



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:38 PM BST

PDB ID : 2C9F
EMDB ID: : EMD-1178
Title : THE QUASI-ATOMIC MODEL OF THE ADENOVIRUS TYPE 3 PENTON
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 : 2005-12-12
Resolution : 16.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

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

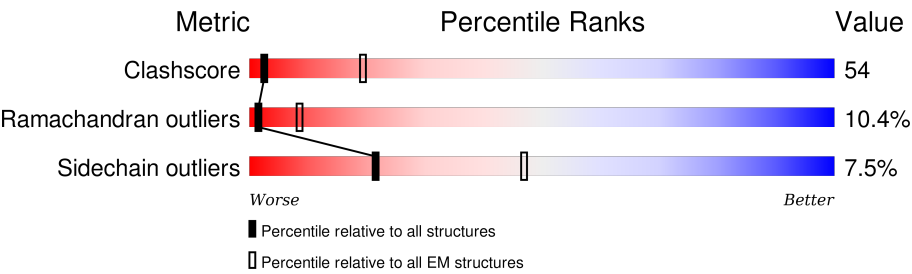
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 16.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 ≥ 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	30% 42% 11% • 16%
1	B	523	30% 43% 11% 16%
1	C	523	30% 43% 11% • 16%
1	D	523	31% 42% 11% • 16%
1	E	523	30% 43% 11% • 16%
2	S	19	21% 26% 5% 47%
2	T	19	26% 21% 5% 47%
2	U	19	21% 26% 5% 47%
2	V	19	21% 26% 5% 47%

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Mol	Chain	Length	Quality of chain
2	W	19	<div> <div></div> <div>26%</div> <div>21%</div> <div>5%</div> <div>47%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18025 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.

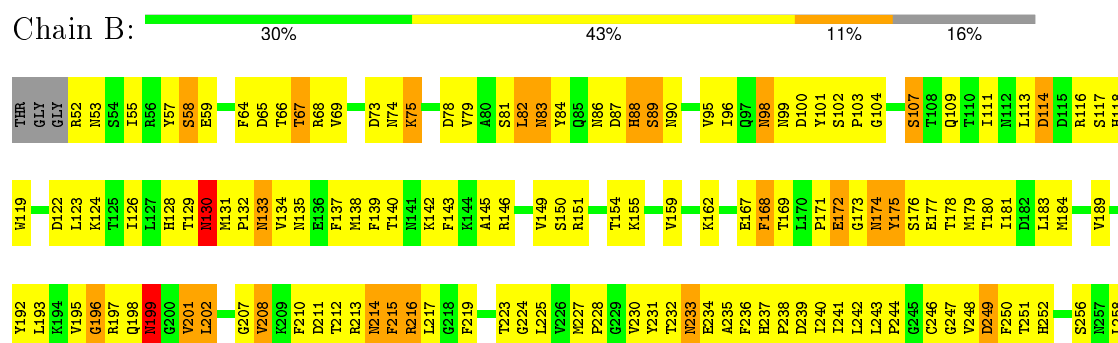
- Molecule 1 is a protein called PENTON PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	440	Total	C	N	O	S	0	0
			3519	2227	608	672	12		
1	B	440	Total	C	N	O	S	0	0
			3519	2227	608	672	12		
1	C	440	Total	C	N	O	S	0	0
			3519	2227	608	672	12		
1	D	440	Total	C	N	O	S	0	0
			3519	2227	608	672	12		
1	E	440	Total	C	N	O	S	0	0
			3519	2227	608	672	12		

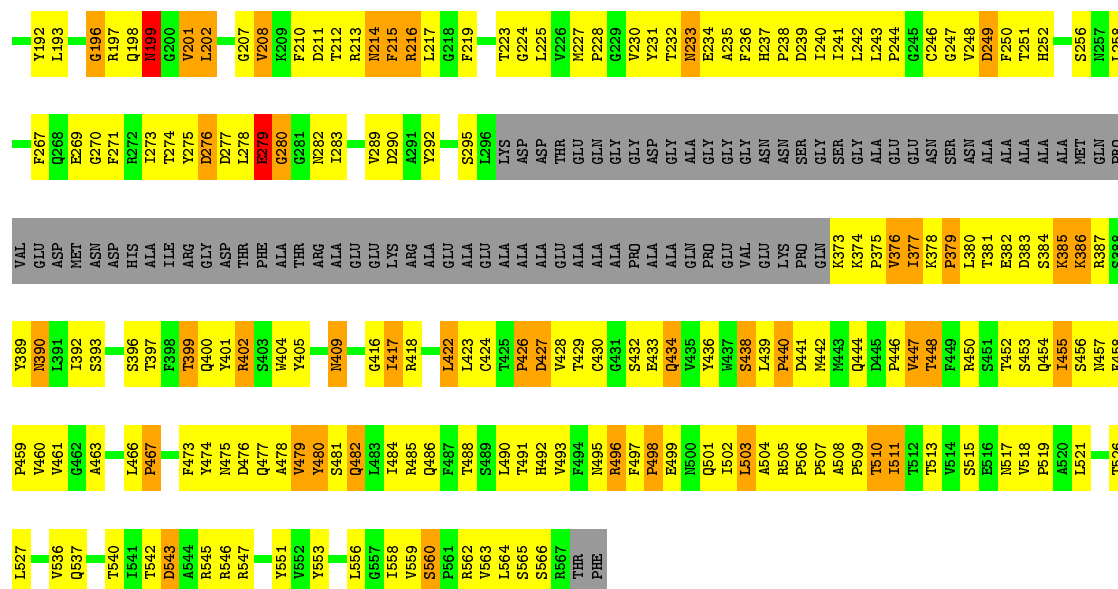
- Molecule 2 is a protein called FIBER.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	S	10	Total	C	N	O	0	0
			86	58	11	17		
2	T	10	Total	C	N	O	0	0
			86	58	11	17		
2	U	10	Total	C	N	O	0	0
			86	58	11	17		
2	V	10	Total	C	N	O	0	0
			86	58	11	17		
2	W	10	Total	C	N	O	0	0
			86	58	11	17		

