.49	0.93
1:B:89:GLY:H	1:B:241:ARG:HH21	1.07	0.93
1:C:183:ARG:HA	1:C:217:LEU:HA	1.49	0.93
1:B:183:ARG:HA	1:B:217:LEU:HA	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:89:GLY:H	1:F:241:ARG:HH21	1.07	0.92
1:F:183:ARG:HA	1:F:217:LEU:HA	1.49	0.92
1:C:15:ASP:HB3	1:C:18:LEU:HB3	1.52	0.92
1:A:89:GLY:H	1:A:241:ARG:HH21	1.07	0.92
1:F:15:ASP:HB3	1:F:18:LEU:HB3	1.52	0.92
1:A:183:ARG:HA	1:A:217:LEU:HA	1.49	0.92
1:A:74:GLU:HB2	1:A:288:LYS:HE2	1.53	0.91
1:E:76:LEU:HD11	1:E:78:CYS:HB2	1.52	0.91
1:B:15:ASP:HB3	1:B:18:LEU:HB3	1.52	0.91
1:D:15:ASP:HB3	1:D:18:LEU:HB3	1.52	0.91
1:E:265:GLU:OE2	1:F:300:ASN:HB3	1.71	0.91
1:E:74:GLU:HB2	1:E:288:LYS:HE2	1.53	0.91
1:C:74:GLU:HB2	1:C:288:LYS:HE2	1.53	0.90
1:A:15:ASP:HB3	1:A:18:LEU:HB3	1.52	0.90
1:C:76:LEU:HD11	1:C:78:CYS:HB2	1.52	0.90
1:D:74:GLU:HB2	1:D:288:LYS:HE2	1.53	0.90
1:B:74:GLU:HB2	1:B:288:LYS:HE2	1.53	0.90
1:B:76:LEU:HD11	1:B:78:CYS:HB2	1.52	0.90
1:B:382:ILE:HD12	1:B:386:ARG:HD3	1.53	0.90
1:F:74:GLU:HB2	1:F:288:LYS:HE2	1.52	0.90
1:D:76:LEU:HD11	1:D:78:CYS:HB2	1.52	0.90
1:E:382:ILE:HD12	1:E:386:ARG:HD3	1.53	0.90
1:A:76:LEU:HD11	1:A:78:CYS:HB2	1.52	0.89
1:C:382:ILE:HD12	1:C:386:ARG:HD3	1.53	0.89
1:F:382:ILE:HD12	1:F:386:ARG:HD3	1.53	0.89
1:F:76:LEU:HD11	1:F:78:CYS:HB2	1.52	0.89
1:D:382:ILE:HD12	1:D:386:ARG:HD3	1.53	0.89
1:E:15:ASP:HB3	1:E:18:LEU:HB3	1.52	0.88
1:D:263:TYR:O	1:D:266:ARG:HD2	1.74	0.88
1:F:263:TYR:O	1:F:266:ARG:HD2	1.74	0.88
1:A:263:TYR:O	1:A:266:ARG:HD2	1.74	0.88
1:C:263:TYR:O	1:C:266:ARG:HD2	1.74	0.88
1:A:382:ILE:HD12	1:A:386:ARG:HD3	1.53	0.88
1:B:263:TYR:O	1:B:266:ARG:HD2	1.74	0.88
1:F:250:ALA:HB3	1:F:273:MET:SD	2.14	0.88
1:A:382:ILE:HG23	1:A:384:SER:H	1.40	0.87
1:E:382:ILE:HG23	1:E:384:SER:H	1.40	0.87
1:E:250:ALA:HB3	1:E:273:MET:SD	2.14	0.87
1:A:250:ALA:HB3	1:A:273:MET:SD	2.14	0.87
1:E:263:TYR:O	1:E:266:ARG:HD2	1.73	0.87
1:F:382:ILE:HG23	1:F:384:SER:H	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:ILE:HG23	1:C:384:SER:H	1.40	0.87
1:C:250:ALA:HB3	1:C:273:MET:SD	2.14	0.87
1:B:250:ALA:HB3	1:B:273:MET:SD	2.14	0.86
1:B:382:ILE:HG23	1:B:384:SER:H	1.39	0.86
1:D:250:ALA:HB3	1:D:273:MET:SD	2.14	0.86
1:E:274:CYS:SG	1:F:5:MET:HE1	2.13	0.86
1:D:382:ILE:HG23	1:D:384:SER:H	1.40	0.86
1:E:170:PHE:HZ	1:E:204:GLN:HB2	1.41	0.85
1:D:116:ALA:HA	1:D:119:LEU:HD12	1.59	0.85
1:D:197:GLY:HA3	1:D:360:PHE:O	1.77	0.85
1:A:197:GLY:HA3	1:A:360:PHE:O	1.77	0.85
1:F:197:GLY:HA3	1:F:360:PHE:O	1.77	0.85
1:C:197:GLY:HA3	1:C:360:PHE:O	1.77	0.85
1:E:197:GLY:HA3	1:E:360:PHE:O	1.77	0.85
1:C:116:ALA:HA	1:C:119:LEU:HD12	1.59	0.84
1:D:170:PHE:HZ	1:D:204:GLN:HB2	1.41	0.84
1:A:116:ALA:HA	1:A:119:LEU:HD12	1.59	0.84
1:A:170:PHE:HZ	1:A:204:GLN:HB2	1.41	0.84
1:B:170:PHE:HZ	1:B:204:GLN:HB2	1.41	0.84
1:B:197:GLY:HA3	1:B:360:PHE:O	1.77	0.84
1:B:116:ALA:HA	1:B:119:LEU:HD12	1.59	0.84
1:C:170:PHE:HZ	1:C:204:GLN:HB2	1.41	0.84
1:F:170:PHE:HZ	1:F:204:GLN:HB2	1.41	0.84
1:C:219:PRO:HG2	1:C:250:ALA:HA	1.60	0.84
1:D:219:PRO:HG2	1:D:250:ALA:HA	1.60	0.84
1:E:116:ALA:HA	1:E:119:LEU:HD12	1.59	0.84
1:C:170:PHE:CZ	1:C:204:GLN:HB2	2.13	0.83
1:E:170:PHE:CZ	1:E:204:GLN:HB2	2.13	0.83
1:A:170:PHE:CZ	1:A:204:GLN:HB2	2.14	0.83
1:B:219:PRO:HG2	1:B:250:ALA:HA	1.60	0.83
1:E:191:CYS:CB	1:E:236:ASP:HB3	2.08	0.83
1:B:191:CYS:CB	1:B:236:ASP:HB3	2.08	0.83
1:F:170:PHE:CZ	1:F:204:GLN:HB2	2.13	0.83
1:E:263:TYR:CB	1:F:70:TYR:CD2	2.62	0.83
1:C:191:CYS:CB	1:C:236:ASP:HB3	2.08	0.83
1:A:219:PRO:HG2	1:A:250:ALA:HA	1.60	0.83
1:B:170:PHE:CZ	1:B:204:GLN:HB2	2.13	0.83
1:E:225:TYR:HB3	1:E:228:PHE:HD2	1.44	0.83
1:F:191:CYS:CB	1:F:236:ASP:HB3	2.08	0.83
1:A:191:CYS:CB	1:A:236:ASP:HB3	2.08	0.82
1:D:170:PHE:CZ	1:D:204:GLN:HB2	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:PRO:HG2	1:E:250:ALA:HA	1.60	0.82
1:F:116:ALA:HA	1:F:119:LEU:HD12	1.59	0.82
1:D:191:CYS:CB	1:D:236:ASP:HB3	2.08	0.82
1:B:373:LEU:HB3	1:B:379:VAL:HG23	1.62	0.82
1:F:225:TYR:HB3	1:F:228:PHE:HD2	1.44	0.82
1:F:373:LEU:HB3	1:F:379:VAL:HG23	1.62	0.82
1:C:373:LEU:HB3	1:C:379:VAL:HG23	1.62	0.82
1:E:300:ASN:HB3	1:F:265:GLU:OE2	1.79	0.82
1:D:304:GLN:O	1:D:307:ALA:HB3	1.80	0.82
1:F:219:PRO:HG2	1:F:250:ALA:HA	1.60	0.82
1:C:304:GLN:O	1:C:307:ALA:HB3	1.80	0.81
1:F:304:GLN:O	1:F:307:ALA:HB3	1.80	0.81
1:C:260:PHE:HB3	1:C:262:LEU:HD21	1.63	0.81
1:E:260:PHE:HB3	1:E:262:LEU:HD21	1.63	0.81
1:A:225:TYR:HB3	1:A:228:PHE:HD2	1.44	0.81
1:A:260:PHE:HB3	1:A:262:LEU:HD21	1.63	0.81
1:D:260:PHE:HB3	1:D:262:LEU:HD21	1.63	0.81
1:B:260:PHE:HB3	1:B:262:LEU:HD21	1.63	0.81
1:D:373:LEU:HB3	1:D:379:VAL:HG23	1.62	0.81
1:A:373:LEU:HB3	1:A:379:VAL:HG23	1.62	0.81
1:E:304:GLN:O	1:E:307:ALA:HB3	1.80	0.81
1:F:221:LEU:HD23	1:F:240:ILE:HG23	1.63	0.81
1:A:304:GLN:O	1:A:307:ALA:HB3	1.80	0.81
1:C:225:TYR:HB3	1:C:228:PHE:HD2	1.44	0.81
1:F:260:PHE:HB3	1:F:262:LEU:HD21	1.63	0.81
1:B:221:LEU:HD23	1:B:240:ILE:HG23	1.63	0.81
1:D:184:SER:H	1:D:217:LEU:HD23	1.46	0.81
1:B:80:ARG:HA	1:B:83:ILE:HD12	1.63	0.80
1:E:80:ARG:HA	1:E:83:ILE:HD12	1.63	0.80
1:B:59:ARG:HA	1:B:62:ALA:HB3	1.64	0.80
1:B:304:GLN:O	1:B:307:ALA:HB3	1.80	0.80
1:C:59:ARG:HA	1:C:62:ALA:HB3	1.64	0.80
1:E:373:LEU:HB3	1:E:379:VAL:HG23	1.62	0.80
1:A:184:SER:H	1:A:217:LEU:HD23	1.46	0.80
1:A:59:ARG:HA	1:A:62:ALA:HB3	1.64	0.80
1:A:80:ARG:HA	1:A:83:ILE:HD12	1.63	0.80
1:D:80:ARG:HA	1:D:83:ILE:HD12	1.63	0.80
1:A:221:LEU:HD23	1:A:240:ILE:HG23	1.63	0.80
1:C:80:ARG:HA	1:C:83:ILE:HD12	1.63	0.80
1:F:80:ARG:HA	1:F:83:ILE:HD12	1.63	0.80
1:E:59:ARG:HA	1:E:62:ALA:HB3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:59:ARG:HA	1:F:62:ALA:HB3	1.64	0.80
1:F:140:TRP:O	1:F:143:HIS:HB2	1.82	0.80
1:D:59:ARG:HA	1:D:62:ALA:HB3	1.64	0.80
1:C:221:LEU:HD23	1:C:240:ILE:HG23	1.63	0.79
1:B:225:TYR:HB3	1:B:228:PHE:HD2	1.44	0.79
1:D:76:LEU:HG	1:D:79:TYR:H	1.48	0.79
1:E:140:TRP:O	1:E:143:HIS:HB2	1.82	0.79
1:C:140:TRP:O	1:C:143:HIS:HB2	1.82	0.79
1:E:184:SER:H	1:E:217:LEU:HD23	1.46	0.79
1:F:226:GLN:H	1:F:259:ILE:HD12	1.48	0.79
1:C:333:MET:HE3	1:C:393:ASN:HA	1.63	0.79
1:B:140:TRP:O	1:B:143:HIS:HB2	1.82	0.79
1:C:184:SER:H	1:C:217:LEU:HD23	1.46	0.79
1:B:184:SER:H	1:B:217:LEU:HD23	1.46	0.79
1:B:95:LEU:HB3	1:B:96:LYS:HE2	1.65	0.79
1:D:225:TYR:HB3	1:D:228:PHE:HD2	1.44	0.79
1:E:221:LEU:HD23	1:E:240:ILE:HG23	1.63	0.79
1:A:140:TRP:O	1:A:143:HIS:HB2	1.82	0.79
1:B:76:LEU:HG	1:B:79:TYR:H	1.48	0.78
1:A:95:LEU:HB3	1:A:96:LYS:HE2	1.65	0.78
1:F:184:SER:H	1:F:217:LEU:HD23	1.46	0.78
1:F:76:LEU:HG	1:F:79:TYR:H	1.48	0.78
1:D:221:LEU:HD23	1:D:240:ILE:HG23	1.63	0.78
1:C:76:LEU:HG	1:C:79:TYR:H	1.48	0.78
1:C:95:LEU:HB3	1:C:96:LYS:HE2	1.65	0.78
1:D:95:LEU:HB3	1:D:96:LYS:HE2	1.65	0.78
1:E:95:LEU:HB3	1:E:96:LYS:HE2	1.65	0.78
1:D:140:TRP:O	1:D:143:HIS:HB2	1.82	0.78
1:D:307:ALA:O	1:D:309:VAL:N	2.17	0.78
1:E:76:LEU:HG	1:E:79:TYR:H	1.48	0.78
1:A:307:ALA:O	1:A:309:VAL:N	2.17	0.78
1:F:307:ALA:O	1:F:309:VAL:N	2.17	0.77
1:E:307:ALA:O	1:E:309:VAL:N	2.17	0.77
1:B:307:ALA:O	1:B:309:VAL:N	2.17	0.77
1:D:226:GLN:H	1:D:259:ILE:HD12	1.48	0.77
1:A:226:GLN:H	1:A:259:ILE:HD12	1.48	0.77
1:E:226:GLN:H	1:E:259:ILE:HD12	1.48	0.77
1:A:76:LEU:HG	1:A:79:TYR:H	1.48	0.77
1:D:333:MET:HE3	1:D:393:ASN:HA	1.67	0.77
1:B:226:GLN:H	1:B:259:ILE:HD12	1.48	0.77
1:C:226:GLN:H	1:C:259:ILE:HD12	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:ALA:O	1:C:309:VAL:N	2.17	0.77
1:E:263:TYR:HB2	1:F:70:TYR:CD2	2.21	0.76
1:E:272:VAL:HG12	1:E:273:MET:H	1.51	0.76
1:F:95:LEU:HB3	1:F:96:LYS:HE2	1.65	0.76
1:C:42:ASN:HB3	1:C:46:ILE:O	1.85	0.76
1:D:42:ASN:HB3	1:D:46:ILE:O	1.85	0.76
1:E:42:ASN:HB3	1:E:46:ILE:O	1.85	0.76
1:E:274:CYS:SG	1:F:5:MET:CE	2.73	0.76
1:A:42:ASN:HB3	1:A:46:ILE:O	1.85	0.76
1:F:42:ASN:HB3	1:F:46:ILE:O	1.85	0.76
1:B:42:ASN:HB3	1:B:46:ILE:O	1.85	0.76
1:E:243:ILE:O	1:E:247:GLY:HA3	1.86	0.75
1:B:272:VAL:HG12	1:B:273:MET:H	1.51	0.75
1:A:243:ILE:O	1:A:247:GLY:HA3	1.86	0.75
1:F:205:TRP:O	1:F:208:VAL:HB	1.87	0.75
1:F:243:ILE:O	1:F:247:GLY:HA3	1.86	0.75
1:F:272:VAL:HG12	1:F:273:MET:H	1.51	0.75
1:E:205:TRP:O	1:E:208:VAL:HB	1.87	0.75
1:D:272:VAL:HG12	1:D:273:MET:H	1.51	0.75
1:C:243:ILE:O	1:C:247:GLY:HA3	1.86	0.75
1:D:205:TRP:O	1:D:208:VAL:HB	1.87	0.75
1:A:323:VAL:HA	1:A:326:MET:HG3	1.69	0.75
1:C:181:PRO:HG2	1:C:184:SER:OG	1.87	0.75
1:B:181:PRO:HG2	1:B:184:SER:OG	1.87	0.75
1:E:323:VAL:HA	1:E:326:MET:HG3	1.69	0.74
1:F:248:LEU:HB3	1:F:249:PRO:CD	2.17	0.74
1:A:181:PRO:HG2	1:A:184:SER:OG	1.87	0.74
1:C:205:TRP:O	1:C:208:VAL:HB	1.87	0.74
1:E:248:LEU:HB3	1:E:249:PRO:CD	2.17	0.74
1:A:272:VAL:HG12	1:A:273:MET:H	1.51	0.74
1:D:181:PRO:HG2	1:D:184:SER:OG	1.87	0.74
1:B:243:ILE:O	1:B:247:GLY:HA3	1.86	0.74
1:E:89:GLY:N	1:E:241:ARG:HH21	1.85	0.74
1:E:181:PRO:HG2	1:E:184:SER:OG	1.87	0.74
1:D:323:VAL:HA	1:D:326:MET:HG3	1.69	0.74
1:A:205:TRP:O	1:A:208:VAL:HB	1.87	0.74
1:D:243:ILE:O	1:D:247:GLY:HA3	1.86	0.74
1:C:248:LEU:HB3	1:C:249:PRO:CD	2.17	0.74
1:B:205:TRP:O	1:B:208:VAL:HB	1.87	0.74
1:B:248:LEU:HB3	1:B:249:PRO:CD	2.17	0.74
1:B:76:LEU:HG	1:B:79:TYR:N	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:LEU:HB3	1:D:249:PRO:CD	2.17	0.74
1:F:323:VAL:HA	1:F:326:MET:HG3	1.69	0.74
1:F:181:PRO:HG2	1:F:184:SER:OG	1.87	0.73
1:A:248:LEU:HB3	1:A:249:PRO:CD	2.17	0.73
1:C:272:VAL:HG12	1:C:273:MET:H	1.51	0.73
1:C:323:VAL:HA	1:C:326:MET:HG3	1.69	0.73
1:A:89:GLY:N	1:A:241:ARG:HH21	1.85	0.73
1:A:333:MET:HE3	1:A:393:ASN:HA	1.70	0.73
1:B:323:VAL:HA	1:B:326:MET:HG3	1.69	0.73
1:C:169:ARG:HG2	1:C:172:ASP:HB2	1.71	0.73
1:D:76:LEU:HG	1:D:79:TYR:N	2.03	0.73
1:F:333:MET:HE3	1:F:393:ASN:HA	1.69	0.73
1:B:169:ARG:HG2	1:B:172:ASP:HB2	1.71	0.73
1:C:76:LEU:HG	1:C:79:TYR:N	2.03	0.73
1:B:58:ALA:O	1:B:62:ALA:HB2	1.88	0.73
1:C:265:GLU:OE2	1:D:300:ASN:HB3	1.89	0.73
1:F:169:ARG:HG2	1:F:172:ASP:HB2	1.71	0.73
1:A:169:ARG:HG2	1:A:172:ASP:HB2	1.71	0.73
1:A:79:TYR:HE1	1:A:306:VAL:HB	1.54	0.73
1:C:58:ALA:O	1:C:62:ALA:HB2	1.88	0.73
1:D:79:TYR:HE1	1:D:306:VAL:HB	1.54	0.73
1:E:169:ARG:HG2	1:E:172:ASP:HB2	1.71	0.73
1:E:58:ALA:O	1:E:62:ALA:HB2	1.88	0.73
1:A:58:ALA:O	1:A:62:ALA:HB2	1.88	0.73
1:A:76:LEU:HG	1:A:79:TYR:N	2.03	0.73
1:E:79:TYR:HE1	1:E:306:VAL:HB	1.54	0.73
1:E:76:LEU:HG	1:E:79:TYR:N	2.03	0.73
1:B:79:TYR:HE1	1:B:306:VAL:HB	1.54	0.72
1:C:79:TYR:HE1	1:C:306:VAL:HB	1.54	0.72
1:F:58:ALA:O	1:F:62:ALA:HB2	1.88	0.72
1:D:89:GLY:N	1:D:241:ARG:HH21	1.85	0.72
1:D:169:ARG:HG2	1:D:172:ASP:HB2	1.71	0.72
1:F:89:GLY:N	1:F:241:ARG:HH21	1.85	0.72
1:F:79:TYR:HE1	1:F:306:VAL:HB	1.54	0.72
1:B:89:GLY:N	1:B:241:ARG:HH21	1.85	0.72
1:E:72:PRO:C	1:E:74:GLU:H	1.92	0.72
1:D:89:GLY:H	1:D:241:ARG:NH2	1.87	0.72
1:B:337:LEU:O	1:B:341:LEU:HB2	1.90	0.72
1:D:58:ALA:O	1:D:62:ALA:HB2	1.88	0.72
1:C:18:LEU:O	1:C:21:MET:HB2	1.90	0.72
1:C:72:PRO:C	1:C:74:GLU:H	1.92	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:LEU:HG	1:F:79:TYR:N	2.03	0.72
1:A:87:LEU:N	1:A:87:LEU:HD23	2.05	0.71
1:B:72:PRO:C	1:B:74:GLU:H	1.92	0.71
1:D:72:PRO:C	1:D:74:GLU:H	1.92	0.71
1:A:72:PRO:C	1:A:74:GLU:H	1.92	0.71
1:B:18:LEU:O	1:B:21:MET:HB2	1.90	0.71
1:B:369:GLN:O	1:B:373:LEU:HD12	1.91	0.71
1:D:369:GLN:O	1:D:373:LEU:HD12	1.91	0.71
1:E:337:LEU:O	1:E:341:LEU:HB2	1.90	0.71
1:F:18:LEU:O	1:F:21:MET:HB2	1.90	0.71
1:B:87:LEU:HD23	1:B:87:LEU:N	2.05	0.71
1:C:369:GLN:O	1:C:373:LEU:HD12	1.91	0.71
1:C:337:LEU:O	1:C:341:LEU:HB2	1.90	0.71
1:D:18:LEU:O	1:D:21:MET:HB2	1.90	0.71
1:F:186:VAL:HG12	1:F:188:LEU:CD1	2.21	0.71
1:A:393:ASN:O	1:A:397:VAL:HG23	1.90	0.71
1:B:333:MET:HE3	1:B:393:ASN:HA	1.73	0.71
1:C:87:LEU:N	1:C:87:LEU:HD23	2.05	0.71
1:D:393:ASN:O	1:D:397:VAL:HG23	1.90	0.71
1:D:87:LEU:N	1:D:87:LEU:HD23	2.05	0.71
1:E:369:GLN:O	1:E:373:LEU:HD12	1.91	0.71
1:F:337:LEU:O	1:F:341:LEU:HB2	1.90	0.71
1:F:393:ASN:O	1:F:397:VAL:HG23	1.90	0.71
1:B:89:GLY:H	1:B:241:ARG:NH2	1.87	0.71
1:F:369:GLN:O	1:F:373:LEU:HD12	1.91	0.71
1:A:369:GLN:O	1:A:373:LEU:HD12	1.91	0.71
1:C:142:ASN:HD22	1:C:142:ASN:N	1.88	0.71
1:C:393:ASN:O	1:C:397:VAL:HG23	1.90	0.71
1:D:337:LEU:O	1:D:341:LEU:HB2	1.90	0.71
1:D:92:HIS:CD2	1:D:245:SER:HB3	2.26	0.71
1:F:72:PRO:C	1:F:74:GLU:H	1.92	0.71
1:F:92:HIS:CD2	1:F:245:SER:HB3	2.26	0.71
1:B:92:HIS:CD2	1:B:245:SER:HB3	2.26	0.71
1:C:99:ARG:O	1:C:273:MET:HA	1.91	0.71
1:B:99:ARG:O	1:B:273:MET:HA	1.91	0.70
1:A:99:ARG:O	1:A:273:MET:HA	1.91	0.70
1:C:92:HIS:CD2	1:C:245:SER:HB3	2.26	0.70
1:E:99:ARG:O	1:E:273:MET:HA	1.91	0.70
1:F:67:ALA:O	1:F:69:LEU:HG	1.91	0.70
1:B:393:ASN:O	1:B:397:VAL:HG23	1.90	0.70
1:B:67:ALA:O	1:B:69:LEU:HG	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:GLY:H	1:C:241:ARG:NH2	1.87	0.70
1:E:92:HIS:CD2	1:E:245:SER:HB3	2.26	0.70
1:F:89:GLY:H	1:F:241:ARG:NH2	1.87	0.70
1:A:18:LEU:O	1:A:21:MET:HB2	1.90	0.70
1:C:67:ALA:O	1:C:69:LEU:HG	1.92	0.70
1:C:89:GLY:N	1:C:241:ARG:HH21	1.85	0.70
1:E:67:ALA:O	1:E:69:LEU:HG	1.92	0.70
1:F:87:LEU:N	1:F:87:LEU:HD23	2.05	0.70
1:A:142:ASN:HD22	1:A:142:ASN:N	1.88	0.70
1:A:92:HIS:CD2	1:A:245:SER:HB3	2.26	0.70
1:E:393:ASN:O	1:E:397:VAL:HG23	1.90	0.70
1:A:89:GLY:H	1:A:241:ARG:NH2	1.87	0.70
1:E:18:LEU:O	1:E:21:MET:HB2	1.90	0.70
1:E:87:LEU:HD23	1:E:87:LEU:N	2.05	0.70
1:F:99:ARG:O	1:F:273:MET:HA	1.91	0.70
1:D:142:ASN:HD22	1:D:142:ASN:N	1.89	0.69
1:D:99:ARG:O	1:D:273:MET:HA	1.91	0.69
1:E:142:ASN:N	1:E:142:ASN:HD22	1.88	0.69
1:E:195:PRO:HB3	1:E:386:ARG:HD2	1.75	0.69
1:A:195:PRO:HB3	1:A:386:ARG:HD2	1.75	0.69
1:B:195:PRO:HB3	1:B:386:ARG:HD2	1.75	0.69
1:C:195:PRO:HB3	1:C:386:ARG:HD2	1.75	0.69
1:C:5:MET:HE1	1:D:274:CYS:SG	2.33	0.69
1:D:67:ALA:O	1:D:69:LEU:HG	1.92	0.69
1:A:337:LEU:O	1:A:341:LEU:HB2	1.90	0.69
1:B:142:ASN:N	1:B:142:ASN:HD22	1.88	0.69
1:E:186:VAL:HG12	1:E:188:LEU:CD1	2.21	0.69
1:A:67:ALA:O	1:A:69:LEU:HG	1.92	0.69
1:A:279:ALA:C	1:A:281:GLY:H	1.96	0.69
1:D:195:PRO:HB3	1:D:386:ARG:HD2	1.75	0.69
1:A:136:SER:HB2	1:A:138:PRO:O	1.93	0.69
1:A:257:SER:CB	1:A:263:TYR:HA	2.23	0.69
1:F:142:ASN:HD22	1:F:142:ASN:N	1.88	0.69
1:F:195:PRO:HB3	1:F:386:ARG:HD2	1.75	0.69
1:B:136:SER:HB2	1:B:138:PRO:O	1.93	0.68
1:C:257:SER:CB	1:C:263:TYR:HA	2.23	0.68
1:D:257:SER:CB	1:D:263:TYR:HA	2.23	0.68
1:D:338:VAL:HG21	1:D:354:LEU:HG	1.75	0.68
1:E:333:MET:HE3	1:E:393:ASN:HA	1.75	0.68
1:E:338:VAL:HG21	1:E:354:LEU:HG	1.75	0.68
1:F:136:SER:HB2	1:F:138:PRO:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:338:VAL:HG21	1:F:354:LEU:HG	1.75	0.68
1:B:257:SER:CB	1:B:263:TYR:HA	2.23	0.68
1:E:279:ALA:C	1:E:281:GLY:H	1.96	0.68
1:E:89:GLY:H	1:E:241:ARG:NH2	1.87	0.68
1:A:221:LEU:HB3	1:A:252:VAL:HG23	1.76	0.68
1:A:338:VAL:HG21	1:A:354:LEU:HG	1.75	0.68
1:B:279:ALA:C	1:B:281:GLY:H	1.96	0.68
1:C:279:ALA:C	1:C:281:GLY:H	1.96	0.68
1:E:221:LEU:HB3	1:E:252:VAL:HG23	1.76	0.68
1:C:221:LEU:HB3	1:C:252:VAL:HG23	1.76	0.68
1:F:191:CYS:HB3	1:F:236:ASP:HB3	1.76	0.68
1:E:136:SER:HB2	1:E:138:PRO:O	1.93	0.68
1:A:173:LEU:O	1:A:177:LEU:HD12	1.94	0.68
1:D:221:LEU:HB3	1:D:252:VAL:HG23	1.76	0.68
1:B:221:LEU:HB3	1:B:252:VAL:HG23	1.76	0.67
1:B:272:VAL:HG12	1:B:273:MET:N	2.10	0.67
1:E:173:LEU:O	1:E:177:LEU:HD12	1.94	0.67
1:A:186:VAL:HG12	1:A:188:LEU:CD1	2.21	0.67
1:B:325:GLU:HA	1:B:328:THR:HB	1.76	0.67
1:C:173:LEU:O	1:C:177:LEU:HD12	1.94	0.67
1:E:325:GLU:HA	1:E:328:THR:HB	1.76	0.67
1:F:173:LEU:O	1:F:177:LEU:HD12	1.94	0.67
1:C:272:VAL:HG12	1:C:273:MET:N	2.10	0.67
1:F:257:SER:CB	1:F:263:TYR:HA	2.23	0.67
1:B:338:VAL:HG21	1:B:354:LEU:HG	1.75	0.67
1:D:272:VAL:HG12	1:D:273:MET:N	2.10	0.67
1:E:257:SER:CB	1:E:263:TYR:HA	2.23	0.67
1:A:325:GLU:HA	1:A:328:THR:HB	1.76	0.67
1:B:186:VAL:HG12	1:B:188:LEU:CD1	2.21	0.67
1:C:136:SER:HB2	1:C:138:PRO:O	1.93	0.67
1:D:173:LEU:O	1:D:177:LEU:HD12	1.94	0.67
1:D:279:ALA:C	1:D:281:GLY:H	1.96	0.67
1:F:325:GLU:HA	1:F:328:THR:HB	1.76	0.67
1:D:136:SER:HB2	1:D:138:PRO:O	1.93	0.67
1:D:325:GLU:HA	1:D:328:THR:HB	1.76	0.67
1:F:272:VAL:HG12	1:F:273:MET:N	2.10	0.67
1:A:191:CYS:HB3	1:A:236:ASP:HB3	1.76	0.67
1:C:325:GLU:HA	1:C:328:THR:HB	1.76	0.67
1:F:221:LEU:HB3	1:F:252:VAL:HG23	1.76	0.67
1:C:191:CYS:HB3	1:C:236:ASP:HB3	1.76	0.67
1:A:272:VAL:HG12	1:A:273:MET:N	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ARG:HD3	1:B:5:MET:HA	1.75	0.67
1:C:338:VAL:HG21	1:C:354:LEU:HG	1.75	0.67
1:D:186:VAL:HG12	1:D:188:LEU:CD1	2.21	0.67
1:B:173:LEU:O	1:B:177:LEU:HD12	1.94	0.66
1:F:221:LEU:CD2	1:F:240:ILE:HG23	2.25	0.66
1:A:265:GLU:HG3	1:A:302:GLY:HA2	1.78	0.66
1:C:265:GLU:HG3	1:C:302:GLY:HA2	1.78	0.66
1:D:191:CYS:HB3	1:D:236:ASP:HB3	1.76	0.66
1:A:221:LEU:CD2	1:A:240:ILE:HG23	2.25	0.66
1:B:191:CYS:HB3	1:B:236:ASP:HB3	1.76	0.66
1:C:405:ALA:HA	1:C:408:MET:HE3	1.78	0.66
1:E:221:LEU:CD2	1:E:240:ILE:HG23	2.25	0.66
1:F:279:ALA:C	1:F:281:GLY:H	1.96	0.66
1:C:186:VAL:HG12	1:C:188:LEU:CD1	2.21	0.66
1:A:79:TYR:CE1	1:A:306:VAL:HB	2.31	0.66
1:E:191:CYS:HB3	1:E:236:ASP:HB3	1.76	0.66
1:E:272:VAL:HG12	1:E:273:MET:N	2.10	0.66
1:A:322:GLU:O	1:A:326:MET:HG2	1.96	0.66
1:D:265:GLU:HG3	1:D:302:GLY:HA2	1.78	0.66
1:D:322:GLU:O	1:D:326:MET:HG2	1.96	0.66
1:F:34:ASN:O	1:F:35:LEU:HD23	1.96	0.66
1:A:187:LEU:C	1:A:188:LEU:HD12	2.17	0.66
1:B:79:TYR:CE1	1:B:306:VAL:HB	2.31	0.66
1:E:186:VAL:CG1	1:E:188:LEU:HD11	2.24	0.66
1:F:187:LEU:C	1:F:188:LEU:HD12	2.17	0.66
1:F:97:GLN:O	1:F:277:ALA:HB2	1.96	0.66
1:B:322:GLU:O	1:B:326:MET:HG2	1.96	0.66
1:C:221:LEU:CD2	1:C:240:ILE:HG23	2.25	0.66
1:C:79:TYR:CE1	1:C:306:VAL:HB	2.31	0.66
1:D:97:GLN:O	1:D:277:ALA:HB2	1.96	0.66
1:D:34:ASN:O	1:D:35:LEU:HD23	1.96	0.66
1:A:338:VAL:O	1:A:342:SER:HB2	1.96	0.65
1:B:187:LEU:C	1:B:188:LEU:HD12	2.17	0.65
1:D:79:TYR:CE1	1:D:306:VAL:HB	2.31	0.65
1:F:265:GLU:HG3	1:F:302:GLY:HA2	1.78	0.65
1:C:322:GLU:O	1:C:326:MET:HG2	1.96	0.65
1:C:338:VAL:O	1:C:342:SER:HB2	1.96	0.65
1:E:187:LEU:C	1:E:188:LEU:HD12	2.17	0.65
1:E:34:ASN:O	1:E:35:LEU:HD23	1.96	0.65
1:D:221:LEU:CD2	1:D:240:ILE:HG23	2.25	0.65
1:E:338:VAL:O	1:E:342:SER:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:LEU:C	1:C:188:LEU:HD12	2.17	0.65
1:A:186:VAL:CG1	1:A:188:LEU:HD11	2.24	0.65
1:A:370:VAL:HG13	1:A:381:LEU:HD12	1.79	0.65
1:B:97:GLN:O	1:B:277:ALA:HB2	1.96	0.65
1:B:265:GLU:HG3	1:B:302:GLY:HA2	1.78	0.65
1:E:70:TYR:CD2	1:F:263:TYR:HB2	2.32	0.65
1:F:322:GLU:O	1:F:326:MET:HG2	1.96	0.65
1:F:79:TYR:CE1	1:F:306:VAL:HB	2.31	0.65
1:A:216:GLU:O	1:A:217:LEU:HG	1.97	0.65
1:B:99:ARG:HB2	1:B:274:CYS:O	1.97	0.65
1:B:338:VAL:O	1:B:342:SER:HB2	1.96	0.65
1:C:99:ARG:HB2	1:C:274:CYS:O	1.97	0.65
1:E:212:LEU:CD1	1:E:219:PRO:HB3	2.27	0.65
1:E:79:TYR:CE1	1:E:306:VAL:HB	2.31	0.65
1:A:212:LEU:CD1	1:A:219:PRO:HB3	2.27	0.65
1:A:97:GLN:O	1:A:277:ALA:HB2	1.96	0.65
1:A:34:ASN:O	1:A:35:LEU:HD23	1.96	0.65
1:E:322:GLU:O	1:E:326:MET:HG2	1.96	0.65
1:E:370:VAL:HG13	1:E:381:LEU:HD12	1.79	0.65
1:F:118:PHE:O	1:F:121:ARG:N	2.30	0.65
1:D:187:LEU:C	1:D:188:LEU:HD12	2.17	0.65
1:D:338:VAL:O	1:D:342:SER:HB2	1.96	0.65
1:F:99:ARG:HB2	1:F:274:CYS:O	1.97	0.65
1:A:5:MET:HA	1:B:183:ARG:HD3	1.79	0.65
1:F:216:GLU:O	1:F:217:LEU:HG	1.97	0.64
1:A:142:ASN:H	1:A:142:ASN:HD22	1.46	0.64
1:D:212:LEU:CD1	1:D:219:PRO:HB3	2.27	0.64
1:E:97:GLN:O	1:E:277:ALA:HB2	1.96	0.64
1:F:212:LEU:CD1	1:F:219:PRO:HB3	2.27	0.64
1:B:221:LEU:CD2	1:B:240:ILE:HG23	2.25	0.64
1:C:212:LEU:CD1	1:C:219:PRO:HB3	2.27	0.64
1:D:99:ARG:HB2	1:D:274:CYS:O	1.97	0.64
1:A:99:ARG:HB2	1:A:274:CYS:O	1.97	0.64
1:B:216:GLU:O	1:B:217:LEU:HG	1.97	0.64
1:B:34:ASN:O	1:B:35:LEU:HD23	1.96	0.64
1:C:34:ASN:O	1:C:35:LEU:HD23	1.96	0.64
1:E:250:ALA:HB3	1:E:273:MET:CE	2.28	0.64
1:C:97:GLN:O	1:C:277:ALA:HB2	1.96	0.64
1:E:134:TRP:CE3	1:E:156:SER:HB3	2.33	0.64
1:F:225:TYR:HB3	1:F:228:PHE:CD2	2.31	0.64
1:E:142:ASN:H	1:E:142:ASN:HD22	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:TRP:CE3	1:F:156:SER:HB3	2.33	0.64
1:B:212:LEU:CD1	1:B:219:PRO:HB3	2.27	0.64
1:B:370:VAL:HG13	1:B:381:LEU:HD12	1.79	0.64
1:E:62:ALA:C	1:E:64:PRO:HD3	2.18	0.64
1:F:338:VAL:O	1:F:342:SER:HB2	1.96	0.64
1:D:186:VAL:CG1	1:D:188:LEU:HD11	2.24	0.64
1:D:254:ASN:ND2	1:D:255:SER:H	1.96	0.64
1:E:265:GLU:HG3	1:E:302:GLY:HA2	1.78	0.64
1:E:301:PHE:O	1:E:305:VAL:HG22	1.98	0.64
1:F:250:ALA:HB3	1:F:273:MET:CE	2.28	0.64
1:F:62:ALA:C	1:F:64:PRO:HD3	2.18	0.64
1:B:142:ASN:HD22	1:B:142:ASN:H	1.46	0.64
1:B:250:ALA:HB3	1:B:273:MET:CE	2.28	0.64
1:C:250:ALA:HB3	1:C:273:MET:CE	2.28	0.64
1:E:254:ASN:ND2	1:E:255:SER:H	1.95	0.64
1:F:142:ASN:H	1:F:142:ASN:HD22	1.46	0.64
1:B:134:TRP:CE3	1:B:156:SER:HB3	2.33	0.64
1:B:254:ASN:ND2	1:B:255:SER:H	1.96	0.64
1:C:370:VAL:HG13	1:C:381:LEU:HD12	1.79	0.64
1:D:216:GLU:O	1:D:217:LEU:HG	1.97	0.64
1:E:99:ARG:HB2	1:E:274:CYS:O	1.97	0.64
1:D:201:THR:HG22	1:D:204:GLN:OE1	1.98	0.63
1:E:201:THR:HG22	1:E:204:GLN:OE1	1.98	0.63
1:E:225:TYR:HB3	1:E:228:PHE:CD2	2.31	0.63
1:E:373:LEU:HB3	1:E:379:VAL:CG2	2.27	0.63
1:F:373:LEU:HB3	1:F:379:VAL:CG2	2.27	0.63
1:C:216:GLU:O	1:C:217:LEU:HG	1.97	0.63
1:E:216:GLU:O	1:E:217:LEU:HG	1.97	0.63
1:E:70:TYR:CD2	1:F:263:TYR:CB	2.82	0.63
1:C:62:ALA:C	1:C:64:PRO:HD3	2.18	0.63
1:D:62:ALA:C	1:D:64:PRO:HD3	2.18	0.63
1:F:201:THR:HG22	1:F:204:GLN:OE1	1.98	0.63
1:A:254:ASN:ND2	1:A:255:SER:H	1.96	0.63
1:B:201:THR:HG22	1:B:204:GLN:OE1	1.98	0.63
1:C:142:ASN:H	1:C:142:ASN:HD22	1.46	0.63
1:D:370:VAL:HG13	1:D:381:LEU:HD12	1.79	0.63
1:F:254:ASN:ND2	1:F:255:SER:H	1.96	0.63
1:A:134:TRP:CE3	1:A:156:SER:HB3	2.33	0.63
1:A:225:TYR:HB3	1:A:228:PHE:CD2	2.31	0.63
1:D:134:TRP:CE3	1:D:156:SER:HB3	2.33	0.63
1:A:397:VAL:O	1:A:400:VAL:HG23	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ASN:ND2	1:C:255:SER:H	1.96	0.63
1:D:250:ALA:HB3	1:D:273:MET:CE	2.28	0.63
1:D:301:PHE:O	1:D:305:VAL:HG22	1.98	0.63
1:F:397:VAL:O	1:F:400:VAL:HG23	1.98	0.63
1:A:201:THR:HG22	1:A:204:GLN:OE1	1.98	0.63
1:A:250:ALA:HB3	1:A:273:MET:CE	2.28	0.63
1:B:118:PHE:O	1:B:121:ARG:N	2.30	0.63
1:A:265:GLU:OE2	1:B:300:ASN:HB3	1.99	0.63
1:B:397:VAL:O	1:B:400:VAL:HG23	1.98	0.63
1:C:201:THR:HG22	1:C:204:GLN:OE1	1.98	0.63
1:E:118:PHE:O	1:E:121:ARG:N	2.30	0.63
1:E:397:VAL:O	1:E:400:VAL:HG23	1.98	0.63
1:A:62:ALA:C	1:A:64:PRO:HD3	2.18	0.63
1:B:62:ALA:C	1:B:64:PRO:HD3	2.18	0.63
1:C:373:LEU:HB3	1:C:379:VAL:CG2	2.27	0.63
1:A:373:LEU:HB3	1:A:379:VAL:CG2	2.28	0.62
1:C:118:PHE:O	1:C:121:ARG:N	2.30	0.62
1:C:186:VAL:CG1	1:C:188:LEU:HD11	2.24	0.62
1:C:300:ASN:HB3	1:D:265:GLU:OE2	1.98	0.62
1:D:397:VAL:O	1:D:400:VAL:HG23	1.98	0.62
1:E:29:ARG:HD3	1:E:32:LYS:HB3	1.81	0.62
1:F:370:VAL:HG13	1:F:381:LEU:HD12	1.79	0.62
1:B:186:VAL:CG1	1:B:188:LEU:HD11	2.24	0.62
1:D:69:LEU:O	1:D:70:TYR:O	2.18	0.62
1:E:69:LEU:O	1:E:70:TYR:O	2.18	0.62
1:B:71:LEU:HD22	1:B:72:PRO:HD2	1.82	0.62
1:D:225:TYR:HB3	1:D:228:PHE:CD2	2.31	0.62
1:E:104:GLN:HE22	1:E:298:PRO:HB2	1.64	0.62
1:F:301:PHE:O	1:F:305:VAL:HG22	1.98	0.62
1:A:301:PHE:O	1:A:305:VAL:HG22	1.98	0.62
1:A:69:LEU:O	1:A:70:TYR:O	2.18	0.62
1:B:301:PHE:O	1:B:305:VAL:HG22	1.98	0.62
1:D:71:LEU:HD22	1:D:72:PRO:HD2	1.82	0.62
1:F:71:LEU:HD22	1:F:72:PRO:HD2	1.82	0.62
1:A:104:GLN:HE22	1:A:298:PRO:HB2	1.64	0.62
1:B:202:ASN:HB3	1:B:238:TYR:CZ	2.35	0.62
1:C:134:TRP:CE3	1:C:156:SER:HB3	2.33	0.62
1:C:29:ARG:HD3	1:C:32:LYS:HB3	1.81	0.62
1:C:397:VAL:O	1:C:400:VAL:HG23	1.98	0.62
1:C:202:ASN:HB3	1:C:238:TYR:CZ	2.35	0.62
1:D:202:ASN:HB3	1:D:238:TYR:CZ	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:ASN:HB3	1:F:238:TYR:CZ	2.35	0.62
1:A:404:PHE:HA	1:A:407:VAL:HG23	1.82	0.62
1:C:301:PHE:O	1:C:305:VAL:HG22	1.98	0.62
1:C:18:LEU:HD12	1:C:21:MET:HB2	1.82	0.62
1:C:69:LEU:O	1:C:70:TYR:O	2.18	0.62
1:C:71:LEU:HD22	1:C:72:PRO:HD2	1.81	0.62
1:D:142:ASN:HD22	1:D:142:ASN:H	1.46	0.62
1:D:18:LEU:HD12	1:D:21:MET:HB2	1.82	0.62
1:B:18:LEU:HD12	1:B:21:MET:HB2	1.82	0.62
1:B:69:LEU:O	1:B:70:TYR:O	2.18	0.62
1:E:159:PRO:HG2	1:E:173:LEU:HB2	1.82	0.62
1:E:257:SER:OG	1:E:263:TYR:HA	2.00	0.62
1:E:404:PHE:HA	1:E:407:VAL:HG23	1.82	0.62
1:B:257:SER:OG	1:B:263:TYR:HA	2.00	0.62
1:B:84:ALA:N	1:B:85:PRO:HD2	2.15	0.62
1:F:18:LEU:HD12	1:F:21:MET:HB2	1.82	0.62
1:A:115:GLY:O	1:A:119:LEU:HG	2.00	0.61
1:A:18:LEU:HD12	1:A:21:MET:HB2	1.82	0.61
1:A:202:ASN:HB3	1:A:238:TYR:CZ	2.35	0.61
1:A:71:LEU:HD22	1:A:72:PRO:HD2	1.82	0.61
1:C:257:SER:OG	1:C:263:TYR:HA	2.00	0.61
1:A:118:PHE:O	1:A:121:ARG:N	2.30	0.61
1:B:373:LEU:HB3	1:B:379:VAL:CG2	2.28	0.61
1:D:404:PHE:HA	1:D:407:VAL:HG23	1.82	0.61
1:E:115:GLY:O	1:E:119:LEU:HG	2.00	0.61
1:F:84:ALA:N	1:F:85:PRO:HD2	2.15	0.61
1:E:193:HIS:CD2	1:E:194:ASN:H	2.19	0.61
1:F:202:ASN:HB3	1:F:238:TYR:CE2	2.36	0.61
1:F:257:SER:OG	1:F:263:TYR:HA	2.00	0.61
1:C:294:ASN:HA	1:D:113:LYS:HE2	1.81	0.61
1:F:133:VAL:HG12	1:F:134:TRP:H	1.66	0.61
1:C:104:GLN:HE22	1:C:298:PRO:HB2	1.64	0.61
1:C:84:ALA:N	1:C:85:PRO:HD2	2.16	0.61
1:D:373:LEU:HB3	1:D:379:VAL:CG2	2.28	0.61
1:C:282:ARG:HH21	1:D:7:GLN:CA	2.13	0.61
1:F:159:PRO:HG2	1:F:173:LEU:HB2	1.82	0.61
1:A:193:HIS:CD2	1:A:194:ASN:H	2.19	0.61
1:A:257:SER:OG	1:A:263:TYR:HA	2.00	0.61
1:B:133:VAL:HG12	1:B:134:TRP:H	1.66	0.61
1:B:29:ARG:HD3	1:B:32:LYS:HB3	1.81	0.61
1:B:404:PHE:HA	1:B:407:VAL:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:PRO:C	1:B:74:GLU:N	2.54	0.61
1:D:29:ARG:HD3	1:D:32:LYS:HB3	1.81	0.61
1:D:84:ALA:N	1:D:85:PRO:HD2	2.15	0.61
1:F:115:GLY:O	1:F:119:LEU:HG	2.00	0.61
1:A:300:ASN:HB3	1:B:265:GLU:OE2	1.99	0.61
1:A:29:ARG:HD3	1:A:32:LYS:HB3	1.81	0.61
1:B:104:GLN:HE22	1:B:298:PRO:HB2	1.64	0.61
1:C:159:PRO:HG2	1:C:173:LEU:HB2	1.82	0.61
1:F:404:PHE:HA	1:F:407:VAL:HG23	1.82	0.61
1:A:159:PRO:HG2	1:A:173:LEU:HB2	1.82	0.61
1:A:82:ALA:O	1:A:86:LEU:HG	2.01	0.61
1:C:133:VAL:HG12	1:C:134:TRP:H	1.66	0.61
1:C:404:PHE:HA	1:C:407:VAL:HG23	1.82	0.61
