



# Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Aug 23, 2017 – 11:46 AM EDT

PDB ID : 2C9G  
EMDB ID: : EMD-1178  
Title : THE QUASI-ATOMIC MODEL OF THE ADENOVIRUS TYPE 3 PENTON  
BASE DODECAHEDRON  
Authors : Fuschiotti, P.; Schoehn, G.; Fender, P.; Fabry, C.M.S.; Hewat, E.A.;  
Chroboczek, J.; Ruigrok, R.W.H.; Conway, J.F.  
Deposited on : unknown  
Resolution : 9.30 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

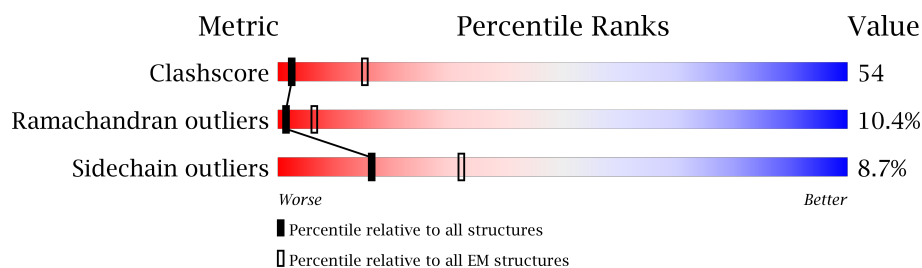
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 9.30 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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

Mol	Chain	Length	Quality of chain
1	A	523	
1	B	523	
1	C	523	
1	D	523	
1	E	523	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17840 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

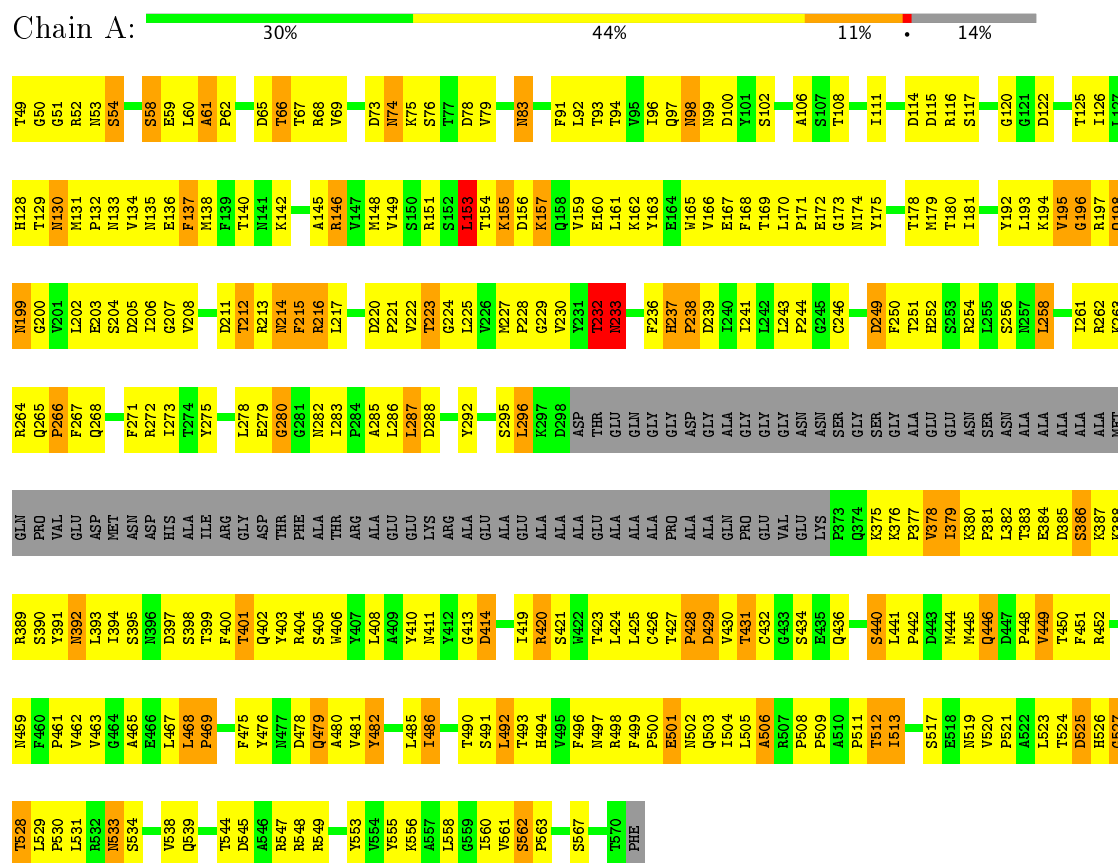
- Molecule 1 is a protein called PENTON PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	448	Total	C	N	O	S	0	1
			3568	2255	618	683	12		
1	B	448	Total	C	N	O	S	0	1
			3568	2255	618	683	12		
1	C	448	Total	C	N	O	S	0	1
			3568	2255	618	683	12		
1	D	448	Total	C	N	O	S	0	1
			3568	2255	618	683	12		
1	E	448	Total	C	N	O	S	0	1
			3568	2255	618	683	12		

### 3 Residue-property plots

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

#### • Molecule 1: PENTON PROTEIN







## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	1849	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	AMPLITUDE, PHASE	Depositor
Microscope	JEOL 2010F	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	51020	Depositor
Image detector	KODAK SO-163 FILM	Depositor

## 5 Model quality [i](#)

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

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.57	0/3652	0.81	2/4971 (0.0%)
1	B	0.57	0/3652	0.81	2/4971 (0.0%)
1	C	0.57	0/3652	0.81	2/4971 (0.0%)
1	D	0.57	0/3652	0.81	2/4971 (0.0%)
1	E	0.57	0/3652	0.81	2/4971 (0.0%)
All	All	0.57	0/18260	0.81	10/24855 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	E	207	GLY	N-CA-C	5.62	127.14	113.10
1	D	207	GLY	N-CA-C	5.60	127.10	113.10
1	A	207	GLY	N-CA-C	5.58	127.06	113.10
1	C	207	GLY	N-CA-C	5.58	127.06	113.10
1	B	207	GLY	N-CA-C	5.58	127.06	113.10
1	C	153	LEU	CB-CG-CD2	5.37	120.13	111.00
1	D	153	LEU	CB-CG-CD2	5.36	120.12	111.00
1	A	153	LEU	CB-CG-CD2	5.36	120.11	111.00
1	B	153	LEU	CB-CG-CD2	5.33	120.06	111.00
1	E	153	LEU	CB-CG-CD2	5.33	120.05	111.00

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	3568	0	3498	414	0
1	B	3568	0	3498	421	0
1	C	3568	0	3498	421	0
1	D	3568	0	3498	424	0
1	E	3568	0	3498	422	0
All	All	17840	0	17490	1895	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 54.