- Molecule 1: PENTON PROTEIN

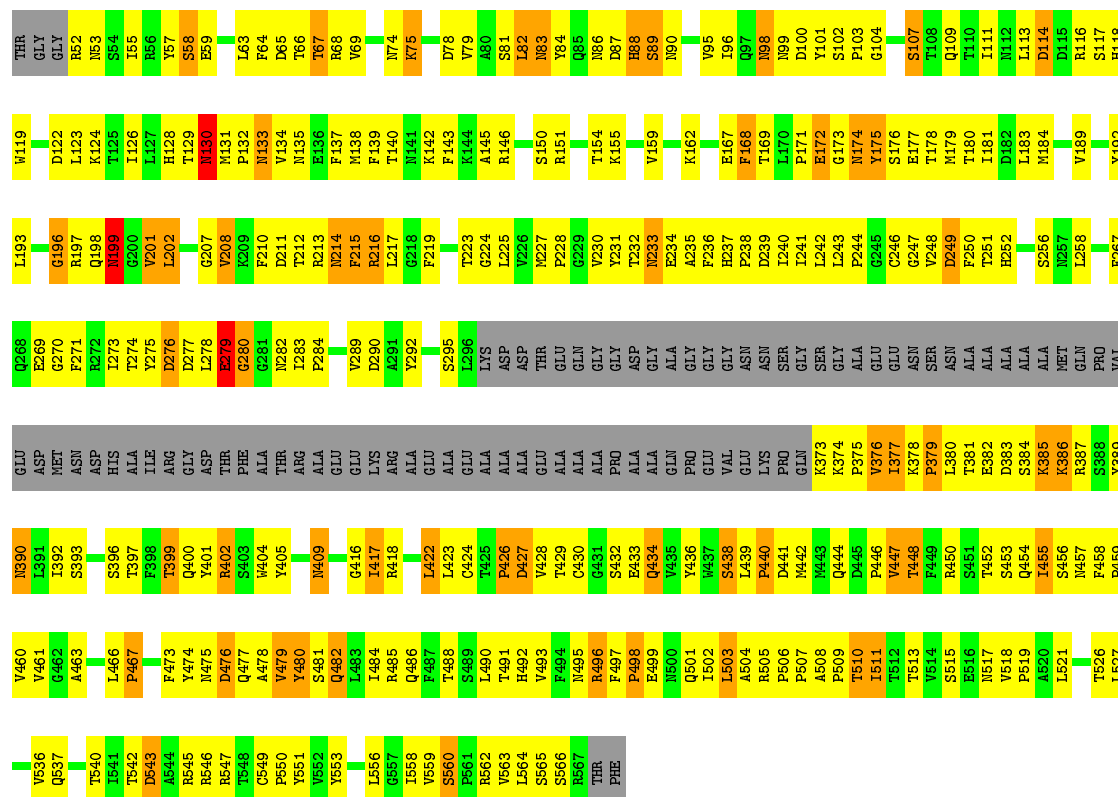






• Molecule 1: PENTON PROTEIN

Chain E: 30% 43% 11% 16%

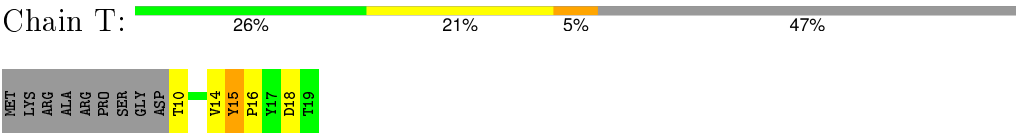


• Molecule 2: FIBER

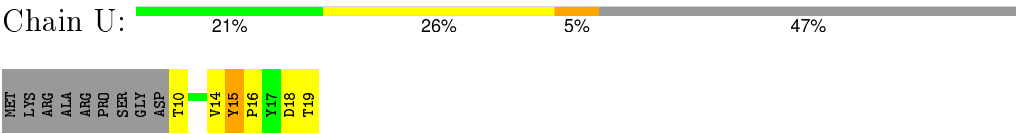
Chain S: 21% 26% 5% 47%



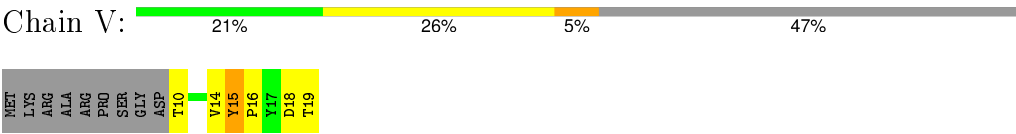
• Molecule 2: FIBER



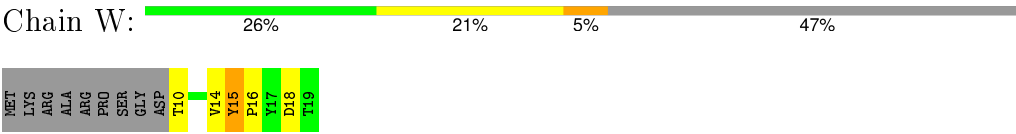
• Molecule 2: FIBER



• Molecule 2: FIBER



• Molecule 2: FIBER



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	AMPLITUDE, PHASE	Depositor
Microscope	FEI/PHILIPS CM200T	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	38000	Depositor
Image detector	KODAK SO163 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	0.61	0/3602	0.81	1/4904 (0.0%)
1	B	0.61	0/3602	0.81	1/4904 (0.0%)
1	C	0.61	0/3602	0.81	1/4904 (0.0%)
1	D	0.61	0/3602	0.81	1/4904 (0.0%)
1	E	0.61	0/3602	0.81	1/4904 (0.0%)
2	S	0.66	0/90	0.69	0/125
2	T	0.66	0/90	0.69	0/125
2	U	0.67	0/90	0.68	0/125
2	V	0.66	0/90	0.69	0/125
2	W	0.66	0/90	0.69	0/125
All	All	0.61	0/18460	0.81	5/25145 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	480	TYR	N-CA-C	-7.27	91.37	111.00
1	A	480	TYR	N-CA-C	-7.26	91.40	111.00
1	D	480	TYR	N-CA-C	-7.26	91.40	111.00
1	B	480	TYR	N-CA-C	-7.25	91.44	111.00
1	E	480	TYR	N-CA-C	-7.24	91.46	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	3519	0	3452	425	0
1	B	3519	0	3452	410	0
1	C	3519	0	3452	414	0
1	D	3519	0	3452	420	0
1	E	3519	0	3452	425	0
2	S	86	0	73	19	0
2	T	86	0	73	16	0
2	U	86	0	73	19	0
2	V	86	0	73	17	0
2	W	86	0	73	18	0
All	All	18025	0	17625	1930	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 (1930) 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:68:ARG:NH1	1:B:560:SER:HB3	1.68	1.09
1:D:68:ARG:NH1	1:D:560:SER:HB3	1.68	1.09
1:C:68:ARG:NH1	1:C:560:SER:HB3	1.68	1.09
1:A:68:ARG:NH1	1:A:560:SER:HB3	1.68	1.08
1:E:68:ARG:NH1	1:E:560:SER:HB3	1.68	1.08
1:B:197:ARG:HE	1:B:198:GLN:HE21	1.05	1.03
1:A:477:GLN:O	1:A:481:SER:HB2	1.59	1.03
1:E:477:GLN:O	1:E:481:SER:HB2	1.59	1.02
1:D:466:LEU:HD12	1:D:467:PRO:HD2	1.41	1.02
1:D:477:GLN:O	1:D:481:SER:HB2	1.59	1.01
1:E:197:ARG:HE	1:E:198:GLN:NE2	1.59	1.01
1:D:197:ARG:HE	1:D:198:GLN:NE2	1.59	1.01
1:B:197:ARG:HE	1:B:198:GLN:NE2	1.59	1.01
1:B:477:GLN:O	1:B:481:SER:HB2	1.59	1.01
1:A:197:ARG:HE	1:A:198:GLN:HE21	1.05	1.01
1:C:466:LEU:HD12	1:C:467:PRO:HD2	1.41	1.01
1:A:68:ARG:HG2	1:A:68:ARG:HH11	1.26	1.00
1:C:477:GLN:O	1:C:481:SER:HB2	1.59	1.00
1:A:488:THR:CG2	1:B:479:VAL:HG12	1.91	1.00
1:C:197:ARG:HE	1:C:198:GLN:NE2	1.59	1.00
1:E:481:SER:O	1:E:485:ARG:N	1.95	1.00
1:B:466:LEU:HD12	1:B:467:PRO:HD2	1.41	1.00
1:C:68:ARG:HG2	1:C:68:ARG:HH11	1.26	1.00
1:A:481:SER:O	1:A:485:ARG:N	1.95	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:ARG:HG2	1:D:68:ARG:HH11	1.26	1.00
1:B:481:SER:O	1:B:485:ARG:N	1.95	1.00
1:E:466:LEU:HD12	1:E:467:PRO:HD2	1.41	0.99
1:B:68:ARG:HG2	1:B:68:ARG:HH11	1.26	0.99
1:A:197:ARG:HE	1:A:198:GLN:NE2	1.59	0.99
1:E:68:ARG:HG2	1:E:68:ARG:HH11	1.25	0.99
1:C:481:SER:O	1:C:485:ARG:N	1.95	0.99
1:D:481:SER:O	1:D:485:ARG:N	1.95	0.99
1:A:466:LEU:HD12	1:A:467:PRO:HD2	1.41	0.98
1:C:197:ARG:HE	1:C:198:GLN:HE21	1.05	0.98
1:D:490:LEU:HB2	1:E:230:VAL:HG11	1.45	0.98
1:A:479:VAL:HG12	1:E:488:THR:CG2	1.94	0.98
1:A:484:ILE:HG21	1:B:480:TYR:CE1	1.97	0.98
1:A:479:VAL:HG12	1:E:488:THR:HG23	1.46	0.97
1:C:488:THR:HG23	1:D:479:VAL:HG12	1.45	0.97
1:C:490:LEU:HB2	1:D:230:VAL:HG11	1.47	0.97
1:D:484:ILE:HG21	1:E:480:TYR:CE1	1.99	0.97
1:E:477:GLN:O	1:E:481:SER:CB	2.13	0.97
1:D:477:GLN:O	1:D:481:SER:CB	2.13	0.97
1:C:477:GLN:O	1:C:481:SER:CB	2.13	0.97
1:A:488:THR:HG23	1:B:479:VAL:HG12	1.46	0.96
1:A:477:GLN:O	1:A:481:SER:CB	2.13	0.96
1:B:477:GLN:O	1:B:481:SER:CB	2.13	0.95
1:C:488:THR:CG2	1:D:479:VAL:HG12	1.97	0.95
1:A:480:TYR:CE1	1:E:484:ILE:HG21	2.00	0.95
1:D:488:THR:CG2	1:E:479:VAL:HG12	1.96	0.95
1:E:197:ARG:HE	1:E:198:GLN:HE21	1.05	0.95
1:A:230:VAL:HG11	1:E:490:LEU:HB2	1.48	0.95
1:D:132:PRO:HA	1:D:175:TYR:OH	1.67	0.94
1:D:488:THR:HG23	1:E:479:VAL:HG12	1.49	0.94
1:D:197:ARG:HE	1:D:198:GLN:HE21	1.05	0.94
1:E:132:PRO:HA	1:E:175:TYR:OH	1.67	0.94
1:D:230:VAL:HG13	1:D:501:GLN:NE2	1.83	0.94
1:B:230:VAL:HG13	1:B:501:GLN:NE2	1.83	0.93
1:C:230:VAL:HG13	1:C:501:GLN:NE2	1.83	0.93
1:E:230:VAL:HG13	1:E:501:GLN:NE2	1.83	0.93
1:C:132:PRO:HA	1:C:175:TYR:OH	1.67	0.92
1:B:132:PRO:HA	1:B:175:TYR:OH	1.67	0.92
1:A:230:VAL:HG13	1:A:501:GLN:NE2	1.83	0.92
1:A:132:PRO:HA	1:A:175:TYR:OH	1.67	0.91
1:E:68:ARG:HH12	1:E:560:SER:HB3	1.36	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ILE:CG2	1:B:480:TYR:CE1	2.54	0.91
1:D:274:THR:HG22	1:D:276:ASP:H	1.37	0.90
1:E:274:THR:HG22	1:E:276:ASP:H	1.37	0.90
1:C:68:ARG:HH12	1:C:560:SER:HB3	1.36	0.89
1:B:274:THR:HG22	1:B:276:ASP:H	1.37	0.89
1:B:83:ASN:HA	1:B:86:ASN:HD22	1.38	0.89
1:D:83:ASN:HA	1:D:86:ASN:HD22	1.38	0.88
1:A:68:ARG:HH12	1:A:560:SER:HB3	1.36	0.88
1:C:275:TYR:CE1	1:C:402:ARG:HD3	2.09	0.88
1:B:275:TYR:CE1	1:B:402:ARG:HD3	2.09	0.87
1:C:83:ASN:HA	1:C:86:ASN:HD22	1.38	0.87
1:A:275:TYR:CE1	1:A:402:ARG:HD3	2.09	0.87
1:C:274:THR:HG22	1:C:276:ASP:H	1.37	0.87
1:A:377:ILE:O	1:A:379:PRO:HD3	1.75	0.87
1:C:377:ILE:O	1:C:379:PRO:HD3	1.75	0.87
1:A:217:LEU:HB2	1:A:232:THR:HG21	1.57	0.87
1:E:83:ASN:HA	1:E:86:ASN:HD22	1.38	0.87
1:D:217:LEU:HB2	1:D:232:THR:HG21	1.56	0.87
1:B:377:ILE:O	1:B:379:PRO:HD3	1.75	0.87
1:D:275:TYR:CE1	1:D:402:ARG:HD3	2.09	0.87
1:A:274:THR:HG22	1:A:276:ASP:H	1.37	0.87
1:B:217:LEU:HB2	1:B:232:THR:HG21	1.57	0.87
1:D:68:ARG:HH12	1:D:560:SER:HB3	1.36	0.87
1:E:275:TYR:CE1	1:E:402:ARG:HD3	2.09	0.86
1:C:484:ILE:HG21	1:D:480:TYR:CE1	2.10	0.86
1:C:100:ASP:OD2	1:D:450:ARG:NH1	2.09	0.86
1:A:83:ASN:HA	1:A:86:ASN:HD22	1.38	0.86
1:D:377:ILE:O	1:D:379:PRO:HD3	1.75	0.86
1:E:377:ILE:O	1:E:379:PRO:HD3	1.75	0.86