1:D:193:HIS:CD2	1:D:194:ASN:H	2.19	0.61
1:D:257:SER:OG	1:D:263:TYR:HA	2.00	0.61
1:D:104:GLN:HE22	1:D:298:PRO:HB2	1.64	0.61
1:E:18:LEU:HD12	1:E:21:MET:HB2	1.82	0.61
1:F:29:ARG:HD3	1:F:32:LYS:HB3	1.81	0.61
1:F:69:LEU:O	1:F:70:TYR:O	2.18	0.61
1:B:202:ASN:HB3	1:B:238:TYR:CE2	2.36	0.61
1:B:82:ALA:O	1:B:86:LEU:HG	2.01	0.61
1:C:82:ALA:O	1:C:86:LEU:HG	2.01	0.61
1:D:82:ALA:O	1:D:86:LEU:HG	2.01	0.61
1:E:202:ASN:HB3	1:E:238:TYR:CZ	2.35	0.61
1:E:82:ALA:O	1:E:86:LEU:HG	2.01	0.61
1:A:84:ALA:N	1:A:85:PRO:HD2	2.15	0.60
1:B:115:GLY:O	1:B:119:LEU:HG	2.00	0.60
1:E:71:LEU:HD22	1:E:72:PRO:HD2	1.82	0.60
1:F:193:HIS:CD2	1:F:194:ASN:H	2.19	0.60
1:B:225:TYR:HB3	1:B:228:PHE:CD2	2.31	0.60
1:E:133:VAL:HG12	1:E:134:TRP:H	1.66	0.60
1:E:84:ALA:N	1:E:85:PRO:HD2	2.16	0.60
1:F:72:PRO:C	1:F:74:GLU:N	2.54	0.60
1:A:178:LYS:HG2	1:A:211:ILE:HG21	1.84	0.60
1:C:115:GLY:O	1:C:119:LEU:HG	2.00	0.60
1:D:178:LYS:HG2	1:D:211:ILE:HG21	1.84	0.60
1:A:133:VAL:HG12	1:A:134:TRP:H	1.66	0.60
1:B:178:LYS:HG2	1:B:211:ILE:HG21	1.83	0.60
1:D:115:GLY:O	1:D:119:LEU:HG	2.00	0.60
1:D:202:ASN:HB3	1:D:238:TYR:CE2	2.36	0.60
1:E:202:ASN:HB3	1:E:238:TYR:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PRO:C	1:A:74:GLU:N	2.54	0.60
1:D:118:PHE:O	1:D:121:ARG:N	2.30	0.60
1:D:87:LEU:HD23	1:D:87:LEU:H	1.66	0.60
1:E:227:GLY:HA2	1:E:231:GLY:O	2.02	0.60
1:F:186:VAL:CG1	1:F:188:LEU:HD11	2.24	0.60
1:A:202:ASN:HB3	1:A:238:TYR:CE2	2.36	0.60
1:B:193:HIS:CD2	1:B:194:ASN:H	2.19	0.60
1:C:202:ASN:HB3	1:C:238:TYR:CE2	2.36	0.60
1:C:178:LYS:HG2	1:C:211:ILE:HG21	1.84	0.60
1:D:159:PRO:HG2	1:D:173:LEU:HB2	1.82	0.60
1:C:5:MET:CE	1:D:274:CYS:SG	2.90	0.60
1:F:104:GLN:HE22	1:F:298:PRO:HB2	1.64	0.60
1:F:82:ALA:O	1:F:86:LEU:HG	2.01	0.60
1:A:142:ASN:H	1:A:142:ASN:ND2	2.00	0.60
1:D:133:VAL:HG12	1:D:134:TRP:H	1.66	0.60
1:B:325:GLU:O	1:B:328:THR:HB	2.02	0.60
1:C:225:TYR:HB3	1:C:228:PHE:CD2	2.31	0.60
1:D:142:ASN:ND2	1:D:142:ASN:H	2.00	0.60
1:C:193:HIS:CD2	1:C:194:ASN:H	2.19	0.60
1:C:282:ARG:HH21	1:D:7:GLN:HA	1.67	0.60
1:D:227:GLY:HA2	1:D:231:GLY:O	2.02	0.60
1:D:325:GLU:O	1:D:328:THR:HB	2.02	0.60
1:D:40:TYR:HD1	1:D:359:MET:HE2	1.66	0.60
1:E:371:ASP:HA	1:E:374:ARG:HG2	1.83	0.60
1:F:178:LYS:HG2	1:F:211:ILE:HG21	1.84	0.60
1:F:227:GLY:HA2	1:F:231:GLY:O	2.02	0.60
1:B:142:ASN:ND2	1:B:142:ASN:H	2.00	0.60
1:B:227:GLY:HA2	1:B:231:GLY:O	2.02	0.60
1:B:22:GLU:O	1:B:26:GLU:HG2	2.02	0.60
1:E:22:GLU:O	1:E:26:GLU:HG2	2.02	0.60
1:F:15:ASP:HB3	1:F:18:LEU:CB	2.30	0.60
1:F:22:GLU:O	1:F:26:GLU:HG2	2.02	0.60
1:B:159:PRO:HG2	1:B:173:LEU:HB2	1.82	0.59
1:E:178:LYS:HG2	1:E:211:ILE:HG21	1.84	0.59
1:C:142:ASN:H	1:C:142:ASN:ND2	2.00	0.59
1:C:15:ASP:HB3	1:C:18:LEU:CB	2.30	0.59
1:C:227:GLY:HA2	1:C:231:GLY:O	2.02	0.59
1:C:305:VAL:HG23	1:C:306:VAL:H	1.67	0.59
1:D:22:GLU:O	1:D:26:GLU:HG2	2.02	0.59
1:C:263:TYR:CB	1:D:70:TYR:CD2	2.85	0.59
1:E:305:VAL:HG23	1:E:306:VAL:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLY:HA2	1:A:231:GLY:O	2.02	0.59
1:B:371:ASP:HA	1:B:374:ARG:HG2	1.83	0.59
1:E:325:GLU:O	1:E:328:THR:HB	2.02	0.59
1:F:142:ASN:H	1:F:142:ASN:ND2	2.00	0.59
1:F:371:ASP:HA	1:F:374:ARG:HG2	1.83	0.59
1:A:371:ASP:HA	1:A:374:ARG:HG2	1.83	0.59
1:B:15:ASP:HB3	1:B:18:LEU:CB	2.30	0.59
1:E:142:ASN:ND2	1:E:142:ASN:H	2.00	0.59
1:F:305:VAL:HG23	1:F:306:VAL:H	1.67	0.59
1:F:325:GLU:O	1:F:328:THR:HB	2.02	0.59
1:A:72:PRO:O	1:A:74:GLU:N	2.36	0.59
1:B:43:GLU:C	1:B:45:GLY:H	2.06	0.59
1:B:72:PRO:O	1:B:74:GLU:N	2.36	0.59
1:C:43:GLU:C	1:C:45:GLY:H	2.06	0.59
1:C:72:PRO:O	1:C:74:GLU:N	2.36	0.59
1:C:87:LEU:H	1:C:87:LEU:HD23	1.66	0.59
1:F:43:GLU:C	1:F:45:GLY:H	2.06	0.59
1:F:72:PRO:O	1:F:74:GLU:N	2.36	0.59
1:A:325:GLU:O	1:A:328:THR:HB	2.02	0.59
1:C:282:ARG:NH2	1:D:7:GLN:HA	2.16	0.59
1:E:72:PRO:O	1:E:74:GLU:N	2.36	0.59
1:D:305:VAL:HG23	1:D:306:VAL:H	1.67	0.59
1:D:43:GLU:C	1:D:45:GLY:H	2.06	0.59
1:D:50:LEU:HD23	1:D:322:GLU:HG2	1.85	0.59
1:A:71:LEU:HD12	1:A:298:PRO:O	2.03	0.59
1:E:87:LEU:HD23	1:E:87:LEU:H	1.66	0.59
1:A:212:LEU:HD23	1:A:217:LEU:HB2	1.84	0.59
1:A:22:GLU:O	1:A:26:GLU:HG2	2.02	0.59
1:A:50:LEU:HD23	1:A:322:GLU:HG2	1.85	0.59
1:C:136:SER:HB2	1:C:139:THR:HB	1.85	0.59
1:D:72:PRO:C	1:D:74:GLU:N	2.54	0.59
1:A:43:GLU:C	1:A:45:GLY:H	2.06	0.59
1:B:136:SER:HB2	1:B:139:THR:HB	1.85	0.59
1:C:325:GLU:O	1:C:328:THR:HB	2.02	0.59
1:C:371:ASP:HA	1:C:374:ARG:HG2	1.83	0.59
1:C:50:LEU:HD23	1:C:322:GLU:HG2	1.85	0.59
1:A:136:SER:HB2	1:A:139:THR:HB	1.85	0.58
1:B:50:LEU:HD23	1:B:322:GLU:HG2	1.85	0.58
1:B:87:LEU:H	1:B:87:LEU:HD23	1.66	0.58
1:C:113:LYS:HE2	1:D:294:ASN:HA	1.85	0.58
1:C:22:GLU:O	1:C:26:GLU:HG2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:LEU:HD23	1:D:217:LEU:HB2	1.85	0.58
1:F:136:SER:HB2	1:F:139:THR:HB	1.85	0.58
1:C:249:PRO:O	1:C:250:ALA:HB2	2.03	0.58
1:C:71:LEU:HD12	1:C:298:PRO:O	2.03	0.58
1:D:249:PRO:O	1:D:250:ALA:HB2	2.03	0.58
1:D:371:ASP:HA	1:D:374:ARG:HG2	1.83	0.58
1:A:249:PRO:O	1:A:250:ALA:HB2	2.03	0.58
1:C:72:PRO:C	1:C:74:GLU:N	2.54	0.58
1:F:249:PRO:O	1:F:250:ALA:HB2	2.03	0.58
1:F:50:LEU:HD23	1:F:322:GLU:HG2	1.85	0.58
1:F:71:LEU:HD12	1:F:298:PRO:O	2.03	0.58
1:B:249:PRO:O	1:B:250:ALA:HB2	2.04	0.58
1:C:212:LEU:HD23	1:C:217:LEU:HB2	1.84	0.58
1:D:136:SER:HB2	1:D:139:THR:HB	1.85	0.58
1:B:212:LEU:HD23	1:B:217:LEU:HB2	1.85	0.58
1:B:305:VAL:HG23	1:B:306:VAL:H	1.67	0.58
1:B:71:LEU:HD12	1:B:298:PRO:O	2.03	0.58
1:E:136:SER:HB2	1:E:139:THR:HB	1.85	0.58
1:F:105:THR:HG21	1:F:111:ALA:HA	1.86	0.58
1:D:72:PRO:O	1:D:74:GLU:N	2.36	0.58
1:E:50:LEU:HD23	1:E:322:GLU:HG2	1.85	0.58
1:E:43:GLU:C	1:E:45:GLY:H	2.06	0.58
1:E:71:LEU:HD12	1:E:298:PRO:O	2.03	0.58
1:E:72:PRO:C	1:E:74:GLU:N	2.54	0.58
1:F:212:LEU:HD23	1:F:217:LEU:HB2	1.84	0.58
1:A:305:VAL:HG23	1:A:306:VAL:H	1.67	0.58
1:B:105:THR:HG21	1:B:111:ALA:HA	1.86	0.58
1:D:71:LEU:HD12	1:D:298:PRO:O	2.03	0.58
1:F:135:VAL:HG13	1:F:187:LEU:HD13	1.86	0.58
1:D:57:GLU:HA	1:D:60:LEU:HB2	1.86	0.58
1:E:105:THR:HG21	1:E:111:ALA:HA	1.86	0.58
1:E:5:MET:HE1	1:F:274:CYS:SG	2.44	0.58
1:C:57:GLU:HA	1:C:60:LEU:HB2	1.86	0.57
1:A:87:LEU:H	1:A:87:LEU:HD23	1.66	0.57
1:D:15:ASP:HB3	1:D:18:LEU:CB	2.30	0.57
1:E:212:LEU:HD23	1:E:217:LEU:HB2	1.84	0.57
1:A:105:THR:HG21	1:A:111:ALA:HA	1.86	0.57
1:B:173:LEU:HG	1:B:177:LEU:HD11	1.86	0.57
1:C:105:THR:HG21	1:C:111:ALA:HA	1.86	0.57
1:E:104:GLN:NE2	1:E:298:PRO:HB2	2.20	0.57
1:A:173:LEU:HG	1:A:177:LEU:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:HG21	1:A:41:TYR:HE2	1.69	0.57
1:D:180:LEU:N	1:D:180:LEU:HD23	2.19	0.57
1:B:57:GLU:HA	1:B:60:LEU:HB2	1.86	0.57
1:C:76:LEU:CD1	1:C:78:CYS:H	2.18	0.57
1:D:37:ILE:HG21	1:D:41:TYR:HE2	1.69	0.57
1:E:173:LEU:HG	1:E:177:LEU:HD11	1.87	0.57
1:E:57:GLU:HA	1:E:60:LEU:HB2	1.86	0.57
1:F:57:GLU:HA	1:F:60:LEU:HB2	1.86	0.57
1:A:135:VAL:HG13	1:A:187:LEU:HD13	1.86	0.57
1:A:76:LEU:CD1	1:A:78:CYS:H	2.18	0.57
1:B:180:LEU:N	1:B:180:LEU:HD23	2.19	0.57
1:D:193:HIS:HB3	1:D:197:GLY:N	2.20	0.57
1:E:135:VAL:HG13	1:E:187:LEU:HD13	1.86	0.57
1:E:49:GLN:NE2	1:F:67:ALA:HA	2.19	0.57
1:F:104:GLN:NE2	1:F:298:PRO:HB2	2.20	0.57
1:B:76:LEU:CD1	1:B:78:CYS:H	2.18	0.57
1:C:135:VAL:HG13	1:C:187:LEU:HD13	1.86	0.57
1:C:193:HIS:HB3	1:C:197:GLY:N	2.20	0.57
1:D:76:LEU:CD1	1:D:78:CYS:H	2.18	0.57
1:F:173:LEU:HG	1:F:177:LEU:HD11	1.87	0.57
1:F:87:LEU:H	1:F:87:LEU:HD23	1.66	0.57
1:B:193:HIS:HB3	1:B:197:GLY:N	2.20	0.57
1:E:180:LEU:HD23	1:E:180:LEU:N	2.19	0.57
1:E:249:PRO:O	1:E:250:ALA:HB2	2.03	0.57
1:B:135:VAL:HG13	1:B:187:LEU:HD13	1.86	0.57
1:E:37:ILE:HG21	1:E:41:TYR:HE2	1.69	0.57
1:F:76:LEU:HD23	1:F:79:TYR:HB2	1.86	0.57
1:A:320:LEU:O	1:A:323:VAL:HG12	2.05	0.56
1:A:403:ALA:O	1:A:406:ALA:HB3	2.05	0.56
1:C:180:LEU:N	1:C:180:LEU:HD23	2.19	0.56
1:A:15:ASP:HB3	1:A:18:LEU:CB	2.30	0.56
1:A:193:HIS:HB3	1:A:197:GLY:N	2.20	0.56
1:A:57:GLU:HA	1:A:60:LEU:HB2	1.86	0.56
1:D:105:THR:HG21	1:D:111:ALA:HA	1.86	0.56
1:D:320:LEU:O	1:D:323:VAL:HG12	2.05	0.56
1:E:224:ALA:HA	1:E:255:SER:HB3	1.87	0.56
1:E:76:LEU:CD1	1:E:78:CYS:H	2.18	0.56
1:F:37:ILE:HG21	1:F:41:TYR:HE2	1.69	0.56
1:F:76:LEU:CD1	1:F:78:CYS:H	2.18	0.56
1:A:180:LEU:HD23	1:A:180:LEU:N	2.20	0.56
1:B:104:GLN:NE2	1:B:298:PRO:HB2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LEU:HD12	1:B:77:ASN:N	2.20	0.56
1:C:104:GLN:NE2	1:C:298:PRO:HB2	2.20	0.56
1:C:37:ILE:HG21	1:C:41:TYR:HE2	1.69	0.56
1:D:80:ARG:HG3	1:D:102:THR:HB	1.88	0.56
1:E:6:PHE:HE1	1:F:249:PRO:CB	2.18	0.56
1:C:403:ALA:O	1:C:406:ALA:HB3	2.06	0.56
1:E:403:ALA:O	1:E:406:ALA:HB3	2.05	0.56
1:F:193:HIS:HB3	1:F:197:GLY:N	2.20	0.56
1:F:320:LEU:O	1:F:323:VAL:HG12	2.05	0.56
1:A:80:ARG:HG3	1:A:102:THR:HB	1.88	0.56
1:B:177:LEU:O	1:B:180:LEU:HG	2.06	0.56
1:A:177:LEU:O	1:A:180:LEU:HG	2.06	0.56
1:A:104:GLN:NE2	1:A:298:PRO:HB2	2.20	0.56
1:A:76:LEU:HD23	1:A:79:TYR:HB2	1.86	0.56
1:B:320:LEU:O	1:B:323:VAL:HG12	2.05	0.56
1:C:320:LEU:O	1:C:323:VAL:HG12	2.05	0.56
1:E:204:GLN:O	1:E:208:VAL:HG23	2.06	0.56
1:E:372:ARG:O	1:E:376:GLU:HB2	2.06	0.56
1:A:382:ILE:HG23	1:A:384:SER:N	2.18	0.56
1:A:397:VAL:C	1:A:400:VAL:HG23	2.26	0.56
1:B:204:GLN:O	1:B:208:VAL:HG23	2.06	0.56
1:B:205:TRP:HA	1:B:208:VAL:CG2	2.36	0.56
1:C:76:LEU:HD12	1:C:77:ASN:N	2.20	0.56
1:E:76:LEU:HD12	1:E:77:ASN:N	2.20	0.56
1:F:180:LEU:HD23	1:F:180:LEU:N	2.19	0.56
1:F:224:ALA:HA	1:F:255:SER:HB3	1.87	0.56
1:A:104:GLN:NE2	1:A:298:PRO:CB	2.69	0.56
1:A:224:ALA:HA	1:A:255:SER:HB3	1.87	0.56
1:A:372:ARG:O	1:A:376:GLU:HB2	2.06	0.56
1:C:80:ARG:HG3	1:C:102:THR:HB	1.88	0.56
1:D:135:VAL:HG13	1:D:187:LEU:HD13	1.86	0.56
1:D:382:ILE:HG23	1:D:384:SER:N	2.18	0.56
1:E:80:ARG:HG3	1:E:102:THR:HB	1.88	0.56
1:E:104:GLN:NE2	1:E:298:PRO:CB	2.69	0.56
1:E:382:ILE:HG23	1:E:384:SER:N	2.18	0.56
1:E:397:VAL:C	1:E:400:VAL:HG23	2.26	0.56
1:F:397:VAL:C	1:F:400:VAL:HG23	2.26	0.56
1:F:403:ALA:O	1:F:406:ALA:HB3	2.05	0.56
1:F:76:LEU:HD12	1:F:77:ASN:N	2.21	0.56
1:A:334:ARG:NH2	1:A:357:ARG:HA	2.21	0.56
1:B:403:ALA:O	1:B:406:ALA:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LEU:HD23	1:B:79:TYR:HB2	1.86	0.56
1:D:76:LEU:HD23	1:D:79:TYR:HB2	1.86	0.56
1:D:76:LEU:HD12	1:D:77:ASN:N	2.20	0.56
1:D:205:TRP:HA	1:D:208:VAL:CG2	2.36	0.56
1:D:274:CYS:HB3	1:D:279:ALA:HB3	1.88	0.56
1:E:15:ASP:HB3	1:E:18:LEU:CB	2.30	0.56
1:E:193:HIS:HB3	1:E:197:GLY:N	2.20	0.56
1:E:245:SER:O	1:E:247:GLY:N	2.39	0.56
1:F:40:TYR:HD1	1:F:359:MET:HE2	1.70	0.56
1:A:282:ARG:HB3	1:B:11:ALA:HB2	1.88	0.56
1:B:224:ALA:HA	1:B:255:SER:HB3	1.87	0.56
1:B:397:VAL:C	1:B:400:VAL:HG23	2.26	0.56
1:B:37:ILE:HG21	1:B:41:TYR:HE2	1.69	0.56
1:C:173:LEU:HG	1:C:177:LEU:HD11	1.86	0.56
1:C:177:LEU:O	1:C:180:LEU:HG	2.06	0.56
1:C:205:TRP:HA	1:C:208:VAL:CG2	2.36	0.56
1:D:224:ALA:HA	1:D:255:SER:HB3	1.87	0.56
1:E:177:LEU:O	1:E:180:LEU:HG	2.06	0.56
1:E:195:PRO:HB2	1:E:386:ARG:HB2	1.88	0.56
1:E:257:SER:HB3	1:E:263:TYR:HA	1.88	0.56
1:A:204:GLN:O	1:A:208:VAL:HG23	2.06	0.55
1:B:257:SER:HB3	1:B:263:TYR:HA	1.88	0.55
1:B:372:ARG:O	1:B:376:GLU:HB2	2.06	0.55
1:F:205:TRP:HA	1:F:208:VAL:CG2	2.36	0.55
1:A:103:ILE:O	1:A:103:ILE:HG13	2.06	0.55
1:A:195:PRO:HB2	1:A:386:ARG:HB2	1.88	0.55
1:A:245:SER:O	1:A:247:GLY:N	2.39	0.55
1:A:76:LEU:HD12	1:A:77:ASN:N	2.20	0.55
1:B:245:SER:O	1:B:247:GLY:N	2.39	0.55
1:B:274:CYS:HB3	1:B:279:ALA:HB3	1.88	0.55
1:C:204:GLN:O	1:C:208:VAL:HG23	2.06	0.55
1:C:257:SER:HB3	1:C:263:TYR:HA	1.88	0.55
1:D:204:GLN:O	1:D:208:VAL:HG23	2.06	0.55
1:D:245:SER:O	1:D:247:GLY:N	2.39	0.55
1:D:104:GLN:NE2	1:D:298:PRO:HB2	2.20	0.55
1:E:334:ARG:NH2	1:E:357:ARG:HA	2.21	0.55
1:F:177:LEU:O	1:F:180:LEU:HG	2.06	0.55
1:F:204:GLN:O	1:F:208:VAL:HG23	2.06	0.55
1:F:245:SER:O	1:F:247:GLY:N	2.39	0.55
1:B:104:GLN:NE2	1:B:298:PRO:CB	2.69	0.55
1:D:104:GLN:NE2	1:D:298:PRO:CB	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:397:VAL:C	1:D:400:VAL:HG23	2.26	0.55
1:E:103:ILE:HG13	1:E:103:ILE:O	2.07	0.55
1:E:205:TRP:HA	1:E:208:VAL:CG2	2.36	0.55
1:E:76:LEU:HD23	1:E:79:TYR:HB2	1.86	0.55
1:F:104:GLN:NE2	1:F:298:PRO:CB	2.69	0.55
1:A:256:PHE:HB2	1:A:267:VAL:O	2.07	0.55
1:B:80:ARG:HG3	1:B:102:THR:HB	1.88	0.55
1:C:224:ALA:HA	1:C:255:SER:HB3	1.87	0.55
1:C:104:GLN:NE2	1:C:298:PRO:CB	2.69	0.55
1:C:397:VAL:C	1:C:400:VAL:HG23	2.26	0.55
1:D:177:LEU:O	1:D:180:LEU:HG	2.06	0.55
1:D:403:ALA:O	1:D:406:ALA:HB3	2.05	0.55
1:F:372:ARG:O	1:F:376:GLU:HB2	2.06	0.55
1:B:334:ARG:NH2	1:B:357:ARG:HA	2.21	0.55
1:B:390:ALA:C	1:B:392:LEU:H	2.10	0.55
1:C:190:PRO:HA	1:C:205:TRP:CZ2	2.41	0.55
1:C:276:ASP:O	1:C:279:ALA:N	2.39	0.55
1:D:334:ARG:NH2	1:D:357:ARG:HA	2.21	0.55
1:A:205:TRP:HA	1:A:208:VAL:CG2	2.36	0.55
1:C:40:TYR:HD1	1:C:359:MET:HE2	1.69	0.55
1:E:184:SER:N	1:E:217:LEU:HD23	2.20	0.55
1:E:274:CYS:HB3	1:E:279:ALA:HB3	1.89	0.55
1:F:334:ARG:NH2	1:F:357:ARG:HA	2.21	0.55
1:F:390:ALA:C	1:F:392:LEU:H	2.10	0.55
1:C:76:LEU:HD23	1:C:79:TYR:HB2	1.86	0.55
1:E:125:GLU:HA	1:E:125:GLU:OE1	2.07	0.55
1:F:190:PRO:HA	1:F:205:TRP:CZ2	2.41	0.55
1:A:190:PRO:HA	1:A:205:TRP:CZ2	2.41	0.55
1:C:372:ARG:O	1:C:376:GLU:HB2	2.06	0.55
1:D:173:LEU:HG	1:D:177:LEU:HD11	1.86	0.55
1:D:190:PRO:HA	1:D:205:TRP:CZ2	2.42	0.55
1:E:133:VAL:HG13	1:E:185:ILE:HB	1.89	0.55
1:E:190:PRO:HA	1:E:205:TRP:CZ2	2.41	0.55
1:E:307:ALA:C	1:E:309:VAL:H	2.10	0.55
1:A:166:ASN:HB3	1:A:352:TYR:HB3	1.89	0.55
1:C:274:CYS:HB3	1:C:279:ALA:HB3	1.88	0.55
1:D:195:PRO:HB2	1:D:386:ARG:HB2	1.88	0.55
1:E:320:LEU:O	1:E:323:VAL:HG12	2.05	0.55
1:A:257:SER:HB3	1:A:263:TYR:HA	1.88	0.55
1:B:195:PRO:HB2	1:B:386:ARG:HB2	1.88	0.55
1:B:53:VAL:O	1:B:56:ALA:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:SER:O	1:C:247:GLY:N	2.39	0.55
1:D:125:GLU:HA	1:D:125:GLU:OE1	2.07	0.55
1:E:256:PHE:HB2	1:E:267:VAL:O	2.07	0.55
1:E:390:ALA:C	1:E:392:LEU:H	2.10	0.55
1:A:125:GLU:HA	1:A:125:GLU:OE1	2.07	0.54
1:A:307:ALA:C	1:A:309:VAL:H	2.10	0.54
1:A:405:ALA:HA	1:A:408:MET:CE	2.38	0.54
1:B:133:VAL:HG13	1:B:185:ILE:HB	1.89	0.54
1:B:239:ALA:C	1:B:243:ILE:HD12	2.28	0.54
1:B:256:PHE:HB2	1:B:267:VAL:O	2.07	0.54
1:C:142:ASN:ND2	1:C:142:ASN:N	2.55	0.54
1:D:103:ILE:HG13	1:D:103:ILE:O	2.06	0.54
1:D:256:PHE:HB2	1:D:267:VAL:O	2.07	0.54
1:D:257:SER:HB3	1:D:263:TYR:HA	1.88	0.54
1:D:372:ARG:O	1:D:376:GLU:HB2	2.06	0.54
1:E:405:ALA:HA	1:E:408:MET:CE	2.38	0.54
1:A:390:ALA:C	1:A:392:LEU:H	2.10	0.54
1:B:276:ASP:O	1:B:279:ALA:N	2.39	0.54
1:C:184:SER:N	1:C:217:LEU:HD23	2.20	0.54
1:C:195:PRO:HB2	1:C:386:ARG:HB2	1.88	0.54
1:D:53:VAL:O	1:D:56:ALA:HB3	2.07	0.54
1:E:166:ASN:HB3	1:E:352:TYR:HB3	1.89	0.54
1:F:80:ARG:HG3	1:F:102:THR:HB	1.88	0.54
1:F:195:PRO:HB2	1:F:386:ARG:HB2	1.88	0.54
1:A:274:CYS:HB3	1:A:279:ALA:HB3	1.88	0.54
1:C:334:ARG:NH2	1:C:357:ARG:HA	2.21	0.54
1:D:142:ASN:ND2	1:D:142:ASN:N	2.55	0.54
1:E:239:ALA:C	1:E:243:ILE:HD12	2.28	0.54
1:E:113:LYS:HE2	1:F:294:ASN:HA	1.88	0.54
1:F:239:ALA:C	1:F:243:ILE:HD12	2.28	0.54
1:F:257:SER:HB3	1:F:263:TYR:HA	1.88	0.54
1:F:405:ALA:HA	1:F:408:MET:CE	2.38	0.54
1:B:142:ASN:ND2	1:B:142:ASN:N	2.55	0.54
1:B:190:PRO:HA	1:B:205:TRP:CZ2	2.42	0.54
1:C:256:PHE:HB2	1:C:267:VAL:O	2.07	0.54
1:D:166:ASN:HB3	1:D:352:TYR:HB3	1.90	0.54
1:E:212:LEU:CD2	1:E:217:LEU:HB2	2.38	0.54
1:E:294:ASN:HA	1:F:113:LYS:HE2	1.88	0.54
1:F:125:GLU:HA	1:F:125:GLU:OE1	2.07	0.54
1:F:222:ASP:OD1	1:F:223:ILE:N	2.41	0.54
1:E:263:TYR:HB3	1:F:70:TYR:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ALA:HA	1:A:408:MET:HE3	1.88	0.54
1:B:222:ASP:OD1	1:B:223:ILE:N	2.41	0.54
1:B:382:ILE:HG23	1:B:384:SER:N	2.18	0.54
1:C:125:GLU:HA	1:C:125:GLU:OE1	2.07	0.54
1:C:51:GLN:HE21	1:C:51:GLN:HA	1.73	0.54
1:C:82:ALA:O	1:C:85:PRO:HG2	2.08	0.54
1:D:276:ASP:O	1:D:279:ALA:N	2.39	0.54
1:E:405:ALA:HA	1:E:408:MET:HE3	1.89	0.54
1:F:256:PHE:HB2	1:F:267:VAL:O	2.07	0.54
1:A:82:ALA:O	1:A:85:PRO:HG2	2.08	0.54
1:B:306:VAL:O	1:B:307:ALA:O	2.26	0.54
1:B:51:GLN:HA	1:B:51:GLN:HE21	1.73	0.54
1:C:239:ALA:C	1:C:243:ILE:HD12	2.28	0.54
1:C:306:VAL:O	1:C:307:ALA:O	2.26	0.54
1:C:53:VAL:O	1:C:56:ALA:HB3	2.07	0.54
1:D:212:LEU:CD2	1:D:217:LEU:HB2	2.38	0.54
1:D:390:ALA:C	1:D:392:LEU:H	2.10	0.54
1:F:212:LEU:CD2	1:F:217:LEU:HB2	2.38	0.54
1:F:276:ASP:O	1:F:279:ALA:N	2.39	0.54
1:F:51:GLN:HE21	1:F:51:GLN:HA	1.73	0.54
1:A:222:ASP:OD1	1:A:223:ILE:N	2.41	0.54
1:A:51:GLN:HE21	1:A:51:GLN:HA	1.73	0.54
1:E:211:ILE:HA	1:E:214:ALA:HB3	1.90	0.54
1:E:373:LEU:HA	1:E:377:PHE:HD1	1.73	0.54
1:F:212:LEU:HD11	1:F:219:PRO:HB3	1.90	0.54
1:F:240:ILE:HA	1:F:243:ILE:HD12	1.89	0.54
1:F:274:CYS:HB3	1:F:279:ALA:HB3	1.88	0.54
1:A:212:LEU:CD2	1:A:217:LEU:HB2	2.38	0.54
1:A:40:TYR:HD1	1:A:359:MET:HE2	1.72	0.54
1:B:166:ASN:HB3	1:B:352:TYR:HB3	1.89	0.54
1:B:405:ALA:HA	1:B:408:MET:CE	2.38	0.54
1:D:222:ASP:OD1	1:D:223:ILE:N	2.41	0.54
1:E:222:ASP:OD1	1:E:223:ILE:N	2.41	0.54
1:B:191:CYS:HB2	1:B:236:ASP:HB3	1.90	0.54
1:B:240:ILE:HA	1:B:243:ILE:HD12	1.89	0.54
1:D:306:VAL:O	1:D:307:ALA:O	2.26	0.54
1:D:51:GLN:HA	1:D:51:GLN:HE21	1.73	0.54
1:F:133:VAL:HG13	1:F:185:ILE:HB	1.89	0.54
1:A:306:VAL:O	1:A:307:ALA:O	2.26	0.53
1:A:53:VAL:O	1:A:56:ALA:HB3	2.08	0.53
1:B:184:SER:N	1:B:217:LEU:HD23	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:LEU:CD2	1:C:217:LEU:HB2	2.38	0.53
1:C:320:LEU:O	1:C:320:LEU:HD12	2.08	0.53
1:D:373:LEU:HA	1:D:377:PHE:HD1	1.73	0.53
1:D:400:VAL:HB	1:D:404:PHE:HZ	1.74	0.53
1:F:373:LEU:HA	1:F:377:PHE:HD1	1.73	0.53
1:A:276:ASP:O	1:A:279:ALA:N	2.39	0.53
1:A:373:LEU:HA	1:A:377:PHE:HD1	1.73	0.53
1:A:400:VAL:HB	1:A:404:PHE:HZ	1.74	0.53
1:B:373:LEU:HA	1:B:377:PHE:HD1	1.73	0.53
1:C:166:ASN:HB3	1:C:352:TYR:HB3	1.89	0.53
1:C:212:LEU:HD11	1:C:219:PRO:HB3	1.90	0.53
1:C:274:CYS:SG	1:D:5:MET:HE3	2.44	0.53
1:C:279:ALA:C	1:C:281:GLY:N	2.62	0.53
1:C:382:ILE:HG23	1:C:384:SER:N	2.18	0.53
1:C:405:ALA:HA	1:C:408:MET:CE	2.38	0.53
1:D:239:ALA:C	1:D:243:ILE:HD12	2.28	0.53
1:D:279:ALA:C	1:D:281:GLY:N	2.62	0.53
1:D:405:ALA:HA	1:D:408:MET:CE	2.38	0.53
1:C:282:ARG:NH2	1:D:7:GLN:CA	2.71	0.53
1:E:279:ALA:C	1:E:281:GLY:N	2.62	0.53
1:E:400:VAL:HB	1:E:404:PHE:HZ	1.74	0.53
1:F:320:LEU:HD12	1:F:320:LEU:O	2.08	0.53
1:A:239:ALA:C	1:A:243:ILE:HD12	2.28	0.53
1:B:125:GLU:OE1	1:B:125:GLU:HA	2.07	0.53
1:C:237:ALA:O	1:C:238:TYR:C	2.47	0.53
1:C:400:VAL:HB	1:C:404:PHE:HZ	1.74	0.53
1:E:212:LEU:HD11	1:E:219:PRO:HB3	1.90	0.53
1:E:320:LEU:O	1:E:320:LEU:HD12	2.08	0.53
1:F:53:VAL:O	1:F:56:ALA:HB3	2.08	0.53
1:A:212:LEU:HD11	1:A:219:PRO:HB3	1.90	0.53
1:B:237:ALA:O	1:B:238:TYR:C	2.47	0.53
1:B:400:VAL:HB	1:B:404:PHE:HZ	1.74	0.53
1:C:222:ASP:OD1	1:C:223:ILE:N	2.41	0.53
1:C:307:ALA:C	1:C:309:VAL:H	2.11	0.53
1:E:51:GLN:HA	1:E:51:GLN:HE21	1.73	0.53
1:F:166:ASN:HB3	1:F:352:TYR:HB3	1.89	0.53
1:F:306:VAL:O	1:F:307:ALA:O	2.26	0.53
1:A:133:VAL:HG13	1:A:185:ILE:HB	1.89	0.53
1:A:240:ILE:HA	1:A:243:ILE:HD12	1.89	0.53
1:A:249:PRO:HB2	1:B:6:PHE:HE1	1.71	0.53
1:B:254:ASN:HD22	1:B:255:SER:H	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ALA:O	1:B:85:PRO:HG2	2.08	0.53
1:C:390:ALA:C	1:C:392:LEU:H	2.10	0.53
1:D:305:VAL:O	1:D:309:VAL:HG23	2.09	0.53
1:E:306:VAL:O	1:E:307:ALA:O	2.26	0.53
1:F:237:ALA:O	1:F:238:TYR:C	2.47	0.53
1:A:142:ASN:ND2	1:A:142:ASN:N	2.55	0.53
1:A:184:SER:N	1:A:217:LEU:HD23	2.20	0.53
1:B:307:ALA:C	1:B:309:VAL:H	2.10	0.53
1:E:263:TYR:CG	1:F:70:TYR:CD2	2.96	0.53
1:E:53:VAL:O	1:E:56:ALA:HB3	2.08	0.53
1:F:254:ASN:HD22	1:F:255:SER:H	1.56	0.53
1:F:305:VAL:O	1:F:309:VAL:HG23	2.09	0.53
1:E:263:TYR:CG	1:F:70:TYR:HD2	2.27	0.53
1:A:211:ILE:HA	1:A:214:ALA:HB3	1.90	0.53
1:B:212:LEU:CD2	1:B:217:LEU:HB2	2.38	0.53
1:B:320:LEU:HD12	1:B:320:LEU:O	2.08	0.53
1:C:133:VAL:HG13	1:C:185:ILE:HB	1.89	0.53
1:D:240:ILE:HA	1:D:243:ILE:HD12	1.89	0.53
1:D:307:ALA:C	1:D:309:VAL:H	2.10	0.53
1:F:274:CYS:HB3	1:F:279:ALA:CB	2.39	0.53
1:F:307:ALA:C	1:F:309:VAL:H	2.11	0.53
1:F:82:ALA:O	1:F:85:PRO:HG2	2.08	0.53
1:A:305:VAL:O	1:A:309:VAL:HG23	2.09	0.53
1:B:212:LEU:HD11	1:B:219:PRO:HB3	1.90	0.53
1:C:240:ILE:HA	1:C:243:ILE:HD12	1.89	0.53
1:C:274:CYS:HB3	1:C:279:ALA:CB	2.39	0.53
1:D:274:CYS:HB3	1:D:279:ALA:CB	2.39	0.53
1:D:82:ALA:O	1:D:85:PRO:HG2	2.08	0.53
1:E:240:ILE:HA	1:E:243:ILE:HD12	1.89	0.53
1:F:400:VAL:HB	1:F:404:PHE:HZ	1.73	0.53
1:B:279:ALA:C	1:B:281:GLY:N	2.62	0.53
1:B:40:TYR:HD1	1:B:359:MET:HE2	1.71	0.53
1:D:133:VAL:HG13	1:D:185:ILE:HB	1.89	0.53
1:D:76:LEU:CG	1:D:79:TYR:HB2	2.39	0.53
1:E:142:ASN:ND2	1:E:142:ASN:N	2.55	0.53
1:E:254:ASN:HD22	1:E:255:SER:H	1.56	0.53
1:E:274:CYS:HB3	1:E:279:ALA:CB	2.39	0.53
1:A:191:CYS:HB2	1:A:236:ASP:HB3	1.90	0.52
1:B:305:VAL:O	1:B:309:VAL:HG23	2.09	0.52
1:C:254:ASN:HD22	1:C:255:SER:H	1.56	0.52
1:C:373:LEU:HA	1:C:377:PHE:HD1	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:ASN:HD22	1:D:255:SER:H	1.56	0.52
1:E:27:ASP:OD2	1:E:29:ARG:HD2	2.09	0.52
1:E:82:ALA:O	1:E:85:PRO:HG2	2.08	0.52
1:A:279:ALA:C	1:A:281:GLY:N	2.62	0.52
1:A:274:CYS:HB3	1:A:279:ALA:CB	2.39	0.52
1:C:27:ASP:OD2	1:C:29:ARG:HD2	2.09	0.52
1:E:326:MET:O	1:E:330:ILE:HG13	2.10	0.52
1:F:241:ARG:N	1:F:241:ARG:HD2	2.24	0.52
1:F:279:ALA:C	1:F:281:GLY:N	2.62	0.52
1:A:241:ARG:N	1:A:241:ARG:HD2	2.24	0.52
1:A:27:ASP:OD2	1:A:29:ARG:HD2	2.09	0.52
1:B:274:CYS:HB3	1:B:279:ALA:CB	2.39	0.52
1:D:211:ILE:HA	1:D:214:ALA:HB3	1.90	0.52
1:D:320:LEU:O	1:D:320:LEU:HD12	2.08	0.52
1:D:326:MET:O	1:D:330:ILE:HG13	2.09	0.52
1:E:237:ALA:O	1:E:238:TYR:C	2.47	0.52
1:F:103:ILE:O	1:F:103:ILE:HG13	2.06	0.52
1:F:211:ILE:HA	1:F:214:ALA:HB3	1.90	0.52
1:F:76:LEU:CG	1:F:79:TYR:HB2	2.39	0.52
1:A:320:LEU:HD12	1:A:320:LEU:O	2.08	0.52
1:B:103:ILE:HG13	1:B:103:ILE:O	2.07	0.52
1:C:191:CYS:HB2	1:C:236:ASP:HB3	1.90	0.52
1:C:326:MET:O	1:C:330:ILE:HG13	2.10	0.52
1:D:240:ILE:N	1:D:243:ILE:HD12	2.25	0.52
1:E:240:ILE:N	1:E:243:ILE:HD12	2.25	0.52
1:E:227:GLY:O	1:E:327:ARG:HD3	2.09	0.52
1:F:212:LEU:HD13	1:F:219:PRO:HB3	1.92	0.52
1:B:27:ASP:OD2	1:B:29:ARG:HD2	2.09	0.52
1:C:103:ILE:O	1:C:103:ILE:HG13	2.06	0.52
1:D:184:SER:N	1:D:217:LEU:HD23	2.20	0.52
1:E:118:PHE:HE1	1:E:122:TYR:HD2	1.58	0.52
1:F:326:MET:O	1:F:330:ILE:HG13	2.10	0.52
1:F:382:ILE:HG23	1:F:384:SER:N	2.18	0.52
1:A:111:ALA:HB1	1:A:270:LEU:HB2	1.92	0.52
1:B:340:VAL:HB	1:B:401:ALA:HB1	1.92	0.52
1:C:211:ILE:HA	1:C:214:ALA:HB3	1.90	0.52
1:D:111:ALA:HB1	1:D:270:LEU:HB2	1.92	0.52
1:D:237:ALA:O	1:D:238:TYR:C	2.47	0.52
1:E:76:LEU:CG	1:E:79:TYR:HB2	2.39	0.52
1:E:263:TYR:HB3	1:F:70:TYR:CD2	2.41	0.52
1:A:76:LEU:CG	1:A:79:TYR:HB2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:MET:O	1:B:330:ILE:HG13	2.10	0.52
1:C:263:TYR:HB2	1:D:70:TYR:CD2	2.43	0.52
1:C:305:VAL:O	1:C:309:VAL:HG23	2.09	0.52
1:D:118:PHE:HE1	1:D:122:TYR:HD2	1.58	0.52
1:D:191:CYS:HB2	1:D:236:ASP:HB3	1.90	0.52
1:D:340:VAL:HB	1:D:401:ALA:HB1	1.92	0.52
1:E:305:VAL:O	1:E:309:VAL:HG23	2.09	0.52
1:F:240:ILE:N	1:F:243:ILE:HD12	2.25	0.52
1:A:240:ILE:N	1:A:243:ILE:HD12	2.25	0.52
1:B:76:LEU:CG	1:B:79:TYR:HB2	2.39	0.52
1:C:227:GLY:O	1:C:327:ARG:HD3	2.09	0.52
1:C:340:VAL:HB	1:C:401:ALA:HB1	1.92	0.52
1:D:212:LEU:HD11	1:D:219:PRO:HB3	1.90	0.52
1:F:27:ASP:OD2	1:F:29:ARG:HD2	2.09	0.52
1:A:118:PHE:HE1	1:A:122:TYR:HD2	1.58	0.52
1:A:188:LEU:HD12	1:A:188:LEU:N	2.25	0.52
1:B:240:ILE:N	1:B:243:ILE:HD12	2.25	0.52
1:B:241:ARG:HD2	1:B:241:ARG:N	2.24	0.52
1:B:405:ALA:HA	1:B:408:MET:HE3	1.92	0.52
1:D:27:ASP:OD2	1:D:29:ARG:HD2	2.09	0.52
1:A:212:LEU:HD13	1:A:219:PRO:HB3	1.92	0.52
1:B:227:GLY:O	1:B:327:ARG:HD3	2.09	0.52
1:C:241:ARG:HD2	1:C:241:ARG:N	2.24	0.52
1:D:241:ARG:N	1:D:241:ARG:HD2	2.24	0.52
1:E:266:ARG:O	1:E:267:VAL:HG13	2.10	0.52
1:E:40:TYR:HD1	1:E:359:MET:HE2	1.75	0.52
1:A:66:GLY:O	1:A:67:ALA:HB3	2.10	0.51
1:B:211:ILE:HA	1:B:214:ALA:HB3	1.90	0.51
1:B:66:GLY:O	1:B:67:ALA:HB3	2.10	0.51
1:C:208:VAL:O	1:C:211:ILE:HD12	2.10	0.51
1:C:240:ILE:N	1:C:243:ILE:HD12	2.25	0.51
1:F:340:VAL:HB	1:F:401:ALA:HB1	1.92	0.51
1:A:254:ASN:HD22	1:A:255:SER:H	1.56	0.51
1:A:265:GLU:HG3	1:A:302:GLY:CA	2.40	0.51
1:A:326:MET:O	1:A:330:ILE:HG13	2.10	0.51
1:A:404:PHE:C	1:A:406:ALA:N	2.64	0.51
1:B:118:PHE:HE1	1:B:122:TYR:HD2	1.58	0.51
1:C:382:ILE:HG21	1:C:386:ARG:HB3	1.92	0.51
1:D:227:GLY:O	1:D:327:ARG:HD3	2.09	0.51
1:D:66:GLY:O	1:D:67:ALA:HB3	2.10	0.51
1:E:188:LEU:N	1:E:188:LEU:HD12	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:LEU:HD13	1:E:219:PRO:HB3	1.92	0.51
1:E:276:ASP:O	1:E:279:ALA:N	2.39	0.51
1:E:6:PHE:HE1	1:F:249:PRO:HB2	1.74	0.51
1:F:208:VAL:O	1:F:211:ILE:HD12	2.10	0.51
1:A:266:ARG:O	1:A:267:VAL:HG13	2.10	0.51
1:B:382:ILE:HG21	1:B:386:ARG:HB3	1.92	0.51
1:C:76:LEU:CG	1:C:79:TYR:HB2	2.39	0.51
1:D:188:LEU:HD12	1:D:188:LEU:N	2.25	0.51
1:E:241:ARG:N	1:E:241:ARG:HD2	2.24	0.51
1:E:382:ILE:HG21	1:E:386:ARG:HB3	1.92	0.51
1:A:237:ALA:O	1:A:238:TYR:C	2.47	0.51
1:A:340:VAL:HB	1:A:401:ALA:HB1	1.92	0.51
1:B:212:LEU:HD13	1:B:219:PRO:HB3	1.92	0.51
1:C:111:ALA:HB1	1:C:270:LEU:HB2	1.92	0.51
1:C:66:GLY:O	1:C:67:ALA:HB3	2.10	0.51
1:D:212:LEU:HD13	1:D:219:PRO:HB3	1.92	0.51
1:E:111:ALA:HB1	1:E:270:LEU:HB2	1.92	0.51
1:F:191:CYS:HB2	1:F:236:ASP:HB3	1.90	0.51
1:F:266:ARG:O	1:F:267:VAL:HG13	2.10	0.51
1:C:118:PHE:HE1	1:C:122:TYR:HD2	1.58	0.51
1:C:188:LEU:N	1:C:188:LEU:HD12	2.25	0.51
1:D:382:ILE:HG21	1:D:386:ARG:HB3	1.92	0.51
1:D:405:ALA:HA	1:D:408:MET:HE3	1.92	0.51
1:E:265:GLU:HG3	1:E:302:GLY:CA	2.41	0.51
1:A:227:GLY:O	1:A:327:ARG:HD3	2.09	0.51
1:A:382:ILE:HG21	1:A:386:ARG:HB3	1.92	0.51
1:B:111:ALA:HB1	1:B:270:LEU:HB2	1.92	0.51
1:B:404:PHE:C	1:B:406:ALA:N	2.64	0.51
1:C:404:PHE:C	1:C:406:ALA:N	2.64	0.51
1:F:227:GLY:O	1:F:327:ARG:HD3	2.09	0.51
1:F:382:ILE:HG21	1:F:386:ARG:HB3	1.92	0.51
1:D:208:VAL:O	1:D:211:ILE:HD12	2.10	0.51
1:E:208:VAL:O	1:E:211:ILE:HD12	2.10	0.51