All (1895) 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:B:452:ARG:HH21	1:C:99:ASN:HB3	1.14	1.13
1:C:452:ARG:HH21	1:D:99:ASN:HB3	1.14	1.11
1:D:452:ARG:HH21	1:E:99:ASN:HB3	1.14	1.10
1:A:99:ASN:HB3	1:E:452:ARG:HH21	1.14	1.07
1:A:452:ARG:HH21	1:B:99:ASN:HB3	1.14	1.06
1:D:68:ARG:HG2	1:D:68:ARG:HH11	1.25	1.02
1:A:68:ARG:HG2	1:A:68:ARG:HH11	1.25	1.01
1:E:68:ARG:HG2	1:E:68:ARG:HH11	1.25	0.99
1:B:68:ARG:HG2	1:B:68:ARG:HH11	1.25	0.98
1:C:68:ARG:HG2	1:C:68:ARG:HH11	1.25	0.97
1:C:452:ARG:NH2	1:D:99:ASN:HB3	1.86	0.91
1:B:278:LEU:HD23	1:B:419:ILE:HD12	1.53	0.91
1:A:278:LEU:HD23	1:A:419:ILE:HD12	1.53	0.91
1:A:99:ASN:HB3	1:E:452:ARG:NH2	1.86	0.91
1:B:292:TYR:HA	1:B:377:PRO:CG	2.01	0.90
1:C:292:TYR:HA	1:C:377:PRO:CG	2.01	0.90
1:A:452:ARG:NH2	1:B:99:ASN:HB3	1.86	0.90
1:E:278:LEU:HD23	1:E:419:ILE:HD12	1.53	0.90
1:D:292:TYR:HA	1:D:377:PRO:CG	2.02	0.90
1:E:292:TYR:HA	1:E:377:PRO:CG	2.01	0.90
1:B:452:ARG:NH2	1:C:99:ASN:HB3	1.86	0.90
1:B:295:SER:HB3	1:B:377:PRO:HG3	1.51	0.90
1:C:376:LYS:HB3	1:C:377:PRO:HD2	1.55	0.89
1:D:451:PHE:HD2	1:D:461:PRO:HA	1.38	0.89
1:B:68:ARG:HH12	1:B:562:SER:HB3	1.38	0.89
1:C:295:SER:HB3	1:C:377:PRO:HG3	1.51	0.89
1:D:452:ARG:NH2	1:E:99:ASN:HB3	1.86	0.89
1:B:376:LYS:HB3	1:B:377:PRO:HD2	1.55	0.89
1:D:295:SER:HB3	1:D:377:PRO:HG3	1.51	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:LYS:HB3	1:D:377:PRO:HD2	1.54	0.89
1:D:68:ARG:HH12	1:D:562:SER:HB3	1.38	0.89
1:C:451:PHE:HD2	1:C:461:PRO:HA	1.38	0.89
1:D:278:LEU:HD23	1:D:419:ILE:HD12	1.53	0.89
1:A:295:SER:HB3	1:A:377:PRO:HG3	1.51	0.89
1:E:295:SER:HB3	1:E:377:PRO:HG3	1.50	0.88
1:A:451:PHE:HD2	1:A:461:PRO:HA	1.38	0.88
1:C:278:LEU:HD23	1:C:419:ILE:HD12	1.53	0.88
1:A:292:TYR:HA	1:A:377:PRO:CG	2.02	0.88
1:A:68:ARG:HH12	1:A:562:SER:HB3	1.38	0.88
1:E:376:LYS:HB3	1:E:377:PRO:HD2	1.55	0.88
1:E:451:PHE:HD2	1:E:461:PRO:HA	1.38	0.88
1:A:376:LYS:HB3	1:A:377:PRO:HD2	1.54	0.87
1:C:68:ARG:HH12	1:C:562:SER:HB3	1.38	0.87
1:E:68:ARG:HH12	1:E:562:SER:HB3	1.38	0.87
1:B:262:ARG:NH1	1:C:130:ASN:HD22	1.73	0.87
1:B:211:ASP:HA	1:B:508:PRO:CG	2.05	0.87
1:A:130:ASN:HD22	1:E:262:ARG:NH1	1.73	0.86
1:A:52:ARG:HB3	1:A:117:SER:OG	1.75	0.86
1:D:83:ASN:HD22	1:D:91:PHE:HB2	1.40	0.86
1:D:504:ILE:HG22	1:D:505:LEU:HD23	1.57	0.86
1:E:52:ARG:HB3	1:E:117:SER:OG	1.75	0.86
1:B:504:ILE:HG22	1:B:505:LEU:HD23	1.57	0.86
1:C:211:ASP:HA	1:C:508:PRO:CG	2.05	0.86
1:E:504:ILE:HG22	1:E:505:LEU:HD23	1.57	0.86
1:E:211:ASP:HA	1:E:508:PRO:CG	2.05	0.86
1:D:262:ARG:NH1	1:E:130:ASN:HD22	1.73	0.86
1:B:451:PHE:HD2	1:B:461:PRO:HA	1.38	0.85
1:A:262:ARG:NH1	1:B:130:ASN:HD22	1.74	0.85
1:A:211:ASP:HA	1:A:508:PRO:CG	2.05	0.85
1:A:83:ASN:HD22	1:A:91:PHE:HB2	1.40	0.85
1:C:52:ARG:HB3	1:C:117:SER:OG	1.75	0.85
1:D:211:ASP:HA	1:D:508:PRO:CG	2.05	0.85
1:B:193:LEU:HD11	1:B:498:ARG:HH12	1.41	0.85
1:C:58:SER:O	1:C:60:LEU:N	2.09	0.85
1:B:52:ARG:HB3	1:B:117:SER:OG	1.75	0.85
1:C:262:ARG:NH1	1:D:130:ASN:HD22	1.73	0.85
1:B:58:SER:O	1:B:60:LEU:N	2.09	0.85
1:B:83:ASN:HD22	1:B:91:PHE:HB2	1.40	0.85
1:C:504:ILE:HG22	1:C:505:LEU:HD23	1.57	0.85
1:E:83:ASN:HD22	1:E:91:PHE:HB2	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:ILE:HG22	1:A:505:LEU:HD23	1.58	0.84
1:C:83:ASN:HD22	1:C:91:PHE:HB2	1.40	0.84
1:D:52:ARG:HB3	1:D:117:SER:OG	1.75	0.84
1:E:58:SER:O	1:E:60:LEU:N	2.09	0.84
1:D:178:THR:HG21	1:D:511:PRO:HD2	1.60	0.84
1:D:58:SER:O	1:D:60:LEU:N	2.09	0.84
1:E:156:ASP:O	1:E:157:LYS:HG3	1.78	0.84
1:D:193:LEU:HD11	1:D:498:ARG:HH12	1.41	0.84
1:C:178:THR:HG21	1:C:511:PRO:HD2	1.60	0.84
1:A:58:SER:O	1:A:60:LEU:N	2.09	0.84
1:A:193:LEU:HD11	1:A:498:ARG:HH12	1.41	0.83
1:C:193:LEU:HD11	1:C:498:ARG:HH12	1.41	0.83
1:A:156:ASP:O	1:A:157:LYS:HG3	1.78	0.83
1:C:156:ASP:O	1:C:157:LYS:HG3	1.78	0.83
1:D:468:LEU:HD12	1:D:469:PRO:HD2	1.59	0.83
1:C:49:THR:HG23	1:C:53:ASN:OD1	1.79	0.83
1:B:178:THR:HG21	1:B:511:PRO:HD2	1.59	0.83
1:D:156:ASP:O	1:D:157:LYS:HG3	1.78	0.83
1:E:193:LEU:HD11	1:E:498:ARG:HH12	1.41	0.83
1:E:49:THR:HG23	1:E:53:ASN:OD1	1.79	0.83
1:E:178:THR:HG21	1:E:511:PRO:HD2	1.60	0.82
1:B:156:ASP:O	1:B:157:LYS:HG3	1.78	0.82
1:E:468:LEU:HD12	1:E:469:PRO:HD2	1.59	0.82
1:D:49:THR:HG23	1:D:53:ASN:OD1	1.79	0.82
1:B:49:THR:HG23	1:B:53:ASN:OD1	1.79	0.82
1:A:49:THR:HG23	1:A:53:ASN:OD1	1.79	0.82
1:C:468:LEU:HD12	1:C:469:PRO:HD2	1.60	0.82
1:D:544:THR:CG2	1:D:548:ARG:HA	2.10	0.82
1:B:468:LEU:HD12	1:B:469:PRO:HD2	1.60	0.82
1:A:178:THR:HG21	1:A:511:PRO:HD2	1.60	0.81
1:A:384:GLU:HG2	1:A:390:SER:HA	1.62	0.81
1:A:468:LEU:HD12	1:A:469:PRO:HD2	1.59	0.81
1:B:544:THR:CG2	1:B:548:ARG:HA	2.10	0.81
1:C:544:THR:CG2	1:C:548:ARG:HA	2.10	0.81
1:C:68:ARG:HG2	1:C:68:ARG:NH1	1.92	0.81
1:A:544:THR:CG2	1:A:548:ARG:HA	2.10	0.81
1:B:384:GLU:HG2	1:B:390:SER:HA	1.62	0.80
1:E:544:THR:CG2	1:E:548:ARG:HA	2.10	0.80
1:C:384:GLU:HG2	1:C:390:SER:HA	1.62	0.80
1:B:68:ARG:HG2	1:B:68:ARG:NH1	1.92	0.80
1:E:384:GLU:HG2	1:E:390:SER:HA	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:HIS:CD2	1:C:425:LEU:HD11	2.18	0.79
1:D:389:ARG:HD3	1:D:502:ASN:HD22	1.47	0.79
1:A:68:ARG:HG2	1:A:68:ARG:NH1	1.92	0.79
1:D:214:ASN:HD22	1:D:214:ASN:C	1.86	0.79
1:D:237:HIS:CD2	1:D:425:LEU:HD11	2.18	0.79
1:E:237:HIS:CD2	1:E:425:LEU:HD11	2.18	0.79
1:B:237:HIS:CD2	1:B:425:LEU:HD11	2.17	0.79
1:D:384:GLU:HG2	1:D:390:SER:HA	1.62	0.79
1:A:214:ASN:HD22	1:A:214:ASN:C	1.86	0.79
1:A:237:HIS:CD2	1:A:425:LEU:HD11	2.18	0.78
1:E:214:ASN:HD22	1:E:214:ASN:C	1.86	0.78
1:B:214:ASN:C	1:B:214:ASN:HD22	1.86	0.78
1:B:389:ARG:HD3	1:B:502:ASN:HD22	1.47	0.78
1:A:154:THR:OG1	1:A:160:GLU:HB2	1.84	0.77
1:E:154:THR:OG1	1:E:160:GLU:HB2	1.84	0.77
1:B:154:THR:OG1	1:B:160:GLU:HB2	1.84	0.77
1:C:214:ASN:C	1:C:214:ASN:HD22	1.86	0.77
1:C:379:ILE:O	1:C:381:PRO:HD3	1.85	0.77
1:E:389:ARG:HD3	1:E:502:ASN:HD22	1.47	0.77
1:A:379:ILE:O	1:A:381:PRO:HD3	1.85	0.77
1:D:154:THR:OG1	1:D:160:GLU:HB2	1.84	0.77
1:A:389:ARG:HD3	1:A:502:ASN:HD22	1.48	0.77
1:C:389:ARG:HD3	1:C:502:ASN:HD22	1.47	0.77
1:B:211:ASP:HA	1:B:508:PRO:HG3	1.67	0.77
1:C:154:THR:OG1	1:C:160:GLU:HB2	1.84	0.77
1:C:211:ASP:HA	1:C:508:PRO:HG3	1.67	0.77
1:A:403:TYR:CE1	1:A:504:ILE:HG21	2.21	0.76
1:C:403:TYR:CE1	1:C:504:ILE:HG21	2.21	0.76
1:D:292:TYR:HA	1:D:377:PRO:HG2	1.67	0.76
1:D:403:TYR:CE1	1:D:504:ILE:HG21	2.21	0.76
1:E:379:ILE:O	1:E:381:PRO:HD3	1.85	0.76
1:A:211:ASP:HA	1:A:508:PRO:HG3	1.67	0.76
1:B:403:TYR:CE1	1:B:504:ILE:HG21	2.21	0.76
1:B:379:ILE:O	1:B:381:PRO:HD3	1.85	0.76
1:C:292:TYR:HA	1:C:377:PRO:HG2	1.67	0.76
1:E:292:TYR:HA	1:E:377:PRO:HG2	1.67	0.76
1:C:475:PHE:O	1:C:513:ILE:HA	1.87	0.76
1:B:292:TYR:HA	1:B:377:PRO:HG2	1.67	0.75
1:D:379:ILE:O	1:D:381:PRO:HD3	1.85	0.75
1:E:403:TYR:CE1	1:E:504:ILE:HG21	2.21	0.75
1:C:68:ARG:NH1	1:C:562:SER:HB3	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:PHE:O	1:B:513:ILE:HA	1.87	0.75
1:D:452:ARG:HE	1:E:98:ASN:HD21	1.34	0.75
1:B:451:PHE:CD2	1:B:461:PRO:HA	2.22	0.75
1:D:211:ASP:HA	1:D:508:PRO:HG3	1.67	0.75
1:E:475:PHE:O	1:E:513:ILE:HA	1.87	0.75
1:A:68:ARG:NH1	1:A:562:SER:HB3	2.01	0.75
1:E:211:ASP:HA	1:E:508:PRO:HG3	1.67	0.75
1:D:451:PHE:CD2	1:D:461:PRO:HA	2.22	0.74
1:D:68:ARG:NH1	1:D:562:SER:HB3	2.01	0.74
1:E:68:ARG:NH1	1:E:562:SER:HB3	2.01	0.74
1:A:292:TYR:HA	1:A:377:PRO:HG2	1.67	0.74
1:B:145:ALA:HB3	1:B:168:PHE:HE1	1.53	0.74
1:B:68:ARG:NH1	1:B:562:SER:HB3	2.01	0.74
1:C:295:SER:O	1:C:296:LEU:HB2	1.88	0.74
1:C:451:PHE:CD2	1:C:461:PRO:HA	2.22	0.74
1:E:68:ARG:HG2	1:E:68:ARG:NH1	1.92	0.74
1:E:403:TYR:HD1	1:E:504:ILE:HD13	1.52	0.74
1:A:403:TYR:HD1	1:A:504:ILE:HD13	1.52	0.74
1:A:475:PHE:O	1:A:513:ILE:HA	1.87	0.74
1:C:142:LYS:HG2	1:C:169:THR:HG22	1.70	0.74
1:D:475:PHE:O	1:D:513:ILE:HA	1.86	0.74
1:B:295:SER:O	1:B:296:LEU:HB2	1.88	0.74
1:E:295:SER:O	1:E:296:LEU:HB2	1.88	0.74
1:C:145:ALA:HB3	1:C:168:PHE:HE1	1.53	0.74
1:C:249:ASP:C	1:C:249:ASP:OD1	2.26	0.74
1:D:142:LYS:HG2	1:D:169:THR:HG22	1.70	0.74
1:B:452:ARG:HE	1:C:98:ASN:HD21	1.34	0.73
1:B:243:LEU:HD21	1:B:403:TYR:CE2	2.23	0.73
1:D:249:ASP:C	1:D:249:ASP:OD1	2.26	0.73
1:D:68:ARG:HG2	1:D:68:ARG:NH1	1.92	0.73
1:E:451:PHE:CD2	1:E:461:PRO:HA	2.22	0.73
1:A:145:ALA:HB3	1:A:168:PHE:HE1	1.53	0.73
1:B:403:TYR:HD1	1:B:504:ILE:HD13	1.52	0.73
1:D:243:LEU:HD21	1:D:403:TYR:CE2	2.24	0.73
1:A:249:ASP:OD1	1:A:249:ASP:C	2.26	0.73
1:A:452:ARG:HE	1:B:98:ASN:HD21	1.34	0.73
1:C:403:TYR:HD1	1:C:504:ILE:HD13	1.52	0.73
1:C:452:ARG:HE	1:D:98:ASN:HD21	1.34	0.73
1:D:468:LEU:CD1	1:D:469:PRO:HD2	2.19	0.73
1:A:142:LYS:HG2	1:A:169:THR:HG22	1.70	0.73
1:A:295:SER:O	1:A:296:LEU:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:LEU:HD21	1:C:403:TYR:CE2	2.23	0.73
1:A:244:PRO:HA	1:A:275:TYR:CD2	2.24	0.73
1:D:295:SER:O	1:D:296:LEU:HB2	1.88	0.73
1:D:403:TYR:HD1	1:D:504:ILE:HD13	1.52	0.73
1:E:148:MET:HA	1:E:163:TYR:HD2	1.54	0.73
1:A:98:ASN:HD21	1:E:452:ARG:HE	1.34	0.72
1:D:244:PRO:HA	1:D:275:TYR:CD2	2.24	0.72
1:D:544:THR:HG22	1:D:548:ARG:HA	1.71	0.72
1:A:468:LEU:CD1	1:A:469:PRO:HD2	2.19	0.72
1:B:249:ASP:C	1:B:249:ASP:OD1	2.27	0.72
1:E:145:ALA:HB3	1:E:168:PHE:HE1	1.53	0.72
1:A:197:ARG:HG3	1:A:198:GLN:N	2.05	0.72
1:A:243:LEU:HD21	1:A:403:TYR:CE2	2.23	0.72
1:B:142:LYS:HG2	1:B:169:THR:HG22	1.70	0.72
1:B:148:MET:HA	1:B:163:TYR:HD2	1.54	0.72
1:B:544:THR:HG22	1:B:548:ARG:HA	1.71	0.72
1:D:145:ALA:HB3	1:D:168:PHE:HE1	1.53	0.72
1:E:142:LYS:HG2	1:E:169:THR:HG22	1.70	0.72
1:A:451:PHE:CD2	1:A:461:PRO:HA	2.22	0.72
1:E:197:ARG:HG3	1:E:198:GLN:N	2.05	0.72
1:E:249:ASP:OD1	1:E:249:ASP:C	2.26	0.72
1:B:244:PRO:HA	1:B:275:TYR:CD2	2.24	0.72
1:E:243:LEU:HD21	1:E:403:TYR:CE2	2.23	0.72
1:E:244:PRO:HA	1:E:275:TYR:CD2	2.24	0.72
1:B:468:LEU:CD1	1:B:469:PRO:HD2	2.19	0.72
1:D:148:MET:HA	1:D:163:TYR:HD2	1.54	0.72
1:E:468:LEU:CD1	1:E:469:PRO:HD2	2.19	0.72
1:C:148:MET:HA	1:C:163:TYR:HD2	1.54	0.71
1:C:244:PRO:HA	1:C:275:TYR:CD2	2.24	0.71
1:A:544:THR:HG22	1:A:548:ARG:HA	1.70	0.71
1:C:544:THR:HG22	1:C:548:ARG:HA	1.70	0.71
1:E:544:THR:HG22	1:E:548:ARG:HA	1.71	0.71
1:A:436:GLN:HE22	1:B:74:ASN:ND2	1.88	0.71
1:C:468:LEU:CD1	1:C:469:PRO:HD2	2.19	0.71
1:D:197:ARG:HG3	1:D:198:GLN:N	2.05	0.71
1:A:419:ILE:HG22	1:A:423:THR:CG2	2.21	0.71
1:B:419:ILE:HG22	1:B:423:THR:CG2	2.21	0.71
1:C:197:ARG:HG3	1:C:198:GLN:N	2.05	0.71
1:D:436:GLN:HE22	1:E:74:ASN:ND2	1.88	0.71
1:A:243:LEU:HD21	1:A:403:TYR:CD2	2.26	0.71
1:A:74:ASN:ND2	1:E:436:GLN:HE22	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:MET:HA	1:A:163:TYR:HD2	1.54	0.71
1:B:197:ARG:HG3	1:B:198:GLN:N	2.05	0.71
1:C:419:ILE:HG22	1:C:423:THR:CG2	2.21	0.71
1:E:419:ILE:HG22	1:E:423:THR:CG2	2.21	0.71
1:C:436:GLN:HE22	1:D:74:ASN:ND2	1.89	0.71
1:C:243:LEU:HD21	1:C:403:TYR:CD2	2.26	0.70
1:E:249:ASP:HB2	1:E:272:ARG:HG2	1.73	0.70
1:D:419:ILE:HG22	1:D:423:THR:CG2	2.21	0.70
1:B:436:GLN:HE22	1:C:74:ASN:ND2	1.89	0.70
1:C:122:ASP:OD1	1:C:528:THR:HB	1.91	0.70
1:C:217:LEU:HB2	1:C:232:THR:HG21	1.73	0.70
1:E:243:LEU:HD21	1:E:403:TYR:CD2	2.26	0.70
1:A:122:ASP:OD1	1:A:528:THR:HB	1.91	0.70
1:B:160:GLU:OE2	1:B:162:LYS:HE3	1.91	0.70
1:D:249:ASP:HB2	1:D:272:ARG:HG2	1.73	0.70
1:B:122:ASP:OD1	1:B:528:THR:HB	1.91	0.70
1:A:160:GLU:OE2	1:A:162:LYS:HE3	1.91	0.70
1:B:215:PHE:CE1	1:B:241:ILE:HD11	2.27	0.70
1:D:217:LEU:HB2	1:D:232:THR:HG21	1.73	0.70
1:D:243:LEU:HD21	1:D:403:TYR:CD2	2.26	0.70
1:E:160:GLU:OE2	1:E:162:LYS:HE3	1.91	0.70
1:C:160:GLU:OE2	1:C:162:LYS:HE3	1.91	0.70
1:D:122:ASP:OD1	1:D:528:THR:HB	1.91	0.70
1:E:217:LEU:HB2	1:E:232:THR:HG21	1.73	0.70
1:A:419:ILE:HG22	1:A:423:THR:HG21	1.75	0.69
1:B:249:ASP:HB2	1:B:272:ARG:HG2	1.73	0.69
1:B:243:LEU:HD21	1:B:403:TYR:CD2	2.26	0.69
1:A:249:ASP:HB2	1:A:272:ARG:HG2	1.73	0.69
1:C:444:MET:HG2	1:C:444:MET:O	1.92	0.69
1:D:215:PHE:CE1	1:D:241:ILE:HD11	2.27	0.69
1:C:215:PHE:CE1	1:C:241:ILE:HD11	2.27	0.69
1:C:249:ASP:HB2	1:C:272:ARG:HG2	1.73	0.69
1:E:122:ASP:OD1	1:E:528:THR:HB	1.91	0.69
1:B:419:ILE:HG22	1:B:423:THR:HG21	1.75	0.69
1:D:419:ILE:HG22	1:D:423:THR:HG21	1.75	0.69
1:B:444:MET:O	1:B:444:MET:HG2	1.92	0.69
1:A:215:PHE:CE1	1:A:241:ILE:HD11	2.27	0.69
1:C:441:LEU:HD12	1:C:445:MET:HE1	1.75	0.69
1:D:160:GLU:OE2	1:D:162:LYS:HE3	1.91	0.69
1:E:512:THR:O	1:E:513:ILE:HB	1.93	0.69
1:A:217:LEU:HB2	1:A:232:THR:HG21	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:LEU:HB2	1:B:232:THR:HG21	1.73	0.68
1:D:444:MET:O	1:D:444:MET:HG2	1.92	0.68
1:A:142:LYS:HD3	1:A:167:GLU:OE2	1.93	0.68
1:E:215:PHE:CE1	1:E:241:ILE:HD11	2.27	0.68
1:E:444:MET:O	1:E:444:MET:HG2	1.92	0.68
1:D:142:LYS:HD3	1:D:167:GLU:OE2	1.93	0.68
1:D:512:THR:O	1:D:513:ILE:HB	1.93	0.68
1:E:142:LYS:HD3	1:E:167:GLU:OE2	1.93	0.68
1:A:512:THR:O	1:A:513:ILE:HB	1.93	0.68
1:E:278:LEU:HD22	1:E:406:TRP:HA	1.76	0.68
1:C:419:ILE:HG22	1:C:423:THR:HG21	1.75	0.68
1:A:444:MET:O	1:A:444:MET:HG2	1.92	0.68
1:B:142:LYS:HD3	1:B:167:GLU:OE2	1.94	0.68
1:E:419:ILE:HG22	1:E:423:THR:HG21	1.75	0.68
1:A:146:ARG:O	1:A:246:CYS:HB2	1.94	0.68
1:B:149:VAL:HG23	1:B:195:VAL:HG11	1.76	0.68
1:B:512:THR:O	1:B:513:ILE:HB	1.93	0.68
1:A:386:SER:O	1:A:387:LYS:HB2	1.94	0.67
1:D:217:LEU:HB2	1:D:232:THR:CG2	2.25	0.67
1:E:149:VAL:HG23	1:E:195:VAL:HG11	1.76	0.67
1:C:217:LEU:HB2	1:C:232:THR:CG2	2.25	0.67
1:D:149:VAL:HG23	1:D:195:VAL:HG11	1.76	0.67
1:E:217:LEU:HB2	1:E:232:THR:CG2	2.25	0.67
1:A:278:LEU:HD22	1:A:406:TRP:HA	1.76	0.67
1:D:278:LEU:HD22	1:D:406:TRP:HA	1.76	0.67
1:A:149:VAL:HG23	1:A:195:VAL:HG11	1.76	0.67
1:C:142:LYS:HD3	1:C:167:GLU:OE2	1.94	0.67
1:C:227:MET:HB2	1:C:228:PRO:HD3	1.76	0.67
1:C:512:THR:O	1:C:513:ILE:HB	1.93	0.67
1:C:83:ASN:N	1:C:83:ASN:OD1	2.27	0.67
1:D:386:SER:O	1:D:387:LYS:HB2	1.94	0.67
1:E:386:SER:O	1:E:387:LYS:HB2	1.94	0.67
1:B:217:LEU:HB2	1:B:232:THR:CG2	2.25	0.67
1:A:227:MET:HB2	1:A:228:PRO:HD3	1.76	0.67
1:B:227:MET:HB2	1:B:228:PRO:HD3	1.76	0.67
1:D:227:MET:HB2	1:D:228:PRO:HD3	1.76	0.67
1:C:452:ARG:HH22	1:D:99:ASN:HD22	1.43	0.67
1:D:146:ARG:O	1:D:246:CYS:HB2	1.94	0.67
1:C:146:ARG:O	1:C:246:CYS:HB2	1.94	0.66
1:D:468:LEU:HD12	1:D:469:PRO:CD	2.25	0.66
1:E:146:ARG:O	1:E:246:CYS:HB2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:CYS:HA	1:B:132:PRO:HG3	1.77	0.66
1:B:468:LEU:HD12	1:B:469:PRO:CD	2.26	0.66
1:C:426:CYS:HA	1:D:132:PRO:HG3	1.77	0.66
1:C:430:VAL:HG21	1:C:517:SER:N	2.10	0.66
1:D:452:ARG:HH22	1:E:99:ASN:HD22	1.43	0.66
1:B:278:LEU:HD22	1:B:406:TRP:HA	1.76	0.66
1:C:149:VAL:HG23	1:C:195:VAL:HG11	1.76	0.66
1:B:146:ARG:O	1:B:246:CYS:HB2	1.94	0.66
1:B:386:SER:O	1:B:387:LYS:HB2	1.94	0.66
1:D:441:LEU:HD12	1:D:445:MET:HE1	1.77	0.66
1:A:217:LEU:HB2	1:A:232:THR:CG2	2.25	0.66
1:A:468:LEU:HD12	1:A:469:PRO:CD	2.26	0.66
1:C:278:LEU:HD22	1:C:406:TRP:HA	1.76	0.66
1:C:386:SER:O	1:C:387:LYS:HB2	1.94	0.66
1:D:430:VAL:HG21	1:D:517:SER:N	2.11	0.66
1:A:452:ARG:HH22	1:B:99:ASN:HD22	1.43	0.66
1:B:426:CYS:HA	1:C:132:PRO:HG3	1.77	0.66
1:C:468:LEU:HD12	1:C:469:PRO:CD	2.26	0.66
1:E:227:MET:HB2	1:E:228:PRO:HD3	1.76	0.66
1:A:99:ASN:HD22	1:E:452:ARG:HH22	1.43	0.65
1:A:132:PRO:HG3	1:E:426:CYS:HA	1.77	0.65
1:B:430:VAL:HG21	1:B:517:SER:N	2.10	0.65
1:B:393:LEU:HD12	1:B:393:LEU:N	2.12	0.65
1:D:60:LEU:O	1:D:61:ALA:HB3	1.97	0.65
1:E:430:VAL:HG21	1:E:517:SER:N	2.11	0.65
1:D:193:LEU:HD11	1:D:498:ARG:NH1	2.12	0.65
1:D:426:CYS:HA	1:E:132:PRO:HG3	1.77	0.65
1:A:393:LEU:N	1:A:393:LEU:HD12	2.12	0.65
1:A:430:VAL:HG21	1:A:517:SER:N	2.10	0.65
1:B:60:LEU:O	1:B:61:ALA:HB3	1.97	0.65
1:C:60:LEU:O	1:C:61:ALA:HB3	1.97	0.65
1:A:436:GLN:HE22	1:B:74:ASN:HD21	1.45	0.65
1:B:452:ARG:HH22	1:C:99:ASN:HD22	1.43	0.65
1:D:393:LEU:N	1:D:393:LEU:HD12	2.12	0.65
1:E:133:ASN:HB2	1:E:174:ASN:OD1	1.97	0.65
1:D:436:GLN:NE2	1:E:74:ASN:HD21	1.95	0.65
1:A:211:ASP:O	1:A:212:THR:HG22	1.97	0.64
1:C:193:LEU:HD11	1:C:498:ARG:NH1	2.12	0.64
1:C:211:ASP:O	1:C:212:THR:HG22	1.97	0.64
1:D:436:GLN:HE22	1:E:74:ASN:HD21	1.45	0.64
1:C:513:ILE:HG22	1:C:513:ILE:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:468:LEU:HD12	1:E:469:PRO:CD	2.26	0.64
1:C:393:LEU:N	1:C:393:LEU:HD12	2.12	0.64
1:E:60:LEU:O	1:E:61:ALA:HB3	1.97	0.64
1:B:436:GLN:NE2	1:C:74:ASN:HD21	1.95	0.64
1:E:393:LEU:HD12	1:E:393:LEU:N	2.12	0.64
1:B:278:LEU:O	1:B:404:ARG:HD3	1.98	0.64
1:B:436:GLN:HE22	1:C:74:ASN:HD21	1.46	0.64
1:E:513:ILE:HG22	1:E:513:ILE:O	1.97	0.64
1:D:513:ILE:HG22	1:D:513:ILE:O	1.97	0.64
1:C:436:GLN:NE2	1:D:74:ASN:HD21	1.96	0.64
1:A:133:ASN:HB2	1:A:174:ASN:OD1	1.97	0.64
1:E:278:LEU:O	1:E:404:ARG:HD3	1.98	0.64
1:E:493:THR:HG21	1:E:497:ASN:O	1.99	0.64
1:E:499:PHE:N	1:E:500:PRO:HD3	2.13	0.64
1:A:74:ASN:HD21	1:E:436:GLN:NE2	1.95	0.63
1:B:133:ASN:HB2	1:B:174:ASN:OD1	1.97	0.63
1:C:133:ASN:HB2	1:C:174:ASN:OD1	1.97	0.63
1:B:493:THR:HG21	1:B:497:ASN:O	1.99	0.63
1:B:513:ILE:HG22	1:B:513:ILE:O	1.97	0.63
1:A:436:GLN:NE2	1:B:74:ASN:HD21	1.95	0.63
1:C:499:PHE:N	1:C:500:PRO:HD3	2.13	0.63
1:C:436:GLN:HE22	1:D:74:ASN:HD21	1.45	0.63
1:B:211:ASP:O	1:B:212:THR:HG22	1.97	0.63
1:B:499:PHE:N	1:B:500:PRO:HD3	2.13	0.63
1:D:211:ASP:O	1:D:212:THR:HG22	1.97	0.63
1:D:278:LEU:O	1:D:404:ARG:HD3	1.98	0.63
1:D:499:PHE:N	1:D:500:PRO:HD3	2.13	0.63
1:E:441:LEU:HD12	1:E:445:MET:HE1	1.81	0.63
1:A:60:LEU:O	1:A:61:ALA:HB3	1.97	0.63
1:E:211:ASP:O	1:E:212:THR:HG22	1.97	0.63
1:C:493:THR:HG21	1:C:497:ASN:O	1.98	0.63
1:A:493:THR:HG21	1:A:497:ASN:O	1.98	0.63
1:C:278:LEU:O	1:C:404:ARG:HD3	1.98	0.63
1:D:133:ASN:HB2	1:D:174:ASN:OD1	1.97	0.63
1:A:134:VAL:HA	1:A:140:THR:OG1	1.99	0.63
1:E:134:VAL:HA	1:E:140:THR:OG1	1.99	0.63
1:E:148:MET:HA	1:E:163:TYR:CD2	2.34	0.63
1:E:83:ASN:OD1	1:E:83:ASN:N	2.26	0.63
1:A:499:PHE:N	1:A:500:PRO:HD3	2.13	0.62
1:B:193:LEU:HD11	1:B:498:ARG:NH1	2.12	0.62
1:D:134:VAL:HA	1:D:140:THR:OG1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:ILE:HG22	1:A:513:ILE:O	1.97	0.62
1:B:134:VAL:HA	1:B:140:THR:OG1	1.99	0.62
1:B:441:LEU:HD12	1:B:445:MET:HE1	1.79	0.62
1:D:148:MET:HA	1:D:163:TYR:CD2	2.34	0.62
1:D:544:THR:HG21	1:D:548:ARG:HD2	1.81	0.62
1:A:278:LEU:O	1:A:404:ARG:HD3	1.98	0.62
1:C:378:VAL:HG12	1:C:379:ILE:N	2.14	0.62
1:D:125:THR:HG23	1:D:524:THR:CG2	2.29	0.62
1:A:378:VAL:HG12	1:A:379:ILE:N	2.15	0.62
1:B:125:THR:HG23	1:B:524:THR:CG2	2.29	0.62
1:A:544:THR:HG21	1:A:548:ARG:HD2	1.81	0.62
1:D:258:LEU:O	1:D:258:LEU:HD12	2.00	0.62
1:E:544:THR:HG21	1:E:548:ARG:HD2	1.81	0.62
1:A:258:LEU:HD12	1:A:258:LEU:O	2.00	0.62
1:A:125:THR:HG23	1:A:524:THR:CG2	2.29	0.62
1:B:178:THR:CG2	1:B:511:PRO:HD2	2.29	0.62
1:B:544:THR:HG21	1:B:548:ARG:HD2	1.81	0.62
1:A:148:MET:HA	1:A:163:TYR:CD2	2.34	0.62
1:B:148:MET:HA	1:B:163:TYR:CD2	2.34	0.62
1:D:493:THR:HG21	1:D:497:ASN:O	1.99	0.62
1:B:125:THR:CG2	1:B:526:HIS:NE2	2.63	0.62
1:C:125:THR:HG23	1:C:524:THR:CG2	2.29	0.62
1:C:134:VAL:HA	1:C:140:THR:OG1	1.99	0.62
1:C:148:MET:HA	1:C:163:TYR:CD2	2.34	0.62
1:E:125:THR:HG23	1:E:524:THR:CG2	2.29	0.62
1:A:125:THR:CG2	1:A:526:HIS:NE2	2.63	0.62
1:B:60:LEU:O	1:B:60:LEU:HG	2.00	0.62
1:D:125:THR:CG2	1:D:526:HIS:NE2	2.63	0.61
1:E:378:VAL:HG12	1:E:379:ILE:N	2.15	0.61
1:B:394:ILE:HG23	1:B:398:SER:HB2	1.82	0.61
1:D:60:LEU:HG	1:D:60:LEU:O	2.00	0.61
1:E:125:THR:CG2	1:E:526:HIS:NE2	2.63	0.61
1:A:193:LEU:HD11	1:A:498:ARG:NH1	2.12	0.61
1:A:394:ILE:HG23	1:A:398:SER:HB2	1.82	0.61
1:E:220:ASP:OD1	1:E:222:VAL:HG12	2.00	0.61
1:B:220:ASP:OD1	1:B:222:VAL:HG12	2.00	0.61
1:D:394:ILE:HG23	1:D:398:SER:HB2	1.82	0.61
1:E:60:LEU:O	1:E:60:LEU:HG	2.00	0.61
1:B:378:VAL:HG12	1:B:379:ILE:N	2.15	0.61
1:C:220:ASP:OD1	1:C:222:VAL:HG12	2.00	0.61
1:E:444:MET:HB2	1:E:539:GLN:OE1	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:ASP:OD1	1:D:222:VAL:HG12	2.00	0.61
1:A:74:ASN:HD21	1:E:436:GLN:HE22	1.46	0.61
1:B:258:LEU:O	1:B:258:LEU:HD12	2.00	0.61
1:C:258:LEU:O	1:C:258:LEU:HD12	2.00	0.61
1:C:444:MET:HB2	1:C:539:GLN:OE1	2.00	0.61
1:C:394:ILE:HG23	1:C:398:SER:HB2	1.82	0.61
1:C:74:ASN:ND2	1:C:556:LYS:HZ1	1.98	0.61
1:D:178:THR:CG2	1:D:511:PRO:HD2	2.30	0.61
1:E:193:LEU:HD11	1:E:498:ARG:NH1	2.12	0.61
1:A:220:ASP:OD1	1:A:222:VAL:HG12	2.00	0.61
1:B:444:MET:HB2	1:B:539:GLN:OE1	2.01	0.61
1:C:125:THR:CG2	1:C:526:HIS:NE2	2.63	0.61
1:C:544:THR:HG21	1:C:548:ARG:HD2	1.81	0.61
1:D:378:VAL:HG12	1:D:379:ILE:N	2.15	0.61
1:C:178:THR:CG2	1:C:511:PRO:HD2	2.30	0.60
1:D:444:MET:HB2	1:D:539:GLN:OE1	2.01	0.60
1:E:258:LEU:O	1:E:258:LEU:HD12	2.00	0.60
1:C:440:SER:HB3	1:C:461:PRO:O	2.02	0.60
1:D:440:SER:HB3	1:D:461:PRO:O	2.01	0.60
1:A:263:LYS:NZ	1:A:268:GLN:HB2	2.16	0.60
1:A:383:THR:HG22	1:A:384:GLU:HG3	1.84	0.60
1:B:125:THR:HG21	1:B:526:HIS:NE2	2.17	0.60
1:B:394:ILE:HG23	1:B:395:SER:H	1.67	0.60
1:C:60:LEU:O	1:C:60:LEU:HG	2.00	0.60
1:E:263:LYS:NZ	1:E:268:GLN:HB2	2.16	0.60
1:B:425:LEU:HD23	1:C:172:GLU:HB3	1.83	0.60
1:D:125:THR:HG21	1:D:526:HIS:NE2	2.16	0.60
1:E:383:THR:HG22	1:E:384:GLU:HG3	1.83	0.60
1:A:125:THR:HG21	1:A:526:HIS:NE2	2.17	0.60