1:B:68:ARG:HH12	1:B:560:SER:HB3	1.36	0.86
1:B:100:ASP:OD2	1:C:450:ARG:NH1	2.09	0.85
1:E:217:LEU:HB2	1:E:232:THR:HG21	1.57	0.85
1:A:473:PHE:O	1:A:511:ILE:HA	1.77	0.85
1:C:217:LEU:HB2	1:C:232:THR:HG21	1.57	0.85
1:D:473:PHE:O	1:D:511:ILE:HA	1.77	0.85
1:D:442:MET:HE3	1:D:559:VAL:HG21	1.58	0.85
1:E:526:THR:HG21	1:E:562:ARG:HH21	1.42	0.84
1:E:473:PHE:O	1:E:511:ILE:HA	1.77	0.84
1:C:526:THR:HG21	1:C:562:ARG:HH21	1.42	0.84
1:E:442:MET:HE3	1:E:559:VAL:HG21	1.60	0.84
1:A:484:ILE:HG21	1:B:480:TYR:CD1	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:THR:HG21	1:B:562:ARG:HH21	1.42	0.84
1:C:473:PHE:O	1:C:511:ILE:HA	1.77	0.83
1:D:526:THR:HG21	1:D:562:ARG:HH21	1.42	0.83
1:B:473:PHE:O	1:B:511:ILE:HA	1.77	0.83
1:A:526:THR:HG21	1:A:562:ARG:HH21	1.42	0.82
1:A:488:THR:HG23	1:B:479:VAL:O	1.78	0.82
1:C:485:ARG:NE	1:D:234:GLU:OE2	2.12	0.82
1:B:542:THR:CG2	1:B:546:ARG:HA	2.10	0.81
1:C:67:THR:HG21	1:D:447:VAL:HG22	1.61	0.81
1:D:542:THR:CG2	1:D:546:ARG:HA	2.10	0.81
1:A:484:ILE:CG2	1:B:480:TYR:CD1	2.63	0.81
1:A:490:LEU:HB2	1:B:230:VAL:HG11	1.62	0.81
1:C:542:THR:CG2	1:C:546:ARG:HA	2.10	0.81
1:B:488:THR:HG23	1:C:479:VAL:HG12	1.62	0.81
1:D:485:ARG:NE	1:E:234:GLU:OE2	2.12	0.81
1:E:197:ARG:NE	1:E:198:GLN:HE21	1.80	0.80
1:C:197:ARG:NE	1:C:198:GLN:HE21	1.80	0.80
1:E:542:THR:CG2	1:E:546:ARG:HA	2.10	0.80
1:D:490:LEU:CB	1:E:230:VAL:HG11	2.12	0.80
1:C:490:LEU:CB	1:D:230:VAL:HG11	2.11	0.80
1:A:542:THR:CG2	1:A:546:ARG:HA	2.10	0.80
1:A:234:GLU:OE2	1:E:485:ARG:NE	2.14	0.80
1:A:197:ARG:NE	1:A:198:GLN:HE21	1.80	0.80
1:B:197:ARG:NE	1:B:198:GLN:HE21	1.80	0.79
1:A:480:TYR:CE1	1:E:484:ILE:CG2	2.65	0.79
1:B:466:LEU:HD12	1:B:467:PRO:CD	2.12	0.79
1:D:197:ARG:NE	1:D:198:GLN:HE21	1.80	0.79
1:E:466:LEU:HD12	1:E:467:PRO:CD	2.12	0.79
1:C:466:LEU:HD12	1:C:467:PRO:CD	2.12	0.79
1:D:104:GLY:O	1:D:107:SER:HB3	1.83	0.79
1:D:68:ARG:HG2	1:D:68:ARG:NH1	1.97	0.79
1:D:466:LEU:HD12	1:D:467:PRO:CD	2.12	0.78
1:A:466:LEU:HD12	1:A:467:PRO:CD	2.12	0.78
1:E:104:GLY:O	1:E:107:SER:HB3	1.83	0.78
1:A:401:TYR:CD1	1:A:502:ILE:HG12	2.19	0.78
1:D:230:VAL:HG13	1:D:501:GLN:HE22	1.47	0.78
1:D:100:ASP:OD2	1:E:450:ARG:NH1	2.15	0.78
1:A:230:VAL:HG11	1:E:490:LEU:CB	2.13	0.78
1:E:401:TYR:CD1	1:E:502:ILE:HG12	2.19	0.78
1:D:401:TYR:CD1	1:D:502:ILE:HG12	2.19	0.78
1:A:104:GLY:O	1:A:107:SER:HB3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:ARG:HG2	1:E:68:ARG:NH1	1.97	0.77
1:A:217:LEU:HB2	1:A:232:THR:CG2	2.14	0.77
1:C:217:LEU:HB2	1:C:232:THR:CG2	2.14	0.77
1:B:104:GLY:O	1:B:107:SER:HB3	1.83	0.77
1:B:488:THR:CG2	1:C:479:VAL:HG12	2.14	0.77
1:A:230:VAL:HG13	1:A:501:GLN:HE22	1.47	0.77
1:B:401:TYR:CD1	1:B:502:ILE:HG12	2.19	0.77
1:C:401:TYR:CD1	1:C:502:ILE:HG12	2.19	0.77
1:C:104:GLY:O	1:C:107:SER:HB3	1.83	0.77
1:D:217:LEU:HB2	1:D:232:THR:CG2	2.14	0.77
1:A:480:TYR:CD1	1:E:484:ILE:HG21	2.19	0.77
1:C:230:VAL:HG13	1:C:501:GLN:HE22	1.47	0.77
1:D:484:ILE:CG2	1:E:480:TYR:CE1	2.66	0.77
1:B:145:ALA:HB3	1:B:168:PHE:HE1	1.50	0.77
1:B:217:LEU:HB2	1:B:232:THR:CG2	2.14	0.76
1:E:376:VAL:HG23	1:E:377:ILE:N	2.01	0.76
1:D:145:ALA:HB3	1:D:168:PHE:HE1	1.50	0.76
1:E:217:LEU:HB2	1:E:232:THR:CG2	2.14	0.76
1:C:376:VAL:HG23	1:C:377:ILE:N	2.01	0.76
1:E:230:VAL:HG13	1:E:501:GLN:HE22	1.47	0.76
1:E:145:ALA:HB3	1:E:168:PHE:HE1	1.50	0.76
1:A:67:THR:HG21	1:B:447:VAL:HG22	1.65	0.76
1:B:376:VAL:HG23	1:B:377:ILE:N	2.01	0.76
1:C:145:ALA:HB3	1:C:168:PHE:HE1	1.50	0.76
1:B:111:ILE:HD13	1:C:447:VAL:HG11	1.67	0.76
1:C:135:ASN:HA	1:C:172:GLU:HG2	1.68	0.76
1:A:145:ALA:HB3	1:A:168:PHE:HE1	1.50	0.76
1:A:376:VAL:HG23	1:A:377:ILE:N	2.01	0.76
1:D:376:VAL:HG23	1:D:377:ILE:N	2.01	0.76
1:D:135:ASN:HA	1:D:172:GLU:HG2	1.68	0.76
1:B:96:ILE:HG22	1:B:98:ASN:H	1.51	0.75
1:B:230:VAL:HG13	1:B:501:GLN:HE22	1.47	0.75
1:B:542:THR:HG22	1:B:546:ARG:HA	1.69	0.75
1:B:134:VAL:HG13	1:B:140:THR:O	1.87	0.75
1:D:134:VAL:HG13	1:D:140:THR:O	1.87	0.75
1:A:96:ILE:HG22	1:A:98:ASN:H	1.51	0.75
1:B:526:THR:HG21	1:B:562:ARG:NH2	2.02	0.75
1:A:526:THR:HG21	1:A:562:ARG:NH2	2.02	0.75
1:A:135:ASN:HA	1:A:172:GLU:HG2	1.68	0.75
1:B:146:ARG:O	1:B:246:CYS:HB2	1.87	0.75
1:C:68:ARG:HG2	1:C:68:ARG:NH1	1.97	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ASN:HA	1:B:172:GLU:HG2	1.68	0.74
1:C:96:ILE:HG22	1:C:98:ASN:H	1.51	0.74
1:E:135:ASN:HA	1:E:172:GLU:HG2	1.68	0.74
1:C:551:TYR:CE2	1:D:422:LEU:HD21	2.22	0.74
1:D:484:ILE:HG21	1:E:480:TYR:CD1	2.22	0.74
1:E:526:THR:HG21	1:E:562:ARG:NH2	2.02	0.74
1:E:542:THR:HG22	1:E:546:ARG:HA	1.68	0.74
1:B:277:ASP:HB3	1:B:417:ILE:HD11	1.70	0.74
1:E:146:ARG:O	1:E:246:CYS:HB2	1.87	0.74
1:D:146:ARG:O	1:D:246:CYS:HB2	1.87	0.74
1:A:277:ASP:HB3	1:A:417:ILE:HD11	1.70	0.74
1:A:134:VAL:HG13	1:A:140:THR:O	1.87	0.74
1:C:134:VAL:HG13	1:C:140:THR:O	1.87	0.74
1:D:542:THR:HG22	1:D:546:ARG:HA	1.69	0.74
1:E:134:VAL:HG13	1:E:140:THR:O	1.87	0.74
1:C:146:ARG:O	1:C:246:CYS:HB2	1.87	0.74
1:D:96:ILE:HG22	1:D:98:ASN:H	1.51	0.74
1:D:510:THR:O	1:D:511:ILE:HB	1.88	0.73
1:A:542:THR:HG22	1:A:546:ARG:HA	1.69	0.73
1:C:277:ASP:HB3	1:C:417:ILE:HD11	1.70	0.73
1:D:277:ASP:HB3	1:D:417:ILE:HD11	1.70	0.73
1:E:277:ASP:HB3	1:E:417:ILE:HD11	1.70	0.73
1:D:526:THR:HG21	1:D:562:ARG:NH2	2.02	0.73
1:A:510:THR:O	1:A:511:ILE:HB	1.88	0.73
1:B:510:THR:O	1:B:511:ILE:HB	1.88	0.73
1:C:526:THR:HG21	1:C:562:ARG:NH2	2.02	0.73
1:A:146:ARG:O	1:A:246:CYS:HB2	1.87	0.73
1:C:542:THR:HG22	1:C:546:ARG:HA	1.69	0.73
1:A:450:ARG:NH1	1:E:100:ASP:OD2	2.22	0.73
1:A:447:VAL:HG22	1:E:67:THR:HG21	1.70	0.72
1:A:488:THR:HG22	1:B:479:VAL:HG12	1.70	0.72
1:B:484:ILE:HG21	1:C:480:TYR:CE1	2.24	0.72
2:U:10:THR:HG22	2:U:10:THR:O	1.89	0.72
2:V:10:THR:HG22	2:V:10:THR:O	1.89	0.72
1:E:96:ILE:HG22	1:E:98:ASN:H	1.51	0.72
1:C:510:THR:O	1:C:511:ILE:HB	1.88	0.72
1:C:193:LEU:HD11	1:C:496:ARG:HH12	1.54	0.72
1:B:154:THR:HG22	1:B:155:LYS:HG3	1.71	0.72