1:E:66:GLY:O	1:E:67:ALA:HB3	2.10	0.51
1:A:11:ALA:HB2	1:B:282:ARG:HB3	1.93	0.51
1:B:208:VAL:O	1:B:211:ILE:HD12	2.10	0.51
1:B:266:ARG:O	1:B:267:VAL:HG13	2.10	0.51
1:D:404:PHE:C	1:D:406:ALA:N	2.64	0.51
1:E:102:THR:HA	1:E:271:SER:HB3	1.93	0.51
1:F:118:PHE:HE1	1:F:122:TYR:HD2	1.58	0.51
1:F:66:GLY:O	1:F:67:ALA:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:VAL:O	1:A:211:ILE:HD12	2.10	0.51
1:A:336:GLU:O	1:A:340:VAL:HG22	2.11	0.51
1:A:77:ASN:O	1:A:81:HIS:HB2	2.11	0.51
1:C:102:THR:HA	1:C:271:SER:HB3	1.93	0.51
1:C:265:GLU:HG3	1:C:302:GLY:CA	2.40	0.51
1:C:308:ALA:HA	1:C:311:ASN:HB2	1.93	0.51
1:E:205:TRP:HA	1:E:208:VAL:HG21	1.93	0.51
1:E:191:CYS:HB2	1:E:236:ASP:HB3	1.90	0.51
1:E:340:VAL:HB	1:E:401:ALA:HB1	1.92	0.51
1:A:102:THR:HA	1:A:271:SER:HB3	1.93	0.50
1:B:336:GLU:O	1:B:340:VAL:HG22	2.11	0.50
1:C:212:LEU:HD13	1:C:219:PRO:HB3	1.92	0.50
1:C:401:ALA:HA	1:C:404:PHE:CE2	2.46	0.50
1:C:77:ASN:O	1:C:81:HIS:HB2	2.11	0.50
1:D:102:THR:HA	1:D:271:SER:HB3	1.93	0.50
1:D:308:ALA:HA	1:D:311:ASN:HB2	1.93	0.50
1:E:77:ASN:O	1:E:81:HIS:HB2	2.11	0.50
1:B:265:GLU:HG3	1:B:302:GLY:CA	2.41	0.50
1:E:76:LEU:HD12	1:E:77:ASN:H	1.77	0.50
1:F:102:THR:HA	1:F:271:SER:HB3	1.93	0.50
1:F:140:TRP:HE3	1:F:143:HIS:HD2	1.59	0.50
1:B:102:THR:HA	1:B:271:SER:HB3	1.93	0.50
1:C:266:ARG:O	1:C:267:VAL:HG13	2.10	0.50
1:D:266:ARG:O	1:D:267:VAL:HG13	2.10	0.50
1:D:401:ALA:HA	1:D:404:PHE:CE2	2.46	0.50
1:E:401:ALA:HA	1:E:404:PHE:CE2	2.46	0.50
1:A:190:PRO:HB3	1:A:239:ALA:CB	2.42	0.50
1:A:308:ALA:HA	1:A:311:ASN:HB2	1.93	0.50
1:D:77:ASN:O	1:D:81:HIS:HB2	2.11	0.50
1:F:190:PRO:HB3	1:F:239:ALA:CB	2.42	0.50
1:F:336:GLU:O	1:F:340:VAL:HG22	2.11	0.50
1:A:205:TRP:HA	1:A:208:VAL:HG21	1.93	0.50
1:B:190:PRO:HB3	1:B:239:ALA:CB	2.42	0.50
1:E:177:LEU:C	1:E:179:THR:H	2.15	0.50
1:E:190:PRO:HB3	1:E:239:ALA:CB	2.42	0.50
1:F:111:ALA:HB1	1:F:270:LEU:HB2	1.92	0.50
1:F:188:LEU:HD12	1:F:188:LEU:N	2.25	0.50
1:A:177:LEU:C	1:A:179:THR:H	2.15	0.50
1:A:401:ALA:HA	1:A:404:PHE:CE2	2.46	0.50
1:A:76:LEU:HD12	1:A:77:ASN:H	1.77	0.50
1:B:188:LEU:N	1:B:188:LEU:HD12	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ALA:HA	1:B:311:ASN:HB2	1.93	0.50
1:D:190:PRO:HB3	1:D:239:ALA:CB	2.42	0.50
1:B:77:ASN:O	1:B:81:HIS:HB2	2.12	0.50
1:F:265:GLU:HG3	1:F:302:GLY:CA	2.40	0.50
1:F:401:ALA:HA	1:F:404:PHE:CE2	2.46	0.50
1:F:86:LEU:HB2	1:F:87:LEU:HD23	1.94	0.50
1:B:185:ILE:H	1:B:185:ILE:HD13	1.77	0.50
1:E:185:ILE:H	1:E:185:ILE:HD13	1.77	0.50
1:E:185:ILE:N	1:E:185:ILE:HD13	2.27	0.50
1:E:40:TYR:HB2	1:E:359:MET:HE1	1.94	0.50
1:E:274:CYS:SG	1:F:5:MET:HE3	2.52	0.50
1:F:209:ILE:O	1:F:212:LEU:N	2.45	0.50
1:A:185:ILE:N	1:A:185:ILE:HD13	2.27	0.49
1:B:140:TRP:HE3	1:B:143:HIS:HD2	1.59	0.49
1:C:185:ILE:HD13	1:C:185:ILE:N	2.27	0.49
1:C:205:TRP:HA	1:C:208:VAL:HG21	1.93	0.49
1:F:205:TRP:HA	1:F:208:VAL:HG21	1.93	0.49
1:F:242:ALA:HA	1:F:246:ALA:HB3	1.95	0.49
1:F:76:LEU:HD12	1:F:77:ASN:H	1.77	0.49
1:B:401:ALA:HA	1:B:404:PHE:CE2	2.46	0.49
1:C:86:LEU:HB2	1:C:87:LEU:HD23	1.94	0.49
1:D:336:GLU:O	1:D:340:VAL:HG22	2.11	0.49
1:A:6:PHE:HE1	1:B:249:PRO:HB2	1.76	0.49
1:B:93:PRO:O	1:B:97:GLN:HB2	2.13	0.49
1:C:382:ILE:CG2	1:C:385:GLY:H	2.25	0.49
1:C:76:LEU:HD12	1:C:77:ASN:H	1.77	0.49
1:C:93:PRO:O	1:C:97:GLN:HB2	2.13	0.49
1:D:171:ASN:O	1:D:173:LEU:N	2.45	0.49
1:D:177:LEU:C	1:D:179:THR:H	2.15	0.49
1:D:185:ILE:H	1:D:185:ILE:CD1	2.24	0.49
1:D:185:ILE:HD13	1:D:185:ILE:H	1.77	0.49
1:D:205:TRP:HA	1:D:208:VAL:HG21	1.93	0.49
1:E:372:ARG:HD3	1:E:407:VAL:HG13	1.94	0.49
1:F:382:ILE:CD1	1:F:386:ARG:HD3	2.36	0.49
1:F:77:ASN:O	1:F:81:HIS:HB2	2.11	0.49
1:A:145:ALA:O	1:A:149:GLY:N	2.46	0.49
1:B:171:ASN:O	1:B:173:LEU:N	2.45	0.49
1:B:185:ILE:N	1:B:185:ILE:HD13	2.27	0.49
1:B:247:GLY:O	1:B:248:LEU:HB2	2.12	0.49
1:B:223:ILE:HG23	1:B:254:ASN:ND2	2.27	0.49
1:C:223:ILE:HG23	1:C:254:ASN:ND2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:ARG:HD3	1:D:407:VAL:HG13	1.94	0.49
1:E:145:ALA:O	1:E:149:GLY:N	2.45	0.49
1:E:171:ASN:O	1:E:173:LEU:N	2.45	0.49
1:E:336:GLU:O	1:E:340:VAL:HG22	2.11	0.49
1:F:382:ILE:CG2	1:F:385:GLY:H	2.25	0.49
1:A:140:TRP:HE3	1:A:143:HIS:HD2	1.59	0.49
1:A:247:GLY:O	1:A:248:LEU:HB2	2.12	0.49
1:A:42:ASN:ND2	1:A:44:ASP:HB2	2.28	0.49
1:A:86:LEU:HB2	1:A:87:LEU:HD23	1.94	0.49
1:B:372:ARG:HD3	1:B:407:VAL:HG13	1.94	0.49
1:B:86:LEU:HB2	1:B:87:LEU:HD23	1.94	0.49
1:C:185:ILE:H	1:C:185:ILE:HD13	1.77	0.49
1:C:190:PRO:HB3	1:C:239:ALA:CB	2.42	0.49
1:C:242:ALA:HA	1:C:246:ALA:HB3	1.95	0.49
1:C:247:GLY:O	1:C:248:LEU:HB2	2.12	0.49
1:C:336:GLU:O	1:C:340:VAL:HG22	2.11	0.49
1:C:42:ASN:ND2	1:C:44:ASP:HB2	2.28	0.49
1:D:42:ASN:ND2	1:D:44:ASP:HB2	2.28	0.49
1:D:86:LEU:HB2	1:D:87:LEU:HD23	1.94	0.49
1:E:308:ALA:HA	1:E:311:ASN:HB2	1.93	0.49
1:E:382:ILE:CG2	1:E:385:GLY:H	2.25	0.49
1:F:185:ILE:H	1:F:185:ILE:HD13	1.77	0.49
1:F:247:GLY:O	1:F:248:LEU:HB2	2.12	0.49
1:F:405:ALA:HA	1:F:408:MET:HE3	1.94	0.49
1:B:238:TYR:O	1:B:239:ALA:C	2.51	0.49
1:B:242:ALA:HA	1:B:246:ALA:HB3	1.94	0.49
1:C:140:TRP:HE3	1:C:143:HIS:HD2	1.59	0.49
1:C:177:LEU:C	1:C:179:THR:H	2.15	0.49
1:D:76:LEU:HD12	1:D:77:ASN:H	1.76	0.49
1:E:209:ILE:O	1:E:212:LEU:N	2.45	0.49
1:E:247:GLY:O	1:E:248:LEU:HB2	2.12	0.49
1:F:171:ASN:O	1:F:173:LEU:N	2.45	0.49
1:F:185:ILE:N	1:F:185:ILE:HD13	2.27	0.49
1:F:238:TYR:O	1:F:239:ALA:C	2.51	0.49
1:D:238:TYR:O	1:D:239:ALA:C	2.51	0.49
1:D:223:ILE:HG23	1:D:254:ASN:ND2	2.27	0.49
1:D:382:ILE:CG2	1:D:385:GLY:H	2.25	0.49
1:E:223:ILE:HG23	1:E:254:ASN:ND2	2.27	0.49
1:F:177:LEU:C	1:F:179:THR:H	2.15	0.49
1:F:308:ALA:HA	1:F:311:ASN:HB2	1.93	0.49
1:B:145:ALA:O	1:B:149:GLY:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:TRP:HA	1:B:208:VAL:HG21	1.93	0.49
1:B:42:ASN:ND2	1:B:44:ASP:HB2	2.28	0.49
1:D:140:TRP:HE3	1:D:143:HIS:HD2	1.59	0.49
1:C:282:ARG:HH21	1:D:7:GLN:C	2.15	0.49
1:E:140:TRP:HE3	1:E:143:HIS:HD2	1.59	0.49
1:F:93:PRO:O	1:F:97:GLN:HB2	2.13	0.49
1:A:171:ASN:O	1:A:173:LEU:N	2.45	0.49
1:A:185:ILE:CD1	1:A:185:ILE:H	2.24	0.49
1:A:185:ILE:H	1:A:185:ILE:HD13	1.77	0.49
1:A:200:LEU:HB2	1:A:204:GLN:CD	2.33	0.49
1:B:382:ILE:CG2	1:B:385:GLY:H	2.25	0.49
1:C:372:ARG:HD3	1:C:407:VAL:HG13	1.95	0.49
1:D:145:ALA:O	1:D:149:GLY:N	2.45	0.49
1:D:93:PRO:O	1:D:97:GLN:HB2	2.13	0.49
1:E:142:ASN:O	1:E:143:HIS:C	2.51	0.49
1:E:200:LEU:HB2	1:E:204:GLN:CD	2.33	0.49
1:B:279:ALA:O	1:B:281:GLY:N	2.46	0.49
1:C:142:ASN:O	1:C:143:HIS:C	2.51	0.49
1:C:145:ALA:O	1:C:149:GLY:N	2.46	0.49
1:C:171:ASN:O	1:C:173:LEU:N	2.45	0.49
1:C:279:ALA:O	1:C:281:GLY:N	2.46	0.49
1:C:228:PHE:HD1	1:C:327:ARG:HB2	1.78	0.49
1:D:228:PHE:HD1	1:D:327:ARG:HB2	1.78	0.49
1:F:145:ALA:O	1:F:149:GLY:N	2.46	0.49
1:F:223:ILE:HG23	1:F:254:ASN:ND2	2.28	0.49
1:A:228:PHE:HD1	1:A:327:ARG:HB2	1.78	0.48
1:B:177:LEU:C	1:B:179:THR:H	2.15	0.48
1:D:185:ILE:HD13	1:D:185:ILE:N	2.27	0.48
1:D:242:ALA:HA	1:D:246:ALA:HB3	1.95	0.48
1:D:279:ALA:O	1:D:281:GLY:N	2.46	0.48
1:E:279:ALA:O	1:E:281:GLY:N	2.46	0.48
1:E:93:PRO:O	1:E:97:GLN:HB2	2.13	0.48
1:A:242:ALA:HA	1:A:246:ALA:HB3	1.95	0.48
1:B:228:PHE:HD1	1:B:327:ARG:HB2	1.78	0.48
1:B:76:LEU:HD12	1:B:77:ASN:H	1.77	0.48
1:C:382:ILE:CD1	1:C:386:ARG:HD3	2.36	0.48
1:D:200:LEU:HB2	1:D:204:GLN:CD	2.33	0.48
1:D:265:GLU:HG3	1:D:302:GLY:CA	2.40	0.48
1:A:142:ASN:O	1:A:143:HIS:C	2.51	0.48
1:A:209:ILE:O	1:A:212:LEU:N	2.45	0.48
1:A:93:PRO:O	1:A:97:GLN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LEU:CD2	1:B:47:ILE:HG13	2.43	0.48
1:C:200:LEU:HB2	1:C:204:GLN:CD	2.33	0.48
1:C:396:ASN:ND2	1:C:396:ASN:H	2.12	0.48
1:C:92:HIS:CG	1:C:93:PRO:HD2	2.49	0.48
1:E:100:VAL:HG23	1:E:100:VAL:O	2.14	0.48
1:E:404:PHE:C	1:E:406:ALA:N	2.64	0.48
1:E:86:LEU:HB2	1:E:87:LEU:HD23	1.94	0.48
1:F:142:ASN:O	1:F:143:HIS:C	2.51	0.48
1:F:146:ILE:H	1:F:146:ILE:HG13	1.34	0.48
1:F:261:SER:O	1:F:262:LEU:HD23	2.13	0.48
1:F:42:ASN:ND2	1:F:44:ASP:HB2	2.28	0.48
1:A:223:ILE:HG23	1:A:254:ASN:ND2	2.27	0.48
1:B:142:ASN:O	1:B:143:HIS:C	2.51	0.48
1:B:200:LEU:HB2	1:B:204:GLN:CD	2.33	0.48
1:B:396:ASN:H	1:B:396:ASN:ND2	2.12	0.48
1:C:282:ARG:NH2	1:D:7:GLN:O	2.45	0.48
1:D:142:ASN:O	1:D:143:HIS:C	2.51	0.48
1:D:247:GLY:O	1:D:248:LEU:HB2	2.12	0.48
1:D:393:ASN:HB3	1:D:396:ASN:HD21	1.79	0.48
1:D:92:HIS:CG	1:D:93:PRO:HD2	2.49	0.48
1:E:261:SER:O	1:E:262:LEU:HD23	2.13	0.48
1:F:118:PHE:O	1:F:121:ARG:HB2	2.14	0.48
1:F:184:SER:N	1:F:217:LEU:HD23	2.20	0.48
1:A:279:ALA:O	1:A:281:GLY:N	2.46	0.48
1:A:92:HIS:CG	1:A:93:PRO:HD2	2.49	0.48
1:B:100:VAL:HG23	1:B:100:VAL:O	2.13	0.48
1:C:114:VAL:O	1:C:115:GLY:C	2.52	0.48
1:C:238:TYR:O	1:C:239:ALA:C	2.51	0.48
1:C:256:PHE:HA	1:C:259:ILE:HG22	1.96	0.48
1:D:400:VAL:O	1:D:403:ALA:N	2.45	0.48
1:E:118:PHE:O	1:E:121:ARG:HB2	2.14	0.48
1:F:372:ARG:HD3	1:F:407:VAL:HG13	1.94	0.48
1:F:393:ASN:HB3	1:F:396:ASN:HD21	1.79	0.48
1:A:238:TYR:O	1:A:239:ALA:C	2.51	0.48
1:A:256:PHE:HA	1:A:259:ILE:HG22	1.96	0.48
1:A:400:VAL:HB	1:A:404:PHE:CZ	2.49	0.48
1:B:256:PHE:HA	1:B:259:ILE:HG22	1.96	0.48
1:B:400:VAL:HB	1:B:404:PHE:CZ	2.49	0.48
1:B:372:ARG:CD	1:B:407:VAL:HG13	2.43	0.48
1:C:136:SER:CB	1:C:139:THR:HB	2.43	0.48
1:C:400:VAL:HB	1:C:404:PHE:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:SER:CB	1:D:139:THR:HB	2.43	0.48
1:E:136:SER:CB	1:E:139:THR:HB	2.43	0.48
1:E:185:ILE:CD1	1:E:185:ILE:H	2.24	0.48
1:E:42:ASN:ND2	1:E:44:ASP:HB2	2.28	0.48
1:F:228:PHE:HD1	1:F:327:ARG:HB2	1.78	0.48
1:F:396:ASN:ND2	1:F:396:ASN:H	2.12	0.48
1:A:118:PHE:O	1:A:121:ARG:HB2	2.14	0.48
1:A:136:SER:CB	1:A:139:THR:HB	2.43	0.48
1:A:372:ARG:HD3	1:A:407:VAL:HG13	1.94	0.48
1:B:133:VAL:HG12	1:B:134:TRP:N	2.29	0.48
1:B:261:SER:O	1:B:262:LEU:HD23	2.13	0.48
1:C:185:ILE:CD1	1:C:185:ILE:H	2.24	0.48
1:C:372:ARG:CD	1:C:407:VAL:HG13	2.43	0.48
1:D:256:PHE:HA	1:D:259:ILE:HG22	1.96	0.48
1:E:223:ILE:HG23	1:E:254:ASN:HD22	1.79	0.48
1:F:136:SER:CB	1:F:139:THR:HB	2.43	0.48
1:A:100:VAL:HG23	1:A:100:VAL:O	2.13	0.48
1:C:58:ALA:O	1:C:62:ALA:CB	2.62	0.48
1:D:400:VAL:HB	1:D:404:PHE:CZ	2.49	0.48
1:F:200:LEU:HB2	1:F:204:GLN:CD	2.34	0.48
1:F:279:ALA:O	1:F:281:GLY:N	2.46	0.48
1:A:382:ILE:CG2	1:A:385:GLY:H	2.25	0.48
1:B:92:HIS:CG	1:B:93:PRO:HD2	2.49	0.48
1:C:118:PHE:O	1:C:121:ARG:HB2	2.14	0.48
1:D:100:VAL:O	1:D:100:VAL:HG23	2.13	0.48
1:E:400:VAL:HB	1:E:404:PHE:CZ	2.49	0.48
1:F:100:VAL:HG23	1:F:100:VAL:O	2.13	0.48
1:F:404:PHE:C	1:F:406:ALA:N	2.64	0.48
1:B:136:SER:CB	1:B:139:THR:HB	2.43	0.48
1:D:396:ASN:ND2	1:D:396:ASN:H	2.12	0.48
1:E:238:TYR:O	1:E:239:ALA:C	2.51	0.48
1:E:242:ALA:HA	1:E:246:ALA:HB3	1.95	0.48
1:E:372:ARG:CD	1:E:407:VAL:HG13	2.43	0.48
1:E:92:HIS:CG	1:E:93:PRO:HD2	2.49	0.48
1:B:223:ILE:HG23	1:B:254:ASN:HD22	1.79	0.47
1:B:393:ASN:HB3	1:B:396:ASN:HD21	1.79	0.47
1:C:393:ASN:HB3	1:C:396:ASN:HD21	1.79	0.47
1:D:345:MET:HB2	1:D:350:PHE:HZ	1.79	0.47
1:D:372:ARG:CD	1:D:407:VAL:HG13	2.43	0.47
1:E:137:ASP:H	1:E:160:TRP:HB3	1.79	0.47
1:F:372:ARG:CD	1:F:407:VAL:HG13	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLN:OE1	1:A:49:GLN:HA	2.14	0.47
1:C:133:VAL:HG12	1:C:134:TRP:N	2.29	0.47
1:C:261:SER:O	1:C:262:LEU:HD23	2.14	0.47
1:D:114:VAL:O	1:D:115:GLY:C	2.52	0.47
1:D:118:PHE:O	1:D:121:ARG:HB2	2.14	0.47
1:E:228:PHE:HD1	1:E:327:ARG:HB2	1.78	0.47
1:F:223:ILE:HG23	1:F:254:ASN:HD22	1.79	0.47
1:A:209:ILE:HG13	1:A:209:ILE:H	1.38	0.47
1:B:400:VAL:O	1:B:403:ALA:N	2.45	0.47
1:E:345:MET:HB2	1:E:350:PHE:HZ	1.79	0.47
1:E:393:ASN:HB3	1:E:396:ASN:HD21	1.79	0.47
1:F:114:VAL:O	1:F:115:GLY:C	2.52	0.47
1:F:256:PHE:HA	1:F:259:ILE:HG22	1.96	0.47
1:A:249:PRO:HB2	1:B:6:PHE:CE1	2.49	0.47
1:A:94:VAL:HG12	1:A:99:ARG:HG3	1.97	0.47
1:B:118:PHE:O	1:B:121:ARG:HB2	2.14	0.47
1:B:355:ASN:O	1:B:357:ARG:N	2.48	0.47
1:C:100:VAL:O	1:C:100:VAL:HG23	2.13	0.47
1:C:146:ILE:H	1:C:146:ILE:HG13	1.34	0.47
1:A:223:ILE:HG23	1:A:254:ASN:HD22	1.79	0.47
1:A:261:SER:O	1:A:262:LEU:HD23	2.14	0.47
1:A:372:ARG:CD	1:A:407:VAL:HG13	2.43	0.47
1:A:58:ALA:O	1:A:62:ALA:CB	2.62	0.47
1:B:47:ILE:HD13	1:B:47:ILE:N	2.30	0.47
1:C:355:ASN:O	1:C:357:ARG:N	2.48	0.47
1:D:223:ILE:HG23	1:D:254:ASN:HD22	1.79	0.47
1:D:261:SER:O	1:D:262:LEU:HD23	2.13	0.47
1:D:49:GLN:HA	1:D:49:GLN:OE1	2.14	0.47
1:F:260:PHE:HB3	1:F:262:LEU:CD2	2.40	0.47
1:A:334:ARG:HH22	1:A:358:GLY:H	1.63	0.47
1:A:396:ASN:H	1:A:396:ASN:ND2	2.12	0.47
1:B:135:VAL:HG23	1:B:156:SER:O	2.15	0.47
1:C:223:ILE:HG23	1:C:254:ASN:HD22	1.79	0.47
1:D:355:ASN:O	1:D:357:ARG:N	2.48	0.47
1:E:256:PHE:HA	1:E:259:ILE:HG22	1.96	0.47
1:E:260:PHE:HB3	1:E:262:LEU:CD2	2.40	0.47
1:E:49:GLN:HA	1:E:49:GLN:OE1	2.14	0.47
1:F:135:VAL:HG23	1:F:156:SER:O	2.15	0.47
1:F:265:GLU:C	1:F:266:ARG:HG2	2.35	0.47
1:F:400:VAL:HB	1:F:404:PHE:CZ	2.49	0.47
1:F:47:ILE:HD13	1:F:47:ILE:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:TYR:HB2	1:A:359:MET:HE1	1.97	0.47
1:A:7:GLN:C	1:A:9:VAL:H	2.18	0.47
1:B:49:GLN:OE1	1:B:49:GLN:HA	2.14	0.47
1:C:135:VAL:HG23	1:C:156:SER:O	2.15	0.47
1:C:94:VAL:HG12	1:C:99:ARG:HG3	1.97	0.47
1:D:94:VAL:HG12	1:D:99:ARG:HG3	1.97	0.47
1:E:114:VAL:O	1:E:115:GLY:C	2.52	0.47
1:E:334:ARG:HH22	1:E:358:GLY:H	1.63	0.47
1:E:7:GLN:C	1:E:9:VAL:H	2.18	0.47
1:F:137:ASP:H	1:F:160:TRP:HB3	1.79	0.47
1:F:92:HIS:CG	1:F:93:PRO:HD2	2.49	0.47
1:A:345:MET:HB2	1:A:350:PHE:HZ	1.79	0.47
1:E:17:ILE:HG12	1:E:141:GLU:OE2	2.15	0.47
1:E:401:ALA:HA	1:E:404:PHE:HE2	1.80	0.47
1:F:17:ILE:HG12	1:F:141:GLU:OE2	2.15	0.47
1:F:209:ILE:H	1:F:209:ILE:HG13	1.38	0.47
1:A:393:ASN:HB3	1:A:396:ASN:HD21	1.79	0.47
1:B:144:VAL:O	1:B:145:ALA:C	2.53	0.47
1:D:401:ALA:HA	1:D:404:PHE:HE2	1.80	0.47
1:E:47:ILE:HD13	1:E:47:ILE:N	2.30	0.47
1:F:94:VAL:HG12	1:F:99:ARG:HG3	1.97	0.47
1:A:47:ILE:HD13	1:A:47:ILE:N	2.30	0.47
1:D:133:VAL:HG12	1:D:134:TRP:N	2.29	0.47
1:D:17:ILE:HG12	1:D:141:GLU:OE2	2.15	0.47
1:D:37:ILE:HG21	1:D:41:TYR:CE2	2.50	0.47
1:D:55:GLU:O	1:D:59:ARG:HD3	2.15	0.47
1:E:144:VAL:O	1:E:145:ALA:C	2.53	0.47
1:E:355:ASN:O	1:E:357:ARG:N	2.48	0.47
1:E:55:GLU:O	1:E:59:ARG:HD3	2.15	0.47
1:A:114:VAL:O	1:A:115:GLY:C	2.52	0.47
1:A:355:ASN:O	1:A:357:ARG:N	2.48	0.47
1:B:209:ILE:H	1:B:209:ILE:HG13	1.37	0.47
1:B:334:ARG:HH22	1:B:358:GLY:H	1.63	0.47
1:B:40:TYR:CG	1:B:41:TYR:N	2.83	0.47
1:D:265:GLU:C	1:D:266:ARG:HG2	2.35	0.47
1:D:47:ILE:HD13	1:D:47:ILE:N	2.30	0.47
1:F:355:ASN:O	1:F:357:ARG:N	2.48	0.47
1:F:401:ALA:HA	1:F:404:PHE:HE2	1.80	0.47
1:B:137:ASP:H	1:B:160:TRP:HB3	1.79	0.46
1:B:17:ILE:HG12	1:B:141:GLU:OE2	2.15	0.46
1:B:401:ALA:HA	1:B:404:PHE:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:VAL:HG12	1:B:99:ARG:HG3	1.97	0.46
1:C:17:ILE:HG12	1:C:141:GLU:OE2	2.15	0.46
1:C:265:GLU:C	1:C:266:ARG:HG2	2.35	0.46
1:C:47:ILE:N	1:C:47:ILE:HD13	2.30	0.46
1:D:105:THR:HG21	1:D:110:GLY:C	2.36	0.46
1:D:310:LEU:HG	1:D:310:LEU:H	1.52	0.46
1:D:334:ARG:HH22	1:D:358:GLY:H	1.63	0.46
1:E:94:VAL:HG12	1:E:99:ARG:HG3	1.97	0.46
1:F:133:VAL:HG12	1:F:134:TRP:N	2.29	0.46
1:F:144:VAL:O	1:F:145:ALA:C	2.53	0.46
1:F:49:GLN:HA	1:F:49:GLN:OE1	2.14	0.46
1:A:37:ILE:HG21	1:A:41:TYR:CE2	2.50	0.46
1:B:40:TYR:HB2	1:B:359:MET:HE1	1.97	0.46
1:C:144:VAL:O	1:C:145:ALA:C	2.54	0.46
1:C:49:GLN:OE1	1:C:49:GLN:HA	2.14	0.46
1:D:89:GLY:N	1:D:241:ARG:NH2	2.55	0.46
1:E:133:VAL:HG12	1:E:134:TRP:N	2.29	0.46
1:F:272:VAL:CG1	1:F:273:MET:H	2.26	0.46
1:A:105:THR:HG21	1:A:110:GLY:C	2.36	0.46
1:B:170:PHE:O	1:B:173:LEU:HD23	2.15	0.46
1:B:265:GLU:C	1:B:266:ARG:HG2	2.35	0.46
1:B:337:LEU:O	1:B:341:LEU:HD12	2.16	0.46
1:B:7:GLN:C	1:B:9:VAL:H	2.18	0.46
1:C:169:ARG:HG2	1:C:172:ASP:CB	2.45	0.46
1:C:334:ARG:HH22	1:C:358:GLY:H	1.63	0.46
1:D:337:LEU:O	1:D:341:LEU:HD12	2.16	0.46
1:E:170:PHE:O	1:E:173:LEU:HD23	2.15	0.46
1:E:396:ASN:ND2	1:E:396:ASN:H	2.12	0.46
1:E:40:TYR:CG	1:E:41:TYR:N	2.83	0.46
1:F:170:PHE:O	1:F:173:LEU:HD23	2.15	0.46
1:C:259:ILE:HG12	1:C:259:ILE:O	2.16	0.46
1:C:55:GLU:O	1:C:59:ARG:HD3	2.15	0.46
1:D:137:ASP:H	1:D:160:TRP:HB3	1.79	0.46
1:F:345:MET:HB2	1:F:350:PHE:HZ	1.79	0.46
1:A:133:VAL:HG12	1:A:134:TRP:N	2.29	0.46
1:A:135:VAL:HG23	1:A:156:SER:O	2.15	0.46
1:A:235:GLU:OE1	1:A:235:GLU:HA	2.16	0.46
1:B:310:LEU:H	1:B:310:LEU:HG	1.53	0.46
1:B:55:GLU:O	1:B:59:ARG:HD3	2.15	0.46
1:C:325:GLU:CA	1:C:328:THR:HB	2.45	0.46
1:C:337:LEU:O	1:C:341:LEU:HD12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:ILE:O	1:D:212:LEU:N	2.45	0.46
1:F:334:ARG:HH22	1:F:358:GLY:H	1.63	0.46
1:A:144:VAL:O	1:A:145:ALA:C	2.54	0.46
1:A:259:ILE:HG12	1:A:259:ILE:O	2.16	0.46
1:B:259:ILE:HG12	1:B:259:ILE:O	2.16	0.46
1:C:40:TYR:CG	1:C:41:TYR:N	2.83	0.46
1:D:135:VAL:HG23	1:D:156:SER:O	2.15	0.46
1:D:40:TYR:CG	1:D:41:TYR:N	2.83	0.46
1:D:7:GLN:C	1:D:9:VAL:H	2.18	0.46
1:E:105:THR:HG21	1:E:110:GLY:C	2.36	0.46
1:E:265:GLU:C	1:E:266:ARG:HG2	2.35	0.46
1:F:104:GLN:OE1	1:F:303:ALA:HB2	2.16	0.46
1:F:233:MET:C	1:F:235:GLU:H	2.19	0.46
1:F:238:TYR:C	1:F:238:TYR:CD1	2.89	0.46
1:F:37:ILE:HG21	1:F:41:TYR:CE2	2.50	0.46
1:F:55:GLU:O	1:F:59:ARG:HD3	2.15	0.46
1:A:337:LEU:O	1:A:341:LEU:HD12	2.16	0.46
1:A:40:TYR:CG	1:A:41:TYR:N	2.83	0.46
1:A:55:GLU:O	1:A:59:ARG:HD3	2.15	0.46
1:B:105:THR:HG21	1:B:110:GLY:C	2.36	0.46
1:B:105:THR:HG21	1:B:110:GLY:O	2.16	0.46
1:B:169:ARG:HG2	1:B:172:ASP:CB	2.45	0.46
1:B:235:GLU:HA	1:B:235:GLU:OE1	2.16	0.46
1:B:345:MET:HB2	1:B:350:PHE:HZ	1.80	0.46
1:C:209:ILE:O	1:C:212:LEU:N	2.45	0.46
1:C:7:GLN:C	1:C:9:VAL:H	2.18	0.46
1:D:169:ARG:HG2	1:D:172:ASP:CB	2.45	0.46
1:D:259:ILE:O	1:D:259:ILE:HG12	2.16	0.46
1:E:89:GLY:N	1:E:241:ARG:NH2	2.55	0.46
1:F:147:PHE:C	1:F:149:GLY:N	2.69	0.46
1:F:72:PRO:HG2	1:F:75:GLY:H	1.81	0.46
1:A:108:GLY:O	1:A:111:ALA:HB3	2.16	0.46
1:A:169:ARG:HG2	1:A:172:ASP:CB	2.45	0.46
1:A:223:ILE:O	1:A:223:ILE:HG23	2.16	0.46
1:C:105:THR:HG21	1:C:110:GLY:C	2.36	0.46
1:C:137:ASP:H	1:C:160:TRP:HB3	1.79	0.46
1:C:238:TYR:C	1:C:238:TYR:CD1	2.89	0.46
1:C:89:GLY:N	1:C:241:ARG:NH2	2.55	0.46
1:E:259:ILE:HG12	1:E:259:ILE:O	2.16	0.46
1:E:76:LEU:CD2	1:E:79:TYR:HB2	2.46	0.46
1:F:235:GLU:OE1	1:F:235:GLU:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:337:LEU:O	1:F:341:LEU:HD12	2.16	0.46
1:F:400:VAL:O	1:F:403:ALA:N	2.45	0.46
1:F:40:TYR:CG	1:F:41:TYR:N	2.83	0.46
1:F:7:GLN:C	1:F:9:VAL:H	2.18	0.46
1:A:105:THR:HG21	1:A:110:GLY:O	2.16	0.46
1:A:137:ASP:H	1:A:160:TRP:HB3	1.79	0.46
1:A:233:MET:C	1:A:235:GLU:H	2.19	0.46
1:A:242:ALA:O	1:A:246:ALA:HB3	2.16	0.46
1:A:245:SER:C	1:A:247:GLY:N	2.69	0.46
1:A:401:ALA:HA	1:A:404:PHE:HE2	1.80	0.46
1:A:72:PRO:HG2	1:A:75:GLY:H	1.81	0.46
1:B:104:GLN:OE1	1:B:303:ALA:HB2	2.16	0.46
1:B:223:ILE:HG23	1:B:223:ILE:O	2.16	0.46
1:B:238:TYR:C	1:B:238:TYR:CD1	2.89	0.46
1:B:272:VAL:CG1	1:B:273:MET:H	2.26	0.46
1:C:108:GLY:O	1:C:111:ALA:HB3	2.16	0.46
1:C:170:PHE:O	1:C:173:LEU:HD23	2.15	0.46
1:C:263:TYR:N	1:C:263:TYR:CD1	2.70	0.46
1:D:170:PHE:O	1:D:173:LEU:HD23	2.15	0.46
1:E:135:VAL:HG23	1:E:156:SER:O	2.15	0.46
1:F:105:THR:HG21	1:F:110:GLY:O	2.16	0.46
1:F:223:ILE:HG23	1:F:223:ILE:O	2.16	0.46
1:A:325:GLU:CA	1:A:328:THR:HB	2.45	0.46
1:B:108:GLY:O	1:B:111:ALA:HB3	2.16	0.46
1:D:233:MET:C	1:D:235:GLU:H	2.19	0.46
1:E:140:TRP:CZ3	1:E:142:ASN:HB2	2.51	0.46
1:E:147:PHE:C	1:E:149:GLY:N	2.69	0.46
1:A:104:GLN:OE1	1:A:303:ALA:HB2	2.16	0.45
1:A:170:PHE:O	1:A:173:LEU:HD23	2.15	0.45
1:A:265:GLU:C	1:A:266:ARG:HG2	2.35	0.45
1:A:47:ILE:HG13	1:B:69:LEU:CD2	2.45	0.45
1:A:79:TYR:CD2	1:A:83:ILE:HD11	2.52	0.45
1:B:233:MET:C	1:B:235:GLU:H	2.19	0.45
1:C:401:ALA:HA	1:C:404:PHE:HE2	1.80	0.45
1:D:144:VAL:O	1:D:145:ALA:C	2.53	0.45
1:D:235:GLU:HA	1:D:235:GLU:OE1	2.16	0.45
1:D:79:TYR:CD2	1:D:83:ILE:HD11	2.52	0.45
1:E:298:PRO:HB3	1:E:299:PRO:HD2	1.98	0.45
1:F:108:GLY:O	1:F:111:ALA:HB3	2.16	0.45
1:F:140:TRP:CZ3	1:F:142:ASN:HB2	2.51	0.45
1:F:252:VAL:HG13	1:F:253:SER:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ILE:HG12	1:A:141:GLU:OE2	2.15	0.45
1:B:209:ILE:O	1:B:212:LEU:N	2.45	0.45
1:B:37:ILE:HG21	1:B:41:TYR:CE2	2.50	0.45
1:C:104:GLN:OE1	1:C:303:ALA:HB2	2.16	0.45
1:C:76:LEU:CD2	1:C:79:TYR:HB2	2.46	0.45
1:C:79:TYR:CD2	1:C:83:ILE:HD11	2.51	0.45
1:E:173:LEU:O	1:E:176:THR:N	2.49	0.45
1:E:245:SER:C	1:E:247:GLY:N	2.69	0.45
1:E:272:VAL:CG1	1:E:273:MET:H	2.26	0.45
1:E:337:LEU:O	1:E:341:LEU:HD12	2.16	0.45
1:E:72:PRO:HG2	1:E:75:GLY:H	1.81	0.45
1:F:105:THR:HG21	1:F:110:GLY:C	2.36	0.45
1:F:58:ALA:O	1:F:62:ALA:CB	2.62	0.45
1:A:298:PRO:HB3	1:A:299:PRO:HD2	1.98	0.45
1:A:266:ARG:HH12	2:A:500:PLP:P	2.40	0.45
1:C:235:GLU:OE1	1:C:235:GLU:HA	2.16	0.45
1:C:242:ALA:O	1:C:246:ALA:HB3	2.16	0.45
1:C:278:GLU:OE1	1:C:279:ALA:N	2.50	0.45
1:C:345:MET:HB2	1:C:350:PHE:HZ	1.79	0.45
1:D:108:GLY:O	1:D:111:ALA:HB3	2.16	0.45
1:E:105:THR:HG21	1:E:110:GLY:O	2.16	0.45
1:E:223:ILE:O	1:E:223:ILE:HG23	2.16	0.45
1:E:224:ALA:HB3	1:E:225:TYR:CE2	2.52	0.45
1:E:235:GLU:OE1	1:E:235:GLU:HA	2.16	0.45
1:E:242:ALA:O	1:E:246:ALA:HB3	2.16	0.45
1:E:252:VAL:HG13	1:E:253:SER:N	2.31	0.45
1:E:278:GLU:OE1	1:E:279:ALA:N	2.50	0.45
1:E:79:TYR:CD2	1:E:83:ILE:HD11	2.52	0.45
1:E:6:PHE:CE1	1:F:249:PRO:CB	2.98	0.45
1:A:173:LEU:O	1:A:176:THR:N	2.49	0.45
1:A:286:GLN:OE1	1:B:12:TYR:HD1	1.99	0.45
1:B:242:ALA:O	1:B:246:ALA:HB3	2.16	0.45
1:B:72:PRO:HG2	1:B:75:GLY:H	1.81	0.45
1:C:105:THR:HG21	1:C:110:GLY:O	2.16	0.45
1:C:140:TRP:CZ3	1:C:142:ASN:HB2	2.51	0.45
1:C:234:GLU:H	1:C:234:GLU:HG2	1.63	0.45
1:C:266:ARG:HH12	2:C:500:PLP:P	2.40	0.45
1:C:272:VAL:CG1	1:C:273:MET:N	2.80	0.45
1:D:104:GLN:OE1	1:D:303:ALA:HB2	2.16	0.45
1:D:238:TYR:CD1	1:D:238:TYR:C	2.89	0.45
1:D:325:GLU:CA	1:D:328:THR:HB	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:GLY:O	1:E:111:ALA:HB3	2.16	0.45
1:E:325:GLU:CA	1:E:328:THR:HB	2.45	0.45
1:E:29:ARG:HB2	1:E:32:LYS:HD3	1.99	0.45
1:F:89:GLY:N	1:F:241:ARG:NH2	2.55	0.45
1:F:76:LEU:CD2	1:F:79:TYR:HB2	2.46	0.45
1:A:147:PHE:C	1:A:149:GLY:N	2.69	0.45
1:A:194:ASN:ND2	1:A:360:PHE:CE2	2.85	0.45
1:C:173:LEU:O	1:C:176:THR:N	2.49	0.45
1:C:72:PRO:HG2	1:C:75:GLY:H	1.81	0.45
1:D:278:GLU:OE1	1:D:279:ALA:N	2.50	0.45
1:D:287:LEU:C	1:D:289:ALA:N	2.70	0.45
1:D:72:PRO:HG2	1:D:75:GLY:H	1.81	0.45
1:E:169:ARG:HG2	1:E:172:ASP:CB	2.45	0.45
1:E:104:GLN:OE1	1:E:303:ALA:HB2	2.16	0.45
1:E:338:VAL:HG21	1:E:354:LEU:CG	2.45	0.45
1:F:79:TYR:CD2	1:F:83:ILE:HD11	2.52	0.45
1:A:140:TRP:CZ3	1:A:142:ASN:HB2	2.51	0.45
1:A:238:TYR:CD1	1:A:238:TYR:C	2.89	0.45
1:A:71:LEU:HB2	1:A:297:SER:HB2	1.99	0.45
1:B:301:PHE:O	1:B:303:ALA:N	2.50	0.45
1:B:325:GLU:CA	1:B:328:THR:HB	2.45	0.45
1:B:396:ASN:O	1:B:398:GLN:N	2.50	0.45
1:A:249:PRO:CB	1:B:6:PHE:CE1	3.00	0.45
1:B:79:TYR:CD2	1:B:83:ILE:HD11	2.52	0.45
1:D:140:TRP:CZ3	1:D:142:ASN:HB2	2.51	0.45
1:D:298:PRO:HB3	1:D:299:PRO:HD2	1.98	0.45
1:D:76:LEU:CD2	1:D:79:TYR:HB2	2.46	0.45
1:E:238:TYR:CD1	1:E:238:TYR:C	2.89	0.45
1:E:266:ARG:HH12	2:E:500:PLP:P	2.40	0.45
1:E:65:HIS:HB3	1:E:66:GLY:H	1.58	0.45
1:F:242:ALA:O	1:F:246:ALA:HB3	2.16	0.45
1:A:224:ALA:HB3	1:A:225:TYR:CE2	2.52	0.45
1:A:278:GLU:OE1	1:A:279:ALA:N	2.50	0.45
1:A:382:ILE:CD1	1:A:386:ARG:HD3	2.36	0.45
1:B:76:LEU:CD2	1:B:79:TYR:HB2	2.46	0.45
1:C:223:ILE:O	1:C:223:ILE:HG23	2.16	0.45
1:C:301:PHE:O	1:C:303:ALA:N	2.50	0.45
1:C:37:ILE:HG21	1:C:41:TYR:CE2	2.50	0.45
1:D:252:VAL:HG13	1:D:253:SER:N	2.31	0.45
1:D:43:GLU:C	1:D:45:GLY:N	2.70	0.45
1:D:266:ARG:HH12	2:D:500:PLP:P	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:LEU:HB2	1:E:297:SER:HB2	1.99	0.45
1:E:393:ASN:C	1:E:395:ALA:H	2.20	0.45
1:F:278:GLU:OE1	1:F:279:ALA:N	2.50	0.45
1:A:287:LEU:C	1:A:289:ALA:N	2.70	0.45
1:A:29:ARG:HB2	1:A:32:LYS:HD3	1.99	0.45
1:A:396:ASN:O	1:A:398:GLN:N	2.50	0.45
1:B:114:VAL:O	1:B:115:GLY:C	2.52	0.45
1:B:173:LEU:O	1:B:176:THR:N	2.49	0.45
1:B:382:ILE:CD1	1:B:386:ARG:HD3	2.36	0.45
1:B:43:GLU:C	1:B:45:GLY:N	2.70	0.45
1:B:47:ILE:HD13	1:B:47:ILE:H	1.82	0.45
1:C:224:ALA:HB3	1:C:225:TYR:CE2	2.52	0.45
1:C:74:GLU:HB2	1:C:288:LYS:CE	2.37	0.45
1:D:173:LEU:O	1:D:176:THR:N	2.49	0.45
1:F:259:ILE:HG12	1:F:259:ILE:O	2.16	0.45
1:A:400:VAL:HG12	1:A:404:PHE:CE1	2.52	0.45
1:B:140:TRP:CZ3	1:B:142:ASN:HB2	2.51	0.45
1:B:194:ASN:ND2	1:B:360:PHE:CE2	2.85	0.45
1:A:249:PRO:CB	1:B:6:PHE:HE1	2.30	0.45
1:C:252:VAL:HG13	1:C:253:SER:N	2.31	0.45
1:D:382:ILE:CD1	1:D:386:ARG:HD3	2.36	0.45
1:D:404:PHE:C	1:D:406:ALA:H	2.21	0.45
1:E:233:MET:C	1:E:235:GLU:H	2.19	0.45
1:E:254:ASN:ND2	1:E:255:SER:N	2.64	0.45
1:E:301:PHE:O	1:E:303:ALA:N	2.50	0.45
1:E:71:LEU:CD2	1:E:72:PRO:HD2	2.47	0.45
1:F:396:ASN:O	1:F:398:GLN:N	2.50	0.45
1:A:17:ILE:HG13	1:A:17:ILE:H	1.66	0.45
1:A:312:ASP:HB3	1:A:315:LEU:HG	1.99	0.45
1:A:393:ASN:O	1:A:395:ALA:N	2.50	0.45
1:B:287:LEU:C	1:B:289:ALA:N	2.70	0.45
1:B:225:TYR:OH	1:B:360:PHE:HE2	2.01	0.45
1:D:242:ALA:O	1:D:246:ALA:HB3	2.16	0.45
1:D:396:ASN:O	1:D:398:GLN:N	2.50	0.45
1:E:209:ILE:HG13	1:E:209:ILE:H	1.38	0.45
1:E:295:TYR:O	1:E:296:SER:CB	2.65	0.45
1:E:297:SER:HA	1:E:298:PRO:HD3	1.87	0.45
1:E:396:ASN:O	1:E:398:GLN:N	2.50	0.45
1:E:400:VAL:O	1:E:403:ALA:N	2.45	0.45
1:F:245:SER:C	1:F:247:GLY:N	2.69	0.45
1:F:266:ARG:HH12	2:F:500:PLP:P	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:VAL:HG21	1:A:354:LEU:CG	2.45	0.44
1:A:400:VAL:O	1:A:403:ALA:N	2.45	0.44
1:A:404:PHE:C	1:A:406:ALA:H	2.21	0.44
1:A:76:LEU:CD2	1:A:79:TYR:HB2	2.46	0.44
1:B:404:PHE:C	1:B:406:ALA:H	2.21	0.44
1:C:287:LEU:C	1:C:289:ALA:N	2.70	0.44
1:C:51:GLN:O	1:C:54:ALA:HB3	2.17	0.44
1:C:7:GLN:O	1:D:282:ARG:NH2	2.43	0.44
1:D:400:VAL:HG12	1:D:404:PHE:CE1	2.52	0.44
1:D:71:LEU:CD2	1:D:72:PRO:HD2	2.47	0.44
1:E:329:ARG:NH2	1:E:333:MET:HE3	2.31	0.44
1:E:225:TYR:OH	1:E:360:PHE:HE2	2.00	0.44
1:E:393:ASN:O	1:E:395:ALA:N	2.50	0.44
1:F:338:VAL:HG21	1:F:354:LEU:CG	2.45	0.44