1:A:394:ILE:HG23	1:A:395:SER:H	1.67	0.60
1:B:220:ASP:HB2	1:B:227:MET:HG2	1.84	0.60
1:C:383:THR:HG22	1:C:384:GLU:HG3	1.84	0.60
1:E:394:ILE:HG23	1:E:395:SER:H	1.66	0.60
1:A:440:SER:HB3	1:A:461:PRO:O	2.02	0.60
1:A:60:LEU:O	1:A:60:LEU:HG	2.00	0.60
1:D:383:THR:HG22	1:D:384:GLU:HG3	1.84	0.60
1:A:444:MET:HB2	1:A:539:GLN:OE1	2.01	0.60
1:B:278:LEU:CD2	1:B:406:TRP:HA	2.32	0.60
1:E:125:THR:HG21	1:E:526:HIS:NE2	2.17	0.60
1:D:449:VAL:CG2	1:E:67:THR:HG21	2.32	0.60
1:A:220:ASP:HB2	1:A:227:MET:HG2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:VAL:CG2	1:B:67:THR:HG21	2.32	0.60
1:C:410:TYR:CD1	1:C:420:ARG:HA	2.37	0.60
1:A:172:GLU:HB3	1:E:425:LEU:HD23	1.83	0.60
1:A:436:GLN:NE2	1:B:556:LYS:HZ3	2.00	0.60
1:B:214:ASN:C	1:B:214:ASN:ND2	2.55	0.60
1:C:394:ILE:HG23	1:C:395:SER:H	1.67	0.60
1:C:243:LEU:HD11	1:C:403:TYR:HE2	1.67	0.60
1:C:449:VAL:CG2	1:D:67:THR:HG21	2.32	0.60
1:E:278:LEU:CD2	1:E:406:TRP:HA	2.32	0.60
1:A:425:LEU:HD23	1:B:172:GLU:HB3	1.84	0.59
1:C:389:ARG:NH1	1:C:389:ARG:HG2	2.17	0.59
1:D:389:ARG:HG2	1:D:389:ARG:NH1	2.17	0.59
1:D:278:LEU:CD2	1:D:406:TRP:HA	2.32	0.59
1:D:410:TYR:CD1	1:D:420:ARG:HA	2.37	0.59
1:D:425:LEU:HD23	1:E:172:GLU:HB3	1.84	0.59
1:A:67:THR:HG21	1:E:449:VAL:CG2	2.32	0.59
1:C:220:ASP:HB2	1:C:227:MET:HG2	1.84	0.59
1:E:282:ASN:HD21	1:E:404:ARG:HE	1.51	0.59
1:E:389:ARG:HG2	1:E:389:ARG:NH1	2.17	0.59
1:A:389:ARG:HG2	1:A:389:ARG:NH1	2.17	0.59
1:B:263:LYS:NZ	1:B:268:GLN:HB2	2.16	0.59
1:B:410:TYR:CD1	1:B:420:ARG:HA	2.37	0.59
1:D:214:ASN:C	1:D:214:ASN:ND2	2.55	0.59
1:D:220:ASP:HB2	1:D:227:MET:HG2	1.84	0.59
1:E:278:LEU:HD23	1:E:419:ILE:CD1	2.30	0.59
1:E:394:ILE:HG23	1:E:398:SER:HB2	1.82	0.59
1:E:440:SER:HB3	1:E:461:PRO:O	2.01	0.59
1:A:410:TYR:CD1	1:A:420:ARG:HA	2.37	0.59
1:B:449:VAL:CG2	1:C:67:THR:HG21	2.32	0.59
1:D:243:LEU:HD11	1:D:403:TYR:HE2	1.67	0.59
1:E:243:LEU:HD11	1:E:403:TYR:HE2	1.67	0.59
1:A:378:VAL:O	1:A:380:LYS:N	2.35	0.59
1:B:383:THR:HG22	1:B:384:GLU:HG3	1.83	0.59
1:E:378:VAL:O	1:E:380:LYS:N	2.36	0.59
1:E:410:TYR:CD1	1:E:420:ARG:HA	2.37	0.59
1:B:282:ASN:HD21	1:B:404:ARG:HE	1.50	0.59
1:C:378:VAL:O	1:C:380:LYS:N	2.36	0.59
1:D:243:LEU:CD2	1:D:403:TYR:CD2	2.86	0.59
1:B:243:LEU:CD2	1:B:403:TYR:CD2	2.86	0.59
1:C:263:LYS:NZ	1:C:268:GLN:HB2	2.16	0.59
1:C:425:LEU:HD23	1:D:172:GLU:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:GLY:O	1:B:399:THR:HB	2.03	0.59
1:C:125:THR:HG21	1:C:526:HIS:NE2	2.17	0.59
1:C:520:VAL:CG2	1:C:521:PRO:HD2	2.33	0.59
1:A:278:LEU:CD2	1:A:406:TRP:HA	2.32	0.59
1:A:178:THR:CG2	1:A:511:PRO:HD2	2.30	0.59
1:C:214:ASN:C	1:C:214:ASN:ND2	2.55	0.59
1:E:520:VAL:CG2	1:E:521:PRO:HD2	2.33	0.59
1:C:278:LEU:CD2	1:C:406:TRP:HA	2.32	0.59
1:D:287:LEU:HD23	1:D:287:LEU:C	2.24	0.59
1:A:197:ARG:HG3	1:A:198:GLN:CG	2.33	0.58
1:B:197:ARG:HG3	1:B:198:GLN:CG	2.33	0.58
1:B:243:LEU:HD11	1:B:403:TYR:HE2	1.67	0.58
1:C:243:LEU:CD2	1:C:403:TYR:CD2	2.86	0.58
1:C:282:ASN:HD21	1:C:404:ARG:HE	1.50	0.58
1:B:378:VAL:O	1:B:380:LYS:N	2.35	0.58
1:B:389:ARG:HG2	1:B:389:ARG:NH1	2.17	0.58
1:C:224:GLY:O	1:C:399:THR:HB	2.03	0.58
1:E:224:GLY:O	1:E:399:THR:HB	2.03	0.58
1:E:220:ASP:HB2	1:E:227:MET:HG2	1.84	0.58
1:B:278:LEU:HD23	1:B:419:ILE:CD1	2.30	0.58
1:C:197:ARG:HG3	1:C:198:GLN:CG	2.33	0.58
1:D:154:THR:HG22	1:D:155:LYS:N	2.19	0.58
1:D:263:LYS:NZ	1:D:268:GLN:HB2	2.16	0.58
1:D:394:ILE:HG23	1:D:395:SER:H	1.67	0.58
1:E:243:LEU:CD2	1:E:403:TYR:CD2	2.86	0.58
1:A:224:GLY:O	1:A:399:THR:HB	2.03	0.58
1:A:282:ASN:HD21	1:A:404:ARG:HE	1.50	0.58
1:B:154:THR:HG22	1:B:155:LYS:N	2.19	0.58
1:D:282:ASN:HD21	1:D:404:ARG:HE	1.50	0.58
1:E:154:THR:HG22	1:E:155:LYS:N	2.18	0.58
1:A:243:LEU:CD2	1:A:403:TYR:CD2	2.86	0.58
1:B:440:SER:HB3	1:B:461:PRO:O	2.02	0.58
1:C:278:LEU:HD23	1:C:419:ILE:CD1	2.30	0.58
1:C:287:LEU:C	1:C:287:LEU:HD23	2.24	0.58
1:E:178:THR:CG2	1:E:511:PRO:HD2	2.30	0.58
1:A:520:VAL:CG2	1:A:521:PRO:HD2	2.33	0.58
1:B:211:ASP:O	1:B:212:THR:CG2	2.52	0.58
1:C:410:TYR:HE2	1:D:172:GLU:OE1	1.87	0.58
1:D:211:ASP:O	1:D:212:THR:CG2	2.52	0.58
1:A:172:GLU:OE1	1:E:410:TYR:HE2	1.87	0.58
1:C:211:ASP:O	1:C:212:THR:CG2	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:ASN:ND2	1:E:214:ASN:C	2.55	0.58
1:A:278:LEU:HD23	1:A:419:ILE:CD1	2.30	0.58
1:C:494:HIS:C	1:C:496:PHE:H	2.07	0.58
1:E:211:ASP:O	1:E:212:THR:CG2	2.52	0.58
1:A:154:THR:HG22	1:A:155:LYS:N	2.19	0.58
1:A:211:ASP:O	1:A:212:THR:CG2	2.52	0.58
1:B:287:LEU:HD23	1:B:287:LEU:C	2.24	0.58
1:D:378:VAL:O	1:D:380:LYS:N	2.35	0.58
1:A:287:LEU:C	1:A:287:LEU:HD23	2.24	0.57
1:C:154:THR:HG22	1:C:155:LYS:N	2.18	0.57
1:A:243:LEU:HD11	1:A:403:TYR:HE2	1.67	0.57
1:A:282:ASN:ND2	1:A:404:ARG:HE	2.03	0.57
1:A:410:TYR:HE2	1:B:172:GLU:OE1	1.87	0.57
1:B:410:TYR:HE2	1:C:172:GLU:OE1	1.87	0.57
1:E:287:LEU:C	1:E:287:LEU:HD23	2.24	0.57
1:B:282:ASN:ND2	1:B:404:ARG:HE	2.03	0.57
1:C:479:GLN:O	1:C:479:GLN:HG2	2.05	0.57
1:D:197:ARG:HG3	1:D:198:GLN:CG	2.33	0.57
1:D:224:GLY:O	1:D:399:THR:HB	2.03	0.57
1:D:410:TYR:HE2	1:E:172:GLU:OE1	1.87	0.57
1:E:197:ARG:HG3	1:E:198:GLN:CG	2.33	0.57
1:B:520:VAL:CG2	1:B:521:PRO:HD2	2.33	0.57
1:D:403:TYR:CD1	1:D:504:ILE:HD13	2.39	0.57
1:A:233:ASN:O	1:A:233:ASN:CG	2.43	0.57
1:D:282:ASN:ND2	1:D:404:ARG:HE	2.03	0.57
1:D:482:TYR:CE1	1:D:486:ILE:HD12	2.40	0.57
1:D:520:VAL:CG2	1:D:521:PRO:HD2	2.33	0.57
1:A:441:LEU:HD12	1:A:445:MET:HE1	1.87	0.57
1:B:479:GLN:O	1:B:479:GLN:HG2	2.05	0.57
1:C:567:SER:HB2	1:D:49:THR:HG21	1.87	0.57
1:B:482:TYR:CE1	1:B:486:ILE:HD12	2.40	0.57
1:E:444:MET:HE3	1:E:561:VAL:HG21	1.87	0.57
1:E:233:ASN:CG	1:E:233:ASN:O	2.43	0.57
1:A:134:VAL:HG22	1:A:173:GLY:O	2.05	0.56
1:C:436:GLN:NE2	1:D:556:LYS:HZ3	2.03	0.56
1:E:134:VAL:HG22	1:E:173:GLY:O	2.05	0.56
1:E:282:ASN:ND2	1:E:404:ARG:HE	2.03	0.56
1:A:482:TYR:CE1	1:A:486:ILE:HD12	2.40	0.56
1:B:233:ASN:O	1:B:233:ASN:CG	2.43	0.56
1:A:567:SER:HB2	1:B:49:THR:HG21	1.87	0.56
1:B:392:ASN:HB3	1:B:402:GLN:NE2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ASN:ND2	1:C:404:ARG:HE	2.02	0.56
1:E:479:GLN:O	1:E:479:GLN:HG2	2.05	0.56
1:B:134:VAL:HG22	1:B:173:GLY:O	2.05	0.56
1:B:434:SER:N	1:C:555:TYR:HE2	2.04	0.56
1:B:494:HIS:C	1:B:496:PHE:H	2.08	0.56
1:D:479:GLN:O	1:D:479:GLN:HG2	2.05	0.56
1:E:273:ILE:O	1:E:273:ILE:HG23	2.05	0.56
1:C:125:THR:CG2	1:C:524:THR:HG23	2.36	0.56
1:A:434:SER:N	1:B:555:TYR:HE2	2.04	0.56
1:C:233:ASN:O	1:C:233:ASN:CG	2.43	0.56
1:C:392:ASN:HB3	1:C:402:GLN:NE2	2.21	0.56
1:D:392:ASN:HB3	1:D:402:GLN:NE2	2.21	0.56
1:D:567:SER:HB2	1:E:49:THR:HG21	1.87	0.56
1:E:392:ASN:HB3	1:E:402:GLN:NE2	2.21	0.56
1:A:125:THR:CG2	1:A:524:THR:HG23	2.35	0.56
1:B:403:TYR:CD1	1:B:504:ILE:HD13	2.39	0.56
1:C:482:TYR:CE1	1:C:486:ILE:HD12	2.40	0.56
1:D:273:ILE:O	1:D:273:ILE:HG23	2.05	0.56
1:E:493:THR:HG22	1:E:494:HIS:N	2.21	0.56
1:E:74:ASN:ND2	1:E:556:LYS:HZ1	2.04	0.56
1:A:392:ASN:HB3	1:A:402:GLN:NE2	2.21	0.56
1:A:67:THR:O	1:A:68:ARG:HG2	2.06	0.56
1:B:273:ILE:O	1:B:273:ILE:HG23	2.05	0.56
1:B:419:ILE:O	1:B:423:THR:HG22	2.06	0.56
1:B:567:SER:HB2	1:C:49:THR:HG21	1.87	0.56
1:C:428:PRO:O	1:C:429:ASP:HB3	2.06	0.56
1:D:134:VAL:HG22	1:D:173:GLY:O	2.05	0.56
1:D:494:HIS:C	1:D:496:PHE:H	2.07	0.56
1:E:482:TYR:CE1	1:E:486:ILE:HD12	2.40	0.56
1:A:273:ILE:O	1:A:273:ILE:HG23	2.05	0.56
1:E:125:THR:CG2	1:E:524:THR:HG23	2.35	0.56
1:A:493:THR:HG22	1:A:494:HIS:N	2.21	0.56
1:A:68:ARG:NH1	1:A:68:ARG:CG	2.66	0.56
1:C:403:TYR:CD1	1:C:504:ILE:HD13	2.39	0.56
1:A:555:TYR:HE2	1:E:434:SER:N	2.04	0.55
1:C:283:ILE:O	1:C:401:THR:HG23	2.07	0.55
1:C:434:SER:N	1:D:555:TYR:HE2	2.04	0.55
1:D:67:THR:O	1:D:68:ARG:HG2	2.06	0.55
1:A:479:GLN:HG2	1:A:479:GLN:O	2.05	0.55
1:A:494:HIS:C	1:A:496:PHE:H	2.08	0.55
1:A:49:THR:HG21	1:E:567:SER:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:THR:CG2	1:B:524:THR:HG23	2.36	0.55
1:B:403:TYR:HD1	1:B:504:ILE:CD1	2.20	0.55
1:B:501:GLU:H	1:B:501:GLU:CD	2.10	0.55
1:D:233:ASN:O	1:D:233:ASN:CG	2.42	0.55
1:A:283:ILE:O	1:A:401:THR:HG23	2.07	0.55
1:A:440:SER:C	1:A:442:PRO:HD3	2.27	0.55
1:B:283:ILE:O	1:B:401:THR:HG23	2.07	0.55
1:C:197:ARG:HG3	1:C:198:GLN:H	1.71	0.55
1:C:440:SER:C	1:C:442:PRO:HD3	2.27	0.55
1:D:419:ILE:O	1:D:423:THR:HG22	2.06	0.55
1:D:403:TYR:HD1	1:D:504:ILE:CD1	2.19	0.55
1:D:68:ARG:CG	1:D:68:ARG:HH11	2.07	0.55
1:E:283:ILE:O	1:E:401:THR:HG23	2.06	0.55
1:A:428:PRO:O	1:A:429:ASP:HB3	2.06	0.55
1:B:493:THR:HG22	1:B:494:HIS:N	2.21	0.55
1:A:419:ILE:O	1:A:423:THR:HG22	2.06	0.55
1:C:449:VAL:HG22	1:D:67:THR:HG21	1.89	0.55
1:A:214:ASN:C	1:A:214:ASN:ND2	2.55	0.55
1:A:501:GLU:H	1:A:501:GLU:CD	2.10	0.55
1:B:428:PRO:O	1:B:429:ASP:HB3	2.06	0.55
1:C:67:THR:O	1:C:68:ARG:HG2	2.06	0.55
1:D:440:SER:C	1:D:442:PRO:HD3	2.27	0.55
1:D:125:THR:CG2	1:D:524:THR:HG23	2.35	0.55
1:E:494:HIS:C	1:E:496:PHE:H	2.08	0.55
1:E:501:GLU:H	1:E:501:GLU:CD	2.10	0.55
1:E:67:THR:O	1:E:68:ARG:HG2	2.06	0.55
1:A:444:MET:HE3	1:A:561:VAL:HG21	1.88	0.55
1:C:134:VAL:HG22	1:C:173:GLY:O	2.05	0.55
1:B:449:VAL:HG22	1:C:67:THR:HG21	1.88	0.55
1:D:449:VAL:HG22	1:E:67:THR:HG21	1.89	0.55
1:A:449:VAL:HG22	1:B:67:THR:HG21	1.89	0.55
1:B:67:THR:O	1:B:68:ARG:HG2	2.06	0.55
1:C:136:GLU:O	1:C:137:PHE:HB2	2.07	0.55
1:D:493:THR:HG22	1:D:494:HIS:N	2.21	0.55
1:E:197:ARG:HG3	1:E:198:GLN:H	1.71	0.55
1:A:197:ARG:HG3	1:A:198:GLN:H	1.71	0.55
1:C:273:ILE:HG23	1:C:273:ILE:O	2.05	0.55
1:D:215:PHE:HE1	1:D:241:ILE:HD11	1.71	0.55
1:A:529:LEU:HD21	1:B:68:ARG:NE	2.22	0.55
1:B:136:GLU:O	1:B:137:PHE:HB2	2.07	0.55
1:E:419:ILE:O	1:E:423:THR:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:434:SER:N	1:E:555:TYR:HE2	2.04	0.55
1:A:403:TYR:CD1	1:A:504:ILE:HD13	2.39	0.54
1:A:74:ASN:ND2	1:A:556:LYS:HZ1	2.05	0.54
1:B:440:SER:C	1:B:442:PRO:HD3	2.27	0.54
1:B:525:ASP:C	1:B:525:ASP:OD1	2.45	0.54
1:C:419:ILE:O	1:C:423:THR:HG22	2.06	0.54
1:D:83:ASN:OD1	1:D:83:ASN:N	2.26	0.54
1:C:544:THR:HG21	1:C:548:ARG:HA	1.89	0.54
1:D:278:LEU:HD23	1:D:419:ILE:CD1	2.30	0.54
1:D:283:ILE:O	1:D:401:THR:HG23	2.07	0.54
1:A:505:LEU:O	1:A:506:ALA:O	2.26	0.54
1:B:263:LYS:HZ3	1:B:268:GLN:HB2	1.73	0.54
1:D:136:GLU:O	1:D:137:PHE:HB2	2.07	0.54
1:E:428:PRO:O	1:E:429:ASP:HB3	2.07	0.54
1:A:263:LYS:HZ3	1:A:268:GLN:HB2	1.73	0.54
1:B:529:LEU:HD21	1:C:68:ARG:NE	2.23	0.54
1:C:501:GLU:H	1:C:501:GLU:CD	2.10	0.54
1:D:428:PRO:O	1:D:429:ASP:HB3	2.06	0.54
1:C:211:ASP:CG	1:C:212:THR:H	2.10	0.54
1:C:525:ASP:C	1:C:525:ASP:OD1	2.45	0.54
1:D:385:ASP:O	1:D:386:SER:C	2.45	0.54
1:D:463:VAL:HB	1:D:529:LEU:CD1	2.38	0.54
1:D:501:GLU:H	1:D:501:GLU:CD	2.10	0.54
1:E:211:ASP:CG	1:E:212:THR:H	2.10	0.54
1:E:440:SER:C	1:E:442:PRO:HD3	2.27	0.54
1:D:525:ASP:OD1	1:D:525:ASP:C	2.45	0.54
1:E:215:PHE:HE1	1:E:241:ILE:HD11	1.71	0.54
1:A:525:ASP:C	1:A:525:ASP:OD1	2.45	0.54
1:B:203:GLU:C	1:B:205:ASP:H	2.11	0.54
1:E:192:TYR:CZ	1:E:197:ARG:HB3	2.43	0.54
1:E:208:VAL:HG23	1:E:208:VAL:O	2.08	0.54
1:E:389:ARG:HG2	1:E:389:ARG:HH11	1.73	0.54
1:E:505:LEU:O	1:E:506:ALA:O	2.26	0.54
1:A:136:GLU:O	1:A:137:PHE:HB2	2.07	0.54
1:B:192:TYR:CZ	1:B:197:ARG:HB3	2.43	0.54
1:C:505:LEU:O	1:C:506:ALA:O	2.26	0.54
1:D:197:ARG:HG3	1:D:198:GLN:H	1.71	0.54
1:D:505:LEU:O	1:D:506:ALA:O	2.26	0.54
1:E:463:VAL:HB	1:E:529:LEU:CD1	2.38	0.54
1:E:525:ASP:C	1:E:525:ASP:OD1	2.45	0.54
1:A:68:ARG:NE	1:E:529:LEU:HD21	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:TYR:CZ	1:A:197:ARG:HB3	2.43	0.54
1:A:239:ASP:OD1	1:A:239:ASP:C	2.46	0.54
1:B:208:VAL:O	1:B:208:VAL:HG23	2.08	0.54
1:B:385:ASP:O	1:B:386:SER:C	2.45	0.54
1:C:192:TYR:CZ	1:C:197:ARG:HB3	2.43	0.54
1:C:385:ASP:O	1:C:386:SER:C	2.45	0.54
1:C:493:THR:HG22	1:C:494:HIS:N	2.21	0.54
1:D:192:TYR:CZ	1:D:197:ARG:HB3	2.43	0.54
1:A:203:GLU:C	1:A:205:ASP:H	2.11	0.54
1:A:67:THR:HG21	1:E:449:VAL:HG22	1.89	0.54
1:E:136:GLU:O	1:E:137:PHE:HB2	2.07	0.54
1:A:385:ASP:O	1:A:386:SER:C	2.45	0.53
1:B:197:ARG:HG3	1:B:198:GLN:H	1.71	0.53
1:C:239:ASP:OD1	1:C:239:ASP:C	2.45	0.53
1:D:211:ASP:CG	1:D:212:THR:H	2.10	0.53
1:E:239:ASP:C	1:E:239:ASP:OD1	2.46	0.53
1:E:385:ASP:O	1:E:386:SER:C	2.46	0.53
1:E:544:THR:HG21	1:E:548:ARG:HA	1.89	0.53
1:A:478:ASP:C	1:A:480:ALA:H	2.12	0.53
1:B:544:THR:HG21	1:B:548:ARG:HA	1.89	0.53
1:C:203:GLU:C	1:C:205:ASP:H	2.11	0.53
1:D:449:VAL:HG12	1:D:450:THR:N	2.23	0.53
1:D:478:ASP:C	1:D:480:ALA:H	2.12	0.53
1:E:403:TYR:HD1	1:E:504:ILE:CD1	2.19	0.53
1:B:215:PHE:HE1	1:B:241:ILE:HD11	1.71	0.53
1:B:478:ASP:C	1:B:480:ALA:H	2.12	0.53
1:B:154:THR:CG2	1:B:155:LYS:N	2.72	0.53
1:B:389:ARG:HH11	1:B:389:ARG:HG2	1.73	0.53
1:C:478:ASP:C	1:C:480:ALA:H	2.12	0.53
1:D:151:ARG:HG3	1:D:161:LEU:CD2	2.39	0.53
1:A:295:SER:HB3	1:A:377:PRO:CG	2.33	0.53
1:A:389:ARG:HG2	1:A:389:ARG:HH11	1.73	0.53
1:A:463:VAL:HB	1:A:529:LEU:CD1	2.38	0.53
1:A:93:THR:HG22	1:A:94:THR:N	2.23	0.53
1:C:93:THR:HG22	1:C:94:THR:N	2.23	0.53
1:B:452:ARG:NH2	1:C:99:ASN:HD22	2.07	0.53
1:D:208:VAL:HG23	1:D:208:VAL:O	2.08	0.53
1:D:529:LEU:HD21	1:E:68:ARG:NE	2.23	0.53
1:C:403:TYR:HD1	1:C:504:ILE:CD1	2.19	0.53
1:C:69:VAL:CG2	1:C:561:VAL:HB	2.39	0.53
1:C:529:LEU:HD21	1:D:68:ARG:NE	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:THR:CG2	1:D:155:LYS:N	2.72	0.53
1:E:203:GLU:C	1:E:205:ASP:H	2.11	0.53
1:A:236:PHE:O	1:A:237:HIS:HB3	2.09	0.53
1:B:211:ASP:CG	1:B:212:THR:H	2.10	0.53
1:C:386:SER:O	1:C:387:LYS:CB	2.57	0.53
1:D:151:ARG:HG3	1:D:161:LEU:HD21	1.91	0.53
1:D:389:ARG:HH11	1:D:389:ARG:HG2	1.73	0.53
1:D:69:VAL:CG2	1:D:561:VAL:HB	2.39	0.53
1:D:93:THR:HG22	1:D:94:THR:N	2.23	0.53
1:B:449:VAL:HG12	1:B:450:THR:N	2.23	0.53
1:B:505:LEU:O	1:B:506:ALA:O	2.26	0.53
1:C:154:THR:CG2	1:C:155:LYS:N	2.72	0.53
1:C:151:ARG:HG3	1:C:161:LEU:HD21	1.91	0.53
1:C:236:PHE:O	1:C:237:HIS:HB3	2.09	0.53
1:E:292:TYR:HA	1:E:377:PRO:HG3	1.91	0.53
1:E:69:VAL:CG2	1:E:561:VAL:HB	2.39	0.53
1:B:222:VAL:HG13	1:B:223:THR:N	2.24	0.53
1:E:151:ARG:HG3	1:E:161:LEU:HD21	1.91	0.53
1:A:544:THR:HG21	1:A:548:ARG:HA	1.89	0.52
1:C:197:ARG:CG	1:C:198:GLN:N	2.72	0.52
1:C:208:VAL:HG23	1:C:208:VAL:O	2.08	0.52
1:C:222:VAL:HG13	1:C:223:THR:N	2.24	0.52
1:C:295:SER:HB3	1:C:377:PRO:CG	2.33	0.52
1:E:151:ARG:HG3	1:E:161:LEU:CD2	2.39	0.52
1:E:120:GLY:O	1:E:563:PRO:HA	2.10	0.52
1:A:215:PHE:HE1	1:A:241:ILE:HD11	1.71	0.52
1:A:449:VAL:HG12	1:A:450:THR:N	2.23	0.52
1:B:239:ASP:OD1	1:B:239:ASP:C	2.45	0.52
1:B:69:VAL:CG2	1:B:561:VAL:HB	2.39	0.52
1:C:180:THR:HG21	1:C:258:LEU:CD2	2.40	0.52
1:D:236:PHE:O	1:D:237:HIS:HB3	2.09	0.52
1:D:266:PRO:O	1:D:268:GLN:N	2.43	0.52
1:E:93:THR:HG22	1:E:94:THR:N	2.23	0.52
1:A:154:THR:CG2	1:A:155:LYS:N	2.72	0.52
1:A:151:ARG:HG3	1:A:161:LEU:CD2	2.39	0.52
1:A:211:ASP:CG	1:A:212:THR:H	2.10	0.52
1:A:386:SER:O	1:A:387:LYS:CB	2.57	0.52
1:A:69:VAL:CG2	1:A:561:VAL:HB	2.39	0.52
1:B:120:GLY:O	1:B:563:PRO:HA	2.10	0.52
1:B:151:ARG:HG3	1:B:161:LEU:HD21	1.91	0.52
1:D:180:THR:HG21	1:D:258:LEU:CD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ASN:O	1:D:54:SER:C	2.48	0.52
1:B:180:THR:HG21	1:B:258:LEU:CD2	2.40	0.52
1:B:266:PRO:O	1:B:268:GLN:N	2.43	0.52
1:B:463:VAL:HB	1:B:529:LEU:CD1	2.38	0.52
1:A:452:ARG:NH2	1:B:99:ASN:HD22	2.06	0.52
1:C:151:ARG:HG3	1:C:161:LEU:CD2	2.39	0.52
1:C:389:ARG:HH11	1:C:389:ARG:HG2	1.73	0.52
1:C:449:VAL:HG12	1:C:450:THR:N	2.23	0.52
1:E:171:PRO:O	1:E:175:TYR:OH	2.25	0.52
1:E:180:THR:HG21	1:E:258:LEU:CD2	2.40	0.52
1:E:236:PHE:O	1:E:237:HIS:HB3	2.09	0.52
1:B:197:ARG:CG	1:B:198:GLN:N	2.72	0.52
1:D:197:ARG:CG	1:D:198:GLN:N	2.72	0.52
1:D:441:LEU:N	1:D:442:PRO:HD3	2.24	0.52
1:E:154:THR:CG2	1:E:155:LYS:N	2.71	0.52
1:E:449:VAL:HG12	1:E:450:THR:N	2.23	0.52
1:A:208:VAL:O	1:A:208:VAL:HG23	2.08	0.52
1:A:211:ASP:HA	1:A:508:PRO:HG2	1.89	0.52
1:C:403:TYR:CD1	1:C:504:ILE:HG21	2.45	0.52
1:C:520:VAL:HG23	1:C:521:PRO:HD2	1.92	0.52
1:D:386:SER:O	1:D:387:LYS:CB	2.57	0.52
1:E:197:ARG:CG	1:E:198:GLN:N	2.72	0.52
1:E:478:ASP:C	1:E:480:ALA:H	2.12	0.52
1:E:520:VAL:HG23	1:E:521:PRO:HD2	1.92	0.52
1:A:171:PRO:O	1:A:175:TYR:OH	2.25	0.52
1:A:266:PRO:O	1:A:268:GLN:N	2.43	0.52
1:A:403:TYR:HD1	1:A:504:ILE:CD1	2.20	0.52
1:B:93:THR:HG22	1:B:94:THR:N	2.23	0.52
1:C:463:VAL:HB	1:C:529:LEU:CD1	2.38	0.52
1:C:211:ASP:HA	1:C:508:PRO:HG2	1.89	0.52
1:C:74:ASN:HD22	1:C:556:LYS:HZ1	1.58	0.52
1:C:262:ARG:HH11	1:D:130:ASN:HD22	1.55	0.52
1:E:222:VAL:HG13	1:E:223:THR:N	2.24	0.52
1:E:386:SER:O	1:E:387:LYS:CB	2.57	0.52
1:A:197:ARG:CG	1:A:198:GLN:N	2.72	0.52
1:A:222:VAL:HG13	1:A:223:THR:N	2.24	0.52
1:B:125:THR:HG22	1:B:524:THR:HG23	1.92	0.52
1:B:151:ARG:HG3	1:B:161:LEU:CD2	2.39	0.52
1:B:403:TYR:CD1	1:B:504:ILE:HG21	2.45	0.52
1:D:222:VAL:HG13	1:D:223:THR:N	2.24	0.52
1:D:120:GLY:O	1:D:563:PRO:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ASN:HD22	1:E:452:ARG:NH2	2.07	0.52
1:A:180:THR:HG21	1:A:258:LEU:CD2	2.40	0.52
1:D:151:ARG:HB3	1:D:200:GLY:O	2.10	0.52
1:D:125:THR:CG2	1:D:524:THR:CG2	2.88	0.52
1:C:263:LYS:HZ3	1:C:268:GLN:HB2	1.74	0.52
1:E:295:SER:HB3	1:E:377:PRO:CG	2.33	0.52
1:E:403:TYR:CD1	1:E:504:ILE:HG21	2.45	0.52
1:A:441:LEU:N	1:A:442:PRO:HD3	2.24	0.51
1:C:125:THR:CG2	1:C:524:THR:CG2	2.88	0.51
1:D:452:ARG:NH2	1:E:99:ASN:HD22	2.06	0.51
1:A:53:ASN:O	1:A:54:SER:C	2.48	0.51
1:C:151:ARG:HB3	1:C:200:GLY:O	2.10	0.51
1:C:215:PHE:HE1	1:C:241:ILE:HD11	1.71	0.51
1:C:295:SER:OG	1:C:377:PRO:HD3	2.10	0.51
1:E:151:ARG:HB3	1:E:200:GLY:O	2.10	0.51
1:A:125:THR:CG2	1:A:524:THR:CG2	2.88	0.51
1:B:441:LEU:N	1:B:442:PRO:HD3	2.24	0.51
1:C:436:GLN:CD	1:D:556:LYS:HZ3	2.14	0.51
1:D:138:MET:HB3	1:D:254:ARG:NH1	2.26	0.51
1:D:239:ASP:C	1:D:239:ASP:OD1	2.45	0.51
1:D:295:SER:OG	1:D:377:PRO:HD3	2.10	0.51
1:E:125:THR:CG2	1:E:524:THR:CG2	2.88	0.51
1:A:151:ARG:HB3	1:A:200:GLY:O	2.10	0.51
1:A:151:ARG:HG3	1:A:161:LEU:HD21	1.91	0.51
1:B:53:ASN:O	1:B:54:SER:C	2.48	0.51
1:C:171:PRO:O	1:C:175:TYR:OH	2.25	0.51
1:C:125:THR:HG22	1:C:524:THR:HG23	1.92	0.51
1:C:132:PRO:HD3	1:C:553:TYR:CE2	2.46	0.51
1:D:425:LEU:HD12	1:D:426:CYS:N	2.26	0.51
1:E:494:HIS:C	1:E:496:PHE:N	2.64	0.51
1:E:53:ASN:O	1:E:54:SER:C	2.48	0.51
1:E:132:PRO:HD3	1:E:553:TYR:CE2	2.46	0.51
1:A:120:GLY:O	1:A:563:PRO:HA	2.10	0.51
1:A:295:SER:OG	1:A:377:PRO:HD3	2.10	0.51
1:B:211:ASP:HA	1:B:508:PRO:HG2	1.89	0.51
1:B:125:THR:CG2	1:B:524:THR:CG2	2.88	0.51
1:B:444:MET:HE3	1:B:561:VAL:HG21	1.93	0.51
1:D:125:THR:HG22	1:D:524:THR:HG23	1.92	0.51
1:D:203:GLU:C	1:D:205:ASP:H	2.11	0.51
1:E:264:ARG:NH1	1:E:424:LEU:HD13	2.26	0.51
1:A:520:VAL:HG23	1:A:521:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:PRO:HD3	1:B:553:TYR:CE2	2.46	0.51
1:B:151:ARG:HB3	1:B:200:GLY:O	2.10	0.51
1:B:138:MET:HB3	1:B:254:ARG:NH1	2.26	0.51
1:B:264:ARG:NH1	1:B:424:LEU:HD13	2.26	0.51
1:B:295:SER:OG	1:B:377:PRO:HD3	2.10	0.51
1:C:120:GLY:O	1:C:563:PRO:HA	2.10	0.51
1:D:547:ARG:O	1:D:548:ARG:HB2	2.11	0.51
1:D:132:PRO:HD3	1:D:553:TYR:CE2	2.46	0.51
1:C:451:PHE:CE1	1:D:97:GLN:HB2	2.46	0.51
1:E:425:LEU:HD12	1:E:426:CYS:N	2.25	0.51
1:A:60:LEU:O	1:A:61:ALA:CB	2.59	0.51
1:B:295:SER:HB3	1:B:377:PRO:CG	2.33	0.51
1:C:138:MET:HB3	1:C:254:ARG:NH1	2.26	0.51
1:C:395:SER:C	1:C:397:ASP:H	2.14	0.51
1:C:441:LEU:N	1:C:442:PRO:HD3	2.24	0.51
1:C:494:HIS:C	1:C:496:PHE:N	2.64	0.51
1:C:60:LEU:O	1:C:61:ALA:CB	2.59	0.51
1:D:295:SER:HB3	1:D:377:PRO:CG	2.33	0.51
1:D:494:HIS:C	1:D:496:PHE:N	2.64	0.51
1:D:544:THR:HG21	1:D:548:ARG:HA	1.89	0.51
1:E:263:LYS:HZ3	1:E:268:GLN:HB2	1.75	0.51
1:E:403:TYR:CD1	1:E:504:ILE:HD13	2.39	0.51
1:A:556:LYS:HZ3	1:E:436:GLN:NE2	2.08	0.51
1:E:125:THR:HG22	1:E:524:THR:HG23	1.92	0.51
1:A:403:TYR:CD1	1:A:504:ILE:HG21	2.45	0.51
1:A:264:ARG:NH1	1:A:424:LEU:HD13	2.26	0.51
1:B:451:PHE:CE1	1:C:97:GLN:HB2	2.46	0.51
1:B:520:VAL:HG23	1:B:521:PRO:HD2	1.92	0.51
1:C:491:SER:O	1:C:492:LEU:O	2.29	0.51
1:C:53:ASN:O	1:C:54:SER:C	2.48	0.51
1:D:403:TYR:CD1	1:D:504:ILE:HG21	2.45	0.51
1:D:430:VAL:HG23	1:D:517:SER:HB2	1.93	0.51
1:E:197:ARG:HG3	1:E:198:GLN:HG2	1.93	0.51
1:A:97:GLN:HB2	1:E:451:PHE:CE1	2.46	0.51
1:C:425:LEU:HD12	1:C:426:CYS:N	2.25	0.51
1:D:264:ARG:NH1	1:D:424:LEU:HD13	2.26	0.51
1:E:295:SER:OG	1:E:377:PRO:HD3	2.10	0.51
1:E:441:LEU:N	1:E:442:PRO:HD3	2.24	0.51
1:A:138:MET:HB3	1:A:254:ARG:NH1	2.26	0.51
1:A:132:PRO:HD3	1:A:553:TYR:CE2	2.46	0.51
1:B:236:PHE:O	1:B:237:HIS:HB3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:PHE:CE1	1:B:97:GLN:HB2	2.46	0.51
1:C:264:ARG:NH1	1:C:424:LEU:HD13	2.26	0.51
1:C:547:ARG:O	1:C:548:ARG:HB2	2.11	0.51
1:D:451:PHE:CE1	1:E:97:GLN:HB2	2.46	0.51
1:C:452:ARG:NH2	1:D:99:ASN:HD22	2.07	0.51
1:A:494:HIS:C	1:A:496:PHE:N	2.64	0.50
1:A:125:THR:HG22	1:A:524:THR:HG23	1.92	0.50
1:B:135:ASN:HA	1:B:172:GLU:HG2	1.93	0.50
1:A:556:LYS:HZ3	1:E:436:GLN:CD	2.14	0.50
1:B:427:THR:HG23	1:B:428:PRO:HD2	1.94	0.50
1:B:451:PHE:CE1	1:C:97:GLN:HG3	2.47	0.50
1:C:266:PRO:C	1:C:268:GLN:H	2.15	0.50
1:C:567:SER:CB	1:D:49:THR:HG21	2.41	0.50
1:D:233:ASN:O	1:D:233:ASN:OD1	2.30	0.50
1:D:520:VAL:HG23	1:D:521:PRO:HD2	1.92	0.50