1:D:193:LEU:HD11	1:D:496:ARG:HH12	1.54	0.72
1:A:193:LEU:HD11	1:A:496:ARG:HH12	1.54	0.72
2:T:10:THR:O	2:T:10:THR:HG22	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:PHE:O	1:C:216:ARG:HB2	1.89	0.72
1:B:68:ARG:HG2	1:B:68:ARG:NH1	1.97	0.72
1:A:488:THR:CG2	1:B:479:VAL:CG1	2.66	0.72
1:B:214:ASN:C	1:B:214:ASN:HD22	1.93	0.72
1:C:111:ILE:HD13	1:D:447:VAL:HG11	1.71	0.71
1:D:154:THR:HG22	1:D:155:LYS:HG3	1.72	0.71
1:A:214:ASN:HD22	1:A:214:ASN:C	1.93	0.71
1:B:215:PHE:O	1:B:216:ARG:HB2	1.89	0.71
1:C:154:THR:HG22	1:C:155:LYS:HG3	1.72	0.71
1:E:214:ASN:HD22	1:E:214:ASN:C	1.93	0.71
1:E:154:THR:HG22	1:E:155:LYS:HG3	1.72	0.71
1:B:193:LEU:HD11	1:B:496:ARG:HH12	1.54	0.71
1:B:275:TYR:CZ	1:B:402:ARG:HD3	2.26	0.71
1:C:484:ILE:HG21	1:D:480:TYR:CD1	2.25	0.71
1:E:510:THR:O	1:E:511:ILE:HB	1.88	0.71
1:C:275:TYR:CZ	1:C:402:ARG:HD3	2.26	0.71
1:B:274:THR:HG22	1:B:276:ASP:N	2.06	0.71
1:A:422:LEU:HD23	1:A:423:LEU:N	2.06	0.71
1:D:214:ASN:HD22	1:D:214:ASN:C	1.93	0.71
1:E:193:LEU:HD11	1:E:496:ARG:HH12	1.54	0.71
1:D:215:PHE:O	1:D:216:ARG:HB2	1.90	0.70
2:W:10:THR:HG22	2:W:10:THR:O	1.89	0.70
1:D:275:TYR:CZ	1:D:402:ARG:HD3	2.26	0.70
1:C:502:ILE:HG22	1:C:503:LEU:N	2.06	0.70
1:D:422:LEU:HD23	1:D:423:LEU:N	2.06	0.70
1:E:376:VAL:O	1:E:378:LYS:N	2.25	0.70
1:A:275:TYR:CZ	1:A:402:ARG:HD3	2.26	0.70
1:A:488:THR:HG22	1:B:479:VAL:CG1	2.21	0.70
2:S:10:THR:O	2:S:10:THR:HG22	1.89	0.70
1:A:479:VAL:O	1:E:488:THR:HG23	1.91	0.70
1:C:376:VAL:O	1:C:378:LYS:N	2.25	0.70
1:E:376:VAL:HG23	1:E:377:ILE:H	1.57	0.70
1:B:376:VAL:O	1:B:378:LYS:N	2.25	0.70
1:C:214:ASN:C	1:C:214:ASN:HD22	1.93	0.70
1:A:215:PHE:O	1:A:216:ARG:HB2	1.89	0.70
1:D:376:VAL:O	1:D:378:LYS:N	2.24	0.70
1:B:422:LEU:HD23	1:B:423:LEU:N	2.06	0.70
1:C:484:ILE:CG2	1:D:480:TYR:CE1	2.75	0.70
1:A:154:THR:HG22	1:A:155:LYS:HG3	1.72	0.70
1:C:442:MET:HE3	1:C:559:VAL:HG21	1.73	0.70
1:A:98:ASN:HD22	1:A:99:ASN:N	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:422:LEU:HD23	1:E:423:LEU:N	2.06	0.70
1:B:98:ASN:HD22	1:B:99:ASN:N	1.90	0.69
1:C:422:LEU:HD23	1:C:423:LEU:N	2.06	0.69
1:A:376:VAL:O	1:A:378:LYS:N	2.25	0.69
1:A:479:VAL:CG1	1:E:488:THR:CG2	2.70	0.69
1:A:502:ILE:HG22	1:A:503:LEU:N	2.06	0.69
1:D:98:ASN:HD22	1:D:99:ASN:N	1.90	0.69
1:A:485:ARG:NE	1:B:234:GLU:OE2	2.25	0.69
1:D:274:THR:HG22	1:D:276:ASP:N	2.06	0.69
1:B:376:VAL:HG23	1:B:377:ILE:H	1.57	0.69
1:C:98:ASN:HD22	1:C:99:ASN:N	1.90	0.69
1:A:68:ARG:HG2	1:A:68:ARG:NH1	1.97	0.69
1:A:376:VAL:HG23	1:A:377:ILE:H	1.57	0.69
1:E:274:THR:HG22	1:E:276:ASP:N	2.06	0.69
1:E:275:TYR:CZ	1:E:402:ARG:HD3	2.26	0.69
1:A:274:THR:HG22	1:A:276:ASP:N	2.06	0.69
1:E:98:ASN:HD22	1:E:99:ASN:N	1.90	0.69
1:B:442:MET:HE3	1:B:559:VAL:HG21	1.75	0.69
1:E:283:ILE:O	1:E:399:THR:HG23	1.93	0.69
1:B:502:ILE:HG22	1:B:503:LEU:N	2.06	0.69
1:C:488:THR:CG2	1:D:479:VAL:CG1	2.71	0.69
1:B:490:LEU:HB2	1:C:230:VAL:HG11	1.74	0.69
1:E:215:PHE:O	1:E:216:ARG:HB2	1.89	0.69
1:A:442:MET:HE3	1:A:559:VAL:HG21	1.73	0.69
1:D:67:THR:HG21	1:E:447:VAL:HG22	1.73	0.69
1:C:455:ILE:HD12	1:C:456:SER:H	1.58	0.69
1:B:283:ILE:O	1:B:399:THR:HG23	1.93	0.69
1:C:376:VAL:HG23	1:C:377:ILE:H	1.57	0.69
1:A:83:ASN:HA	1:A:86:ASN:ND2	2.09	0.68
1:A:283:ILE:O	1:A:399:THR:HG23	1.93	0.68
1:C:274:THR:HG22	1:C:276:ASP:N	2.05	0.68
1:A:211:ASP:OD1	1:A:213:ARG:HG2	1.94	0.68
1:C:211:ASP:OD1	1:C:213:ARG:HG2	1.93	0.68
1:E:502:ILE:HG22	1:E:503:LEU:N	2.06	0.68
1:D:488:THR:HG23	1:E:479:VAL:O	1.93	0.68
1:C:283:ILE:O	1:C:399:THR:HG23	1.93	0.68
1:E:83:ASN:HA	1:E:86:ASN:ND2	2.09	0.68
1:D:211:ASP:OD1	1:D:213:ARG:HG2	1.93	0.68
1:E:426:PRO:O	1:E:427:ASP:HB3	1.93	0.68
1:A:497:PHE:HD1	1:A:503:LEU:HB3	1.59	0.68
1:B:426:PRO:O	1:B:427:ASP:HB3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:502:ILE:HG22	1:D:503:LEU:N	2.06	0.68
1:D:455:ILE:HD12	1:D:456:SER:H	1.58	0.68
1:B:455:ILE:HD12	1:B:456:SER:H	1.58	0.68
1:A:480:TYR:CD1	1:E:484:ILE:CG2	2.77	0.67
1:B:83:ASN:HA	1:B:86:ASN:ND2	2.09	0.67
1:C:556:LEU:HD21	1:D:434:GLN:HG2	1.75	0.67
1:D:426:PRO:O	1:D:427:ASP:HB3	1.94	0.67
1:E:455:ILE:HD12	1:E:456:SER:H	1.58	0.67
1:B:274:THR:HG22	1:B:275:TYR:N	2.10	0.67
1:A:455:ILE:HD12	1:A:456:SER:H	1.59	0.67
1:D:283:ILE:O	1:D:399:THR:HG23	1.93	0.67
1:E:497:PHE:HD1	1:E:503:LEU:HB3	1.59	0.67
1:A:422:LEU:HD21	1:E:551:TYR:CE2	2.30	0.67
1:B:214:ASN:HD21	1:B:216:ARG:HB3	1.60	0.67
1:C:497:PHE:HD1	1:C:503:LEU:HB3	1.59	0.67
1:C:214:ASN:HD21	1:C:216:ARG:HB3	1.60	0.67
1:A:183:LEU:HD21	1:B:236:PHE:HE2	1.59	0.67
1:B:211:ASP:OD1	1:B:213:ARG:HG2	1.93	0.67
1:D:217:LEU:CB	1:D:232:THR:HG21	2.24	0.67
1:D:215:PHE:HB3	1:D:283:ILE:HG23	1.77	0.67
1:D:130:ASN:HA	1:D:517:ASN:CG	2.16	0.67
1:C:274:THR:HG22	1:C:275:TYR:N	2.10	0.67
1:E:211:ASP:OD1	1:E:213:ARG:HG2	1.94	0.67
1:E:214:ASN:HD21	1:E:216:ARG:HB3	1.60	0.66
1:D:497:PHE:HD1	1:D:503:LEU:HB3	1.59	0.66
1:A:217:LEU:CB	1:A:232:THR:HG21	2.25	0.66
1:C:217:LEU:CB	1:C:232:THR:HG21	2.24	0.66
1:B:145:ALA:HB3	1:B:168:PHE:CE1	2.31	0.66
1:C:215:PHE:HB3	1:C:283:ILE:HG23	1.77	0.66
1:E:130:ASN:HA	1:E:517:ASN:CG	2.16	0.66
1:C:83:ASN:HA	1:C:86:ASN:ND2	2.09	0.66
1:E:217:LEU:CB	1:E:232:THR:HG21	2.25	0.66
1:E:215:PHE:HB3	1:E:283:ILE:HG23	1.77	0.66
1:A:426:PRO:O	1:A:427:ASP:HB3	1.94	0.66
1:B:497:PHE:HD1	1:B:503:LEU:HB3	1.59	0.66
1:C:426:PRO:O	1:C:427:ASP:HB3	1.94	0.66
1:D:551:TYR:CE2	1:E:422:LEU:HD21	2.31	0.66
1:A:145:ALA:HB3	1:A:168:PHE:CE1	2.31	0.66
1:D:376:VAL:HG23	1:D:377:ILE:H	1.57	0.66
1:D:133:ASN:HB2	1:D:175:TYR:CD2	2.32	0.65
1:D:488:THR:CG2	1:E:479:VAL:CG1	2.73	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASN:HA	1:A:517:ASN:CG	2.16	0.65
1:A:274:THR:HG22	1:A:275:TYR:N	2.10	0.65
1:A:438:SER:HB3	1:A:459:PRO:O	1.97	0.65
1:C:133:ASN:HB2	1:C:175:TYR:CD2	2.32	0.65
1:A:214:ASN:HD21	1:A:216:ARG:HB3	1.60	0.65
1:A:438:SER:C	1:A:440:PRO:HD3	2.17	0.65