1:F:400:VAL:HG12	1:F:404:PHE:CE1	2.52	0.44
1:A:260:PHE:HB3	1:A:262:LEU:CD2	2.40	0.44
1:A:301:PHE:O	1:A:303:ALA:N	2.50	0.44
1:A:51:GLN:O	1:A:54:ALA:HB3	2.17	0.44
1:B:17:ILE:H	1:B:17:ILE:HG13	1.66	0.44
1:B:224:ALA:HB3	1:B:225:TYR:CE2	2.52	0.44
1:B:266:ARG:HH12	2:B:500:PLP:P	2.40	0.44
1:B:71:LEU:CD2	1:B:72:PRO:HD2	2.47	0.44
1:C:400:VAL:HG12	1:C:404:PHE:CE1	2.52	0.44
1:C:47:ILE:HD13	1:C:47:ILE:H	1.82	0.44
1:D:105:THR:HG21	1:D:110:GLY:O	2.16	0.44
1:D:223:ILE:HG23	1:D:223:ILE:O	2.16	0.44
1:D:71:LEU:HB2	1:D:297:SER:HB2	1.99	0.44
1:D:51:GLN:O	1:D:54:ALA:HB3	2.17	0.44
1:D:65:HIS:HB3	1:D:66:GLY:H	1.58	0.44
1:E:47:ILE:H	1:E:47:ILE:HD13	1.82	0.44
1:F:224:ALA:HB3	1:F:225:TYR:CE2	2.52	0.44
1:F:287:LEU:C	1:F:289:ALA:N	2.70	0.44
1:F:312:ASP:HB3	1:F:315:LEU:HG	1.99	0.44
1:F:29:ARG:HB2	1:F:32:LYS:HD3	1.99	0.44
1:F:393:ASN:C	1:F:395:ALA:H	2.20	0.44
1:A:272:VAL:CG1	1:A:273:MET:N	2.80	0.44
1:B:147:PHE:C	1:B:149:GLY:N	2.69	0.44
1:B:252:VAL:HG13	1:B:253:SER:N	2.31	0.44
1:B:338:VAL:HG21	1:B:354:LEU:CG	2.45	0.44
1:B:393:ASN:O	1:B:395:ALA:N	2.50	0.44
1:C:245:SER:C	1:C:247:GLY:N	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:ASP:HB3	1:C:315:LEU:HG	2.00	0.44
1:E:116:ALA:C	1:E:118:PHE:N	2.71	0.44
1:E:51:GLN:O	1:E:54:ALA:HB3	2.17	0.44
1:F:40:TYR:HB2	1:F:359:MET:HE1	1.99	0.44
1:F:404:PHE:C	1:F:406:ALA:H	2.21	0.44
1:F:43:GLU:C	1:F:45:GLY:N	2.70	0.44
1:A:192:CYS:N	1:A:199:ASP:OD1	2.51	0.44
1:A:295:TYR:O	1:A:296:SER:CB	2.65	0.44
1:A:393:ASN:C	1:A:395:ALA:H	2.20	0.44
1:A:43:GLU:C	1:A:45:GLY:N	2.70	0.44
1:B:278:GLU:OE1	1:B:279:ALA:N	2.50	0.44
1:B:51:GLN:O	1:B:54:ALA:HB3	2.17	0.44
1:C:147:PHE:C	1:C:149:GLY:N	2.69	0.44
1:C:404:PHE:C	1:C:406:ALA:H	2.21	0.44
1:D:194:ASN:ND2	1:D:360:PHE:CE2	2.85	0.44
1:D:224:ALA:HB3	1:D:225:TYR:CE2	2.52	0.44
1:D:393:ASN:O	1:D:395:ALA:N	2.50	0.44
1:E:37:ILE:HG21	1:E:41:TYR:CE2	2.50	0.44
1:E:400:VAL:HG12	1:E:404:PHE:CE1	2.52	0.44
1:F:325:GLU:CA	1:F:328:THR:HB	2.45	0.44
1:F:194:ASN:ND2	1:F:360:PHE:CE2	2.85	0.44
1:B:89:GLY:N	1:B:241:ARG:NH2	2.55	0.44
1:B:295:TYR:O	1:B:296:SER:CB	2.65	0.44
1:B:29:ARG:HB2	1:B:32:LYS:HD3	1.99	0.44
1:C:233:MET:C	1:C:235:GLU:H	2.19	0.44
1:C:393:ASN:O	1:C:395:ALA:N	2.50	0.44
1:C:40:TYR:HB2	1:C:359:MET:HE1	2.00	0.44
1:D:245:SER:C	1:D:247:GLY:N	2.69	0.44
1:D:251:LEU:HD13	1:D:272:VAL:HG22	2.00	0.44
1:D:301:PHE:O	1:D:303:ALA:N	2.50	0.44
1:D:312:ASP:HB3	1:D:315:LEU:HG	1.99	0.44
1:D:29:ARG:HB2	1:D:32:LYS:HD3	1.99	0.44
1:D:38:GLY:C	1:D:39:LEU:HD23	2.38	0.44
1:F:297:SER:HA	1:F:298:PRO:HD3	1.87	0.44
1:A:252:VAL:HG13	1:A:253:SER:N	2.31	0.44
1:A:347:GLU:HB3	1:E:402:LYS:CE	2.47	0.44
1:B:251:LEU:HD13	1:B:272:VAL:HG22	2.00	0.44
1:B:312:ASP:HB3	1:B:315:LEU:HG	1.99	0.44
1:B:400:VAL:HG12	1:B:404:PHE:CE1	2.52	0.44
1:C:194:ASN:ND2	1:C:360:PHE:CE2	2.85	0.44
1:D:192:CYS:N	1:D:199:ASP:OD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:ILE:H	1:D:47:ILE:HD13	1.82	0.44
1:E:194:ASN:ND2	1:E:360:PHE:CE2	2.85	0.44
1:F:173:LEU:O	1:F:176:THR:N	2.49	0.44
1:F:377:PHE:N	1:F:377:PHE:CD1	2.86	0.44
1:A:228:PHE:HA	1:A:327:ARG:HB2	2.00	0.44
1:A:38:GLY:C	1:A:39:LEU:HD23	2.38	0.44
1:B:116:ALA:C	1:B:118:PHE:N	2.71	0.44
1:B:71:LEU:HB2	1:B:297:SER:HB2	1.99	0.44
1:B:393:ASN:C	1:B:395:ALA:H	2.20	0.44
1:D:272:VAL:CG1	1:D:273:MET:H	2.26	0.44
1:D:377:PHE:N	1:D:377:PHE:CD1	2.86	0.44
1:E:228:PHE:HA	1:E:327:ARG:HB2	2.00	0.44
1:E:393:ASN:C	1:E:395:ALA:N	2.71	0.44
1:E:43:GLU:O	1:E:45:GLY:N	2.51	0.44
1:E:82:ALA:C	1:E:85:PRO:HG2	2.38	0.44
1:F:256:PHE:HA	1:F:259:ILE:CG2	2.48	0.44
1:E:11:ALA:HB2	1:F:282:ARG:HB3	1.99	0.44
1:A:225:TYR:OH	1:A:360:PHE:HE2	2.00	0.44
1:A:82:ALA:C	1:A:85:PRO:HG2	2.38	0.44
1:B:298:PRO:HB3	1:B:299:PRO:HD2	1.98	0.44
1:B:82:ALA:C	1:B:85:PRO:HG2	2.38	0.44
1:C:396:ASN:O	1:C:398:GLN:N	2.50	0.44
1:C:43:GLU:C	1:C:45:GLY:N	2.70	0.44
1:C:71:LEU:HB2	1:C:297:SER:HB2	1.99	0.44
1:D:147:PHE:C	1:D:149:GLY:N	2.69	0.44
1:E:251:LEU:HD13	1:E:272:VAL:HG22	2.00	0.44
1:E:287:LEU:C	1:E:289:ALA:N	2.70	0.44
1:F:38:GLY:C	1:F:39:LEU:HD23	2.38	0.44
1:F:71:LEU:HB2	1:F:297:SER:HB2	1.99	0.44
1:A:47:ILE:HD13	1:A:47:ILE:H	1.82	0.44
1:B:147:PHE:C	1:B:149:GLY:H	2.22	0.44
1:B:263:TYR:N	1:B:263:TYR:CD1	2.70	0.44
1:C:298:PRO:HB3	1:C:299:PRO:HD2	1.99	0.44
1:C:38:GLY:C	1:C:39:LEU:HD23	2.38	0.44
1:C:400:VAL:O	1:C:403:ALA:N	2.45	0.44
1:D:71:LEU:HD11	1:D:300:ASN:HA	2.00	0.44
1:E:58:ALA:O	1:E:62:ALA:CB	2.62	0.44
1:F:116:ALA:C	1:F:118:PHE:N	2.71	0.44
1:F:192:CYS:N	1:F:199:ASP:OD1	2.51	0.44
1:F:251:LEU:HD13	1:F:272:VAL:HG22	2.00	0.44
1:F:393:ASN:O	1:F:395:ALA:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:GLU:O	1:F:45:GLY:N	2.51	0.44
1:F:47:ILE:HD13	1:F:47:ILE:H	1.82	0.44
1:F:74:GLU:HB2	1:F:288:LYS:CE	2.37	0.44
1:A:116:ALA:C	1:A:118:PHE:N	2.71	0.43
1:A:89:GLY:N	1:A:241:ARG:NH2	2.55	0.43
1:B:245:SER:C	1:B:247:GLY:N	2.69	0.43
1:C:116:ALA:C	1:C:118:PHE:N	2.71	0.43
1:C:29:ARG:HB2	1:C:32:LYS:HD3	1.99	0.43
1:C:71:LEU:HD11	1:C:300:ASN:HA	2.00	0.43
1:C:84:ALA:N	1:C:85:PRO:CD	2.81	0.43
1:D:82:ALA:C	1:D:85:PRO:HG2	2.38	0.43
1:F:301:PHE:O	1:F:303:ALA:N	2.50	0.43
1:F:51:GLN:O	1:F:54:ALA:HB3	2.17	0.43
1:F:88:PHE:CE1	1:F:244:ALA:HB2	2.53	0.43
1:A:393:ASN:C	1:A:395:ALA:N	2.71	0.43
1:A:84:ALA:N	1:A:85:PRO:CD	2.81	0.43
1:B:71:LEU:HD11	1:B:300:ASN:HA	2.00	0.43
1:B:38:GLY:C	1:B:39:LEU:HD23	2.38	0.43
1:B:84:ALA:N	1:B:85:PRO:CD	2.81	0.43
1:C:256:PHE:HA	1:C:259:ILE:CG2	2.48	0.43
1:D:393:ASN:C	1:D:395:ALA:H	2.20	0.43
1:E:256:PHE:HA	1:E:259:ILE:CG2	2.48	0.43
1:F:193:HIS:HB3	1:F:197:GLY:CA	2.49	0.43
1:F:82:ALA:C	1:F:85:PRO:HG2	2.38	0.43
1:A:147:PHE:C	1:A:149:GLY:H	2.22	0.43
1:B:107:GLY:H	1:B:267:VAL:C	2.22	0.43
1:B:192:CYS:N	1:B:199:ASP:OD1	2.51	0.43
1:C:377:PHE:N	1:C:377:PHE:CD1	2.86	0.43
1:C:82:ALA:C	1:C:85:PRO:HG2	2.38	0.43
1:D:256:PHE:HA	1:D:259:ILE:CG2	2.48	0.43
1:D:295:TYR:O	1:D:296:SER:CB	2.65	0.43
1:D:225:TYR:OH	1:D:360:PHE:HE2	2.00	0.43
1:F:107:GLY:H	1:F:267:VAL:C	2.22	0.43
1:F:225:TYR:OH	1:F:360:PHE:HE2	2.01	0.43
1:F:84:ALA:N	1:F:85:PRO:CD	2.81	0.43
1:F:87:LEU:O	1:F:241:ARG:NE	2.52	0.43
1:A:71:LEU:HD11	1:A:300:ASN:HA	2.00	0.43
1:A:71:LEU:CD2	1:A:72:PRO:HD2	2.47	0.43
1:B:165:THR:C	1:B:167:GLY:N	2.72	0.43
1:B:377:PHE:N	1:B:377:PHE:CD1	2.86	0.43
1:C:147:PHE:C	1:C:149:GLY:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ILE:HG13	1:C:209:ILE:H	1.38	0.43
1:E:147:PHE:C	1:E:149:GLY:H	2.22	0.43
1:E:87:LEU:O	1:E:241:ARG:NE	2.52	0.43
1:E:38:GLY:C	1:E:39:LEU:HD23	2.38	0.43
1:F:298:PRO:HB3	1:F:299:PRO:HD2	1.98	0.43
1:F:393:ASN:C	1:F:395:ALA:N	2.71	0.43
1:F:67:ALA:O	1:F:69:LEU:N	2.52	0.43
1:A:256:PHE:HA	1:A:259:ILE:CG2	2.48	0.43
1:A:303:ALA:O	1:A:304:GLN:C	2.57	0.43
1:A:325:GLU:HA	1:A:328:THR:CB	2.48	0.43
1:B:193:HIS:HB3	1:B:197:GLY:CA	2.49	0.43
1:B:43:GLU:O	1:B:45:GLY:N	2.51	0.43
1:C:295:TYR:O	1:C:296:SER:CB	2.65	0.43
1:C:393:ASN:C	1:C:395:ALA:N	2.71	0.43
1:D:116:ALA:C	1:D:118:PHE:N	2.71	0.43
1:D:193:HIS:HB3	1:D:197:GLY:CA	2.49	0.43
1:D:228:PHE:HA	1:D:327:ARG:HB2	2.00	0.43
1:D:334:ARG:HH22	1:D:358:GLY:N	2.17	0.43
1:E:192:CYS:N	1:E:199:ASP:OD1	2.51	0.43
1:E:377:PHE:N	1:E:377:PHE:CD1	2.86	0.43
1:F:71:LEU:HD11	1:F:300:ASN:HA	2.00	0.43
1:B:174:LEU:O	1:B:178:LYS:HG3	2.19	0.43
1:B:58:ALA:O	1:B:62:ALA:CB	2.62	0.43
1:C:43:GLU:O	1:C:45:GLY:N	2.51	0.43
1:D:17:ILE:H	1:D:17:ILE:HG13	1.66	0.43
1:D:256:PHE:O	1:D:257:SER:C	2.57	0.43
1:D:303:ALA:O	1:D:304:GLN:C	2.57	0.43
1:D:341:LEU:C	1:D:343:THR:H	2.22	0.43
1:E:107:GLY:H	1:E:267:VAL:C	2.22	0.43
1:E:165:THR:C	1:E:167:GLY:N	2.72	0.43
1:E:170:PHE:HB3	1:E:171:ASN:H	1.67	0.43
1:E:278:GLU:OE1	1:E:282:ARG:NH1	2.52	0.43
1:E:312:ASP:HB3	1:E:315:LEU:HG	2.00	0.43
1:F:118:PHE:CD1	1:F:118:PHE:C	2.92	0.43
1:A:165:THR:C	1:A:167:GLY:N	2.72	0.43
1:C:260:PHE:HB3	1:C:262:LEU:CD2	2.41	0.43
1:C:334:ARG:HH22	1:C:358:GLY:N	2.17	0.43
1:C:393:ASN:C	1:C:395:ALA:H	2.20	0.43
1:D:107:GLY:H	1:D:267:VAL:C	2.22	0.43
1:D:209:ILE:O	1:D:210:GLU:C	2.57	0.43
1:D:278:GLU:OE1	1:D:282:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:LEU:O	1:E:178:LYS:HG3	2.19	0.43
1:F:107:GLY:H	1:F:267:VAL:CA	2.32	0.43
1:F:295:TYR:O	1:F:296:SER:CB	2.65	0.43
1:F:334:ARG:HH22	1:F:358:GLY:N	2.17	0.43
1:A:174:LEU:O	1:A:178:LYS:HG3	2.19	0.43
1:A:209:ILE:O	1:A:210:GLU:C	2.57	0.43
1:A:251:LEU:HD13	1:A:272:VAL:HG22	2.00	0.43
1:A:341:LEU:C	1:A:343:THR:H	2.22	0.43
1:A:377:PHE:CD1	1:A:377:PHE:N	2.86	0.43
1:A:87:LEU:O	1:A:241:ARG:NE	2.52	0.43
1:B:107:GLY:H	1:B:267:VAL:CA	2.32	0.43
1:B:118:PHE:C	1:B:118:PHE:CD1	2.92	0.43
1:B:256:PHE:HA	1:B:259:ILE:CG2	2.48	0.43
1:B:278:GLU:OE1	1:B:282:ARG:NH1	2.52	0.43
1:A:12:TYR:HD1	1:B:286:GLN:OE1	2.02	0.43
1:B:334:ARG:HH22	1:B:358:GLY:N	2.17	0.43
1:B:393:ASN:C	1:B:395:ALA:N	2.71	0.43
1:B:88:PHE:CE1	1:B:244:ALA:CB	3.02	0.43
1:C:192:CYS:N	1:C:199:ASP:OD1	2.51	0.43
1:C:193:HIS:HB3	1:C:197:GLY:CA	2.49	0.43
1:C:256:PHE:O	1:C:257:SER:C	2.57	0.43
1:C:107:GLY:H	1:C:267:VAL:CA	2.32	0.43
1:C:65:HIS:HB3	1:C:66:GLY:H	1.58	0.43
1:E:234:GLU:H	1:E:234:GLU:HG2	1.63	0.43
1:E:71:LEU:HD11	1:E:300:ASN:HA	2.00	0.43
1:E:325:GLU:HA	1:E:328:THR:CB	2.48	0.43
1:E:99:ARG:O	1:E:280:ALA:HB2	2.19	0.43
1:F:147:PHE:C	1:F:149:GLY:H	2.22	0.43
1:F:88:PHE:CE1	1:F:244:ALA:CB	3.02	0.43
1:F:228:PHE:HA	1:F:327:ARG:HB2	2.00	0.43
1:A:278:GLU:OE1	1:A:282:ARG:NH1	2.52	0.43
1:B:303:ALA:O	1:B:304:GLN:C	2.57	0.43
1:B:228:PHE:HA	1:B:327:ARG:HB2	2.00	0.43
1:C:174:LEU:O	1:C:178:LYS:HG3	2.19	0.43
1:D:147:PHE:C	1:D:149:GLY:H	2.22	0.43
1:D:220:PHE:CD1	1:D:220:PHE:C	2.92	0.43
1:D:393:ASN:C	1:D:395:ALA:N	2.71	0.43
1:E:347:GLU:HG3	1:E:347:GLU:H	1.62	0.43
1:F:165:THR:C	1:F:167:GLY:N	2.72	0.43
1:F:278:GLU:OE1	1:F:282:ARG:NH1	2.52	0.43
1:A:43:GLU:O	1:A:45:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:GLU:C	1:B:217:LEU:HG	2.40	0.43
1:C:15:ASP:OD1	1:C:17:ILE:HD11	2.19	0.43
1:C:303:ALA:O	1:C:304:GLN:C	2.57	0.43
1:C:228:PHE:HA	1:C:327:ARG:HB2	2.00	0.43
1:C:225:TYR:OH	1:C:360:PHE:HE2	2.00	0.43
1:D:174:LEU:O	1:D:178:LYS:HG3	2.19	0.43
1:D:107:GLY:H	1:D:267:VAL:CA	2.32	0.43
1:D:338:VAL:HG21	1:D:354:LEU:CG	2.45	0.43
1:D:43:GLU:O	1:D:45:GLY:N	2.51	0.43
1:E:272:VAL:CG1	1:E:273:MET:N	2.80	0.43
1:E:303:ALA:O	1:E:304:GLN:C	2.57	0.43
1:E:404:PHE:C	1:E:406:ALA:H	2.21	0.43
1:F:303:ALA:O	1:F:304:GLN:C	2.57	0.43
1:B:87:LEU:O	1:B:241:ARG:NE	2.52	0.42
1:A:6:PHE:CE1	1:B:249:PRO:HB2	2.54	0.42
1:B:297:SER:HA	1:B:298:PRO:HD3	1.87	0.42
1:B:341:LEU:C	1:B:343:THR:H	2.22	0.42
1:B:67:ALA:O	1:B:69:LEU:N	2.52	0.42
1:C:88:PHE:CE1	1:C:244:ALA:CB	3.02	0.42
1:C:251:LEU:HD13	1:C:272:VAL:HG22	2.00	0.42
1:C:80:ARG:HG3	1:C:102:THR:O	2.19	0.42
1:D:88:PHE:CE1	1:D:244:ALA:HB2	2.54	0.42
1:E:220:PHE:C	1:E:220:PHE:CD1	2.92	0.42
1:E:252:VAL:O	1:E:270:LEU:HA	2.19	0.42
1:E:276:ASP:C	1:E:278:GLU:N	2.72	0.42
1:F:310:LEU:H	1:F:310:LEU:HG	1.52	0.42
1:F:341:LEU:C	1:F:343:THR:H	2.22	0.42
1:A:107:GLY:H	1:A:267:VAL:C	2.22	0.42
1:A:254:ASN:ND2	1:A:255:SER:N	2.64	0.42
1:A:99:ARG:O	1:A:280:ALA:HB2	2.19	0.42
1:B:220:PHE:CD1	1:B:220:PHE:C	2.92	0.42
1:B:325:GLU:HA	1:B:328:THR:CB	2.48	0.42
1:C:220:PHE:CD1	1:C:220:PHE:C	2.92	0.42
1:C:99:ARG:O	1:C:280:ALA:HB2	2.19	0.42
1:C:340:VAL:HB	1:C:401:ALA:CB	2.50	0.42
1:D:234:GLU:H	1:D:234:GLU:HG2	1.63	0.42
1:D:340:VAL:HB	1:D:401:ALA:CB	2.50	0.42
1:D:46:ILE:HG12	1:D:47:ILE:N	2.34	0.42
1:E:88:PHE:CE1	1:E:244:ALA:HB2	2.53	0.42
1:F:254:ASN:ND2	1:F:255:SER:N	2.64	0.42
1:F:256:PHE:O	1:F:257:SER:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:252:VAL:O	1:F:270:LEU:HA	2.19	0.42
1:A:113:LYS:HD3	1:A:146:ILE:HG22	2.02	0.42
1:A:107:GLY:H	1:A:267:VAL:CA	2.32	0.42
1:A:312:ASP:HB3	1:A:315:LEU:CD1	2.49	0.42
1:B:88:PHE:CE1	1:B:244:ALA:HB2	2.53	0.42
1:C:165:THR:C	1:C:167:GLY:N	2.72	0.42
1:C:209:ILE:O	1:C:210:GLU:C	2.57	0.42
1:C:278:GLU:OE1	1:C:282:ARG:NH1	2.52	0.42
1:C:312:ASP:HB3	1:C:315:LEU:CD1	2.49	0.42
1:C:88:PHE:CE1	1:C:244:ALA:HB2	2.53	0.42
1:D:84:ALA:N	1:D:85:PRO:CD	2.81	0.42
1:E:107:GLY:H	1:E:267:VAL:CA	2.32	0.42
1:E:173:LEU:HA	1:E:176:THR:OG1	2.20	0.42
1:E:210:GLU:O	1:E:214:ALA:HB2	2.19	0.42
1:E:382:ILE:CD1	1:E:386:ARG:HD3	2.36	0.42
1:E:43:GLU:C	1:E:45:GLY:N	2.70	0.42
1:F:220:PHE:C	1:F:220:PHE:CD1	2.92	0.42
1:F:240:ILE:H	1:F:240:ILE:HG13	1.31	0.42
1:A:216:GLU:C	1:A:217:LEU:HG	2.40	0.42
1:A:256:PHE:O	1:A:257:SER:C	2.57	0.42
1:A:276:ASP:C	1:A:278:GLU:N	2.72	0.42
1:B:15:ASP:OD1	1:B:17:ILE:HD11	2.19	0.42
1:B:256:PHE:O	1:B:257:SER:C	2.57	0.42
1:B:260:PHE:HB3	1:B:262:LEU:CD2	2.41	0.42
1:B:5:MET:HE2	1:B:5:MET:HB3	1.98	0.42
1:C:113:LYS:HD3	1:C:146:ILE:HG22	2.02	0.42
1:D:113:LYS:HD3	1:D:146:ILE:HG22	2.02	0.42
1:D:99:ARG:O	1:D:280:ALA:HB2	2.19	0.42
1:D:87:LEU:O	1:D:241:ARG:NE	2.52	0.42
1:E:233:MET:HB3	1:E:234:GLU:H	1.70	0.42
1:E:240:ILE:CA	1:E:243:ILE:HD12	2.50	0.42
1:F:210:GLU:O	1:F:214:ALA:HB2	2.19	0.42
1:F:216:GLU:C	1:F:217:LEU:HG	2.40	0.42
1:F:340:VAL:HB	1:F:401:ALA:CB	2.50	0.42
1:F:46:ILE:HG12	1:F:47:ILE:N	2.34	0.42
1:F:71:LEU:CD2	1:F:72:PRO:HD2	2.47	0.42
1:A:340:VAL:HB	1:A:401:ALA:CB	2.50	0.42
1:C:216:GLU:C	1:C:217:LEU:HG	2.40	0.42
1:C:87:LEU:O	1:C:241:ARG:NE	2.52	0.42
1:E:15:ASP:OD1	1:E:17:ILE:HD11	2.19	0.42
1:E:74:GLU:HB2	1:E:288:LYS:CE	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:234:GLU:HG2	1:F:234:GLU:H	1.63	0.42
1:F:99:ARG:O	1:F:280:ALA:HB2	2.19	0.42
1:F:380:TYR:C	1:F:381:LEU:HG	2.39	0.42
1:A:240:ILE:CA	1:A:243:ILE:HD12	2.50	0.42
1:A:334:ARG:HH22	1:A:358:GLY:N	2.17	0.42
1:A:393:ASN:ND2	1:A:395:ALA:CB	2.83	0.42
1:A:67:ALA:O	1:A:69:LEU:N	2.52	0.42
1:B:340:VAL:HB	1:B:401:ALA:CB	2.50	0.42
1:B:80:ARG:HG3	1:B:102:THR:O	2.19	0.42
1:C:107:GLY:H	1:C:267:VAL:C	2.22	0.42
1:C:341:LEU:C	1:C:343:THR:H	2.22	0.42
1:C:46:ILE:HG12	1:C:47:ILE:N	2.34	0.42
1:D:118:PHE:CD1	1:D:118:PHE:C	2.92	0.42
1:D:15:ASP:OD1	1:D:17:ILE:HD11	2.19	0.42
1:D:216:GLU:C	1:D:217:LEU:HG	2.40	0.42
1:E:193:HIS:HB3	1:E:197:GLY:CA	2.49	0.42
1:E:209:ILE:O	1:E:210:GLU:C	2.57	0.42
1:E:312:ASP:HB3	1:E:315:LEU:CD1	2.49	0.42
1:F:169:ARG:HG2	1:F:172:ASP:CB	2.45	0.42
1:F:209:ILE:O	1:F:210:GLU:C	2.57	0.42
1:F:263:TYR:CD1	1:F:263:TYR:N	2.70	0.42
1:F:276:ASP:C	1:F:278:GLU:N	2.72	0.42
1:F:393:ASN:ND2	1:F:395:ALA:CB	2.83	0.42
1:A:193:HIS:HB3	1:A:197:GLY:CA	2.49	0.42
1:A:210:GLU:O	1:A:214:ALA:HB2	2.19	0.42
1:A:252:VAL:O	1:A:270:LEU:HA	2.19	0.42
1:A:88:PHE:CE1	1:A:244:ALA:HB2	2.53	0.42
1:B:113:LYS:HD3	1:B:146:ILE:HG22	2.02	0.42
1:B:386:ARG:HG2	1:B:387:MET:N	2.35	0.42
1:C:240:ILE:CA	1:C:243:ILE:HD12	2.50	0.42
1:C:252:VAL:O	1:C:270:LEU:HA	2.19	0.42
1:C:390:ALA:C	1:C:392:LEU:N	2.73	0.42
1:C:71:LEU:CD2	1:C:72:PRO:HD2	2.47	0.42
1:E:67:ALA:O	1:E:69:LEU:N	2.52	0.42
1:F:80:ARG:HG3	1:F:102:THR:O	2.19	0.42
1:A:220:PHE:CD1	1:A:220:PHE:C	2.92	0.42
1:A:46:ILE:HG12	1:A:47:ILE:N	2.34	0.42
1:B:209:ILE:O	1:B:210:GLU:C	2.57	0.42
1:B:393:ASN:ND2	1:B:395:ALA:CB	2.83	0.42
1:C:67:ALA:O	1:C:69:LEU:N	2.52	0.42
1:D:312:ASP:HB3	1:D:315:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:ALA:O	1:D:69:LEU:N	2.52	0.42
1:E:334:ARG:HH22	1:E:358:GLY:N	2.17	0.42
1:E:393:ASN:ND2	1:E:395:ALA:CB	2.83	0.42
1:F:118:PHE:C	1:F:120:LYS:N	2.73	0.42
1:F:23:ARG:HG3	1:F:374:ARG:CZ	2.50	0.42
1:E:5:MET:CE	1:F:274:CYS:SG	3.07	0.42
1:F:5:MET:HE2	1:F:5:MET:HB3	1.97	0.42
1:A:88:PHE:CE1	1:A:244:ALA:CB	3.02	0.42
1:B:234:GLU:H	1:B:234:GLU:HG2	1.63	0.42
1:B:245:SER:O	1:B:246:ALA:C	2.59	0.42
1:B:276:ASP:C	1:B:278:GLU:N	2.72	0.42
1:B:79:TYR:O	1:B:80:ARG:C	2.59	0.42
1:C:118:PHE:C	1:C:120:LYS:N	2.73	0.42
1:D:80:ARG:HG3	1:D:102:THR:O	2.19	0.42
1:D:211:ILE:HG13	1:D:211:ILE:H	1.48	0.42
1:D:276:ASP:C	1:D:278:GLU:N	2.72	0.42
1:D:88:PHE:CE1	1:D:244:ALA:CB	3.02	0.42
1:E:88:PHE:CE1	1:E:244:ALA:CB	3.02	0.42
1:E:245:SER:O	1:E:246:ALA:C	2.59	0.42
1:E:256:PHE:O	1:E:257:SER:C	2.57	0.42
1:E:341:LEU:C	1:E:343:THR:H	2.22	0.42
1:E:380:TYR:C	1:E:381:LEU:HG	2.39	0.42
1:E:46:ILE:HG12	1:E:47:ILE:N	2.34	0.42
1:F:174:LEU:O	1:F:178:LYS:HG3	2.19	0.42
1:A:118:PHE:CD1	1:A:118:PHE:C	2.92	0.42
1:A:380:TYR:C	1:A:381:LEU:HG	2.39	0.42
1:B:254:ASN:ND2	1:B:255:SER:N	2.64	0.42
1:B:312:ASP:HB3	1:B:315:LEU:CD1	2.49	0.42
1:B:329:ARG:NH2	1:B:333:MET:HE3	2.33	0.42
1:B:46:ILE:HG12	1:B:47:ILE:N	2.34	0.42
1:C:286:GLN:O	1:C:289:ALA:HB3	2.20	0.42
1:C:338:VAL:HG21	1:C:354:LEU:CD2	2.50	0.42
1:D:165:THR:C	1:D:167:GLY:N	2.72	0.42
1:D:380:TYR:C	1:D:381:LEU:HG	2.39	0.42
1:E:118:PHE:C	1:E:118:PHE:CD1	2.92	0.42
1:E:113:LYS:HD3	1:E:146:ILE:HG22	2.02	0.42
1:E:238:TYR:O	1:E:241:ARG:HB2	2.20	0.42
1:E:396:ASN:HB2	1:E:397:VAL:H	1.75	0.42
1:F:96:LYS:H	1:F:96:LYS:HG2	1.64	0.42
1:A:80:ARG:HG3	1:A:102:THR:O	2.19	0.41
1:A:245:SER:O	1:A:246:ALA:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:TYR:O	1:A:47:ILE:HG23	2.20	0.41
1:B:238:TYR:O	1:B:241:ARG:HB2	2.20	0.41
1:B:312:ASP:CG	1:B:315:LEU:HG	2.40	0.41
1:C:254:ASN:ND2	1:C:255:SER:N	2.64	0.41
1:D:286:GLN:O	1:D:289:ALA:HB3	2.20	0.41
1:D:312:ASP:CG	1:D:315:LEU:HG	2.40	0.41
1:D:66:GLY:O	1:D:67:ALA:CB	2.68	0.41
1:F:245:SER:O	1:F:246:ALA:C	2.59	0.41
1:F:312:ASP:HB3	1:F:315:LEU:CD1	2.49	0.41
1:F:66:GLY:O	1:F:67:ALA:CB	2.68	0.41
1:A:5:MET:HB3	1:A:5:MET:HE2	1.83	0.41
1:A:6:PHE:HE1	1:B:249:PRO:CB	2.33	0.41
1:B:233:MET:HB3	1:B:234:GLU:H	1.70	0.41
1:B:99:ARG:O	1:B:280:ALA:HB2	2.19	0.41
1:C:210:GLU:O	1:C:214:ALA:HB2	2.20	0.41
1:C:380:TYR:C	1:C:381:LEU:HG	2.39	0.41
1:C:393:ASN:ND2	1:C:395:ALA:CB	2.83	0.41
1:D:254:ASN:ND2	1:D:255:SER:N	2.64	0.41
1:D:338:VAL:HG21	1:D:354:LEU:CD2	2.50	0.41
1:D:40:TYR:O	1:D:47:ILE:CG2	2.69	0.41
1:E:386:ARG:HG2	1:E:387:MET:N	2.35	0.41
1:E:80:ARG:HG3	1:E:102:THR:O	2.19	0.41
1:F:113:LYS:HD3	1:F:146:ILE:HG22	2.02	0.41
1:F:15:ASP:OD1	1:F:17:ILE:HD11	2.19	0.41
1:F:312:ASP:CG	1:F:315:LEU:HG	2.40	0.41
1:A:286:GLN:O	1:A:289:ALA:HB3	2.20	0.41
1:B:252:VAL:O	1:B:270:LEU:HA	2.19	0.41
1:B:286:GLN:O	1:B:289:ALA:HB3	2.20	0.41
1:B:40:TYR:O	1:B:47:ILE:CG2	2.69	0.41
1:C:173:LEU:HA	1:C:176:THR:OG1	2.20	0.41
1:C:312:ASP:CG	1:C:315:LEU:HG	2.40	0.41
1:C:40:TYR:O	1:C:47:ILE:CG2	2.69	0.41
1:D:238:TYR:O	1:D:241:ARG:HB2	2.20	0.41
1:D:40:TYR:O	1:D:47:ILE:HG23	2.20	0.41
1:D:79:TYR:O	1:D:80:ARG:C	2.59	0.41
1:E:168:VAL:HG13	1:E:168:VAL:O	2.21	0.41
1:E:340:VAL:HB	1:E:401:ALA:CB	2.50	0.41
1:E:23:ARG:HG3	1:E:374:ARG:CZ	2.50	0.41
1:F:173:LEU:HA	1:F:176:THR:OG1	2.20	0.41
1:F:245:SER:OG	1:F:246:ALA:N	2.53	0.41
1:F:286:GLN:O	1:F:289:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:393:ASN:HB3	1:F:396:ASN:ND2	2.36	0.41
1:A:173:LEU:HA	1:A:176:THR:OG1	2.20	0.41
1:A:23:ARG:HG3	1:A:374:ARG:CZ	2.50	0.41
1:B:338:VAL:HG21	1:B:354:LEU:CD2	2.50	0.41
1:B:87:LEU:CD2	1:B:87:LEU:N	2.75	0.41
1:C:276:ASP:C	1:C:278:GLU:N	2.72	0.41
1:C:79:TYR:O	1:C:80:ARG:C	2.59	0.41
1:D:252:VAL:O	1:D:270:LEU:HA	2.19	0.41
1:D:23:ARG:HG3	1:D:374:ARG:CZ	2.50	0.41
1:E:338:VAL:HG21	1:E:354:LEU:CD2	2.50	0.41
1:E:363:THR:OG1	1:E:385:GLY:HA2	2.21	0.41
1:E:390:ALA:C	1:E:392:LEU:N	2.73	0.41
1:F:336:GLU:O	1:F:340:VAL:CG2	2.69	0.41
1:A:338:VAL:HG21	1:A:354:LEU:CD2	2.50	0.41
1:B:173:LEU:HA	1:B:176:THR:OG1	2.20	0.41
1:B:240:ILE:CA	1:B:243:ILE:HD12	2.50	0.41
1:C:107:GLY:O	1:C:108:GLY:C	2.58	0.41
1:C:168:VAL:HG21	1:C:200:LEU:HD22	2.03	0.41
1:C:23:ARG:HG3	1:C:374:ARG:CZ	2.50	0.41
1:C:338:VAL:HG21	1:C:354:LEU:CG	2.45	0.41
1:C:66:GLY:O	1:C:67:ALA:CB	2.68	0.41
1:C:73:MET:HB2	1:C:288:LYS:HD3	2.03	0.41
1:E:312:ASP:CG	1:E:315:LEU:HG	2.40	0.41
1:E:336:GLU:O	1:E:340:VAL:CG2	2.69	0.41
1:F:238:TYR:O	1:F:241:ARG:HB2	2.20	0.41
1:F:79:TYR:O	1:F:80:ARG:C	2.59	0.41
1:A:15:ASP:OD1	1:A:17:ILE:HD11	2.19	0.41
1:A:73:MET:HB2	1:A:288:LYS:HD3	2.03	0.41
1:B:185:ILE:CD1	1:B:185:ILE:H	2.24	0.41
1:B:210:GLU:O	1:B:214:ALA:HB2	2.19	0.41
1:B:23:ARG:HG3	1:B:374:ARG:CZ	2.50	0.41
1:B:380:TYR:C	1:B:381:LEU:HG	2.39	0.41
1:D:168:VAL:HG21	1:D:200:LEU:HD22	2.03	0.41
1:D:210:GLU:O	1:D:214:ALA:HB2	2.19	0.41
1:D:58:ALA:O	1:D:62:ALA:CB	2.62	0.41
1:F:40:TYR:O	1:F:47:ILE:HG23	2.20	0.41
1:A:6:PHE:CE1	1:B:249:PRO:CB	3.04	0.41
1:D:168:VAL:HG13	1:D:168:VAL:O	2.20	0.41
1:D:240:ILE:H	1:D:240:ILE:HG13	1.31	0.41
1:D:73:MET:HB2	1:D:288:LYS:HD3	2.03	0.41
1:E:286:GLN:O	1:E:289:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:VAL:HG13	1:F:168:VAL:O	2.20	0.41
1:A:118:PHE:C	1:A:120:LYS:N	2.73	0.41
1:A:336:GLU:O	1:A:340:VAL:CG2	2.69	0.41
1:B:200:LEU:CB	1:B:204:GLN:NE2	2.84	0.41
1:E:216:GLU:C	1:E:217:LEU:HG	2.40	0.41
1:E:40:TYR:O	1:E:47:ILE:CG2	2.69	0.41
1:F:107:GLY:O	1:F:108:GLY:C	2.58	0.41
1:F:363:THR:OG1	1:F:385:GLY:HA2	2.21	0.41
1:A:168:VAL:O	1:A:168:VAL:HG13	2.21	0.41
1:A:297:SER:HA	1:A:298:PRO:HD3	1.87	0.41
1:A:87:LEU:CD2	1:A:87:LEU:N	2.75	0.41
1:B:73:MET:HB2	1:B:288:LYS:HD3	2.03	0.41
1:B:323:VAL:CG1	1:B:324:GLU:N	2.84	0.41
1:B:40:TYR:O	1:B:47:ILE:HG23	2.20	0.41
1:B:50:LEU:HD12	1:B:260:PHE:O	2.21	0.41
1:B:66:GLY:O	1:B:67:ALA:CB	2.68	0.41
1:C:211:ILE:HG13	1:C:211:ILE:H	1.48	0.41
1:C:40:TYR:O	1:C:47:ILE:HG23	2.20	0.41
1:C:96:LYS:H	1:C:96:LYS:HG2	1.64	0.41
1:D:118:PHE:C	1:D:120:LYS:N	2.73	0.41
1:D:173:LEU:HA	1:D:176:THR:OG1	2.20	0.41
1:D:245:SER:O	1:D:246:ALA:C	2.59	0.41
1:D:336:GLU:O	1:D:340:VAL:CG2	2.69	0.41
1:D:355:ASN:O	1:D:356:GLN:C	2.60	0.41
1:D:393:ASN:ND2	1:D:395:ALA:CB	2.83	0.41
1:E:200:LEU:CB	1:E:204:GLN:NE2	2.84	0.41
1:E:73:MET:HB2	1:E:288:LYS:HD3	2.03	0.41
1:E:40:TYR:O	1:E:47:ILE:HG23	2.20	0.41
1:E:66:GLY:O	1:E:67:ALA:CB	2.68	0.41
1:F:325:GLU:HA	1:F:328:THR:CB	2.48	0.41
1:A:263:TYR:N	1:A:263:TYR:CD1	2.70	0.41
1:B:336:GLU:O	1:B:340:VAL:CG2	2.69	0.41
1:B:355:ASN:O	1:B:356:GLN:C	2.59	0.41
1:D:50:LEU:HD12	1:D:260:PHE:O	2.21	0.41
1:E:84:ALA:N	1:E:85:PRO:CD	2.81	0.41
1:F:168:VAL:HG21	1:F:200:LEU:HD22	2.03	0.41
1:F:200:LEU:CB	1:F:204:GLN:NE2	2.84	0.41
1:F:323:VAL:CG1	1:F:324:GLU:N	2.84	0.41
1:F:338:VAL:HG21	1:F:354:LEU:CD2	2.50	0.41
1:A:393:ASN:HB3	1:A:396:ASN:ND2	2.36	0.41
1:C:238:TYR:O	1:C:241:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:SER:O	1:C:246:ALA:C	2.59	0.41
1:C:50:LEU:HD12	1:C:260:PHE:O	2.21	0.41
1:E:226:GLN:NE2	1:E:237:ALA:HB2	2.36	0.41
1:F:240:ILE:CA	1:F:243:ILE:HD12	2.50	0.41
1:F:308:ALA:O	1:F:315:LEU:HD12	2.21	0.41
1:F:386:ARG:HG2	1:F:387:MET:N	2.35	0.41
1:A:107:GLY:O	1:A:108:GLY:C	2.58	0.40
1:A:308:ALA:O	1:A:315:LEU:HD12	2.21	0.40
1:A:312:ASP:CG	1:A:315:LEU:HG	2.40	0.40
1:A:79:TYR:O	1:A:80:ARG:C	2.59	0.40
1:B:107:GLY:O	1:B:108:GLY:C	2.58	0.40
1:B:308:ALA:O	1:B:315:LEU:HD12	2.21	0.40
1:D:107:GLY:O	1:D:108:GLY:C	2.58	0.40
1:D:308:ALA:O	1:D:315:LEU:HD12	2.21	0.40
1:E:118:PHE:C	1:E:120:LYS:N	2.73	0.40
1:E:393:ASN:HB3	1:E:396:ASN:ND2	2.36	0.40
1:A:238:TYR:O	1:A:241:ARG:HB2	2.20	0.40
1:A:323:VAL:CG1	1:A:324:GLU:N	2.84	0.40
1:A:40:TYR:O	1:A:47:ILE:CG2	2.69	0.40
1:B:154:GLU:O	1:B:155:VAL:C	2.59	0.40
1:B:168:VAL:HG13	1:B:168:VAL:O	2.20	0.40
1:C:168:VAL:O	1:C:168:VAL:HG13	2.21	0.40
1:C:200:LEU:CB	1:C:204:GLN:NE2	2.84	0.40
1:C:336:GLU:O	1:C:340:VAL:CG2	2.69	0.40
1:C:355:ASN:O	1:C:356:GLN:C	2.60	0.40
1:C:393:ASN:HB3	1:C:396:ASN:ND2	2.36	0.40
1:D:146:ILE:H	1:D:146:ILE:HG13	1.34	0.40
1:D:226:GLN:NE2	1:D:237:ALA:HB2	2.36	0.40
1:D:76:LEU:HG	1:D:79:TYR:HB2	2.03	0.40
1:E:154:GLU:O	1:E:155:VAL:C	2.59	0.40
1:E:168:VAL:HG21	1:E:200:LEU:HD22	2.03	0.40
1:E:245:SER:OG	1:E:246:ALA:N	2.53	0.40
1:A:226:GLN:NE2	1:A:237:ALA:HB2	2.36	0.40
1:A:310:LEU:H	1:A:310:LEU:HG	1.52	0.40
1:A:386:ARG:HG2	1:A:387:MET:N	2.35	0.40
1:A:50:LEU:HD12	1:A:260:PHE:O	2.21	0.40
1:A:66:GLY:O	1:A:67:ALA:CB	2.68	0.40
1:B:118:PHE:C	1:B:120:LYS:N	2.73	0.40
1:B:400:VAL:O	1:B:403:ALA:HB3	2.22	0.40
1:C:118:PHE:CD1	1:C:118:PHE:C	2.92	0.40
1:C:211:ILE:O	1:C:215:ARG:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:ASN:HA	1:D:195:PRO:HA	1.92	0.40
1:D:220:PHE:C	1:D:220:PHE:HD1	2.25	0.40
1:D:400:VAL:O	1:D:403:ALA:HB3	2.22	0.40
1:E:294:ASN:HB3	1:E:295:TYR:H	1.77	0.40
1:F:154:GLU:O	1:F:155:VAL:C	2.59	0.40
1:F:211:ILE:O	1:F:215:ARG:HB2	2.22	0.40
1:F:183:ARG:C	1:F:218:ILE:HD12	2.42	0.40
1:F:218:ILE:HA	1:F:219:PRO:HD3	1.95	0.40
1:F:50:LEU:HD12	1:F:260:PHE:O	2.21	0.40
1:F:355:ASN:O	1:F:356:GLN:C	2.60	0.40
1:A:363:THR:OG1	1:A:385:GLY:HA2	2.21	0.40
1:B:226:GLN:NE2	1:B:237:ALA:HB2	2.37	0.40
1:C:154:GLU:O	1:C:155:VAL:C	2.59	0.40
1:C:226:GLN:NE2	1:C:237:ALA:HB2	2.36	0.40
1:C:282:ARG:H	1:C:282:ARG:HG2	1.67	0.40
1:C:297:SER:HA	1:C:298:PRO:HD3	1.87	0.40
1:C:308:ALA:O	1:C:315:LEU:HD12	2.21	0.40
1:C:363:THR:OG1	1:C:385:GLY:HA2	2.21	0.40
1:D:233:MET:HB3	1:D:234:GLU:H	1.70	0.40
1:D:99:ARG:H	1:D:99:ARG:HG2	1.71	0.40
1:F:40:TYR:O	1:F:47:ILE:CG2	2.69	0.40
1:A:174:LEU:HD23	1:A:174:LEU:HA	1.91	0.40
1:A:200:LEU:CB	1:A:204:GLN:NE2	2.84	0.40
1:A:220:PHE:C	1:A:220:PHE:HD1	2.25	0.40
1:A:305:VAL:HG22	1:A:305:VAL:H	1.61	0.40
1:A:355:ASN:O	1:A:356:GLN:C	2.60	0.40
1:C:323:VAL:CG1	1:C:324:GLU:N	2.84	0.40
1:C:70:TYR:CD2	1:D:263:TYR:HB2	2.56	0.40
1:D:154:GLU:O	1:D:155:VAL:C	2.59	0.40
1:D:294:ASN:OD1	1:D:295:TYR:HD1	2.05	0.40
1:E:308:ALA:O	1:E:315:LEU:HD12	2.21	0.40
1:E:323:VAL:CG1	1:E:324:GLU:N	2.84	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ASN:CG	1:E:216:GLU:OE1[1_545]	0.69	1.51
1:B:349:ASN:OD1	1:E:216:GLU:OE1[1_545]	0.87	1.33
1:B:349:ASN:OD1	1:E:216:GLU:CD[1_545]	1.22	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:THR:CG2	1:C:215:ARG:NH1[1_445]	1.65	0.55
1:B:349:ASN:CG	1:E:216:GLU:CD[1_545]	1.75	0.45
1:B:349:ASN:CB	1:E:216:GLU:OE1[1_545]	1.77	0.43
1:B:349:ASN:ND2	1:E:216:GLU:OE1[1_545]	1.83	0.37
1:B:351:ASP:OD2	1:E:215:ARG:O[1_545]	1.91	0.29
1:B:349:ASN:OD1	1:E:216:GLU:CG[1_545]	1.95	0.25