1:E:430:VAL:HG23	1:E:517:SER:HB2	1.93	0.50
1:A:98:ASN:ND2	1:E:452:ARG:HE	2.08	0.50
1:D:451:PHE:HE1	1:E:97:GLN:HG3	1.76	0.50
1:A:547:ARG:O	1:A:548:ARG:HB2	2.11	0.50
1:D:197:ARG:HG3	1:D:198:GLN:HG2	1.93	0.50
1:D:243:LEU:CD2	1:D:403:TYR:HD2	2.24	0.50
1:E:138:MET:HB3	1:E:254:ARG:NH1	2.26	0.50
1:A:233:ASN:O	1:A:233:ASN:OD1	2.30	0.50
1:B:60:LEU:O	1:B:61:ALA:CB	2.59	0.50
1:A:451:PHE:HE1	1:B:97:GLN:HG3	1.76	0.50
1:D:60:LEU:O	1:D:61:ALA:CB	2.59	0.50
1:E:192:TYR:CD2	1:E:193:LEU:HD23	2.47	0.50
1:D:436:GLN:CD	1:E:556:LYS:HZ3	2.14	0.50
1:A:197:ARG:HG3	1:A:198:GLN:HG2	1.93	0.50
1:A:451:PHE:CE1	1:B:97:GLN:HG3	2.47	0.50
1:C:135:ASN:HA	1:C:172:GLU:HG2	1.94	0.50
1:C:266:PRO:O	1:C:268:GLN:N	2.43	0.50
1:C:451:PHE:CE1	1:D:97:GLN:HG3	2.47	0.50
1:C:544:THR:HG22	1:C:545:ASP:N	2.27	0.50
1:E:211:ASP:HA	1:E:508:PRO:HG2	1.89	0.50
1:E:243:LEU:CD2	1:E:403:TYR:HD2	2.24	0.50
1:D:567:SER:CB	1:E:49:THR:HG21	2.41	0.50
1:A:243:LEU:CD2	1:A:403:TYR:HD2	2.24	0.50
1:A:266:PRO:C	1:A:268:GLN:H	2.15	0.50
1:A:491:SER:O	1:A:492:LEU:O	2.29	0.50
1:A:97:GLN:HG3	1:E:451:PHE:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:THR:O	1:C:181:ILE:N	2.45	0.50
1:C:192:TYR:CD2	1:C:193:LEU:HD23	2.47	0.50
1:D:192:TYR:CD2	1:D:193:LEU:HD23	2.47	0.50
1:D:427:THR:HG23	1:D:428:PRO:HD2	1.94	0.50
1:E:243:LEU:CD2	1:E:244:PRO:HD3	2.42	0.50
1:E:427:THR:HG23	1:E:428:PRO:HD2	1.94	0.50
1:A:178:THR:O	1:A:181:ILE:N	2.45	0.50
1:A:544:THR:HG22	1:A:545:ASP:N	2.27	0.50
1:A:567:SER:CB	1:B:49:THR:HG21	2.41	0.50
1:B:491:SER:O	1:B:492:LEU:O	2.29	0.50
1:B:544:THR:HG22	1:B:545:ASP:N	2.26	0.50
1:B:547:ARG:O	1:B:548:ARG:HB2	2.11	0.50
1:B:61:ALA:HB1	1:B:62:PRO:CD	2.42	0.50
1:B:567:SER:CB	1:C:49:THR:HG21	2.41	0.50
1:D:237:HIS:ND1	1:D:238:PRO:O	2.45	0.50
1:C:451:PHE:HE1	1:D:97:GLN:HG3	1.77	0.50
1:A:61:ALA:HB1	1:A:62:PRO:CD	2.42	0.50
1:B:243:LEU:CD2	1:B:244:PRO:HD3	2.42	0.50
1:B:266:PRO:C	1:B:268:GLN:H	2.15	0.50
1:B:395:SER:C	1:B:397:ASP:H	2.14	0.50
1:B:425:LEU:HD12	1:B:426:CYS:N	2.26	0.50
1:C:233:ASN:O	1:C:233:ASN:OD1	2.30	0.50
1:C:61:ALA:HB1	1:C:62:PRO:CD	2.42	0.50
1:D:114:ASP:OD1	1:D:115:ASP:N	2.45	0.50
1:D:135:ASN:HA	1:D:172:GLU:HG2	1.94	0.50
1:D:451:PHE:CE1	1:E:97:GLN:HG3	2.47	0.50
1:D:491:SER:O	1:D:492:LEU:O	2.29	0.50
1:E:61:ALA:HB1	1:E:62:PRO:CD	2.42	0.50
1:A:192:TYR:CD2	1:A:193:LEU:HD23	2.47	0.50
1:B:233:ASN:O	1:B:233:ASN:OD1	2.30	0.50
1:B:386:SER:O	1:B:387:LYS:CB	2.57	0.50
1:C:114:ASP:OD1	1:C:115:ASP:N	2.45	0.50
1:C:243:LEU:CD2	1:C:244:PRO:HD3	2.42	0.50
1:B:436:GLN:CD	1:C:556:LYS:HZ3	2.16	0.50
1:D:395:SER:C	1:D:397:ASP:H	2.14	0.50
1:E:178:THR:O	1:E:181:ILE:N	2.45	0.50
1:E:266:PRO:O	1:E:268:GLN:N	2.43	0.50
1:E:266:PRO:C	1:E:268:GLN:H	2.14	0.50
1:E:547:ARG:O	1:E:548:ARG:HB2	2.11	0.50
1:A:425:LEU:HD12	1:A:426:CYS:N	2.26	0.49
1:B:178:THR:O	1:B:181:ILE:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:HIS:C	1:B:496:PHE:N	2.64	0.49
1:D:178:THR:O	1:D:181:ILE:N	2.45	0.49
1:D:197:ARG:HG3	1:D:198:GLN:HG3	1.94	0.49
1:E:544:THR:HG22	1:E:545:ASP:N	2.26	0.49
1:A:49:THR:HG21	1:E:567:SER:CB	2.42	0.49
1:A:126:ILE:HG23	1:A:523:LEU:HD23	1.94	0.49
1:A:394:ILE:HG22	1:A:400:PHE:O	2.12	0.49
1:B:481:VAL:HG21	1:C:482:TYR:OH	2.12	0.49
1:C:197:ARG:HG3	1:C:198:GLN:HG2	1.93	0.49
1:D:243:LEU:HD22	1:D:244:PRO:CD	2.43	0.49
1:D:266:PRO:C	1:D:268:GLN:H	2.15	0.49
1:D:436:GLN:NE2	1:E:556:LYS:HZ3	2.09	0.49
1:A:486:ILE:HD11	1:E:485:LEU:HD11	1.94	0.49
1:B:171:PRO:O	1:B:175:TYR:OH	2.25	0.49
1:B:212:THR:HG23	1:B:508:PRO:HB3	1.94	0.49
1:C:444:MET:HE3	1:C:561:VAL:HG21	1.94	0.49
1:D:243:LEU:CD2	1:D:244:PRO:HD3	2.42	0.49
1:D:212:THR:HG23	1:D:508:PRO:HB3	1.94	0.49
1:D:126:ILE:HG23	1:D:523:LEU:HD23	1.94	0.49
1:D:544:THR:HG22	1:D:545:ASP:N	2.26	0.49
1:E:114:ASP:OD1	1:E:115:ASP:N	2.45	0.49
1:A:243:LEU:CD2	1:A:244:PRO:HD3	2.42	0.49
1:A:395:SER:C	1:A:397:ASP:H	2.14	0.49
1:A:430:VAL:HG23	1:A:517:SER:HB2	1.93	0.49
1:B:129:THR:HG22	1:B:553:TYR:O	2.13	0.49
1:D:61:ALA:HB1	1:D:62:PRO:CD	2.42	0.49
1:E:491:SER:O	1:E:492:LEU:O	2.29	0.49
1:E:444:MET:CE	1:E:561:VAL:HG21	2.43	0.49
1:A:129:THR:HG22	1:A:553:TYR:O	2.13	0.49
1:A:481:VAL:HG21	1:B:482:TYR:OH	2.13	0.49
1:A:485:LEU:HD11	1:B:486:ILE:HD11	1.95	0.49
1:A:436:GLN:CD	1:B:556:LYS:HZ3	2.15	0.49
1:C:237:HIS:ND1	1:C:238:PRO:O	2.45	0.49
1:C:243:LEU:HD22	1:C:244:PRO:CD	2.43	0.49
1:C:91:PHE:N	1:C:91:PHE:CD2	2.81	0.49
1:E:67:THR:OG1	1:E:68:ARG:N	2.45	0.49
1:B:114:ASP:OD1	1:B:115:ASP:N	2.45	0.49
1:B:243:LEU:CD2	1:B:403:TYR:HD2	2.24	0.49
1:B:262:ARG:HH11	1:C:130:ASN:HD22	1.55	0.49
1:C:212:THR:HG23	1:C:508:PRO:HB3	1.94	0.49
1:E:125:THR:HG22	1:E:526:HIS:NE2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:ASN:HA	1:E:172:GLU:HG2	1.94	0.49
1:E:394:ILE:HG22	1:E:400:PHE:O	2.12	0.49
1:E:60:LEU:O	1:E:61:ALA:CB	2.59	0.49
1:A:114:ASP:OD1	1:A:115:ASP:N	2.45	0.49
1:A:262:ARG:HH11	1:B:130:ASN:HD22	1.56	0.49
1:B:197:ARG:HG3	1:B:198:GLN:HG2	1.93	0.49
1:B:394:ILE:HG22	1:B:400:PHE:O	2.12	0.49
1:C:394:ILE:HG22	1:C:400:PHE:O	2.13	0.49
1:D:444:MET:CE	1:D:561:VAL:HG21	2.43	0.49
1:E:129:THR:HG22	1:E:553:TYR:O	2.13	0.49
1:E:243:LEU:HD22	1:E:244:PRO:CD	2.43	0.49
1:A:452:ARG:HE	1:B:98:ASN:ND2	2.08	0.49
1:A:97:GLN:HG3	1:E:451:PHE:HE1	1.77	0.49
1:B:451:PHE:HE1	1:C:97:GLN:HG3	1.76	0.49
1:D:67:THR:OG1	1:D:68:ARG:N	2.45	0.49
1:E:211:ASP:OD1	1:E:213:ARG:HG2	2.13	0.49
1:E:233:ASN:OD1	1:E:233:ASN:O	2.30	0.49
1:E:126:ILE:HG23	1:E:523:LEU:HD23	1.94	0.49
1:B:243:LEU:HD22	1:B:244:PRO:CD	2.43	0.49
1:B:430:VAL:HG23	1:B:517:SER:HB2	1.93	0.49
1:C:197:ARG:HG3	1:C:198:GLN:HG3	1.94	0.49
1:C:430:VAL:HG23	1:C:517:SER:HB2	1.93	0.49
1:E:449:VAL:HG12	1:E:450:THR:HG23	1.95	0.49
1:A:197:ARG:HG3	1:A:198:GLN:HG3	1.94	0.49
1:A:451:PHE:HE2	1:A:462:VAL:HG23	1.78	0.49
1:B:192:TYR:CD2	1:B:193:LEU:HD23	2.47	0.49
1:B:452:ARG:HE	1:C:98:ASN:ND2	2.08	0.49
1:C:427:THR:HG23	1:C:428:PRO:HD2	1.94	0.49
1:D:129:THR:HG22	1:D:553:TYR:O	2.13	0.49
1:D:125:THR:HG22	1:D:526:HIS:NE2	2.28	0.49
1:D:481:VAL:HG21	1:E:482:TYR:OH	2.13	0.49
1:A:212:THR:HG23	1:A:508:PRO:HB3	1.94	0.48
1:A:427:THR:HG23	1:A:428:PRO:HD2	1.94	0.48
1:B:444:MET:CE	1:B:561:VAL:HG21	2.43	0.48
1:C:243:LEU:CD2	1:C:403:TYR:HD2	2.24	0.48
1:D:203:GLU:O	1:D:205:ASP:N	2.46	0.48
1:D:214:ASN:HD21	1:D:216:ARG:HG2	1.78	0.48
1:D:69:VAL:HG22	1:D:561:VAL:HB	1.95	0.48
1:D:444:MET:HE3	1:D:561:VAL:HG21	1.94	0.48
1:A:441:LEU:HB2	1:A:445:MET:HE2	1.95	0.48
1:A:482:TYR:OH	1:E:481:VAL:HG21	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:ASP:OD1	1:B:549:ARG:HG2	2.13	0.48
1:B:98:ASN:HD22	1:B:99:ASN:N	2.11	0.48
1:C:203:GLU:O	1:C:205:ASP:N	2.46	0.48
1:C:449:VAL:HG12	1:C:450:THR:HG23	1.95	0.48
1:C:69:VAL:HG22	1:C:561:VAL:HB	1.95	0.48
1:D:211:ASP:HA	1:D:508:PRO:HG2	1.89	0.48
1:D:66:THR:HA	1:D:563:PRO:O	2.13	0.48
1:E:203:GLU:O	1:E:205:ASP:N	2.46	0.48
1:A:125:THR:HG22	1:A:526:HIS:NE2	2.28	0.48
1:A:243:LEU:HD22	1:A:244:PRO:CD	2.43	0.48
1:A:449:VAL:HG12	1:A:450:THR:HG23	1.95	0.48
1:B:237:HIS:ND1	1:B:238:PRO:O	2.45	0.48
1:B:67:THR:OG1	1:B:68:ARG:N	2.45	0.48
1:C:211:ASP:OD1	1:C:213:ARG:HG2	2.13	0.48
1:C:292:TYR:HA	1:C:377:PRO:HG3	1.90	0.48
1:C:389:ARG:CD	1:C:502:ASN:HD22	2.23	0.48
1:D:91:PHE:CD2	1:D:91:PHE:N	2.81	0.48
1:A:214:ASN:HD21	1:A:216:ARG:HG2	1.78	0.48
1:A:91:PHE:N	1:A:91:PHE:CD2	2.81	0.48
1:C:444:MET:CE	1:C:561:VAL:HG21	2.43	0.48
1:C:451:PHE:HE2	1:C:462:VAL:HG23	1.78	0.48
1:C:481:VAL:HG21	1:D:482:TYR:OH	2.12	0.48
1:D:476:TYR:HD1	1:D:513:ILE:HD12	1.79	0.48
1:D:545:ASP:OD1	1:D:549:ARG:HG2	2.13	0.48
1:A:545:ASP:OD1	1:A:549:ARG:HG2	2.13	0.48
1:A:66:THR:HA	1:A:563:PRO:O	2.14	0.48
1:C:126:ILE:HG23	1:C:523:LEU:HD23	1.94	0.48
1:C:452:ARG:HE	1:D:98:ASN:ND2	2.08	0.48
1:B:485:LEU:HD11	1:C:486:ILE:HD11	1.94	0.48
1:C:66:THR:HA	1:C:563:PRO:O	2.13	0.48
1:D:394:ILE:HG22	1:D:400:PHE:O	2.13	0.48
1:D:452:ARG:HE	1:E:98:ASN:ND2	2.08	0.48
1:E:212:THR:HG23	1:E:508:PRO:HB3	1.94	0.48
1:E:451:PHE:HE2	1:E:462:VAL:HG23	1.78	0.48
1:E:69:VAL:HG22	1:E:561:VAL:HB	1.95	0.48
1:A:67:THR:OG1	1:A:68:ARG:N	2.45	0.48
1:B:197:ARG:HG3	1:B:198:GLN:HG3	1.94	0.48
1:B:211:ASP:OD1	1:B:213:ARG:HG2	2.13	0.48
1:B:292:TYR:HA	1:B:377:PRO:HG3	1.90	0.48
1:C:129:THR:HG22	1:C:553:TYR:O	2.13	0.48
1:D:485:LEU:HD11	1:E:486:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ILE:HD13	1:E:449:VAL:HG11	1.96	0.48
1:A:243:LEU:CD2	1:A:403:TYR:CE2	2.96	0.48
1:A:444:MET:CE	1:A:561:VAL:HG21	2.43	0.48
1:B:197:ARG:C	1:B:199:ASN:H	2.17	0.48
1:B:66:THR:HA	1:B:563:PRO:O	2.13	0.48
1:C:125:THR:HG22	1:C:526:HIS:NE2	2.28	0.48
1:C:545:ASP:OD1	1:C:549:ARG:HG2	2.13	0.48
1:C:98:ASN:HD22	1:C:99:ASN:N	2.11	0.48
1:D:243:LEU:HD22	1:D:244:PRO:HD2	1.96	0.48
1:D:538:VAL:HG23	1:D:538:VAL:O	2.14	0.48
1:E:214:ASN:HD21	1:E:216:ARG:HG2	1.78	0.48
1:E:237:HIS:ND1	1:E:238:PRO:O	2.45	0.48
1:A:135:ASN:HA	1:A:172:GLU:HG2	1.94	0.48
1:A:243:LEU:HD22	1:A:244:PRO:HD2	1.96	0.48
1:A:431:THR:O	1:A:432:CYS:HB2	2.14	0.48
1:B:126:ILE:HG23	1:B:523:LEU:HD23	1.94	0.48
1:E:243:LEU:HD22	1:E:244:PRO:HD2	1.96	0.48
1:E:98:ASN:HD22	1:E:99:ASN:N	2.11	0.48
1:A:389:ARG:CD	1:A:502:ASN:HD22	2.23	0.48
1:B:476:TYR:HD1	1:B:513:ILE:HD12	1.79	0.48
1:B:538:VAL:HG23	1:B:538:VAL:O	2.14	0.48
1:D:171:PRO:O	1:D:175:TYR:OH	2.25	0.48
1:E:395:SER:C	1:E:397:ASP:H	2.14	0.48
1:B:125:THR:HG22	1:B:526:HIS:NE2	2.28	0.48
1:B:203:GLU:O	1:B:205:ASP:N	2.46	0.48
1:B:203:GLU:HA	1:B:206:ILE:HG13	1.96	0.48
1:B:214:ASN:HD21	1:B:216:ARG:HG2	1.79	0.48
1:C:243:LEU:CD2	1:C:403:TYR:CE2	2.96	0.48
1:D:211:ASP:OD1	1:D:213:ARG:HG2	2.13	0.48
1:E:75:LYS:HZ2	1:E:94:THR:HG23	1.79	0.48
1:E:91:PHE:N	1:E:91:PHE:CD2	2.81	0.48
1:A:130:ASN:HD22	1:E:262:ARG:HH11	1.55	0.47
1:A:197:ARG:C	1:A:199:ASN:H	2.17	0.47
1:A:203:GLU:O	1:A:205:ASP:N	2.46	0.47
1:A:538:VAL:HG23	1:A:538:VAL:O	2.14	0.47
1:E:197:ARG:HG3	1:E:198:GLN:HG3	1.94	0.47
1:E:410:TYR:O	1:E:420:ARG:HD3	2.14	0.47
1:E:538:VAL:HG23	1:E:538:VAL:O	2.14	0.47
1:A:436:GLN:N	1:A:436:GLN:OE1	2.38	0.47
1:A:83:ASN:OD1	1:A:83:ASN:N	2.26	0.47
1:A:449:VAL:HG11	1:B:111:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:PHE:N	1:B:500:PRO:CD	2.77	0.47
1:C:214:ASN:HD21	1:C:216:ARG:HG2	1.78	0.47
1:C:410:TYR:O	1:C:420:ARG:HD3	2.14	0.47
1:D:430:VAL:CG2	1:D:431:THR:N	2.77	0.47
1:D:449:VAL:HG12	1:D:450:THR:HG23	1.95	0.47
1:D:499:PHE:N	1:D:500:PRO:CD	2.78	0.47
1:D:508:PRO:HA	1:D:509:PRO:HD3	1.73	0.47
1:E:545:ASP:OD1	1:E:549:ARG:HG2	2.13	0.47
1:A:211:ASP:OD1	1:A:213:ARG:HG2	2.13	0.47
1:A:410:TYR:O	1:A:420:ARG:HD3	2.14	0.47
1:B:243:LEU:HD22	1:B:244:PRO:HD2	1.96	0.47
1:B:431:THR:O	1:B:432:CYS:HB2	2.14	0.47
1:B:451:PHE:HE2	1:B:462:VAL:HG23	1.78	0.47
1:C:243:LEU:HD22	1:C:244:PRO:HD2	1.96	0.47
1:A:203:GLU:HA	1:A:206:ILE:HG13	1.96	0.47
1:A:405:SER:HB3	1:A:408:LEU:HB2	1.97	0.47
1:B:430:VAL:CG2	1:B:431:THR:N	2.77	0.47
1:D:263:LYS:HZ3	1:D:268:GLN:HB2	1.77	0.47
1:D:98:ASN:HD22	1:D:99:ASN:N	2.12	0.47
1:E:476:TYR:HD1	1:E:513:ILE:HD12	1.79	0.47
1:E:66:THR:HA	1:E:563:PRO:O	2.14	0.47
1:A:430:VAL:CG2	1:A:431:THR:N	2.77	0.47
1:A:499:PHE:N	1:A:500:PRO:CD	2.78	0.47
1:C:149:VAL:CG2	1:C:195:VAL:HG11	2.45	0.47
1:C:413:GLY:O	1:C:414:ASP:C	2.53	0.47
1:C:431:THR:O	1:C:432:CYS:HB2	2.14	0.47
1:D:216:ARG:O	1:D:216:ARG:HG3	2.15	0.47
1:C:485:LEU:HD11	1:D:486:ILE:HD11	1.94	0.47
1:E:216:ARG:HG3	1:E:216:ARG:O	2.15	0.47
1:E:243:LEU:CD2	1:E:403:TYR:CE2	2.96	0.47
1:E:431:THR:O	1:E:432:CYS:HB2	2.14	0.47
1:A:216:ARG:O	1:A:216:ARG:HG3	2.15	0.47
1:A:476:TYR:HD1	1:A:513:ILE:HD12	1.79	0.47
1:A:69:VAL:HG22	1:A:561:VAL:HB	1.95	0.47
1:A:78:ASP:OD1	1:A:94:THR:HG22	2.15	0.47
1:A:98:ASN:HD22	1:A:99:ASN:N	2.11	0.47
1:C:558:LEU:HA	1:C:558:LEU:HD23	1.62	0.47
1:D:405:SER:HB3	1:D:408:LEU:HB2	1.97	0.47
1:D:413:GLY:O	1:D:414:ASP:C	2.53	0.47
1:B:216:ARG:O	1:B:216:ARG:HG3	2.15	0.47
1:B:410:TYR:O	1:B:420:ARG:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:VAL:HG11	1:C:111:ILE:HD13	1.95	0.47
1:B:449:VAL:HG12	1:B:450:THR:HG23	1.95	0.47
1:B:69:VAL:HG22	1:B:561:VAL:HB	1.95	0.47
1:C:449:VAL:HG11	1:D:111:ILE:HD13	1.96	0.47
1:C:131:MET:HA	1:C:553:TYR:CD2	2.50	0.47
1:E:74:ASN:HD22	1:E:556:LYS:HZ1	1.61	0.47
1:B:413:GLY:O	1:B:414:ASP:C	2.53	0.47
1:D:410:TYR:O	1:D:420:ARG:HD3	2.14	0.47
1:D:131:MET:HA	1:D:553:TYR:CD2	2.50	0.47
1:E:180:THR:HG21	1:E:258:LEU:HD23	1.97	0.47
1:E:197:ARG:C	1:E:199:ASN:H	2.17	0.47
1:A:74:ASN:HD22	1:A:556:LYS:HZ1	1.62	0.47
1:C:197:ARG:C	1:C:199:ASN:H	2.17	0.47
1:D:449:VAL:HG11	1:E:111:ILE:HD13	1.96	0.47
1:E:261:ILE:HD12	1:E:406:TRP:CE3	2.50	0.47
1:E:131:MET:HA	1:E:553:TYR:CD2	2.50	0.47
1:A:261:ILE:HD12	1:A:406:TRP:CE3	2.50	0.47
1:C:389:ARG:CG	1:C:389:ARG:HH11	2.28	0.47
1:D:451:PHE:HE2	1:D:462:VAL:HG23	1.78	0.47
1:E:389:ARG:CG	1:E:389:ARG:HH11	2.28	0.47
1:E:430:VAL:CG2	1:E:431:THR:N	2.77	0.47
1:A:60:LEU:HD21	1:E:451:PHE:O	2.15	0.47
1:B:233:ASN:OD1	1:B:233:ASN:C	2.54	0.47
1:B:91:PHE:CD2	1:B:91:PHE:N	2.81	0.47
1:C:265:GLN:HA	1:C:266:PRO:HD2	1.57	0.47
1:C:430:VAL:CG2	1:C:431:THR:N	2.78	0.47
1:C:78:ASP:OD1	1:C:94:THR:HG22	2.14	0.47
1:D:203:GLU:HA	1:D:206:ILE:HG13	1.96	0.47
1:D:389:ARG:CG	1:D:389:ARG:HH11	2.28	0.47
1:E:405:SER:HB3	1:E:408:LEU:HB2	1.97	0.47
1:B:405:SER:HB3	1:B:408:LEU:HB2	1.97	0.46
1:B:261:ILE:HD12	1:B:406:TRP:CE3	2.50	0.46
1:B:130:ASN:HA	1:B:519:ASN:CG	2.36	0.46
1:B:131:MET:HA	1:B:553:TYR:CD2	2.50	0.46
1:C:203:GLU:HA	1:C:206:ILE:HG13	1.96	0.46
1:A:237:HIS:ND1	1:A:238:PRO:O	2.45	0.46
1:A:413:GLY:O	1:A:414:ASP:C	2.53	0.46
1:A:450:THR:HG21	1:B:96:ILE:CD1	2.46	0.46
1:A:451:PHE:O	1:B:60:LEU:HD21	2.16	0.46
1:A:130:ASN:HA	1:A:519:ASN:CG	2.36	0.46
1:A:131:MET:HA	1:A:553:TYR:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:476:TYR:HD1	1:C:513:ILE:HD12	1.79	0.46
1:D:138:MET:HB3	1:D:254:ARG:HH11	1.80	0.46
1:D:197:ARG:O	1:D:199:ASN:N	2.43	0.46
1:D:292:TYR:HA	1:D:377:PRO:HG3	1.90	0.46
1:A:180:THR:HG21	1:A:258:LEU:HD23	1.97	0.46
1:A:389:ARG:CG	1:A:389:ARG:HH11	2.29	0.46
1:A:436:GLN:HE22	1:B:556:LYS:HZ3	1.63	0.46
1:B:508:PRO:HA	1:B:509:PRO:HD3	1.73	0.46
1:B:83:ASN:N	1:B:83:ASN:OD1	2.26	0.46
1:C:180:THR:HG21	1:C:258:LEU:HD23	1.97	0.46
1:D:261:ILE:HD12	1:D:406:TRP:CE3	2.50	0.46
1:E:138:MET:HB3	1:E:254:ARG:HH11	1.80	0.46
1:A:96:ILE:CD1	1:E:450:THR:HG21	2.46	0.46
1:B:441:LEU:HB2	1:B:445:MET:HE2	1.98	0.46
1:C:113:LEU:HD23	1:C:113:LEU:HA	1.71	0.46
1:C:130:ASN:HA	1:C:519:ASN:CG	2.36	0.46
1:C:215:PHE:O	1:C:216:ARG:HB3	2.15	0.46
1:D:78:ASP:OD1	1:D:94:THR:HG22	2.14	0.46
1:E:203:GLU:HA	1:E:206:ILE:HG13	1.96	0.46
1:A:51:GLY:HA3	1:A:116:ARG:HH12	1.81	0.46
1:A:513:ILE:HD12	1:A:513:ILE:N	2.31	0.46
1:B:211:ASP:C	1:B:212:THR:CG2	2.84	0.46
1:B:376:LYS:CB	1:B:377:PRO:HD2	2.32	0.46
1:B:68:ARG:CG	1:B:68:ARG:NH1	2.66	0.46
1:D:146:ARG:HE	1:D:246:CYS:HA	1.80	0.46
1:D:450:THR:HG21	1:E:96:ILE:CD1	2.46	0.46
1:C:451:PHE:O	1:D:60:LEU:HD21	2.16	0.46
1:E:146:ARG:HE	1:E:246:CYS:HA	1.79	0.46
1:D:410:TYR:CE2	1:E:172:GLU:OE1	2.69	0.46
1:E:211:ASP:C	1:E:212:THR:CG2	2.84	0.46
1:E:413:GLY:O	1:E:414:ASP:C	2.53	0.46
1:D:451:PHE:O	1:E:60:LEU:HD21	2.16	0.46
1:A:427:THR:HA	1:A:428:PRO:HD3	1.75	0.46
1:B:180:THR:HG21	1:B:258:LEU:HD23	1.97	0.46
1:B:202:LEU:O	1:B:205:ASP:OD1	2.34	0.46
1:B:51:GLY:HA3	1:B:116:ARG:HH12	1.81	0.46
1:B:78:ASP:OD1	1:B:94:THR:HG22	2.15	0.46
1:C:244:PRO:HA	1:C:275:TYR:CE2	2.51	0.46
1:C:51:GLY:HA3	1:C:116:ARG:HH12	1.81	0.46
1:C:538:VAL:O	1:C:538:VAL:HG23	2.14	0.46
1:D:211:ASP:C	1:D:212:THR:CG2	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:ASP:OD1	1:E:94:THR:HG22	2.14	0.46
1:A:178:THR:O	1:A:180:THR:N	2.49	0.46
1:A:146:ARG:HE	1:A:246:CYS:HA	1.80	0.46
1:A:544:THR:HG23	1:A:549:ARG:N	2.31	0.46
1:B:436:GLN:NE2	1:C:556:LYS:HZ3	2.14	0.46
1:B:450:THR:HG21	1:C:96:ILE:CD1	2.45	0.46
1:C:178:THR:O	1:C:180:THR:N	2.49	0.46
1:C:216:ARG:O	1:C:216:ARG:HG3	2.15	0.46
1:C:146:ARG:HE	1:C:246:CYS:HA	1.80	0.46
1:C:138:MET:HB3	1:C:254:ARG:HH11	1.80	0.46
1:D:130:ASN:HA	1:D:519:ASN:CG	2.36	0.46
1:D:178:THR:O	1:D:180:THR:N	2.49	0.46
1:E:215:PHE:O	1:E:216:ARG:HB3	2.15	0.46
1:A:132:PRO:HD3	1:A:553:TYR:CD2	2.51	0.46
1:A:233:ASN:C	1:A:233:ASN:OD1	2.54	0.46
1:A:73:ASP:OD1	1:A:73:ASP:N	2.42	0.46
1:B:135:ASN:HB2	1:B:172:GLU:OE2	2.16	0.46
1:B:151:ARG:NH1	1:B:205:ASP:OD2	2.49	0.46
1:B:215:PHE:O	1:B:216:ARG:HB3	2.15	0.46
1:C:261:ILE:HD12	1:C:406:TRP:CE3	2.50	0.46
1:C:544:THR:HG23	1:C:549:ARG:N	2.31	0.46
1:E:295:SER:CB	1:E:377:PRO:HG3	2.36	0.46
1:A:135:ASN:HB2	1:A:172:GLU:OE2	2.16	0.46
1:A:138:MET:HB3	1:A:254:ARG:HH11	1.80	0.46
1:A:211:ASP:C	1:A:212:THR:CG2	2.84	0.46
1:A:215:PHE:O	1:A:216:ARG:HB3	2.15	0.46
1:A:468:LEU:HA	1:A:469:PRO:HD3	1.76	0.46
1:B:146:ARG:HE	1:B:246:CYS:HA	1.80	0.46
1:B:244:PRO:HA	1:B:275:TYR:CE2	2.51	0.46
1:B:382:LEU:HA	1:B:382:LEU:HD12	1.75	0.46
1:C:211:ASP:C	1:C:212:THR:CG2	2.84	0.46
1:C:513:ILE:N	1:C:513:ILE:HD12	2.31	0.46
1:D:51:GLY:HA3	1:D:116:ARG:HH12	1.81	0.46
1:D:132:PRO:HD3	1:D:553:TYR:CD2	2.51	0.46
1:D:215:PHE:O	1:D:216:ARG:HB3	2.15	0.46
1:D:295:SER:CB	1:D:377:PRO:HG3	2.36	0.46
1:E:202:LEU:O	1:E:205:ASP:OD1	2.34	0.46
1:B:178:THR:O	1:B:180:THR:N	2.49	0.46
1:B:237:HIS:CD2	1:B:425:LEU:CD1	2.97	0.46
1:B:225:LEU:HD22	1:B:285:ALA:O	2.16	0.46
1:B:389:ARG:HH11	1:B:389:ARG:CG	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:ASN:C	1:C:233:ASN:OD1	2.54	0.46
1:C:405:SER:HB3	1:C:408:LEU:HB2	1.97	0.46
1:C:499:PHE:N	1:C:500:PRO:CD	2.77	0.46
1:D:135:ASN:HB2	1:D:172:GLU:OE2	2.16	0.46
1:D:202:LEU:O	1:D:205:ASP:OD1	2.34	0.46
1:E:178:THR:O	1:E:180:THR:N	2.49	0.46
1:A:225:LEU:HD22	1:A:285:ALA:O	2.16	0.45
1:B:132:PRO:HD3	1:B:553:TYR:CD2	2.51	0.45
1:B:493:THR:CG2	1:B:494:HIS:N	2.79	0.45
1:B:513:ILE:N	1:B:513:ILE:HD12	2.31	0.45
1:C:151:ARG:NH1	1:C:205:ASP:OD2	2.49	0.45
1:C:295:SER:CB	1:C:377:PRO:HG3	2.36	0.45
1:C:67:THR:OG1	1:C:68:ARG:N	2.45	0.45
1:D:197:ARG:CG	1:D:198:GLN:H	2.29	0.45
1:D:244:PRO:HA	1:D:275:TYR:CE2	2.51	0.45
1:C:450:THR:HG21	1:D:96:ILE:CD1	2.46	0.45
1:A:151:ARG:NH1	1:A:205:ASP:OD2	2.49	0.45
1:A:493:THR:HG22	1:A:494:HIS:O	2.16	0.45
1:A:93:THR:HG22	1:A:94:THR:O	2.16	0.45
1:B:451:PHE:O	1:C:60:LEU:HD21	2.16	0.45
1:C:135:ASN:HA	1:C:172:GLU:CG	2.46	0.45
1:D:431:THR:O	1:D:432:CYS:HB2	2.14	0.45
1:D:544:THR:HG23	1:D:549:ARG:N	2.31	0.45
1:E:233:ASN:OD1	1:E:233:ASN:C	2.54	0.45
1:E:244:PRO:HA	1:E:275:TYR:CE2	2.51	0.45
1:E:493:THR:HG22	1:E:494:HIS:O	2.16	0.45
1:E:544:THR:HG23	1:E:549:ARG:N	2.31	0.45
1:A:382:LEU:HD12	1:A:382:LEU:HA	1.75	0.45
1:B:135:ASN:HA	1:B:172:GLU:CG	2.47	0.45
1:A:410:TYR:CE2	1:B:172:GLU:OE1	2.69	0.45
1:C:436:GLN:HE21	1:D:558:LEU:HD11	1.81	0.45
1:C:493:THR:HG22	1:C:494:HIS:O	2.16	0.45
1:C:493:THR:CG2	1:C:494:HIS:N	2.80	0.45
1:D:195:VAL:HG12	1:D:196:GLY:N	2.32	0.45
1:D:197:ARG:C	1:D:199:ASN:H	2.17	0.45
1:D:436:GLN:HE21	1:E:558:LEU:HD11	1.81	0.45
1:D:493:THR:CG2	1:D:494:HIS:N	2.80	0.45
1:E:135:ASN:HA	1:E:172:GLU:CG	2.46	0.45
1:E:441:LEU:HB2	1:E:445:MET:HE2	1.97	0.45
1:A:558:LEU:HD11	1:E:436:GLN:HE21	1.81	0.45
1:C:146:ARG:HB2	1:C:165:TRP:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ARG:CG	1:C:198:GLN:H	2.29	0.45
1:E:51:GLY:HA3	1:E:116:ARG:HH12	1.81	0.45
1:E:93:THR:HG22	1:E:94:THR:O	2.16	0.45
1:A:135:ASN:HA	1:A:172:GLU:CG	2.47	0.45
1:A:295:SER:CB	1:A:377:PRO:HG3	2.36	0.45
1:B:135:ASN:N	1:B:140:THR:OG1	2.47	0.45
1:B:265:GLN:HA	1:B:266:PRO:HD2	1.57	0.45
1:C:202:LEU:O	1:C:205:ASP:OD1	2.34	0.45
1:C:237:HIS:CD2	1:C:425:LEU:CD1	2.97	0.45
1:C:225:LEU:HD22	1:C:285:ALA:O	2.16	0.45
1:B:436:GLN:HE21	1:C:558:LEU:HD11	1.81	0.45
1:C:68:ARG:CG	1:C:68:ARG:NH1	2.66	0.45
1:D:135:ASN:HA	1:D:172:GLU:CG	2.47	0.45
1:D:146:ARG:HB2	1:D:165:TRP:CD2	2.52	0.45
1:D:170:LEU:HB3	1:D:171:PRO:HD2	1.99	0.45
1:D:225:LEU:HD22	1:D:285:ALA:O	2.16	0.45
1:D:446:GLN:O	1:D:448:PRO:HD3	2.17	0.45
1:E:170:LEU:HB3	1:E:171:PRO:HD2	1.99	0.45
1:E:195:VAL:HG12	1:E:196:GLY:N	2.32	0.45
1:E:225:LEU:HD22	1:E:285:ALA:O	2.16	0.45
1:E:130:ASN:HA	1:E:519:ASN:CG	2.36	0.45
1:A:146:ARG:HB2	1:A:165:TRP:CD2	2.52	0.45
1:A:202:LEU:O	1:A:205:ASP:OD1	2.34	0.45
1:B:243:LEU:CD2	1:B:403:TYR:CE2	2.96	0.45
1:B:529:LEU:HD21	1:C:68:ARG:HE	1.82	0.45
1:B:93:THR:HG22	1:B:94:THR:O	2.16	0.45
1:D:151:ARG:NH1	1:D:205:ASP:OD2	2.49	0.45
1:D:441:LEU:HB2	1:D:445:MET:HE2	1.99	0.45
1:E:135:ASN:HB2	1:E:172:GLU:OE2	2.16	0.45
1:A:436:GLN:HE21	1:B:558:LEU:HD11	1.81	0.45
1:B:527:GLY:HA3	1:C:68:ARG:NH2	2.32	0.45
1:C:132:PRO:HD3	1:C:553:TYR:CD2	2.51	0.45
1:C:463:VAL:HB	1:C:529:LEU:HD13	1.99	0.45
1:D:180:THR:HG21	1:D:258:LEU:HD23	1.97	0.45
1:D:243:LEU:HD23	1:D:244:PRO:HD3	1.99	0.45
1:D:513:ILE:N	1:D:513:ILE:HD12	2.31	0.45
1:D:74:ASN:ND2	1:D:556:LYS:HZ1	2.13	0.45
1:E:132:PRO:HD3	1:E:553:TYR:CD2	2.51	0.45
1:E:202:LEU:O	1:E:203:GLU:C	2.55	0.45
1:E:446:GLN:O	1:E:448:PRO:HD3	2.17	0.45