1:D:485:ARG:NH1	1:D:505:ARG:NH2	2.44	0.65
1:E:274:THR:HG22	1:E:275:TYR:N	2.10	0.65
1:D:274:THR:HG22	1:D:275:TYR:N	2.10	0.65
1:E:438:SER:C	1:E:440:PRO:HD3	2.17	0.65
1:C:130:ASN:HA	1:C:517:ASN:CG	2.16	0.65
1:A:490:LEU:CB	1:B:230:VAL:HG11	2.27	0.65
1:C:207:GLY:O	1:C:208:VAL:HB	1.97	0.65
1:B:438:SER:C	1:B:440:PRO:HD3	2.17	0.65
1:B:217:LEU:CB	1:B:232:THR:HG21	2.24	0.65
1:E:133:ASN:HB2	1:E:175:TYR:CD2	2.31	0.65
1:B:133:ASN:HB2	1:B:175:TYR:CD2	2.32	0.65
1:B:485:ARG:NH1	1:B:505:ARG:NH2	2.44	0.65
1:B:224:GLY:O	1:B:225:LEU:HD23	1.97	0.65
1:B:130:ASN:HA	1:B:517:ASN:CG	2.16	0.65
1:E:442:MET:CE	1:E:559:VAL:HG21	2.27	0.65
1:B:207:GLY:O	1:B:208:VAL:HB	1.97	0.65
1:A:215:PHE:HB3	1:A:283:ILE:HG23	1.77	0.65
1:C:438:SER:C	1:C:440:PRO:HD3	2.17	0.65
1:A:485:ARG:NH1	1:A:505:ARG:NH2	2.44	0.65
1:E:485:ARG:NH1	1:E:505:ARG:NH2	2.44	0.65
1:E:207:GLY:O	1:E:208:VAL:HB	1.97	0.65
1:A:224:GLY:O	1:A:225:LEU:HD23	1.97	0.64
1:D:484:ILE:CG2	1:E:480:TYR:CD1	2.80	0.64
1:D:214:ASN:HD21	1:D:216:ARG:HB3	1.60	0.64
1:D:224:GLY:O	1:D:225:LEU:HD23	1.97	0.64
1:C:145:ALA:HB3	1:C:168:PHE:CE1	2.31	0.64
2:W:18:ASP:OD1	2:W:18:ASP:O	2.15	0.64
1:C:485:ARG:NH1	1:C:505:ARG:NH2	2.44	0.64
1:B:215:PHE:HB3	1:B:283:ILE:HG23	1.77	0.64
1:A:442:MET:CE	1:A:559:VAL:HG21	2.27	0.64
2:V:18:ASP:O	2:V:18:ASP:OD1	2.15	0.64
1:B:511:ILE:O	1:B:511:ILE:HG22	1.97	0.64
1:A:133:ASN:HB2	1:A:175:TYR:CD2	2.32	0.64
1:E:145:ALA:HB3	1:E:168:PHE:CE1	2.31	0.64
2:S:18:ASP:O	2:S:18:ASP:OD1	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:ARG:HD3	2:U:14:VAL:HG12	1.80	0.64
1:D:83:ASN:HA	1:D:86:ASN:ND2	2.09	0.64
1:D:442:MET:CE	1:D:559:VAL:HG21	2.28	0.64
1:B:64:PHE:HD1	1:C:118:HIS:NE2	1.95	0.64
1:D:496:ARG:HD3	2:V:14:VAL:HG12	1.80	0.64
1:D:145:ALA:HB3	1:D:168:PHE:CE1	2.31	0.64
2:U:18:ASP:OD1	2:U:18:ASP:O	2.15	0.64
2:T:18:ASP:OD1	2:T:18:ASP:O	2.15	0.64
1:C:434:GLN:NE2	1:C:436:TYR:HE2	1.96	0.64
1:B:67:THR:HG21	1:C:447:VAL:HG22	1.80	0.64
1:C:488:THR:HG23	1:D:479:VAL:O	1.97	0.64
1:D:438:SER:C	1:D:440:PRO:HD3	2.17	0.64
1:B:442:MET:CE	1:B:559:VAL:HG21	2.28	0.64
1:C:466:LEU:CD1	1:C:467:PRO:HD2	2.24	0.64
1:B:438:SER:HB3	1:B:459:PRO:O	1.97	0.64
1:E:434:GLN:NE2	1:E:436:TYR:HE2	1.96	0.64
1:E:210:PHE:HD2	1:E:240:ILE:HG22	1.63	0.64
1:E:511:ILE:HG22	1:E:511:ILE:O	1.97	0.64
1:E:224:GLY:O	1:E:225:LEU:HD23	1.97	0.64
1:C:442:MET:CE	1:C:559:VAL:HG21	2.28	0.64
1:E:466:LEU:CD1	1:E:467:PRO:HD2	2.24	0.64
1:D:438:SER:HB3	1:D:459:PRO:O	1.97	0.64
1:C:511:ILE:O	1:C:511:ILE:HG22	1.97	0.64
1:B:68:ARG:NE	1:C:527:LEU:HD21	2.12	0.63
1:D:511:ILE:O	1:D:511:ILE:HG22	1.97	0.63
1:A:542:THR:HG21	1:A:546:ARG:HA	1.80	0.63
1:A:434:GLN:NE2	1:A:436:TYR:HE2	1.96	0.63
1:A:210:PHE:HD2	1:A:240:ILE:HG22	1.63	0.63
1:B:496:ARG:HD3	2:T:14:VAL:HG12	1.80	0.63
1:C:210:PHE:HD2	1:C:240:ILE:HG22	1.63	0.63
1:C:224:GLY:O	1:C:225:LEU:HD23	1.97	0.63
1:E:438:SER:HB3	1:E:459:PRO:O	1.97	0.63
1:E:134:VAL:HA	1:E:140:THR:OG1	1.98	0.63
1:D:434:GLN:NE2	1:D:436:TYR:HE2	1.96	0.63
1:A:207:GLY:O	1:A:208:VAL:HB	1.97	0.63
1:C:558:ILE:HD11	1:D:463:ALA:HB3	1.79	0.63
1:D:228:PRO:HG3	2:U:15:TYR:CE1	2.34	0.63
1:A:134:VAL:HA	1:A:140:THR:OG1	1.99	0.63
1:D:207:GLY:O	1:D:208:VAL:HB	1.97	0.63
1:A:111:ILE:HD13	1:B:447:VAL:HG11	1.81	0.63
1:A:511:ILE:HG22	1:A:511:ILE:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:PRO:O	1:E:174:ASN:ND2	2.32	0.63
1:A:496:ARG:HD3	2:S:14:VAL:HG12	1.80	0.63
1:E:138:MET:O	1:E:139:PHE:HB2	1.98	0.63
1:B:484:ILE:CG2	1:C:480:TYR:CE1	2.82	0.63
1:C:542:THR:HG21	1:C:546:ARG:HA	1.80	0.63
1:A:100:ASP:OD2	1:B:450:ARG:NH1	2.32	0.63
1:D:485:ARG:HH21	1:E:234:GLU:CD	2.02	0.63
1:C:134:VAL:HA	1:C:140:THR:OG1	1.99	0.63
1:B:434:GLN:NE2	1:B:436:TYR:HE2	1.96	0.63
1:D:134:VAL:HA	1:D:140:THR:OG1	1.98	0.62
1:C:138:MET:O	1:C:139:PHE:HB2	1.99	0.62
1:B:138:MET:O	1:B:139:PHE:HB2	1.99	0.62
1:B:542:THR:HG21	1:B:546:ARG:HA	1.80	0.62
1:D:171:PRO:O	1:D:174:ASN:ND2	2.32	0.62
1:D:210:PHE:HD2	1:D:240:ILE:HG22	1.63	0.62
1:A:171:PRO:O	1:A:174:ASN:ND2	2.32	0.62
1:D:556:LEU:HD21	1:E:434:GLN:HG2	1.80	0.62
1:B:134:VAL:HA	1:B:140:THR:OG1	1.98	0.62
1:B:74:ASN:OD1	1:C:434:GLN:OE1	2.17	0.62
1:A:479:VAL:HG12	1:A:479:VAL:O	2.00	0.62
1:C:438:SER:HB3	1:C:459:PRO:O	1.97	0.62
1:E:211:ASP:OD1	1:E:212:THR:N	2.31	0.62
1:E:159:VAL:HG23	1:E:159:VAL:O	2.00	0.62
1:D:138:MET:O	1:D:139:PHE:HB2	1.98	0.62
1:A:551:TYR:CE2	1:B:422:LEU:HD21	2.35	0.62
1:C:171:PRO:O	1:C:174:ASN:ND2	2.32	0.62
1:E:496:ARG:HD3	2:W:14:VAL:HG12	1.80	0.62
1:D:154:THR:HG22	1:D:155:LYS:N	2.14	0.62
1:E:154:THR:HG22	1:E:155:LYS:N	2.14	0.62
1:B:177:GLU:HG3	1:B:178:THR:N	2.15	0.62
1:D:542:THR:HG21	1:D:546:ARG:HA	1.80	0.62
1:B:159:VAL:O	1:B:159:VAL:HG23	2.00	0.62
1:E:177:GLU:HG3	1:E:178:THR:N	2.15	0.62
1:B:210:PHE:HD2	1:B:240:ILE:HG22	1.63	0.62
1:C:475:ASN:C	1:C:477:GLN:N	2.54	0.62
1:E:542:THR:HG21	1:E:546:ARG:HA	1.80	0.62
1:A:383:ASP:OD1	1:A:387:ARG:HD2	2.00	0.62
1:A:177:GLU:HG3	1:A:178:THR:N	2.15	0.62
1:D:475:ASN:C	1:D:477:GLN:H	2.03	0.61
1:B:479:VAL:HG12	1:B:479:VAL:O	2.00	0.61
1:B:171:PRO:O	1:B:174:ASN:ND2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:THR:HG22	1:A:155:LYS:N	2.14	0.61
1:E:475:ASN:C	1:E:477:GLN:H	2.03	0.61
1:C:479:VAL:O	1:C:479:VAL:HG12	2.00	0.61
1:D:292:TYR:CD1	1:D:376:VAL:HG12	2.35	0.61
1:A:159:VAL:HG23	1:A:159:VAL:O	2.00	0.61
1:A:466:LEU:CD1	1:A:467:PRO:HD2	2.24	0.61
1:C:292:TYR:CD1	1:C:376:VAL:HG12	2.35	0.61
1:C:177:GLU:HG3	1:C:178:THR:N	2.15	0.61
1:C:383:ASP:OD1	1:C:387:ARG:HD2	2.00	0.61
1:D:466:LEU:CD1	1:D:467:PRO:HD2	2.24	0.61
1:C:154:THR:HG22	1:C:155:LYS:N	2.14	0.61
1:B:154:THR:HG22	1:B:155:LYS:N	2.14	0.61
1:D:177:GLU:HG3	1:D:178:THR:N	2.15	0.61
1:A:138:MET:O	1:A:139:PHE:HB2	1.98	0.61
1:D:376:VAL:CG2	1:D:377:ILE:H	2.14	0.61
1:D:383:ASP:OD1	1:D:387:ARG:HD2	2.00	0.61
1:C:99:ASN:HB3	1:D:450:ARG:NH2	2.16	0.61