## 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	395/397 (100%)	254 (64%)	91 (23%)	50 (13%)	0	4
1	B	395/397 (100%)	254 (64%)	91 (23%)	50 (13%)	0	4
1	C	395/397 (100%)	254 (64%)	91 (23%)	50 (13%)	0	4
1	D	395/397 (100%)	254 (64%)	91 (23%)	50 (13%)	0	4
1	E	395/397 (100%)	254 (64%)	91 (23%)	50 (13%)	0	4
1	F	395/397 (100%)	254 (64%)	91 (23%)	50 (13%)	0	4
All	All	2370/2382 (100%)	1524 (64%)	546 (23%)	300 (13%)	0	4

All (300) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	70	TYR
1	A	141	GLU
1	A	145	ALA
1	A	170	PHE
1	A	233	MET
1	A	245	SER
1	A	248	LEU
1	A	307	ALA

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Mol	Chain	Res	Type
1	A	308	ALA
1	A	397	VAL
1	B	65	HIS
1	B	70	TYR
1	B	141	GLU
1	B	145	ALA
1	B	170	PHE
1	B	233	MET
1	B	245	SER
1	B	248	LEU
1	B	307	ALA
1	B	308	ALA
1	B	397	VAL
1	C	65	HIS
1	C	70	TYR
1	C	141	GLU
1	C	145	ALA
1	C	170	PHE
1	C	233	MET
1	C	245	SER
1	C	248	LEU
1	C	307	ALA
1	C	308	ALA
1	C	397	VAL
1	D	65	HIS
1	D	70	TYR
1	D	141	GLU
1	D	145	ALA
1	D	170	PHE
1	D	233	MET
1	D	245	SER
1	D	248	LEU
1	D	307	ALA
1	D	308	ALA
1	D	397	VAL
1	E	65	HIS
1	E	70	TYR
1	E	141	GLU
1	E	145	ALA
1	E	170	PHE
1	E	233	MET
1	E	245	SER