1:E:499:PHE:N	1:E:500:PRO:CD	2.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:GLN:O	1:A:448:PRO:HD3	2.17	0.45
1:B:197:ARG:CG	1:B:198:GLN:H	2.30	0.45
1:B:544:THR:HG23	1:B:549:ARG:N	2.31	0.45
1:C:135:ASN:HB2	1:C:172:GLU:OE2	2.16	0.45
1:C:436:GLN:N	1:C:436:GLN:OE1	2.38	0.45
1:D:250:PHE:O	1:D:252:HIS:N	2.50	0.45
1:D:63:LEU:HD12	1:D:63:LEU:HA	1.82	0.45
1:E:258:LEU:C	1:E:258:LEU:HD12	2.37	0.45
1:E:513:ILE:HD12	1:E:513:ILE:N	2.31	0.45
1:E:525:ASP:O	1:E:525:ASP:OD1	2.35	0.45
1:A:243:LEU:HD23	1:A:244:PRO:HD3	1.99	0.45
1:A:292:TYR:HA	1:A:377:PRO:HG3	1.91	0.45
1:B:195:VAL:HG12	1:B:196:GLY:N	2.32	0.45
1:D:233:ASN:C	1:D:233:ASN:OD1	2.54	0.45
1:D:525:ASP:OD1	1:D:525:ASP:O	2.35	0.45
1:E:493:THR:CG2	1:E:494:HIS:N	2.80	0.45
1:B:129:THR:HB	1:B:130:ASN:H	1.65	0.45
1:B:138:MET:HB3	1:B:254:ARG:HH11	1.80	0.45
1:B:149:VAL:CG2	1:B:195:VAL:HG11	2.45	0.45
1:C:195:VAL:HG12	1:C:196:GLY:N	2.32	0.45
1:C:225:LEU:HD13	1:C:287:LEU:HA	1.99	0.45
1:C:533:ASN:OD1	1:C:533:ASN:N	2.50	0.45
1:D:529:LEU:HD21	1:E:68:ARG:HE	1.82	0.45
1:E:476:TYR:HD1	1:E:513:ILE:CD1	2.30	0.45
1:A:197:ARG:O	1:A:199:ASN:N	2.43	0.44
1:A:250:PHE:O	1:A:252:HIS:N	2.50	0.44
1:A:525:ASP:O	1:A:525:ASP:OD1	2.35	0.44
1:A:74:ASN:ND2	1:A:556:LYS:NZ	2.66	0.44
1:A:75:LYS:NZ	1:A:94:THR:HG23	2.33	0.44
1:B:146:ARG:HB2	1:B:165:TRP:CD2	2.52	0.44
1:B:170:LEU:HB3	1:B:171:PRO:HD2	1.99	0.44
1:B:203:GLU:C	1:B:205:ASP:N	2.71	0.44
1:B:295:SER:CB	1:B:377:PRO:HG3	2.36	0.44
1:B:493:THR:HG22	1:B:494:HIS:O	2.16	0.44
1:C:217:LEU:CB	1:C:232:THR:HG21	2.46	0.44
1:C:525:ASP:O	1:C:525:ASP:OD1	2.35	0.44
1:E:151:ARG:NH1	1:E:205:ASP:OD2	2.49	0.44
1:A:172:GLU:OE1	1:E:410:TYR:CE2	2.68	0.44
1:C:229:GLY:O	1:C:286:LEU:HD13	2.18	0.44
1:D:258:LEU:C	1:D:258:LEU:HD12	2.37	0.44
1:D:493:THR:HG22	1:D:494:HIS:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:PHE:O	1:E:252:HIS:N	2.50	0.44
1:E:420:ARG:O	1:E:420:ARG:HG3	2.17	0.44
1:E:389:ARG:CD	1:E:502:ASN:HD22	2.23	0.44
1:E:533:ASN:OD1	1:E:533:ASN:N	2.50	0.44
1:A:476:TYR:HD1	1:A:513:ILE:CD1	2.30	0.44
1:A:529:LEU:HD21	1:B:68:ARG:HE	1.82	0.44
1:B:225:LEU:HD13	1:B:287:LEU:HA	2.00	0.44
1:B:229:GLY:O	1:B:286:LEU:HD13	2.18	0.44
1:D:217:LEU:CB	1:D:232:THR:HG21	2.46	0.44
1:D:389:ARG:CD	1:D:502:ASN:HD22	2.23	0.44
1:D:75:LYS:NZ	1:D:94:THR:HG23	2.32	0.44
1:E:243:LEU:HD23	1:E:244:PRO:HD3	1.99	0.44
1:E:68:ARG:NH1	1:E:68:ARG:CG	2.66	0.44
1:E:75:LYS:NZ	1:E:94:THR:HG23	2.32	0.44
1:A:229:GLY:O	1:A:286:LEU:HD13	2.18	0.44
1:A:441:LEU:HD12	1:A:445:MET:CE	2.48	0.44
1:A:533:ASN:OD1	1:A:533:ASN:N	2.50	0.44
1:B:243:LEU:HD23	1:B:244:PRO:HD3	1.99	0.44
1:B:476:TYR:HD1	1:B:513:ILE:CD1	2.30	0.44
1:C:203:GLU:C	1:C:205:ASP:N	2.70	0.44
1:C:262:ARG:NH1	1:D:130:ASN:ND2	2.55	0.44
1:C:527:GLY:HA3	1:D:68:ARG:NH2	2.32	0.44
1:C:75:LYS:NZ	1:C:94:THR:HG23	2.32	0.44
1:C:93:THR:HG22	1:C:94:THR:O	2.17	0.44
1:C:410:TYR:CE2	1:D:172:GLU:OE1	2.68	0.44
1:D:203:GLU:C	1:D:205:ASP:N	2.70	0.44
1:D:265:GLN:HA	1:D:266:PRO:HD2	1.57	0.44
1:E:63:LEU:HD12	1:E:63:LEU:HA	1.82	0.44
1:A:195:VAL:HG12	1:A:196:GLY:N	2.32	0.44
1:A:203:GLU:C	1:A:205:ASP:N	2.70	0.44
1:A:429:ASP:OD1	1:A:432:CYS:N	2.51	0.44
1:B:250:PHE:O	1:B:252:HIS:N	2.50	0.44
1:B:446:GLN:O	1:B:448:PRO:HD3	2.17	0.44
1:B:74:ASN:ND2	1:B:556:LYS:NZ	2.65	0.44
1:B:75:LYS:NZ	1:B:94:THR:HG23	2.32	0.44
1:C:250:PHE:O	1:C:252:HIS:N	2.50	0.44
1:C:468:LEU:C	1:C:468:LEU:HD12	2.38	0.44
1:C:63:LEU:HA	1:C:63:LEU:HD12	1.82	0.44
1:D:295:SER:O	1:D:296:LEU:CB	2.64	0.44
1:D:429:ASP:OD1	1:D:432:CYS:N	2.51	0.44
1:D:93:THR:HG22	1:D:94:THR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:ARG:HB2	1:E:165:TRP:CD2	2.52	0.44
1:E:229:GLY:O	1:E:286:LEU:HD13	2.18	0.44
1:E:441:LEU:HD12	1:E:445:MET:CE	2.48	0.44
1:B:558:LEU:HD23	1:B:558:LEU:HA	1.62	0.44
1:C:243:LEU:HD23	1:C:244:PRO:HD3	1.99	0.44
1:A:560:ILE:HD11	1:E:465:ALA:HB3	2.00	0.44
1:B:258:LEU:HD12	1:B:258:LEU:C	2.38	0.44
1:B:261:ILE:HD12	1:B:406:TRP:CZ3	2.53	0.44
1:B:436:GLN:N	1:B:436:GLN:OE1	2.39	0.44
1:B:463:VAL:HB	1:B:529:LEU:HD13	1.99	0.44
1:C:264:ARG:O	1:C:264:ARG:HG3	2.18	0.44
1:E:468:LEU:HD12	1:E:468:LEU:C	2.38	0.44
1:E:128:HIS:HD2	1:E:555:TYR:HD2	1.66	0.44
1:A:197:ARG:CG	1:A:198:GLN:H	2.30	0.44
1:A:391:TYR:O	1:A:392:ASN:C	2.57	0.44
1:A:68:ARG:HE	1:E:529:LEU:HD21	1.82	0.44
1:A:83:ASN:ND2	1:A:92:LEU:O	2.51	0.44
1:B:420:ARG:HG3	1:B:420:ARG:O	2.17	0.44
1:C:420:ARG:O	1:C:420:ARG:HG3	2.17	0.44
1:C:128:HIS:HD2	1:C:555:TYR:HD2	1.66	0.44
1:C:83:ASN:ND2	1:C:92:LEU:O	2.51	0.44
1:D:533:ASN:OD1	1:D:533:ASN:N	2.50	0.44
1:E:225:LEU:HD13	1:E:287:LEU:HA	1.99	0.44
1:E:261:ILE:HD12	1:E:406:TRP:CZ3	2.53	0.44
1:A:170:LEU:HB3	1:A:171:PRO:HD2	1.99	0.44
1:A:68:ARG:NH2	1:E:527:GLY:HA3	2.32	0.44
1:B:525:ASP:OD1	1:B:525:ASP:O	2.35	0.44
1:C:170:LEU:HB3	1:C:171:PRO:HD2	1.99	0.44
1:C:446:GLN:O	1:C:448:PRO:HD3	2.17	0.44
1:E:83:ASN:ND2	1:E:92:LEU:O	2.51	0.44
1:A:420:ARG:O	1:A:420:ARG:HG3	2.17	0.43
1:A:493:THR:CG2	1:A:494:HIS:N	2.79	0.43
1:A:527:GLY:HA3	1:B:68:ARG:NH2	2.32	0.43
1:B:467:LEU:HA	1:B:467:LEU:HD12	1.83	0.43
1:C:202:LEU:O	1:C:203:GLU:C	2.55	0.43
1:C:258:LEU:HD12	1:C:258:LEU:C	2.37	0.43
1:C:261:ILE:HD12	1:C:406:TRP:CZ3	2.53	0.43
1:D:106:ALA:C	1:D:108:THR:N	2.71	0.43
1:D:135:ASN:N	1:D:140:THR:OG1	2.47	0.43
1:D:420:ARG:HG3	1:D:420:ARG:O	2.17	0.43
1:D:83:ASN:ND2	1:D:92:LEU:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASN:ND2	1:E:262:ARG:NH1	2.55	0.43
1:E:436:GLN:N	1:E:436:GLN:OE1	2.39	0.43
1:A:202:LEU:O	1:A:203:GLU:C	2.55	0.43
1:A:258:LEU:HD12	1:A:258:LEU:C	2.37	0.43
1:A:264:ARG:O	1:A:264:ARG:HG3	2.18	0.43
1:A:225:LEU:HD13	1:A:287:LEU:HA	1.99	0.43
1:A:468:LEU:C	1:A:468:LEU:HD12	2.38	0.43
1:B:533:ASN:N	1:B:533:ASN:OD1	2.50	0.43
1:D:261:ILE:HD12	1:D:406:TRP:CZ3	2.53	0.43
1:D:468:LEU:HD12	1:D:468:LEU:C	2.38	0.43
1:D:444:MET:HB2	1:D:539:GLN:CD	2.39	0.43
1:D:527:GLY:HA3	1:E:68:ARG:NH2	2.33	0.43
1:E:74:ASN:ND2	1:E:556:LYS:NZ	2.66	0.43
1:A:106:ALA:C	1:A:108:THR:H	2.22	0.43
1:A:244:PRO:HA	1:A:275:TYR:CE2	2.51	0.43
1:A:393:LEU:N	1:A:393:LEU:CD1	2.81	0.43
1:A:467:LEU:HD13	1:B:126:ILE:HG21	2.01	0.43
1:B:83:ASN:ND2	1:B:92:LEU:O	2.51	0.43
1:C:429:ASP:OD1	1:C:432:CYS:N	2.51	0.43
1:C:524:THR:OG1	1:C:525:ASP:N	2.52	0.43
1:E:264:ARG:HG3	1:E:264:ARG:O	2.18	0.43
1:A:463:VAL:HB	1:A:529:LEU:HD13	1.99	0.43
1:B:202:LEU:O	1:B:203:GLU:C	2.55	0.43
1:C:391:TYR:O	1:C:392:ASN:C	2.57	0.43
1:D:225:LEU:HD13	1:D:287:LEU:HA	1.99	0.43
1:D:262:ARG:HH11	1:E:130:ASN:HD22	1.55	0.43
1:E:197:ARG:CG	1:E:198:GLN:H	2.29	0.43
1:E:444:MET:HB2	1:E:539:GLN:CD	2.39	0.43
1:A:237:HIS:CD2	1:A:425:LEU:CD1	2.97	0.43
1:B:411:ASN:OD1	1:C:172:GLU:N	2.52	0.43
1:B:497:ASN:O	1:B:500:PRO:HD3	2.19	0.43
1:B:467:LEU:HD13	1:C:126:ILE:HG21	2.00	0.43
1:C:395:SER:C	1:C:397:ASP:N	2.71	0.43
1:C:419:ILE:C	1:C:421:SER:N	2.72	0.43
1:C:74:ASN:ND2	1:C:556:LYS:NZ	2.66	0.43
1:D:229:GLY:O	1:D:286:LEU:HD13	2.18	0.43
1:A:419:ILE:C	1:A:421:SER:N	2.72	0.43
1:A:481:VAL:O	1:A:482:TYR:C	2.57	0.43
1:A:497:ASN:O	1:A:500:PRO:HD3	2.19	0.43
1:A:524:THR:OG1	1:A:525:ASP:N	2.52	0.43
1:A:527:GLY:HA3	1:B:68:ARG:HH21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:LEU:CD1	1:B:393:LEU:N	2.81	0.43
1:B:419:ILE:C	1:B:421:SER:N	2.72	0.43
1:C:106:ALA:C	1:C:108:THR:N	2.71	0.43
1:C:476:TYR:HD1	1:C:513:ILE:CD1	2.30	0.43
1:B:465:ALA:HB3	1:C:560:ILE:HD11	2.00	0.43
1:D:74:ASN:ND2	1:D:556:LYS:NZ	2.66	0.43
1:C:527:GLY:HA3	1:D:68:ARG:HH21	1.84	0.43
1:E:149:VAL:CG2	1:E:195:VAL:HG11	2.45	0.43
1:A:419:ILE:O	1:A:421:SER:N	2.52	0.43
1:A:508:PRO:HA	1:A:509:PRO:HD3	1.73	0.43
1:A:68:ARG:NH1	1:A:562:SER:CB	2.79	0.43
1:B:262:ARG:NH1	1:C:130:ASN:ND2	2.55	0.43
1:B:429:ASP:OD1	1:B:432:CYS:N	2.51	0.43
1:C:444:MET:HB2	1:C:539:GLN:CD	2.39	0.43
1:D:463:VAL:HB	1:D:529:LEU:HD13	1.99	0.43
1:E:391:TYR:O	1:E:392:ASN:C	2.57	0.43
1:E:427:THR:HA	1:E:428:PRO:HD3	1.75	0.43
1:A:126:ILE:HG21	1:E:467:LEU:HD13	2.00	0.43
1:C:441:LEU:HB2	1:C:445:MET:HE2	2.00	0.43
1:C:529:LEU:HD21	1:D:68:ARG:HE	1.82	0.43
1:D:243:LEU:CD2	1:D:403:TYR:CE2	2.96	0.43
1:D:436:GLN:N	1:D:436:GLN:OE1	2.38	0.43
1:C:465:ALA:HB3	1:D:560:ILE:HD11	2.00	0.43
1:E:106:ALA:C	1:E:108:THR:H	2.22	0.43
1:C:481:VAL:O	1:C:482:TYR:C	2.57	0.43
1:D:393:LEU:N	1:D:393:LEU:CD1	2.81	0.43
1:D:74:ASN:HD22	1:D:556:LYS:HZ1	1.67	0.43
1:E:217:LEU:CB	1:E:232:THR:HG21	2.46	0.43
1:E:463:VAL:HB	1:E:529:LEU:HD13	1.99	0.43
1:A:214:ASN:O	1:A:216:ARG:N	2.50	0.43
1:A:261:ILE:HD12	1:A:406:TRP:CZ3	2.53	0.43
1:A:444:MET:HB2	1:A:539:GLN:CD	2.39	0.43
1:A:128:HIS:HD2	1:A:555:TYR:HD2	1.66	0.43
1:B:264:ARG:O	1:B:264:ARG:HG3	2.18	0.43
1:B:524:THR:OG1	1:B:525:ASP:N	2.52	0.43
1:C:197:ARG:O	1:C:199:ASN:N	2.43	0.43
1:D:264:ARG:O	1:D:264:ARG:HG3	2.18	0.43
1:E:275:TYR:CE1	1:E:404:ARG:HD2	2.54	0.43
1:E:419:ILE:O	1:E:421:SER:N	2.52	0.43
1:E:68:ARG:NH1	1:E:562:SER:CB	2.79	0.43
1:A:279:GLU:O	1:A:280:GLY:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:TYR:O	1:B:392:ASN:C	2.57	0.42
1:B:527:GLY:HA3	1:C:68:ARG:HH21	1.84	0.42
1:C:194:LYS:HG2	1:C:194:LYS:O	2.19	0.42
1:C:419:ILE:O	1:C:421:SER:N	2.52	0.42
1:D:202:LEU:O	1:D:203:GLU:C	2.55	0.42
1:D:394:ILE:HG23	1:D:395:SER:N	2.34	0.42
1:D:65:ASP:O	1:D:66:THR:C	2.57	0.42
1:E:265:GLN:HA	1:E:266:PRO:HD2	1.57	0.42
1:E:481:VAL:O	1:E:482:TYR:C	2.57	0.42
1:E:497:ASN:O	1:E:500:PRO:HD3	2.19	0.42
1:E:65:ASP:O	1:E:66:THR:C	2.58	0.42
1:B:419:ILE:O	1:B:421:SER:N	2.52	0.42
1:B:468:LEU:HD12	1:B:468:LEU:C	2.38	0.42
1:A:451:PHE:CE1	1:B:97:GLN:CB	3.03	0.42
1:D:275:TYR:CE1	1:D:404:ARG:HD2	2.54	0.42
1:D:476:TYR:HD1	1:D:513:ILE:CD1	2.30	0.42
1:D:68:ARG:NH1	1:D:562:SER:CB	2.79	0.42
1:B:106:ALA:C	1:B:108:THR:H	2.22	0.42
1:C:411:ASN:OD1	1:D:172:GLU:N	2.51	0.42
1:C:430:VAL:O	1:C:432:CYS:N	2.53	0.42
1:C:467:LEU:HA	1:C:467:LEU:HD12	1.83	0.42
1:C:65:ASP:O	1:C:66:THR:C	2.58	0.42
1:D:106:ALA:C	1:D:108:THR:H	2.22	0.42
1:D:278:LEU:CD2	1:D:419:ILE:HD12	2.38	0.42
1:D:441:LEU:HD12	1:D:445:MET:CE	2.47	0.42
1:D:128:HIS:HD2	1:D:555:TYR:HD2	1.66	0.42
1:D:75:LYS:HZ2	1:D:94:THR:HG23	1.84	0.42
1:E:106:ALA:C	1:E:108:THR:N	2.71	0.42
1:A:53:ASN:O	1:A:54:SER:O	2.38	0.42
1:B:444:MET:HB2	1:B:539:GLN:CD	2.39	0.42
1:B:481:VAL:O	1:B:482:TYR:C	2.57	0.42
1:B:389:ARG:CD	1:B:502:ASN:HD22	2.23	0.42
1:B:128:HIS:HD2	1:B:555:TYR:HD2	1.66	0.42
1:B:410:TYR:CE2	1:C:172:GLU:OE1	2.68	0.42
1:C:497:ASN:O	1:C:500:PRO:HD3	2.19	0.42
1:C:75:LYS:HZ2	1:C:94:THR:HG23	1.83	0.42
1:D:149:VAL:CG2	1:D:195:VAL:HG11	2.45	0.42
1:D:411:ASN:OD1	1:E:172:GLU:N	2.52	0.42
1:E:203:GLU:HG2	1:E:203:GLU:H	1.69	0.42
1:E:419:ILE:C	1:E:421:SER:N	2.72	0.42
1:A:106:ALA:C	1:A:108:THR:N	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:PHE:CE1	1:C:97:GLN:CB	3.03	0.42
1:C:393:LEU:CD1	1:C:393:LEU:N	2.81	0.42
1:D:419:ILE:O	1:D:421:SER:N	2.52	0.42
1:E:203:GLU:C	1:E:205:ASP:N	2.71	0.42
1:E:237:HIS:CD2	1:E:425:LEU:CD1	2.97	0.42
1:A:172:GLU:N	1:E:411:ASN:OD1	2.52	0.42
1:A:558:LEU:HD23	1:A:558:LEU:HA	1.62	0.42
1:B:194:LYS:HG2	1:B:194:LYS:O	2.19	0.42
1:B:295:SER:O	1:B:296:LEU:CB	2.64	0.42
1:B:275:TYR:CE1	1:B:404:ARG:HD2	2.54	0.42
1:B:230:VAL:HG13	1:B:503:GLN:NE2	2.35	0.42
1:C:275:TYR:CE1	1:C:404:ARG:HD2	2.54	0.42
1:C:478:ASP:C	1:C:480:ALA:N	2.73	0.42
1:C:230:VAL:HG13	1:C:503:GLN:NE2	2.35	0.42
1:D:230:VAL:HG13	1:D:503:GLN:NE2	2.35	0.42
1:D:502:ASN:C	1:D:504:ILE:H	2.23	0.42
1:D:93:THR:CG2	1:D:94:THR:N	2.83	0.42
1:E:135:ASN:N	1:E:140:THR:OG1	2.47	0.42
1:E:230:VAL:HG13	1:E:503:GLN:NE2	2.35	0.42
1:E:53:ASN:O	1:E:54:SER:O	2.38	0.42
1:E:93:THR:CG2	1:E:94:THR:N	2.83	0.42
1:A:395:SER:C	1:A:397:ASP:N	2.71	0.42
1:A:465:ALA:HB3	1:B:560:ILE:HD11	2.00	0.42
1:A:230:VAL:HG13	1:A:503:GLN:NE2	2.35	0.42
1:B:237:HIS:NE2	1:B:425:LEU:CD1	2.83	0.42
1:B:441:LEU:HD12	1:B:445:MET:CE	2.47	0.42
1:C:106:ALA:C	1:C:108:THR:H	2.22	0.42
1:C:502:ASN:C	1:C:504:ILE:H	2.23	0.42
1:D:279:GLU:O	1:D:280:GLY:O	2.37	0.42
1:D:467:LEU:HD13	1:E:126:ILE:HG21	2.01	0.42
1:D:524:THR:OG1	1:D:525:ASP:N	2.52	0.42
1:E:145:ALA:HB3	1:E:168:PHE:CE1	2.44	0.42
1:D:527:GLY:HA3	1:E:68:ARG:HH21	1.84	0.42
1:A:411:ASN:OD1	1:B:172:GLU:N	2.52	0.42
1:A:430:VAL:O	1:A:432:CYS:N	2.53	0.42
1:A:502:ASN:C	1:A:504:ILE:H	2.23	0.42
1:A:65:ASP:O	1:A:66:THR:C	2.58	0.42
1:C:279:GLU:O	1:C:280:GLY:O	2.38	0.42
1:D:406:TRP:HE1	1:D:419:ILE:HG21	1.85	0.42
1:D:497:ASN:O	1:D:500:PRO:HD3	2.19	0.42
1:E:475:PHE:CD1	1:E:475:PHE:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:465:ALA:HB3	1:E:560:ILE:HD11	2.00	0.42
1:D:451:PHE:CE1	1:E:97:GLN:CB	3.03	0.42
1:B:197:ARG:O	1:B:199:ASN:N	2.43	0.42
1:B:279:GLU:O	1:B:280:GLY:O	2.38	0.42
1:B:65:ASP:O	1:B:66:THR:C	2.57	0.42
1:C:441:LEU:HD12	1:C:445:MET:CE	2.48	0.42
1:D:391:TYR:O	1:D:392:ASN:C	2.57	0.42
1:D:53:ASN:O	1:D:54:SER:O	2.38	0.42
1:E:178:THR:C	1:E:180:THR:N	2.73	0.42
1:E:194:LYS:HG2	1:E:194:LYS:O	2.19	0.42
1:A:68:ARG:HH21	1:E:527:GLY:HA3	1.84	0.42
1:A:180:THR:O	1:A:181:ILE:C	2.58	0.42
1:A:237:HIS:NE2	1:A:425:LEU:CD1	2.83	0.42
1:B:475:PHE:CD1	1:B:475:PHE:N	2.88	0.42
1:B:502:ASN:C	1:B:504:ILE:H	2.23	0.42
1:B:68:ARG:NH1	1:B:562:SER:CB	2.79	0.42
1:C:406:TRP:HE1	1:C:419:ILE:HG21	1.85	0.42
1:C:467:LEU:HD13	1:D:126:ILE:HG21	2.01	0.42
1:D:178:THR:C	1:D:180:THR:N	2.73	0.42
1:D:194:LYS:O	1:D:194:LYS:HG2	2.19	0.42
1:D:237:HIS:NE2	1:D:425:LEU:CD1	2.83	0.42
1:E:430:VAL:O	1:E:432:CYS:N	2.53	0.42
1:E:501:GLU:O	1:E:501:GLU:HG2	2.20	0.42
1:E:524:THR:OG1	1:E:525:ASP:N	2.52	0.42
1:A:149:VAL:CG2	1:A:195:VAL:HG11	2.45	0.41
1:D:129:THR:HB	1:D:130:ASN:H	1.65	0.41
1:D:68:ARG:NH1	1:D:68:ARG:CG	2.66	0.41
1:E:131:MET:HA	1:E:132:PRO:HD3	1.87	0.41
1:A:194:LYS:HG2	1:A:194:LYS:O	2.19	0.41
1:B:154:THR:HG1	1:B:160:GLU:HB2	1.83	0.41
1:B:211:ASP:C	1:B:212:THR:HG23	2.41	0.41
1:B:394:ILE:HG23	1:B:395:SER:N	2.34	0.41
1:B:406:TRP:HE1	1:B:419:ILE:HG21	1.85	0.41
1:B:430:VAL:O	1:B:432:CYS:N	2.53	0.41
1:B:468:LEU:HA	1:B:469:PRO:HD3	1.76	0.41
1:B:53:ASN:O	1:B:54:SER:O	2.38	0.41
1:B:75:LYS:HZ2	1:B:94:THR:HG23	1.84	0.41
1:C:180:THR:O	1:C:181:ILE:C	2.58	0.41
1:D:430:VAL:O	1:D:432:CYS:N	2.53	0.41
1:E:279:GLU:O	1:E:280:GLY:O	2.38	0.41
1:E:376:LYS:CB	1:E:377:PRO:HD2	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:THR:HG1	1:A:160:GLU:HB2	1.81	0.41
1:A:178:THR:C	1:A:180:THR:N	2.73	0.41
1:A:275:TYR:CE1	1:A:404:ARG:HD2	2.54	0.41
1:B:93:THR:CG2	1:B:94:THR:N	2.83	0.41
1:C:178:THR:C	1:C:180:THR:N	2.73	0.41
1:C:214:ASN:O	1:C:216:ARG:N	2.50	0.41
1:C:419:ILE:HG22	1:C:423:THR:HG22	2.02	0.41
1:B:450:THR:HG21	1:C:96:ILE:HD13	2.03	0.41
1:D:383:THR:C	1:D:384:GLU:HG3	2.41	0.41
1:D:481:VAL:O	1:D:482:TYR:C	2.57	0.41
1:C:451:PHE:CE1	1:D:97:GLN:CB	3.03	0.41
1:E:149:VAL:HG22	1:E:149:VAL:O	2.21	0.41
1:E:243:LEU:HD23	1:E:243:LEU:HA	1.92	0.41
1:E:406:TRP:HE1	1:E:419:ILE:HG21	1.85	0.41
1:B:180:THR:O	1:B:181:ILE:C	2.58	0.41
1:B:88:HIS:CD2	1:B:555:TYR:O	2.74	0.41
1:C:135:ASN:N	1:C:140:THR:OG1	2.47	0.41
1:C:211:ASP:C	1:C:212:THR:HG23	2.41	0.41
1:C:237:HIS:NE2	1:C:425:LEU:CD1	2.83	0.41
1:C:501:GLU:O	1:C:501:GLU:HG2	2.20	0.41
1:D:501:GLU:HG2	1:D:501:GLU:O	2.20	0.41
1:D:530:PRO:HG3	1:E:66:THR:O	2.21	0.41
1:E:287:LEU:HD23	1:E:288:ASP:C	2.41	0.41
1:E:383:THR:C	1:E:384:GLU:HG3	2.41	0.41
1:E:237:HIS:NE2	1:E:425:LEU:CD1	2.83	0.41
1:A:135:ASN:N	1:A:140:THR:OG1	2.47	0.41
1:B:106:ALA:C	1:B:108:THR:N	2.71	0.41
1:C:382:LEU:HA	1:C:382:LEU:HD12	1.75	0.41
1:C:88:HIS:CD2	1:C:555:TYR:O	2.74	0.41
1:D:214:ASN:O	1:D:216:ARG:N	2.50	0.41
1:D:265:GLN:NE2	1:D:268:GLN:NE2	2.68	0.41
1:D:382:LEU:HA	1:D:382:LEU:HD12	1.75	0.41
1:E:211:ASP:C	1:E:212:THR:HG23	2.41	0.41
1:E:395:SER:C	1:E:397:ASP:N	2.71	0.41
1:B:287:LEU:HD23	1:B:288:ASP:C	2.41	0.41
1:B:395:SER:C	1:B:397:ASP:N	2.71	0.41
1:B:530:PRO:HG3	1:C:66:THR:O	2.21	0.41
1:C:211:ASP:OD1	1:C:212:THR:N	2.35	0.41
1:C:475:PHE:CD1	1:C:475:PHE:N	2.88	0.41
1:E:197:ARG:O	1:E:199:ASN:N	2.43	0.41
1:E:255:LEU:HA	1:E:255:LEU:HD23	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:502:ASN:C	1:E:504:ILE:H	2.23	0.41
1:E:508:PRO:HA	1:E:509:PRO:HD3	1.73	0.41
1:A:153:LEU:HD23	1:A:159:VAL:HG12	2.03	0.41
1:A:203:GLU:H	1:A:203:GLU:HG2	1.69	0.41
1:A:287:LEU:HD23	1:A:288:ASP:C	2.41	0.41
1:A:406:TRP:HE1	1:A:419:ILE:HG21	1.85	0.41
1:A:419:ILE:HG22	1:A:423:THR:HG22	2.02	0.41
1:A:430:VAL:HG23	1:A:431:THR:N	2.36	0.41
1:B:478:ASP:C	1:B:480:ALA:N	2.73	0.41
1:A:530:PRO:HG3	1:B:66:THR:O	2.21	0.41
1:C:149:VAL:HG22	1:C:149:VAL:O	2.21	0.41
1:C:265:GLN:NE2	1:C:268:GLN:NE2	2.68	0.41
1:D:478:ASP:C	1:D:480:ALA:N	2.73	0.41
1:E:214:ASN:O	1:E:216:ARG:N	2.50	0.41
1:E:265:GLN:NE2	1:E:268:GLN:NE2	2.68	0.41
1:E:393:LEU:CD1	1:E:393:LEU:N	2.81	0.41
1:E:429:ASP:OD1	1:E:432:CYS:N	2.51	0.41
1:A:211:ASP:C	1:A:212:THR:HG23	2.41	0.41
1:A:475:PHE:CD1	1:A:475:PHE:N	2.88	0.41
1:B:214:ASN:O	1:B:216:ARG:N	2.50	0.41
1:B:383:THR:C	1:B:384:GLU:HG3	2.41	0.41
1:C:180:THR:HG21	1:C:258:LEU:HD21	2.03	0.41
1:C:430:VAL:HG23	1:C:431:THR:N	2.36	0.41
1:C:450:THR:HG21	1:D:96:ILE:HD13	2.03	0.41
1:D:395:SER:C	1:D:397:ASP:N	2.71	0.41
1:E:113:LEU:HA	1:E:113:LEU:HD23	1.71	0.41
1:A:97:GLN:CB	1:E:451:PHE:CE1	3.03	0.41
1:E:478:ASP:C	1:E:480:ALA:N	2.73	0.41
1:A:265:GLN:NE2	1:A:268:GLN:NE2	2.68	0.41
1:A:501:GLU:HG2	1:A:501:GLU:O	2.20	0.41
1:C:68:ARG:NH1	1:C:562:SER:CB	2.79	0.41
1:D:180:THR:O	1:D:181:ILE:C	2.58	0.41
1:E:129:THR:HB	1:E:130:ASN:H	1.65	0.41
1:E:153:LEU:HD23	1:E:159:VAL:HG12	2.03	0.41
1:E:180:THR:O	1:E:181:ILE:C	2.58	0.41
1:E:88:HIS:CD2	1:E:555:TYR:O	2.74	0.41
1:A:93:THR:CG2	1:A:94:THR:N	2.83	0.41
1:B:113:LEU:HA	1:B:113:LEU:HD23	1.71	0.41
1:B:185:ASN:O	1:B:188:ILE:HB	2.21	0.41
1:B:381:PRO:O	1:B:381:PRO:HG2	2.21	0.41
1:B:243:LEU:CD1	1:B:403:TYR:HE2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:ILE:C	1:C:506:ALA:H	2.25	0.41
1:D:134:VAL:HG21	1:D:175:TYR:CE2	2.56	0.41
1:D:153:LEU:HD23	1:D:159:VAL:HG12	2.03	0.41
1:D:211:ASP:C	1:D:212:THR:HG23	2.41	0.41
1:D:287:LEU:HD23	1:D:288:ASP:C	2.41	0.41
1:D:394:ILE:CG2	1:D:398:SER:HB2	2.51	0.41
1:D:475:PHE:CD1	1:D:475:PHE:N	2.88	0.41
1:A:96:ILE:HD13	1:E:450:THR:HG21	2.03	0.41
1:A:217:LEU:CB	1:A:232:THR:HG21	2.46	0.41
1:A:66:THR:O	1:E:530:PRO:HG3	2.21	0.41
1:B:178:THR:C	1:B:180:THR:N	2.73	0.41
1:B:430:VAL:HG23	1:B:431:THR:N	2.36	0.41
1:C:131:MET:HA	1:C:132:PRO:HD3	1.87	0.41
1:C:53:ASN:O	1:C:54:SER:O	2.38	0.41
1:D:131:MET:HA	1:D:132:PRO:HD3	1.87	0.41
1:D:149:VAL:HG22	1:D:149:VAL:O	2.21	0.41
1:D:290:ASP:O	1:D:291:ALA:C	2.60	0.41
1:D:96:ILE:HA	1:D:96:ILE:HD13	1.87	0.41
1:E:295:SER:O	1:E:296:LEU:CB	2.64	0.41
1:A:383:THR:C	1:A:384:GLU:HG3	2.41	0.40
1:B:153:LEU:HD23	1:B:159:VAL:HG12	2.03	0.40
1:B:501:GLU:HG2	1:B:501:GLU:O	2.20	0.40
1:B:63:LEU:HD12	1:B:63:LEU:HA	1.82	0.40
1:C:93:THR:CG2	1:C:94:THR:N	2.83	0.40
1:C:96:ILE:HG22	1:C:98:ASN:H	1.86	0.40
1:D:430:VAL:HG23	1:D:431:THR:N	2.36	0.40
1:D:542:THR:O	1:D:542:THR:HG22	2.21	0.40
1:D:96:ILE:HG22	1:D:98:ASN:H	1.86	0.40
1:E:468:LEU:HA	1:E:469:PRO:HD3	1.76	0.40
1:A:220:ASP:HA	1:A:221:PRO:HD2	1.89	0.40
1:C:129:THR:HB	1:C:130:ASN:H	1.65	0.40
1:C:153:LEU:HD23	1:C:159:VAL:HG12	2.03	0.40
1:C:383:THR:C	1:C:384:GLU:HG3	2.41	0.40
1:D:180:THR:HG21	1:D:258:LEU:HD21	2.03	0.40
1:D:198:GLN:HG3	1:D:198:GLN:H	1.63	0.40
1:D:419:ILE:C	1:D:421:SER:N	2.72	0.40
1:A:180:THR:HG21	1:A:258:LEU:HD21	2.03	0.40
1:B:132:PRO:HD2	1:B:135:ASN:HD22	1.86	0.40
1:C:508:PRO:HA	1:C:509:PRO:HD3	1.73	0.40
1:C:530:PRO:HG3	1:D:66:THR:O	2.21	0.40
1:D:75:LYS:HB3	1:D:78:ASP:OD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:ASN:O	1:E:188:ILE:HB	2.21	0.40
1:B:265:GLN:NE2	1:B:268:GLN:NE2	2.68	0.40
1:B:75:LYS:HB3	1:B:78:ASP:OD2	2.22	0.40
1:B:96:ILE:HG22	1:B:98:ASN:H	1.86	0.40
1:C:134:VAL:HG21	1:C:175:TYR:CE2	2.56	0.40
1:C:73:ASP:OD1	1:C:73:ASP:N	2.42	0.40
1:D:145:ALA:HB3	1:D:168:PHE:CE1	2.44	0.40
1:E:243:LEU:CG	1:E:403:TYR:CE2	3.05	0.40
1:E:419:ILE:HA	1:E:422:TRP:NE1	2.37	0.40
1:A:134:VAL:HG21	1:A:175:TYR:CE2	2.56	0.40
1:A:149:VAL:HG22	1:A:149:VAL:O	2.21	0.40
1:A:211:ASP:OD1	1:A:212:THR:N	2.35	0.40
1:B:278:LEU:CD2	1:B:419:ILE:HD12	2.38	0.40
1:B:481:VAL:HG13	1:B:482:TYR:N	2.37	0.40
1:C:381:PRO:HG2	1:C:381:PRO:O	2.21	0.40
1:D:113:LEU:HA	1:D:113:LEU:HD23	1.71	0.40
1:D:154:THR:HG1	1:D:160:GLU:HB2	1.83	0.40
1:D:88:HIS:CD2	1:D:555:TYR:O	2.74	0.40
1:E:290:ASP:O	1:E:291:ALA:C	2.60	0.40
1:E:394:ILE:HG23	1:E:395:SER:N	2.34	0.40
1:E:468:LEU:HD12	1:E:469:PRO:N	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	444/523 (85%)	324 (73%)	74 (17%)	46 (10%)	0	10
1	B	444/523 (85%)	324 (73%)	74 (17%)	46 (10%)	0	10
1	C	444/523 (85%)	324 (73%)	74 (17%)	46 (10%)	0	10
1	D	444/523 (85%)	323 (73%)	75 (17%)	46 (10%)	0	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	444/523 (85%)	324 (73%)	74 (17%)	46 (10%)	0	10
All	All	2220/2615 (85%)	1619 (73%)	371 (17%)	230 (10%)	1	10