1:A:475:ASN:C	1:A:477:GLN:N	2.53	0.61
1:E:479:VAL:O	1:E:479:VAL:HG12	2.00	0.61
1:A:428:VAL:HG21	1:A:515:SER:N	2.16	0.61
1:A:479:VAL:CG1	1:E:488:THR:HG22	2.31	0.61
1:A:292:TYR:CD1	1:A:376:VAL:HG12	2.35	0.61
1:D:428:VAL:HG21	1:D:515:SER:N	2.16	0.61
1:D:159:VAL:HG23	1:D:159:VAL:O	2.00	0.61
1:B:292:TYR:CD1	1:B:376:VAL:HG12	2.35	0.61
1:B:428:VAL:HG21	1:B:515:SER:N	2.16	0.61
1:C:183:LEU:HD21	1:D:236:PHE:HE2	1.65	0.61
1:E:475:ASN:C	1:E:477:GLN:N	2.53	0.61
1:D:495:ASN:O	1:D:497:PHE:N	2.34	0.61
1:E:383:ASP:OD1	1:E:387:ARG:HD2	2.00	0.61
1:C:428:VAL:HG21	1:C:515:SER:N	2.16	0.61
1:A:447:VAL:HG11	1:E:111:ILE:HD13	1.83	0.60
1:D:479:VAL:HG12	1:D:479:VAL:O	2.00	0.60
1:A:495:ASN:O	1:A:497:PHE:N	2.34	0.60
1:B:475:ASN:C	1:B:477:GLN:H	2.03	0.60
1:C:376:VAL:CG2	1:C:377:ILE:H	2.14	0.60
1:C:484:ILE:CG2	1:D:480:TYR:CD1	2.83	0.60
1:B:383:ASP:OD1	1:B:387:ARG:HD2	2.00	0.60
1:A:236:PHE:HE2	1:E:183:LEU:HD21	1.66	0.60
1:E:479:VAL:HA	1:E:482:GLN:HB3	1.83	0.60
1:B:376:VAL:CG2	1:B:377:ILE:H	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:TYR:CD1	1:E:376:VAL:HG12	2.35	0.60
1:D:273:ILE:O	1:D:273:ILE:HG23	2.02	0.60
1:E:478:ALA:HB1	1:E:508:ALA:HB3	1.83	0.60
1:C:159:VAL:HG23	1:C:159:VAL:O	2.00	0.60
1:C:68:ARG:NE	1:D:527:LEU:HD21	2.16	0.60
1:B:273:ILE:O	1:B:273:ILE:HG23	2.02	0.60
1:C:67:THR:HG21	1:D:447:VAL:CG2	2.29	0.60
1:D:475:ASN:C	1:D:477:GLN:N	2.53	0.60
1:B:479:VAL:HA	1:B:482:GLN:HB3	1.83	0.60
1:C:495:ASN:O	1:C:497:PHE:N	2.35	0.60
1:A:173:GLY:O	1:A:175:TYR:CD1	2.55	0.60
1:A:57:TYR:O	1:A:58:SER:C	2.40	0.60
1:A:479:VAL:HA	1:A:482:GLN:HB3	1.83	0.60
1:A:491:THR:HB	1:A:493:VAL:HG23	1.84	0.60
1:B:488:THR:HG23	1:C:479:VAL:O	2.02	0.60
1:A:478:ALA:HB1	1:A:508:ALA:HB3	1.83	0.60
1:C:57:TYR:O	1:C:58:SER:C	2.40	0.60
1:D:479:VAL:HA	1:D:482:GLN:HB3	1.83	0.60
1:E:495:ASN:O	1:E:497:PHE:N	2.35	0.60
1:C:479:VAL:HA	1:C:482:GLN:HB3	1.83	0.60
1:C:491:THR:HB	1:C:493:VAL:HG23	1.84	0.60
1:D:488:THR:HG22	1:E:479:VAL:HG12	1.82	0.60
1:E:173:GLY:O	1:E:175:TYR:CD1	2.55	0.60
1:B:475:ASN:C	1:B:477:GLN:N	2.53	0.60
1:A:497:PHE:CD2	1:A:497:PHE:N	2.69	0.60
1:C:475:ASN:C	1:C:477:GLN:H	2.03	0.60
1:A:376:VAL:CG2	1:A:377:ILE:N	2.65	0.60
1:E:52:ARG:N	1:E:116:ARG:HH12	2.00	0.60
1:B:478:ALA:HB1	1:B:508:ALA:HB3	1.83	0.60
1:A:475:ASN:C	1:A:477:GLN:H	2.03	0.60
1:C:488:THR:HG22	1:D:479:VAL:HG12	1.84	0.60
1:B:173:GLY:O	1:B:175:TYR:CD1	2.55	0.60
1:D:211:ASP:OD1	1:D:212:THR:N	2.31	0.60
1:C:173:GLY:O	1:C:175:TYR:CD1	2.55	0.59
1:E:273:ILE:O	1:E:273:ILE:HG23	2.02	0.59
1:E:428:VAL:HG21	1:E:515:SER:N	2.16	0.59
1:C:52:ARG:N	1:C:116:ARG:HH12	2.00	0.59
1:D:57:TYR:O	1:D:58:SER:C	2.40	0.59
1:B:497:PHE:CD2	1:B:497:PHE:N	2.69	0.59
1:D:173:GLY:O	1:D:175:TYR:CD1	2.55	0.59
1:E:376:VAL:CG2	1:E:377:ILE:N	2.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:LEU:HD22	1:D:404:TRP:HA	1.84	0.59
1:D:233:ASN:OD1	1:D:507:PRO:HG3	2.02	0.59
1:D:210:PHE:CD2	1:D:240:ILE:HG22	2.37	0.59
1:B:52:ARG:N	1:B:116:ARG:HH12	2.00	0.59
1:D:491:THR:HB	1:D:493:VAL:HG23	1.84	0.59
1:B:387:ARG:HG2	1:B:387:ARG:HH11	1.68	0.59
1:E:233:ASN:OD1	1:E:507:PRO:HG3	2.02	0.59
1:C:273:ILE:HG23	1:C:273:ILE:O	2.02	0.59
1:C:536:VAL:O	1:C:536:VAL:HG23	2.02	0.59
1:E:237:HIS:CD2	1:E:238:PRO:O	2.56	0.59
1:C:237:HIS:CD2	1:C:238:PRO:O	2.56	0.59
1:C:278:LEU:HD22	1:C:404:TRP:HA	1.84	0.59
1:B:57:TYR:O	1:B:58:SER:C	2.40	0.59
1:B:495:ASN:O	1:B:497:PHE:N	2.34	0.59
1:A:479:VAL:HG12	1:E:488:THR:HG22	1.80	0.59
1:E:491:THR:HB	1:E:493:VAL:HG23	1.83	0.59
1:A:237:HIS:CD2	1:A:238:PRO:O	2.56	0.59
1:D:208:VAL:HG22	1:D:242:LEU:CD2	2.33	0.59
1:C:211:ASP:OD1	1:C:212:THR:N	2.31	0.59
1:E:536:VAL:O	1:E:536:VAL:HG23	2.02	0.59
1:D:111:ILE:HD13	1:E:447:VAL:HG11	1.82	0.59
1:C:488:THR:HG22	1:D:479:VAL:CG1	2.33	0.59
1:C:497:PHE:CD2	1:C:497:PHE:N	2.69	0.59
1:C:490:LEU:HB2	1:D:230:VAL:CG1	2.28	0.59
1:A:376:VAL:CG2	1:A:377:ILE:H	2.14	0.59
1:C:208:VAL:HG22	1:C:242:LEU:CD2	2.33	0.59
1:B:536:VAL:O	1:B:536:VAL:HG23	2.02	0.59
1:D:478:ALA:HB1	1:D:508:ALA:HB3	1.83	0.59
1:E:57:TYR:O	1:E:58:SER:C	2.40	0.59
1:B:409:ASN:N	1:B:409:ASN:OD1	2.36	0.59
1:A:211:ASP:OD1	1:A:212:THR:N	2.31	0.59
1:B:210:PHE:CD2	1:B:240:ILE:HG22	2.37	0.59
1:A:536:VAL:HG23	1:A:536:VAL:O	2.02	0.59
1:D:376:VAL:CG2	1:D:377:ILE:N	2.65	0.59
1:E:376:VAL:CG2	1:E:377:ILE:H	2.14	0.59
1:E:208:VAL:HG22	1:E:242:LEU:CD2	2.33	0.59
1:A:210:PHE:CD2	1:A:240:ILE:HG22	2.37	0.59
1:D:475:ASN:HB3	1:E:474:TYR:CE2	2.38	0.59
1:E:122:ASP:OD1	1:E:526:THR:HG22	2.03	0.59
1:B:278:LEU:HD22	1:B:404:TRP:HA	1.84	0.59
1:E:433:GLU:OE1	1:E:433:GLU:HA	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:VAL:CG2	1:C:377:ILE:N	2.65	0.58
1:C:210:PHE:CD2	1:C:240:ILE:HG22	2.37	0.58
1:D:536:VAL:O	1:D:536:VAL:HG23	2.02	0.58
1:A:233:ASN:OD1	1:A:507:PRO:HG3	2.03	0.58
1:B:477:GLN:O	1:B:481:SER:N	2.36	0.58
1:A:278:LEU:HD22	1:A:404:TRP:HA	1.84	0.58
1:A:208:VAL:HG22	1:A:242:LEU:CD2	2.33	0.58
1:A:52:ARG:N	1:A:116:ARG:HH12	2.00	0.58
1:B:433:GLU:HA	1:B:433:GLU:OE1	2.03	0.58
1:C:478:ALA:HB1	1:C:508:ALA:HB3	1.83	0.58
1:D:57:TYR:CD2	1:E:448:THR:HG22	2.39	0.58
1:B:491:THR:HB	1:B:493:VAL:HG23	1.84	0.58
1:D:496:ARG:O	2:V:16:PRO:HD3	2.03	0.58
1:A:295:SER:OG	1:A:375:PRO:HD3	2.03	0.58
1:B:233:ASN:OD1	1:B:507:PRO:HG3	2.02	0.58
1:C:409:ASN:OD1	1:C:409:ASN:N	2.36	0.58
1:D:183:LEU:HD21	1:E:236:PHE:HE2	1.67	0.58
1:A:68:ARG:NE	1:B:527:LEU:HD21	2.18	0.58
1:B:274:THR:CG2	1:B:275:TYR:N	2.67	0.58
1:A:477:GLN:O	1:A:481:SER:N	2.36	0.58
1:A:234:GLU:CD	1:E:485:ARG:HH21	2.06	0.58
1:B:376:VAL:CG2	1:B:377:ILE:N	2.65	0.58
1:A:434:GLN:HG2	1:E:556:LEU:HD21	1.83	0.58
1:A:556:LEU:HD21	1:B:434:GLN:HG2	1.86	0.58
1:E:387:ARG:HH11	1:E:387:ARG:HG2	1.67	0.58
1:A:433:GLU:HA	1:A:433:GLU:OE1	2.03	0.58
1:A:474:TYR:CE2	1:E:475:ASN:HB3	2.38	0.58
1:E:497:PHE:N	1:E:497:PHE:CD2	2.69	0.58
1:A:401:TYR:HD1	1:A:502:ILE:HG12	1.69	0.58