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Mol	Chain	Res	Type
1	E	248	LEU
1	E	307	ALA
1	E	308	ALA
1	E	397	VAL
1	F	65	HIS
1	F	70	TYR
1	F	141	GLU
1	F	145	ALA
1	F	170	PHE
1	F	233	MET
1	F	245	SER
1	F	248	LEU
1	F	307	ALA
1	F	308	ALA
1	F	397	VAL
1	A	44	ASP
1	A	68	SER
1	A	73	MET
1	A	82	ALA
1	A	140	TRP
1	A	144	VAL
1	A	172	ASP
1	A	199	ASP
1	A	246	ALA
1	A	280	ALA
1	A	302	GLY
1	A	356	GLN
1	B	44	ASP
1	B	68	SER
1	B	73	MET
1	B	82	ALA
1	B	140	TRP
1	B	144	VAL
1	B	172	ASP
1	B	199	ASP
1	B	246	ALA
1	B	280	ALA
1	B	302	GLY
1	B	356	GLN
1	C	44	ASP
1	C	68	SER
1	C	73	MET

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Mol	Chain	Res	Type
1	C	82	ALA
1	C	140	TRP
1	C	144	VAL
1	C	172	ASP
1	C	199	ASP
1	C	246	ALA
1	C	302	GLY
1	C	356	GLN
1	D	44	ASP
1	D	68	SER
1	D	73	MET
1	D	82	ALA
1	D	140	TRP
1	D	144	VAL
1	D	172	ASP
1	D	199	ASP
1	D	246	ALA
1	D	302	GLY
1	D	356	GLN
1	E	44	ASP
1	E	68	SER
1	E	73	MET
1	E	82	ALA
1	E	140	TRP
1	E	144	VAL
1	E	172	ASP
1	E	199	ASP
1	E	246	ALA
1	E	280	ALA
1	E	302	GLY
1	E	356	GLN
1	F	44	ASP
1	F	68	SER
1	F	73	MET
1	F	82	ALA
1	F	140	TRP
1	F	144	VAL
1	F	172	ASP
1	F	199	ASP
1	F	246	ALA
1	F	280	ALA
1	F	302	GLY