All (230) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	SER
1	A	59	GLU
1	A	130	ASN
1	A	137	PHE
1	A	296	LEU
1	A	375	LYS
1	A	378	VAL
1	A	379	ILE
1	A	449	VAL
1	A	469	PRO
1	A	492	LEU
1	A	506	ALA
1	B	54	SER
1	B	59	GLU
1	B	130	ASN
1	B	137	PHE
1	B	296	LEU
1	B	375	LYS
1	B	378	VAL
1	B	379	ILE
1	B	449	VAL
1	B	469	PRO
1	B	492	LEU
1	B	506	ALA
1	C	54	SER
1	C	59	GLU
1	C	130	ASN
1	C	137	PHE
1	C	296	LEU
1	C	375	LYS
1	C	378	VAL
1	C	379	ILE
1	C	449	VAL
1	C	469	PRO
1	C	492	LEU
1	C	506	ALA

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Mol	Chain	Res	Type
1	D	54	SER
1	D	59	GLU
1	D	130	ASN
1	D	137	PHE
1	D	296	LEU
1	D	375	LYS
1	D	378	VAL
1	D	379	ILE
1	D	449	VAL
1	D	469	PRO
1	D	492	LEU
1	D	506	ALA
1	E	54	SER
1	E	59	GLU
1	E	130	ASN
1	E	137	PHE
1	E	296	LEU
1	E	375	LYS
1	E	378	VAL
1	E	379	ILE
1	E	449	VAL
1	E	469	PRO
1	E	492	LEU
1	E	506	ALA
1	A	50	GLY
1	A	79	VAL
1	A	157	LYS
1	A	196	GLY
1	A	204	SER
1	A	212	THR
1	A	216	ARG
1	A	251	THR
1	A	267	PHE
1	A	280	GLY
1	A	386	SER
1	A	527	GLY
1	B	50	GLY
1	B	79	VAL
1	B	157	LYS
1	B	196	GLY
1	B	204	SER
1	B	212	THR