1:D:237:HIS:CD2	1:D:238:PRO:O	2.56	0.58
1:D:295:SER:OG	1:D:375:PRO:HD3	2.03	0.58
1:B:122:ASP:OD1	1:B:526:THR:HG22	2.03	0.58
1:A:409:ASN:N	1:A:409:ASN:OD1	2.36	0.58
1:E:210:PHE:CD2	1:E:240:ILE:HG22	2.37	0.58
1:A:387:ARG:HG2	1:A:387:ARG:HH11	1.67	0.58
1:D:558:ILE:HD11	1:E:463:ALA:HB3	1.86	0.58
1:A:98:ASN:HD22	1:A:98:ASN:C	2.06	0.58
1:B:401:TYR:HD1	1:B:502:ILE:HG12	1.69	0.58
1:E:477:GLN:O	1:E:481:SER:N	2.36	0.58
1:A:496:ARG:O	2:S:16:PRO:HD3	2.03	0.58
1:C:477:GLN:O	1:C:481:SER:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:SER:OG	1:C:375:PRO:HD3	2.03	0.58
1:D:52:ARG:N	1:D:116:ARG:HH12	2.00	0.58
1:C:433:GLU:OE1	1:C:433:GLU:HA	2.03	0.58
1:A:274:THR:CG2	1:A:275:TYR:N	2.67	0.58
1:C:387:ARG:HH11	1:C:387:ARG:HG2	1.68	0.58
1:D:387:ARG:HH11	1:D:387:ARG:HG2	1.67	0.58
2:S:15:TYR:HD2	2:S:16:PRO:N	2.02	0.58
1:C:496:ARG:O	2:U:16:PRO:HD3	2.03	0.58
1:D:98:ASN:C	1:D:98:ASN:HD22	2.06	0.58
1:C:233:ASN:OD1	1:C:507:PRO:HG3	2.02	0.58
1:D:274:THR:CG2	1:D:275:TYR:N	2.67	0.58
1:B:237:HIS:CD2	1:B:238:PRO:O	2.56	0.58
1:C:122:ASP:OD1	1:C:526:THR:HG22	2.04	0.58
1:B:211:ASP:OD1	1:B:212:THR:N	2.31	0.58
1:D:433:GLU:HA	1:D:433:GLU:OE1	2.03	0.58
1:A:502:ILE:O	1:A:504:ALA:N	2.36	0.58
1:B:295:SER:OG	1:B:375:PRO:HD3	2.03	0.58
1:E:278:LEU:HD22	1:E:404:TRP:HA	1.84	0.58
2:T:15:TYR:HD2	2:T:16:PRO:N	2.02	0.57
1:D:477:GLN:O	1:D:481:SER:N	2.36	0.57
2:W:15:TYR:HD2	2:W:16:PRO:N	2.02	0.57
1:D:496:ARG:C	1:D:497:PHE:HD2	2.07	0.57
1:C:274:THR:CG2	1:C:275:TYR:N	2.67	0.57
1:E:295:SER:OG	1:E:375:PRO:HD3	2.03	0.57
1:D:439:LEU:N	1:D:440:PRO:HD3	2.19	0.57
1:E:98:ASN:C	1:E:98:ASN:HD22	2.06	0.57
1:B:99:ASN:HB3	1:C:450:ARG:NH2	2.19	0.57
1:B:496:ARG:O	2:T:16:PRO:HD3	2.03	0.57
1:C:502:ILE:O	1:C:504:ALA:N	2.37	0.57
1:E:496:ARG:O	2:W:16:PRO:HD3	2.03	0.57
1:D:498:PRO:HG2	1:D:499:GLU:OE2	2.04	0.57
1:D:122:ASP:OD1	1:D:526:THR:HG22	2.03	0.57
1:A:475:ASN:HB3	1:B:474:TYR:CE2	2.39	0.57
1:E:502:ILE:O	1:E:504:ALA:N	2.37	0.57
1:D:497:PHE:N	1:D:497:PHE:CD2	2.69	0.57
1:A:496:ARG:C	1:A:497:PHE:HD2	2.08	0.57
1:A:498:PRO:HG2	1:A:499:GLU:OE2	2.04	0.57
1:B:208:VAL:HG22	1:B:242:LEU:CD2	2.33	0.57
1:B:484:ILE:HG21	1:C:480:TYR:CD1	2.39	0.57
1:E:409:ASN:OD1	1:E:409:ASN:N	2.36	0.57
1:E:518:VAL:HG23	1:E:519:PRO:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:VAL:HG23	1:A:519:PRO:HD2	1.87	0.57
1:C:475:ASN:HB3	1:D:474:TYR:CE2	2.39	0.57
1:A:122:ASP:OD1	1:A:526:THR:HG22	2.03	0.57
1:D:214:ASN:C	1:D:214:ASN:ND2	2.58	0.57
1:D:502:ILE:O	1:D:504:ALA:N	2.37	0.57
1:C:496:ARG:C	1:C:497:PHE:HD2	2.07	0.57
1:B:466:LEU:CD1	1:B:467:PRO:HD2	2.24	0.57
1:A:484:ILE:HG23	1:B:480:TYR:CE1	2.40	0.57
1:C:175:TYR:CD1	1:C:175:TYR:N	2.72	0.57
1:B:100:ASP:CG	1:C:450:ARG:HH12	2.07	0.57
1:B:498:PRO:HG2	1:B:499:GLU:OE2	2.05	0.57
1:E:496:ARG:C	1:E:497:PHE:CD2	2.78	0.57
1:E:496:ARG:C	1:E:497:PHE:HD2	2.08	0.57
1:C:485:ARG:HH21	1:D:234:GLU:CD	2.08	0.57
1:C:498:PRO:HG2	1:C:499:GLU:OE2	2.04	0.57
2:U:15:TYR:HD2	2:U:16:PRO:N	2.02	0.57
1:B:175:TYR:HD1	1:B:175:TYR:H	1.52	0.57
1:B:496:ARG:C	1:B:497:PHE:HD2	2.07	0.57
1:B:502:ILE:O	1:B:504:ALA:N	2.37	0.57
1:E:498:PRO:HG2	1:E:499:GLU:OE2	2.05	0.57
1:B:175:TYR:CD1	1:B:175:TYR:N	2.72	0.57
1:A:273:ILE:HG23	1:A:273:ILE:O	2.02	0.57
1:E:258:LEU:CD1	1:E:428:VAL:HA	2.35	0.57
1:E:274:THR:CG2	1:E:275:TYR:N	2.67	0.57
2:V:15:TYR:HD2	2:V:16:PRO:N	2.02	0.57
1:A:496:ARG:C	1:A:497:PHE:CD2	2.78	0.57
2:S:15:TYR:HD2	2:S:16:PRO:CD	2.18	0.57
2:U:15:TYR:HD2	2:U:16:PRO:CD	2.18	0.57
1:B:490:LEU:CB	1:C:230:VAL:HG11	2.34	0.57
1:C:214:ASN:C	1:C:214:ASN:ND2	2.58	0.57
1:A:88:HIS:ND1	1:A:553:TYR:O	2.38	0.57
1:A:175:TYR:CD1	1:A:175:TYR:N	2.72	0.57
1:B:258:LEU:CD1	1:B:428:VAL:HA	2.35	0.57
1:B:88:HIS:ND1	1:B:553:TYR:O	2.38	0.57
1:C:68:ARG:NH1	1:C:68:ARG:CG	2.67	0.56
1:A:99:ASN:HB3	1:B:450:ARG:NH2	2.20	0.56
1:B:496:ARG:C	1:B:497:PHE:CD2	2.78	0.56
1:E:401:TYR:HD1	1:E:502:ILE:HG12	1.69	0.56
1:A:258:LEU:CD1	1:A:428:VAL:HA	2.35	0.56
1:B:429:THR:O	1:B:430:CYS:HB2	2.05	0.56
1:B:98:ASN:C	1:B:98:ASN:HD22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:TYR:H	1:A:175:TYR:HD1	1.52	0.56
1:D:409:ASN:OD1	1:D:409:ASN:N	2.36	0.56
1:A:463:ALA:HB3	1:E:558:ILE:HD11	1.88	0.56
1:D:88:HIS:ND1	1:D:553:TYR:O	2.38	0.56
1:C:98:ASN:C	1:C:98:ASN:HD22	2.06	0.56
1:D:461:VAL:HB	1:D:527:LEU:HD13	1.88	0.56
1:B:461:VAL:HB	1:B:527:LEU:HD13	1.87	0.56
2:V:15:TYR:HD2	2:V:16:PRO:CD	2.18	0.56
1:C:496:ARG:C	1:C:497:PHE:CD2	2.78	0.56
1:D:488:THR:HG22	1:E:479:VAL:CG1	2.34	0.56
1:E:175:TYR:N	1:E:175:TYR:CD1	2.72	0.56
1:E:439:LEU:N	1:E:440:PRO:HD3	2.19	0.56
1:E:69:VAL:CG2	1:E:559:VAL:HB	2.36	0.56
1:A:130:ASN:HA	1:A:517:ASN:ND2	2.21	0.56
1:C:258:LEU:CD1	1:C:428:VAL:HA	2.35	0.56
1:A:151:ARG:HB3	1:A:201:VAL:H	1.70	0.56
1:E:151:ARG:HB3	1:E:201:VAL:H	1.70	0.56
1:C:439:LEU:N	1:C:440:PRO:HD3	2.19	0.56
1:C:130:ASN:HA	1:C:517:ASN:ND2	2.21	0.56
1:D:496:ARG:C	1:D:497:PHE:CD2	2.78	0.56
1:E:214:ASN:ND2	1:E:214:ASN:C	2.58	0.56
1:E:130:ASN:HA	1:E:517:ASN:ND2	2.21	0.56
1:A:429:THR:O	1:A:430:CYS:HB2	2.05	0.56
1:D:429:THR:O	1:D:430:CYS:HB2	2.05	0.56
1:C:461:VAL:HB	1:C:527:LEU:HD13	1.88	0.56
1:A:243:LEU:HG	1:A:401:TYR:HE2	1.71	0.56
1:D:132:PRO:HD2	1:D:551:TYR:CE2	2.41	0.56
1:C:132:PRO:HD2	1:C:551:TYR:CE2	2.41	0.56
1:C:86:ASN:HB3	1:C:90:ASN:O	2.06	0.56
1:B:154:THR:CG2	1:B:155:LYS:N	2.69	0.56
1:D:154:THR:CG2	1:D:155:LYS:N	2.69	0.56
1:A:214:ASN:C	1:A:214:ASN:ND2	2.58	0.56
1:D:258:LEU:CD1	1:D:428:VAL:HA	2.35	0.56
1:A:128:HIS:CE1	1:B:432:SER:HG	2.24	0.56
1:C:151:ARG:HB3	1:C:201:VAL:H	1.70	0.56
1:E:429:THR:O	1:E:430:CYS:HB2	2.05	0.56
1:D:67:THR:OG1	1:D:68:ARG:N	2.39	0.56
1:E:132:PRO:HD2	1:E:551:TYR:CE2	2.41	0.56
1:B:86:ASN:HB3	1:B:90:ASN:O	2.06	0.56
1:E:86:ASN:HB3	1:E:90:ASN:O	2.06	0.56
1:C:69:VAL:CG2	1:C:559:VAL:HB	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:ASN:HA	1:D:517:ASN:ND2	2.21	0.56