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Mol	Chain	Res	Type
1	F	356	GLN
1	A	9	VAL
1	A	51	GLN
1	A	67	ALA
1	A	113	LYS
1	A	169	ARG
1	A	178	LYS
1	A	183	ARG
1	A	239	ALA
1	A	241	ARG
1	A	294	ASN
1	B	9	VAL
1	B	51	GLN
1	B	67	ALA
1	B	113	LYS
1	B	169	ARG
1	B	178	LYS
1	B	183	ARG
1	B	239	ALA
1	B	241	ARG
1	B	294	ASN
1	B	386	ARG
1	C	9	VAL
1	C	51	GLN
1	C	67	ALA
1	C	113	LYS
1	C	169	ARG
1	C	178	LYS
1	C	183	ARG
1	C	239	ALA
1	C	241	ARG
1	C	280	ALA
1	C	294	ASN
1	D	9	VAL
1	D	51	GLN
1	D	67	ALA
1	D	113	LYS
1	D	169	ARG
1	D	178	LYS
1	D	183	ARG
1	D	239	ALA
1	D	241	ARG

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Mol	Chain	Res	Type
1	D	280	ALA
1	D	294	ASN
1	D	386	ARG
1	E	9	VAL
1	E	51	GLN
1	E	67	ALA
1	E	113	LYS
1	E	136	SER
1	E	169	ARG
1	E	178	LYS
1	E	183	ARG
1	E	239	ALA
1	E	241	ARG
1	E	294	ASN
1	F	9	VAL
1	F	51	GLN
1	F	67	ALA
1	F	113	LYS
1	F	169	ARG
1	F	178	LYS
1	F	183	ARG
1	F	239	ALA
1	F	241	ARG
1	F	294	ASN
1	A	136	SER
1	A	181	PRO
1	A	386	ARG
1	A	393	ASN
1	A	394	THR
1	B	136	SER
1	B	181	PRO
1	B	393	ASN
1	B	394	THR
1	C	136	SER
1	C	181	PRO
1	C	386	ARG
1	C	393	ASN
1	C	394	THR
1	D	136	SER
1	D	181	PRO
1	D	393	ASN
1	D	394	THR