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Mol	Chain	Res	Type
1	B	216	ARG
1	B	251	THR
1	B	267	PHE
1	B	280	GLY
1	B	386	SER
1	B	527	GLY
1	C	50	GLY
1	C	79	VAL
1	C	157	LYS
1	C	196	GLY
1	C	204	SER
1	C	212	THR
1	C	216	ARG
1	C	251	THR
1	C	267	PHE
1	C	280	GLY
1	C	386	SER
1	C	527	GLY
1	D	50	GLY
1	D	79	VAL
1	D	157	LYS
1	D	196	GLY
1	D	204	SER
1	D	212	THR
1	D	216	ARG
1	D	251	THR
1	D	267	PHE
1	D	280	GLY
1	D	386	SER
1	D	527	GLY
1	E	50	GLY
1	E	79	VAL
1	E	157	LYS
1	E	196	GLY
1	E	204	SER
1	E	212	THR
1	E	216	ARG
1	E	251	THR
1	E	267	PHE
1	E	280	GLY
1	E	386	SER
1	E	527	GLY

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Mol	Chain	Res	Type
1	A	66	THR
1	A	74	ASN
1	A	198	GLN
1	A	199	ASN
1	A	215	PHE
1	A	233	ASN
1	A	392	ASN
1	A	414	ASP
1	A	428	PRO
1	A	431	THR
1	A	479	GLN
1	B	66	THR
1	B	74	ASN
1	B	198	GLN
1	B	199	ASN
1	B	215	PHE
1	B	233	ASN
1	B	392	ASN
1	B	414	ASP
1	B	428	PRO
1	B	431	THR
1	B	479	GLN
1	C	66	THR
1	C	74	ASN
1	C	198	GLN
1	C	199	ASN
1	C	215	PHE
1	C	233	ASN
1	C	392	ASN
1	C	414	ASP
1	C	428	PRO
1	C	431	THR
1	C	479	GLN
1	D	66	THR
1	D	74	ASN
1	D	198	GLN
1	D	199	ASN
1	D	215	PHE
1	D	233	ASN
1	D	392	ASN
1	D	414	ASP
1	D	428	PRO

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Mol	Chain	Res	Type
1	D	431	THR
1	D	479	GLN
1	E	66	THR
1	E	74	ASN
1	E	198	GLN
1	E	199	ASN
1	E	215	PHE
1	E	233	ASN
1	E	392	ASN
1	E	414	ASP
1	E	428	PRO
1	E	431	THR
1	E	479	GLN
1	A	388	LYS
1	B	388	LYS
1	C	388	LYS
1	D	388	LYS
1	E	388	LYS
1	A	155	LYS
1	A	179	MET
1	A	232	THR
1	A	490	THR
1	A	513	ILE
1	B	155	LYS
1	B	179	MET
1	B	232	THR
1	B	490	THR
1	B	513	ILE
1	C	155	LYS
1	C	179	MET
1	C	266	PRO
1	C	490	THR
1	C	513	ILE
1	D	155	LYS
1	D	179	MET
1	D	490	THR
1	D	513	ILE
1	E	155	LYS
1	E	179	MET
1	E	490	THR
1	E	513	ILE
1	A	61	ALA

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Mol	Chain	Res	Type
1	A	237	HIS
1	A	266	PRO
1	B	61	ALA
1	B	237	HIS
1	B	266	PRO
1	C	61	ALA
1	C	232	THR
1	C	237	HIS
1	D	61	ALA
1	D	232	THR
1	D	237	HIS
1	D	266	PRO
1	E	61	ALA
1	E	232	THR
1	E	237	HIS
1	E	266	PRO
1	A	486	ILE
1	B	486	ILE
1	C	486	ILE
1	D	486	ILE
1	E	486	ILE
1	B	195	VAL
1	C	195	VAL
1	D	195	VAL
1	A	195	VAL
1	E	195	VAL

### 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 PDB entries followed by that with respect to all EM entries.

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	404/451 (90%)	369 (91%)	35 (9%)	12	40
1	B	404/451 (90%)	369 (91%)	35 (9%)	12	40
1	C	404/451 (90%)	369 (91%)	35 (9%)	12	40
1	D	404/451 (90%)	369 (91%)	35 (9%)	12	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	404/451 (90%)	369 (91%)	35 (9%)	12	40
All	All	2020/2255 (90%)	1845 (91%)	175 (9%)	16	40

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	76	SER
1	A	83	ASN
1	A	98	ASN
1	A	100	ASP
1	A	102	SER
1	A	146	ARG
1	A	153	LEU
1	A	166	VAL
1	A	214	ASN
1	A	223	THR
1	A	232	THR
1	A	233	ASN
1	A	238	PRO
1	A	249	ASP
1	A	256	SER
1	A	258	LEU
1	A	271	PHE
1	A	287	LEU
1	A	401	THR
1	A	420	ARG
1	A	429	ASP
1	A	440	SER
1	A	446	GLN
1	A	459	ASN
1	A	468	LEU
1	A	482	TYR
1	A	501	GLU
1	A	512	THR
1	A	525	ASP
1	A	528	THR
1	A	531	LEU
1	A	533	ASN
1	A	534	SER
1	A	562	SER
1	B	58	SER

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Mol	Chain	Res	Type
1	B	76	SER
1	B	83	ASN
1	B	98	ASN
1	B	100	ASP
1	B	102	SER
1	B	146	ARG
1	B	153	LEU
1	B	166	VAL
1	B	214	ASN
1	B	223	THR
1	B	232	THR
1	B	233	ASN
1	B	238	PRO
1	B	249	ASP
1	B	256	SER
1	B	258	LEU
1	B	271	PHE
1	B	287	LEU
1	B	401	THR
1	B	420	ARG
1	B	429	ASP
1	B	440	SER
1	B	446	GLN
1	B	459	ASN
1	B	468	LEU
1	B	482	TYR
1	B	501	GLU
1	B	512	THR
1	B	525	ASP
1	B	528	THR
1	B	531	LEU
1	B	533	ASN
1	B	534	SER
1	B	562	SER
1	C	58	SER
1	C	76	SER
1	C	83	ASN
1	C	98	ASN
1	C	100	ASP
1	C	102	SER
1	C	146	ARG
1	C	153	LEU

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Mol	Chain	Res	Type
1	C	166	VAL
1	C	214	ASN
1	C	223	THR
1	C	232	THR
1	C	233	ASN
1	C	238	PRO
1	C	249	ASP
1	C	256	SER
1	C	258	LEU
1	C	271	PHE
1	C	287	LEU
1	C	401	THR
1	C	420	ARG
1	C	429	ASP
1	C	440	SER
1	C	446	GLN
1	C	459	ASN
1	C	468	LEU
1	C	482	TYR
1	C	501	GLU
1	C	512	THR
1	C	525	ASP
1	C	528	THR
1	C	531	LEU
1	C	533	ASN
1	C	534	SER
1	C	562	SER
1	D	58	SER
1	D	76	SER
1	D	83	ASN
1	D	98	ASN
1	D	100	ASP
1	D	102	SER
1	D	146	ARG
1	D	153	LEU
1	D	166	VAL
1	D	214	ASN
1	D	223	THR
1	D	232	THR
1	D	233	ASN
1	D	238	PRO
1	D	249	ASP

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Mol	Chain	Res	Type
1	D	256	SER
1	D	258	LEU
1	D	271	PHE
1	D	287	LEU
1	D	401	THR
1	D	420	ARG
1	D	429	ASP
1	D	440	SER
1	D	446	GLN
1	D	459	ASN
1	D	468	LEU
1	D	482	TYR
1	D	501	GLU
1	D	512	THR
1	D	525	ASP
1	D	528	THR
1	D	531	LEU
1	D	533	ASN
1	D	534	SER
1	D	562	SER
1	E	58	SER
1	E	76	SER
1	E	83	ASN
1	E	98	ASN
1	E	100	ASP
1	E	102	SER
1	E	146	ARG
1	E	153	LEU
1	E	166	VAL
1	E	214	ASN
1	E	223	THR
1	E	232	THR
1	E	233	ASN
1	E	238	PRO
1	E	249	ASP
1	E	256	SER
1	E	258	LEU
1	E	271	PHE
1	E	287	LEU
1	E	401	THR
1	E	420	ARG
1	E	429	ASP

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Mol	Chain	Res	Type
1	E	440	SER
1	E	446	GLN
1	E	459	ASN
1	E	468	LEU
1	E	482	TYR
1	E	501	GLU
1	E	512	THR
1	E	525	ASP
1	E	528	THR
1	E	531	LEU
1	E	533	ASN
1	E	534	SER
1	E	562	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	86	ASN
1	A	98	ASN
1	A	99	ASN
1	A	128	HIS
1	A	130	ASN
1	A	214	ASN
1	A	265	GLN
1	A	282	ASN
1	A	402	GLN
1	A	459	ASN
1	A	471	HIS
1	B	74	ASN
1	B	86	ASN
1	B	98	ASN
1	B	99	ASN
1	B	128	HIS
1	B	130	ASN
1	B	214	ASN
1	B	265	GLN
1	B	282	ASN
1	B	402	GLN
1	B	459	ASN
1	B	471	HIS
1	C	74	ASN

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Mol	Chain	Res	Type
1	C	86	ASN
1	C	98	ASN
1	C	99	ASN
1	C	128	HIS
1	C	130	ASN
1	C	214	ASN
1	C	265	GLN
1	C	282	ASN
1	C	402	GLN
1	C	459	ASN
1	C	471	HIS
1	D	74	ASN
1	D	86	ASN
1	D	98	ASN
1	D	99	ASN
1	D	128	HIS
1	D	130	ASN
1	D	199	ASN
1	D	214	ASN
1	D	265	GLN
1	D	282	ASN
1	D	402	GLN
1	D	459	ASN
1	D	471	HIS
1	E	74	ASN
1	E	86	ASN
1	E	98	ASN
1	E	99	ASN
1	E	128	HIS
1	E	130	ASN
1	E	214	ASN
1	E	265	GLN
1	E	282	ASN
1	E	402	GLN
1	E	459	ASN
1	E	471	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.