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Mol	Chain	Res	Type
1	E	181	PRO
1	E	386	ARG
1	E	393	ASN
1	E	394	THR
1	F	136	SER
1	F	181	PRO
1	F	386	ARG
1	F	393	ASN
1	F	394	THR
1	A	164	ALA
1	A	244	ALA
1	A	257	SER
1	A	296	SER
1	B	164	ALA
1	B	244	ALA
1	B	257	SER
1	B	296	SER
1	C	164	ALA
1	C	244	ALA
1	C	257	SER
1	C	296	SER
1	D	164	ALA
1	D	244	ALA
1	D	257	SER
1	D	296	SER
1	E	164	ALA
1	E	244	ALA
1	E	257	SER
1	E	296	SER
1	F	164	ALA
1	F	244	ALA
1	F	257	SER
1	F	296	SER
1	A	89	GLY
1	B	89	GLY
1	C	89	GLY
1	D	89	GLY
1	E	89	GLY
1	F	89	GLY
1	A	107	GLY
1	A	146	ILE
1	A	155	VAL

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Mol	Chain	Res	Type
1	A	298	PRO
1	B	107	GLY
1	B	146	ILE
1	B	155	VAL
1	B	298	PRO
1	C	107	GLY
1	C	146	ILE
1	C	155	VAL
1	C	298	PRO
1	D	107	GLY
1	D	146	ILE
1	D	155	VAL
1	D	298	PRO
1	E	107	GLY
1	E	155	VAL
1	F	107	GLY
1	F	146	ILE
1	F	155	VAL
1	F	298	PRO
1	A	83	ILE
1	B	83	ILE
1	C	83	ILE
1	D	83	ILE
1	E	83	ILE
1	E	146	ILE
1	E	298	PRO
1	F	83	ILE
1	A	66	GLY
1	B	66	GLY
1	C	66	GLY
1	D	66	GLY
1	E	66	GLY
1	F	66	GLY
1	B	138	PRO
1	C	138	PRO
1	A	138	PRO
1	D	138	PRO
1	E	138	PRO
1	F	138	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	316/316 (100%)	196 (62%)	120 (38%)	0	1
1	B	316/316 (100%)	196 (62%)	120 (38%)	0	1
1	C	316/316 (100%)	196 (62%)	120 (38%)	0	1
1	D	316/316 (100%)	196 (62%)	120 (38%)	0	1
1	E	316/316 (100%)	196 (62%)	120 (38%)	0	1
1	F	316/316 (100%)	196 (62%)	120 (38%)	0	1
All	All	1896/1896 (100%)	1176 (62%)	720 (38%)	0	1

All (720) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	7	GLN
1	A	8	LYS
1	A	9	VAL
1	A	10	ASP
1	A	12	TYR
1	A	15	ASP
1	A	21	MET
1	A	23	ARG
1	A	39	LEU
1	A	43	GLU
1	A	44	ASP
1	A	47	ILE
1	A	50	LEU
1	A	51	GLN
1	A	57	GLU
1	A	59	ARG
1	A	60	LEU
1	A	63	GLN
1	A	65	HIS
1	A	70	TYR
1	A	77	ASN

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Mol	Chain	Res	Type
1	A	80	ARG
1	A	87	LEU
1	A	91	ASP
1	A	92	HIS
1	A	94	VAL
1	A	95	LEU
1	A	96	LYS
1	A	99	ARG
1	A	102	THR
1	A	103	ILE
1	A	104	GLN
1	A	105	THR
1	A	114	VAL
1	A	117	ASP
1	A	118	PHE
1	A	135	VAL
1	A	136	SER
1	A	139	THR
1	A	142	ASN
1	A	143	HIS
1	A	146	ILE
1	A	156	SER
1	A	157	THR
1	A	170	PHE
1	A	173	LEU
1	A	183	ARG
1	A	185	ILE
1	A	187	LEU
1	A	189	HIS
1	A	199	ASP
1	A	200	LEU
1	A	201	THR
1	A	202	ASN
1	A	203	ASP
1	A	204	GLN
1	A	209	ILE
1	A	210	GLU
1	A	211	ILE
1	A	212	LEU
1	A	213	LYS
1	A	220	PHE
1	A	225	TYR

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Mol	Chain	Res	Type
1	A	226	GLN
1	A	228	PHE
1	A	240	ILE
1	A	241	ARG
1	A	248	LEU
1	A	251	LEU
1	A	252	VAL
1	A	254	ASN
1	A	255	SER
1	A	258	LYS
1	A	261	SER
1	A	262	LEU
1	A	263	TYR
1	A	265	GLU
1	A	266	ARG
1	A	270	LEU
1	A	271	SER
1	A	273	MET
1	A	276	ASP
1	A	278	GLU
1	A	282	ARG
1	A	284	LEU
1	A	288	LYS
1	A	296	SER
1	A	304	GLN
1	A	305	VAL
1	A	310	LEU
1	A	318	SER
1	A	325	GLU
1	A	327	ARG
1	A	328	THR
1	A	329	ARG
1	A	331	LEU
1	A	333	MET
1	A	336	GLU
1	A	337	LEU
1	A	339	LYS
1	A	340	VAL
1	A	342	SER
1	A	345	MET
1	A	347	GLU
1	A	348	ARG

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Mol	Chain	Res	Type
1	A	353	LEU
1	A	355	ASN
1	A	362	TYR
1	A	374	ARG
1	A	379	VAL
1	A	381	LEU
1	A	386	ARG
1	A	387	MET
1	A	394	THR
1	A	396	ASN
1	A	398	GLN
1	A	400	VAL
1	A	404	PHE
1	A	408	MET
1	B	5	MET
1	B	7	GLN
1	B	8	LYS
1	B	9	VAL
1	B	10	ASP
1	B	12	TYR
1	B	15	ASP
1	B	21	MET
1	B	23	ARG
1	B	39	LEU
1	B	43	GLU
1	B	44	ASP
1	B	47	ILE
1	B	50	LEU
1	B	51	GLN
1	B	57	GLU
1	B	59	ARG
1	B	60	LEU
1	B	63	GLN
1	B	65	HIS
1	B	70	TYR
1	B	77	ASN
1	B	80	ARG
1	B	87	LEU
1	B	91	ASP
1	B	92	HIS
1	B	94	VAL
1	B	95	LEU

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Mol	Chain	Res	Type
1	B	96	LYS
1	B	99	ARG
1	B	102	THR
1	B	103	ILE
1	B	104	GLN
1	B	105	THR
1	B	114	VAL
1	B	117	ASP
1	B	118	PHE
1	B	135	VAL
1	B	136	SER
1	B	139	THR
1	B	142	ASN
1	B	143	HIS
1	B	146	ILE
1	B	156	SER
1	B	157	THR
1	B	170	PHE
1	B	173	LEU
1	B	183	ARG
1	B	185	ILE
1	B	187	LEU
1	B	189	HIS
1	B	199	ASP
1	B	200	LEU
1	B	201	THR
1	B	202	ASN
1	B	203	ASP
1	B	204	GLN
1	B	209	ILE
1	B	210	GLU
1	B	211	ILE
1	B	212	LEU
1	B	213	LYS
1	B	220	PHE
1	B	225	TYR
1	B	226	GLN
1	B	228	PHE
1	B	240	ILE
1	B	241	ARG
1	B	248	LEU
1	B	251	LEU

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Mol	Chain	Res	Type
1	B	252	VAL
1	B	254	ASN
1	B	255	SER
1	B	258	LYS
1	B	261	SER
1	B	262	LEU
1	B	263	TYR
1	B	265	GLU
1	B	266	ARG
1	B	270	LEU
1	B	271	SER
1	B	273	MET
1	B	276	ASP
1	B	278	GLU
1	B	282	ARG
1	B	284	LEU
1	B	288	LYS
1	B	296	SER
1	B	304	GLN
1	B	305	VAL
1	B	310	LEU
1	B	318	SER
1	B	325	GLU
1	B	327	ARG
1	B	328	THR
1	B	329	ARG
1	B	331	LEU
1	B	333	MET
1	B	336	GLU
1	B	337	LEU
1	B	339	LYS
1	B	340	VAL
1	B	342	SER
1	B	345	MET
1	B	347	GLU
1	B	348	ARG
1	B	353	LEU
1	B	355	ASN
1	B	362	TYR
1	B	374	ARG
1	B	379	VAL
1	B	381	LEU

*Continued on next page...*

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Mol	Chain	Res	Type
1	B	386	ARG
1	B	387	MET
1	B	394	THR
1	B	396	ASN
1	B	398	GLN
1	B	400	VAL
1	B	404	PHE
1	B	408	MET
1	C	5	MET
1	C	7	GLN
1	C	8	LYS
1	C	9	VAL
1	C	10	ASP
1	C	12	TYR
1	C	15	ASP
1	C	21	MET
1	C	23	ARG
1	C	39	LEU
1	C	43	GLU
1	C	44	ASP
1	C	47	ILE
1	C	50	LEU
1	C	51	GLN
1	C	57	GLU
1	C	59	ARG
1	C	60	LEU
1	C	63	GLN
1	C	65	HIS
1	C	70	TYR
1	C	77	ASN
1	C	80	ARG
1	C	87	LEU
1	C	91	ASP
1	C	92	HIS
1	C	94	VAL
1	C	95	LEU
1	C	96	LYS
1	C	99	ARG
1	C	102	THR
1	C	103	ILE
1	C	104	GLN
1	C	105	THR

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Mol	Chain	Res	Type
1	C	114	VAL
1	C	117	ASP
1	C	118	PHE
1	C	135	VAL
1	C	136	SER
1	C	139	THR
1	C	142	ASN
1	C	143	HIS
1	C	146	ILE
1	C	156	SER
1	C	157	THR
1	C	170	PHE
1	C	173	LEU
1	C	183	ARG
1	C	185	ILE
1	C	187	LEU
1	C	189	HIS
1	C	199	ASP
1	C	200	LEU
1	C	201	THR
1	C	202	ASN
1	C	203	ASP
1	C	204	GLN
1	C	209	ILE
1	C	210	GLU
1	C	211	ILE
1	C	212	LEU
1	C	213	LYS
1	C	220	PHE
1	C	225	TYR
1	C	226	GLN
1	C	228	PHE
1	C	240	ILE
1	C	241	ARG
1	C	248	LEU
1	C	251	LEU
1	C	252	VAL
1	C	254	ASN
1	C	255	SER
1	C	258	LYS
1	C	261	SER
1	C	262	LEU

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Mol	Chain	Res	Type
1	C	263	TYR
1	C	265	GLU
1	C	266	ARG
1	C	270	LEU
1	C	271	SER
1	C	273	MET
1	C	276	ASP
1	C	278	GLU
1	C	282	ARG
1	C	284	LEU
1	C	288	LYS
1	C	296	SER
1	C	304	GLN
1	C	305	VAL
1	C	310	LEU
1	C	318	SER
1	C	325	GLU
1	C	327	ARG
1	C	328	THR
1	C	329	ARG
1	C	331	LEU
1	C	333	MET
1	C	336	GLU
1	C	337	LEU
1	C	339	LYS
1	C	340	VAL
1	C	342	SER
1	C	345	MET
1	C	347	GLU
1	C	348	ARG
1	C	353	LEU
1	C	355	ASN
1	C	362	TYR
1	C	374	ARG
1	C	379	VAL
1	C	381	LEU
1	C	386	ARG
1	C	387	MET
1	C	394	THR
1	C	396	ASN
1	C	398	GLN
1	C	400	VAL

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Mol	Chain	Res	Type
1	C	404	PHE
1	C	408	MET
1	D	5	MET
1	D	7	GLN
1	D	8	LYS
1	D	9	VAL
1	D	10	ASP
1	D	12	TYR
1	D	15	ASP
1	D	21	MET
1	D	23	ARG
1	D	39	LEU
1	D	43	GLU
1	D	44	ASP
1	D	47	ILE
1	D	50	LEU
1	D	51	GLN
1	D	57	GLU
1	D	59	ARG
1	D	60	LEU
1	D	63	GLN
1	D	65	HIS
1	D	70	TYR
1	D	77	ASN
1	D	80	ARG
1	D	87	LEU
1	D	91	ASP
1	D	92	HIS
1	D	94	VAL
1	D	95	LEU
1	D	96	LYS
1	D	99	ARG
1	D	102	THR
1	D	103	ILE
1	D	104	GLN
1	D	105	THR
1	D	114	VAL
1	D	117	ASP
1	D	118	PHE
1	D	135	VAL
1	D	136	SER
1	D	139	THR

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Mol	Chain	Res	Type
1	D	142	ASN
1	D	143	HIS
1	D	146	ILE
1	D	156	SER
1	D	157	THR
1	D	170	PHE
1	D	173	LEU
1	D	183	ARG
1	D	185	ILE
1	D	187	LEU
1	D	189	HIS
1	D	199	ASP
1	D	200	LEU
1	D	201	THR
1	D	202	ASN
1	D	203	ASP
1	D	204	GLN
1	D	209	ILE
1	D	210	GLU
1	D	211	ILE
1	D	212	LEU
1	D	213	LYS
1	D	220	PHE
1	D	225	TYR
1	D	226	GLN
1	D	228	PHE
1	D	240	ILE
1	D	241	ARG
1	D	248	LEU
1	D	251	LEU
1	D	252	VAL
1	D	254	ASN
1	D	255	SER
1	D	258	LYS
1	D	261	SER
1	D	262	LEU
1	D	263	TYR
1	D	265	GLU
1	D	266	ARG
1	D	270	LEU
1	D	271	SER
1	D	273	MET

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Mol	Chain	Res	Type
1	D	276	ASP
1	D	278	GLU
1	D	282	ARG
1	D	284	LEU
1	D	288	LYS
1	D	296	SER
1	D	304	GLN
1	D	305	VAL
1	D	310	LEU
1	D	318	SER
1	D	325	GLU
1	D	327	ARG
1	D	328	THR
1	D	329	ARG
1	D	331	LEU
1	D	333	MET
1	D	336	GLU
1	D	337	LEU
1	D	339	LYS
1	D	340	VAL
1	D	342	SER
1	D	345	MET
1	D	347	GLU
1	D	348	ARG
1	D	353	LEU
1	D	355	ASN
1	D	362	TYR
1	D	374	ARG
1	D	379	VAL
1	D	381	LEU
1	D	386	ARG
1	D	387	MET
1	D	394	THR
1	D	396	ASN
1	D	398	GLN
1	D	400	VAL
1	D	404	PHE
1	D	408	MET
1	E	5	MET
1	E	7	GLN
1	E	8	LYS
1	E	9	VAL

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Mol	Chain	Res	Type
1	E	10	ASP
1	E	12	TYR
1	E	15	ASP
1	E	21	MET
1	E	23	ARG
1	E	39	LEU
1	E	43	GLU
1	E	44	ASP
1	E	47	ILE
1	E	50	LEU
1	E	51	GLN
1	E	57	GLU
1	E	59	ARG
1	E	60	LEU
1	E	63	GLN
1	E	65	HIS
1	E	70	TYR
1	E	77	ASN
1	E	80	ARG
1	E	87	LEU
1	E	91	ASP
1	E	92	HIS
1	E	94	VAL
1	E	95	LEU
1	E	96	LYS
1	E	99	ARG
1	E	102	THR
1	E	103	ILE
1	E	104	GLN
1	E	105	THR
1	E	114	VAL
1	E	117	ASP
1	E	118	PHE
1	E	135	VAL
1	E	136	SER
1	E	139	THR
1	E	142	ASN
1	E	143	HIS
1	E	146	ILE
1	E	156	SER
1	E	157	THR
1	E	170	PHE

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Mol	Chain	Res	Type
1	E	173	LEU
1	E	183	ARG
1	E	185	ILE
1	E	187	LEU
1	E	189	HIS
1	E	199	ASP
1	E	200	LEU
1	E	201	THR
1	E	202	ASN
1	E	203	ASP
1	E	204	GLN
1	E	209	ILE
1	E	210	GLU
1	E	211	ILE
1	E	212	LEU
1	E	213	LYS
1	E	220	PHE
1	E	225	TYR
1	E	226	GLN
1	E	228	PHE
1	E	240	ILE
1	E	241	ARG
1	E	248	LEU
1	E	251	LEU
1	E	252	VAL
1	E	254	ASN
1	E	255	SER
1	E	258	LYS
1	E	261	SER
1	E	262	LEU
1	E	263	TYR
1	E	265	GLU
1	E	266	ARG
1	E	270	LEU
1	E	271	SER
1	E	273	MET
1	E	276	ASP
1	E	278	GLU
1	E	282	ARG
1	E	284	LEU
1	E	288	LYS
1	E	296	SER

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Mol	Chain	Res	Type
1	E	304	GLN
1	E	305	VAL
1	E	310	LEU
1	E	318	SER
1	E	325	GLU
1	E	327	ARG
1	E	328	THR
1	E	329	ARG
1	E	331	LEU
1	E	333	MET
1	E	336	GLU
1	E	337	LEU
1	E	339	LYS
1	E	340	VAL
1	E	342	SER
1	E	345	MET
1	E	347	GLU
1	E	348	ARG
1	E	353	LEU
1	E	355	ASN
1	E	362	TYR
1	E	374	ARG
1	E	379	VAL
1	E	381	LEU
1	E	386	ARG
1	E	387	MET
1	E	394	THR
1	E	396	ASN
1	E	398	GLN
1	E	400	VAL
1	E	404	PHE
1	E	408	MET
1	F	5	MET
1	F	7	GLN
1	F	8	LYS
1	F	9	VAL
1	F	10	ASP
1	F	12	TYR
1	F	15	ASP
1	F	21	MET
1	F	23	ARG
1	F	39	LEU

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Mol	Chain	Res	Type
1	F	43	GLU
1	F	44	ASP
1	F	47	ILE
1	F	50	LEU
1	F	51	GLN
1	F	57	GLU
1	F	59	ARG
1	F	60	LEU
1	F	63	GLN
1	F	65	HIS
1	F	70	TYR
1	F	77	ASN
1	F	80	ARG
1	F	87	LEU
1	F	91	ASP
1	F	92	HIS
1	F	94	VAL
1	F	95	LEU
1	F	96	LYS
1	F	99	ARG
1	F	102	THR
1	F	103	ILE
1	F	104	GLN
1	F	105	THR
1	F	114	VAL
1	F	117	ASP
1	F	118	PHE
1	F	135	VAL
1	F	136	SER
1	F	139	THR
1	F	142	ASN
1	F	143	HIS
1	F	146	ILE
1	F	156	SER
1	F	157	THR
1	F	170	PHE
1	F	173	LEU
1	F	183	ARG
1	F	185	ILE
1	F	187	LEU
1	F	189	HIS
1	F	199	ASP

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Mol	Chain	Res	Type
1	F	200	LEU
1	F	201	THR
1	F	202	ASN
1	F	203	ASP
1	F	204	GLN
1	F	209	ILE
1	F	210	GLU
1	F	211	ILE
1	F	212	LEU
1	F	213	LYS
1	F	220	PHE
1	F	225	TYR
1	F	226	GLN
1	F	228	PHE
1	F	240	ILE
1	F	241	ARG
1	F	248	LEU
1	F	251	LEU
1	F	252	VAL
1	F	254	ASN
1	F	255	SER
1	F	258	LYS
1	F	261	SER
1	F	262	LEU
1	F	263	TYR
1	F	265	GLU
1	F	266	ARG
1	F	270	LEU
1	F	271	SER
1	F	273	MET
1	F	276	ASP
1	F	278	GLU
1	F	282	ARG
1	F	284	LEU
1	F	288	LYS
1	F	296	SER
1	F	304	GLN
1	F	305	VAL
1	F	310	LEU
1	F	318	SER
1	F	325	GLU
1	F	327	ARG

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Mol	Chain	Res	Type
1	F	328	THR
1	F	329	ARG
1	F	331	LEU
1	F	333	MET
1	F	336	GLU
1	F	337	LEU
1	F	339	LYS
1	F	340	VAL
1	F	342	SER
1	F	345	MET
1	F	347	GLU
1	F	348	ARG
1	F	353	LEU
1	F	355	ASN
1	F	362	TYR
1	F	374	ARG
1	F	379	VAL
1	F	381	LEU
1	F	386	ARG
1	F	387	MET
1	F	394	THR
1	F	396	ASN
1	F	398	GLN
1	F	400	VAL
1	F	404	PHE
1	F	408	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	42	ASN
1	A	51	GLN
1	A	61	ASN
1	A	104	GLN
1	A	142	ASN
1	A	166	ASN
1	A	194	ASN
1	A	226	GLN
1	A	254	ASN
1	A	311	ASN
1	A	356	GLN

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Mol	Chain	Res	Type
1	A	398	GLN
1	B	7	GLN
1	B	42	ASN
1	B	51	GLN
1	B	61	ASN
1	B	104	GLN
1	B	142	ASN
1	B	166	ASN
1	B	194	ASN
1	B	226	GLN
1	B	254	ASN
1	B	311	ASN
1	B	356	GLN
1	B	398	GLN
1	C	7	GLN
1	C	42	ASN
1	C	51	GLN
1	C	61	ASN
1	C	104	GLN
1	C	142	ASN
1	C	166	ASN
1	C	194	ASN
1	C	226	GLN
1	C	254	ASN
1	C	311	ASN
1	C	356	GLN
1	C	398	GLN
1	D	7	GLN
1	D	42	ASN
1	D	51	GLN
1	D	61	ASN
1	D	104	GLN
1	D	142	ASN
1	D	166	ASN
1	D	194	ASN
1	D	226	GLN
1	D	254	ASN
1	D	311	ASN
1	D	356	GLN
1	D	398	GLN
1	E	7	GLN
1	E	42	ASN

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Mol	Chain	Res	Type
1	E	51	GLN
1	E	61	ASN
1	E	104	GLN
1	E	142	ASN
1	E	166	ASN
1	E	194	ASN
1	E	226	GLN
1	E	254	ASN
1	E	311	ASN
1	E	356	GLN
1	E	398	GLN
1	F	7	GLN
1	F	42	ASN
1	F	51	GLN
1	F	61	ASN
1	F	104	GLN
1	F	142	ASN
1	F	166	ASN
1	F	194	ASN
1	F	226	GLN
1	F	254	ASN
1	F	311	ASN
1	F	356	GLN
1	F	398	GLN

### 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 ⓘ

6 ligands are modelled in this entry.

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$
2	PLP	E	500	1	15,15,16	2.15	4 (26%)	20,22,23	2.36	4 (20%)
2	PLP	C	500	1	15,15,16	2.16	4 (26%)	20,22,23	2.36	4 (20%)
2	PLP	B	500	1	15,15,16	2.15	4 (26%)	20,22,23	2.35	4 (20%)
2	PLP	F	500	1	15,15,16	2.16	4 (26%)	20,22,23	2.35	4 (20%)
2	PLP	D	500	1	15,15,16	2.17	4 (26%)	20,22,23	2.37	4 (20%)
2	PLP	A	500	1	15,15,16	2.15	4 (26%)	20,22,23	2.35	4 (20%)

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
2	PLP	E	500	1	-	5/6/6/8	0/1/1/1
2	PLP	C	500	1	-	5/6/6/8	0/1/1/1
2	PLP	B	500	1	-	5/6/6/8	0/1/1/1
2	PLP	F	500	1	-	5/6/6/8	0/1/1/1
2	PLP	D	500	1	-	5/6/6/8	0/1/1/1
2	PLP	A	500	1	-	5/6/6/8	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	PLP	C4A-C4	6.28	1.64	1.51
2	C	500	PLP	C4A-C4	6.26	1.64	1.51
2	A	500	PLP	C4A-C4	6.24	1.64	1.51
2	F	500	PLP	C4A-C4	6.23	1.64	1.51
2	E	500	PLP	C4A-C4	6.22	1.64	1.51
2	B	500	PLP	C4A-C4	6.20	1.64	1.51
2	F	500	PLP	C3-C2	-2.88	1.38	1.40
2	D	500	PLP	C3-C2	-2.87	1.38	1.40
2	E	500	PLP	C3-C2	-2.84	1.38	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	500	PLP	C6-C5	-2.84	1.31	1.37
2	A	500	PLP	C3-C2	-2.83	1.38	1.40
2	B	500	PLP	C3-C2	-2.82	1.38	1.40
2	E	500	PLP	C6-C5	-2.81	1.31	1.37
2	D	500	PLP	C6-C5	-2.81	1.31	1.37
2	C	500	PLP	C6-C5	-2.81	1.31	1.37
2	A	500	PLP	C6-C5	-2.81	1.31	1.37
2	B	500	PLP	C6-C5	-2.80	1.31	1.37
2	C	500	PLP	C3-C2	-2.77	1.38	1.40
2	B	500	PLP	P-O3P	-2.11	1.46	1.54
2	D	500	PLP	P-O3P	-2.11	1.46	1.54
2	A	500	PLP	P-O3P	-2.11	1.46	1.54
2	C	500	PLP	P-O3P	-2.10	1.46	1.54
2	F	500	PLP	P-O3P	-2.10	1.46	1.54
2	E	500	PLP	P-O3P	-2.09	1.46	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	PLP	O4P-C5A-C5	8.03	124.66	109.35
2	E	500	PLP	O4P-C5A-C5	8.02	124.64	109.35
2	C	500	PLP	O4P-C5A-C5	8.02	124.62	109.35
2	F	500	PLP	O4P-C5A-C5	8.02	124.62	109.35
2	A	500	PLP	O4P-C5A-C5	8.00	124.60	109.35
2	B	500	PLP	O4P-C5A-C5	7.99	124.58	109.35
2	D	500	PLP	C5A-C5-C6	-3.66	113.35	119.37
2	E	500	PLP	C5A-C5-C6	-3.66	113.36	119.37
2	A	500	PLP	C5A-C5-C6	-3.64	113.39	119.37
2	B	500	PLP	C5A-C5-C6	-3.64	113.39	119.37
2	C	500	PLP	C5A-C5-C6	-3.64	113.39	119.37
2	F	500	PLP	C5A-C5-C6	-3.61	113.43	119.37
2	E	500	PLP	C6-C5-C4	2.69	120.28	118.16
2	D	500	PLP	C6-C5-C4	2.67	120.26	118.16
2	E	500	PLP	O3P-P-O1P	2.64	121.02	110.68
2	D	500	PLP	O3P-P-O1P	2.64	121.01	110.68
2	A	500	PLP	O3P-P-O1P	2.64	121.00	110.68
2	F	500	PLP	O3P-P-O1P	2.63	120.99	110.68
2	C	500	PLP	O3P-P-O1P	2.63	120.98	110.68
2	B	500	PLP	O3P-P-O1P	2.63	120.97	110.68
2	F	500	PLP	C6-C5-C4	2.61	120.22	118.16
2	A	500	PLP	C6-C5-C4	2.61	120.21	118.16
2	C	500	PLP	C6-C5-C4	2.61	120.21	118.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	PLP	C6-C5-C4	2.58	120.19	118.16

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	500	PLP	C4-C5-C5A-O4P
2	E	500	PLP	C6-C5-C5A-O4P
2	E	500	PLP	C5A-O4P-P-O1P
2	E	500	PLP	C5A-O4P-P-O2P
2	E	500	PLP	C5A-O4P-P-O3P
2	C	500	PLP	C4-C5-C5A-O4P
2	C	500	PLP	C6-C5-C5A-O4P
2	C	500	PLP	C5A-O4P-P-O1P
2	C	500	PLP	C5A-O4P-P-O2P
2	C	500	PLP	C5A-O4P-P-O3P
2	B	500	PLP	C4-C5-C5A-O4P
2	B	500	PLP	C6-C5-C5A-O4P
2	B	500	PLP	C5A-O4P-P-O1P
2	B	500	PLP	C5A-O4P-P-O2P
2	B	500	PLP	C5A-O4P-P-O3P
2	F	500	PLP	C4-C5-C5A-O4P
2	F	500	PLP	C6-C5-C5A-O4P
2	F	500	PLP	C5A-O4P-P-O1P
2	F	500	PLP	C5A-O4P-P-O2P
2	F	500	PLP	C5A-O4P-P-O3P
2	D	500	PLP	C4-C5-C5A-O4P
2	D	500	PLP	C6-C5-C5A-O4P
2	D	500	PLP	C5A-O4P-P-O1P
2	D	500	PLP	C5A-O4P-P-O2P
2	D	500	PLP	C5A-O4P-P-O3P
2	A	500	PLP	C4-C5-C5A-O4P
2	A	500	PLP	C6-C5-C5A-O4P
2	A	500	PLP	C5A-O4P-P-O1P
2	A	500	PLP	C5A-O4P-P-O2P
2	A	500	PLP	C5A-O4P-P-O3P

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	500	PLP	1	0
2	C	500	PLP	1	0
2	B	500	PLP	1	0
2	F	500	PLP	1	0
2	D	500	PLP	1	0
2	A	500	PLP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.