1:B:439:LEU:N	1:B:440:PRO:HD3	2.19	0.56
1:B:130:ASN:HA	1:B:517:ASN:ND2	2.21	0.56
2:W:18:ASP:O	2:W:18:ASP:CG	2.44	0.56
1:A:67:THR:OG1	1:B:447:VAL:HG23	2.06	0.56
1:A:447:VAL:CG2	1:E:67:THR:HG21	2.36	0.56
1:B:132:PRO:HD2	1:B:551:TYR:CE2	2.41	0.56
1:A:86:ASN:HB3	1:A:90:ASN:O	2.06	0.56
1:E:279:GLU:O	1:E:280:GLY:O	2.24	0.56
1:A:154:THR:CG2	1:A:155:LYS:N	2.69	0.56
1:D:518:VAL:HG23	1:D:519:PRO:HD2	1.87	0.56
1:D:150:SER:HB3	1:D:199:ASN:HD22	1.71	0.56
1:A:179:MET:HE3	1:A:485:ARG:HH22	1.71	0.56
1:C:243:LEU:HG	1:C:401:TYR:HE2	1.71	0.56
1:C:279:GLU:O	1:C:280:GLY:O	2.24	0.56
1:A:69:VAL:CG2	1:A:559:VAL:HB	2.36	0.56
1:D:151:ARG:HB3	1:D:201:VAL:H	1.70	0.56
2:W:15:TYR:HD2	2:W:16:PRO:CD	2.18	0.56
1:E:175:TYR:HD1	1:E:175:TYR:H	1.52	0.56
1:D:86:ASN:HB3	1:D:90:ASN:O	2.06	0.56
1:C:88:HIS:HD2	1:D:267:PHE:CZ	2.24	0.56
1:C:67:THR:OG1	1:C:68:ARG:N	2.39	0.55
1:C:197:ARG:HG3	1:C:198:GLN:HG3	1.88	0.55
1:B:69:VAL:CG2	1:B:559:VAL:HB	2.36	0.55
2:T:15:TYR:HD2	2:T:16:PRO:CD	2.18	0.55
1:E:243:LEU:HG	1:E:401:TYR:HE2	1.71	0.55
1:A:132:PRO:HD2	1:A:551:TYR:CE2	2.41	0.55
1:A:279:GLU:O	1:A:280:GLY:O	2.24	0.55
1:E:154:THR:CG2	1:E:155:LYS:N	2.69	0.55
1:C:150:SER:HB3	1:C:199:ASN:HD22	1.71	0.55
1:B:65:ASP:O	1:B:66:THR:HB	2.06	0.55
1:B:518:VAL:HG23	1:B:519:PRO:HD2	1.87	0.55
1:B:150:SER:HB3	1:B:199:ASN:HD22	1.71	0.55
1:B:151:ARG:HB3	1:B:201:VAL:H	1.71	0.55
1:A:461:VAL:HB	1:A:527:LEU:HD13	1.88	0.55
1:D:197:ARG:HG3	1:D:198:GLN:HG3	1.89	0.55
1:D:69:VAL:CG2	1:D:559:VAL:HB	2.36	0.55
2:T:18:ASP:O	2:T:18:ASP:CG	2.44	0.55
1:E:65:ASP:O	1:E:66:THR:HB	2.06	0.55
1:A:150:SER:HB3	1:A:199:ASN:HD22	1.71	0.55
1:D:243:LEU:HG	1:D:401:TYR:HE2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:THR:CG2	1:C:155:LYS:N	2.69	0.55
2:S:18:ASP:O	2:S:18:ASP:CG	2.44	0.55
1:D:65:ASP:O	1:D:66:THR:HB	2.06	0.55
1:C:518:VAL:HG23	1:C:519:PRO:HD2	1.87	0.55
1:D:175:TYR:HD1	1:D:175:TYR:H	1.52	0.55
2:V:18:ASP:CG	2:V:18:ASP:O	2.44	0.55
2:U:18:ASP:O	2:U:18:ASP:CG	2.44	0.55
1:E:88:HIS:ND1	1:E:553:TYR:O	2.38	0.55
1:C:65:ASP:O	1:C:66:THR:HB	2.06	0.55
1:A:67:THR:OG1	1:A:68:ARG:N	2.39	0.55
1:C:175:TYR:HD1	1:C:175:TYR:H	1.52	0.55
1:A:404:TRP:NE1	1:A:417:ILE:HG21	2.22	0.55
1:E:150:SER:HB3	1:E:199:ASN:HD22	1.71	0.55
1:E:461:VAL:HB	1:E:527:LEU:HD13	1.88	0.55
1:C:444:GLN:O	1:C:446:PRO:HD3	2.07	0.55
1:B:444:GLN:O	1:B:446:PRO:HD3	2.07	0.55
1:E:444:GLN:O	1:E:446:PRO:HD3	2.07	0.55
1:D:401:TYR:HD1	1:D:502:ILE:HG12	1.69	0.55
1:D:175:TYR:CD1	1:D:175:TYR:N	2.72	0.55
1:E:279:GLU:O	1:E:280:GLY:C	2.45	0.55
1:B:214:ASN:C	1:B:214:ASN:ND2	2.58	0.55
1:E:67:THR:OG1	1:E:68:ARG:N	2.39	0.55
1:A:439:LEU:N	1:A:440:PRO:HD3	2.19	0.55
1:C:429:THR:O	1:C:430:CYS:HB2	2.05	0.55
1:B:197:ARG:HG3	1:B:198:GLN:HG3	1.89	0.54
1:C:375:PRO:O	1:C:377:ILE:N	2.40	0.54
1:B:279:GLU:O	1:B:280:GLY:O	2.24	0.54
1:A:444:GLN:O	1:A:446:PRO:HD3	2.07	0.54
1:B:67:THR:OG1	1:B:68:ARG:N	2.39	0.54
1:E:197:ARG:HG3	1:E:198:GLN:HG3	1.88	0.54
1:A:228:PRO:HG3	2:W:15:TYR:CE1	2.42	0.54
1:A:375:PRO:O	1:A:377:ILE:N	2.40	0.54
1:E:375:PRO:O	1:E:377:ILE:N	2.41	0.54
1:B:122:ASP:OD1	1:B:526:THR:CG2	2.56	0.54
1:A:122:ASP:OD1	1:A:526:THR:CG2	2.56	0.54
1:B:428:VAL:CG1	1:B:513:THR:HB	2.38	0.54
1:E:495:ASN:O	1:E:498:PRO:HD3	2.08	0.54
1:C:171:PRO:HG2	1:C:174:ASN:ND2	2.23	0.54
1:E:52:ARG:N	1:E:116:ARG:NH1	2.56	0.54
1:B:52:ARG:N	1:B:116:ARG:NH1	2.56	0.54
1:D:279:GLU:O	1:D:280:GLY:C	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:PRO:O	1:B:377:ILE:N	2.40	0.54
1:C:542:THR:CG2	1:C:547:ARG:N	2.70	0.54
1:E:404:TRP:NE1	1:E:417:ILE:HG21	2.22	0.54
1:C:428:VAL:CG1	1:C:513:THR:HB	2.38	0.54
1:A:495:ASN:O	1:A:498:PRO:HD3	2.08	0.54
1:D:171:PRO:HG2	1:D:174:ASN:ND2	2.23	0.54
1:C:404:TRP:NE1	1:C:417:ILE:HG21	2.22	0.54
1:B:484:ILE:CG2	1:C:480:TYR:CD1	2.90	0.54
1:B:556:LEU:HD21	1:C:434:GLN:HG2	1.89	0.54
1:D:428:VAL:CG1	1:D:513:THR:HB	2.38	0.54
1:A:563:VAL:HG12	1:A:564:LEU:N	2.23	0.54
1:B:495:ASN:O	1:B:498:PRO:HD3	2.08	0.54
1:D:179:MET:HE3	1:D:485:ARG:HH22	1.72	0.54
1:E:214:ASN:O	1:E:216:ARG:N	2.41	0.54
1:C:88:HIS:ND1	1:C:553:TYR:O	2.38	0.54
1:D:67:THR:HG21	1:E:447:VAL:CG2	2.37	0.54
1:B:243:LEU:HG	1:B:401:TYR:HE2	1.71	0.54
1:B:404:TRP:NE1	1:B:417:ILE:HG21	2.22	0.54
1:C:122:ASP:OD1	1:C:526:THR:CG2	2.56	0.54
1:B:542:THR:CG2	1:B:547:ARG:N	2.70	0.54
1:E:428:VAL:CG1	1:E:513:THR:HB	2.38	0.54
1:A:65:ASP:O	1:A:66:THR:HB	2.06	0.54
1:D:563:VAL:HG12	1:D:564:LEU:N	2.23	0.54
1:B:96:ILE:O	1:C:448:THR:HB	2.07	0.54
1:B:485:ARG:NE	1:C:234:GLU:OE2	2.38	0.54
1:E:542:THR:CG2	1:E:547:ARG:N	2.70	0.54
1:A:542:THR:CG2	1:A:547:ARG:N	2.71	0.54
1:E:171:PRO:HG2	1:E:174:ASN:ND2	2.23	0.54
1:D:404:TRP:HE1	1:D:417:ILE:HG21	1.73	0.54
1:C:214:ASN:O	1:C:216:ARG:N	2.41	0.54
1:A:52:ARG:N	1:A:116:ARG:NH1	2.56	0.54
1:B:243:LEU:HG	1:B:401:TYR:CE2	2.43	0.54
1:C:223:THR:HG21	1:C:227:MET:SD	2.48	0.54
1:B:214:ASN:O	1:B:216:ARG:N	2.41	0.54
1:B:64:PHE:CD1	1:C:118:HIS:NE2	2.76	0.54
1:B:177:GLU:CG	1:B:178:THR:N	2.71	0.54
1:D:243:LEU:HG	1:D:401:TYR:CE2	2.43	0.53
1:D:375:PRO:O	1:D:377:ILE:N	2.40	0.53
1:E:122:ASP:OD1	1:E:526:THR:CG2	2.55	0.53
1:B:279:GLU:O	1:B:280:GLY:C	2.45	0.53
1:A:404:TRP:HE1	1:A:417:ILE:HG21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:GLU:O	1:D:280:GLY:O	2.24	0.53
1:E:243:LEU:HG	1:E:401:TYR:CE2	2.44	0.53
1:B:223:THR:HG21	1:B:227:MET:SD	2.49	0.53
1:D:122:ASP:OD1	1:D:526:THR:CG2	2.56	0.53
1:D:542:THR:CG2	1:D:547:ARG:N	2.71	0.53
1:D:52:ARG:N	1:D:116:ARG:NH1	2.56	0.53
1:A:558:ILE:HD11	1:B:463:ALA:HB3	1.90	0.53
1:C:563:VAL:HG12	1:C:564:LEU:N	2.23	0.53
1:C:228:PRO:HG3	2:T:15:TYR:CE1	2.43	0.53
1:A:171:PRO:HG2	1:A:174:ASN:ND2	2.23	0.53
1:A:279:GLU:O	1:A:280:GLY:C	2.45	0.53
1:D:404:TRP:NE1	1:D:417:ILE:HG21	2.22	0.53
1:A:197:ARG:HG3	1:A:198:GLN:HG3	1.89	0.53
1:C:495:ASN:O	1:C:498:PRO:HD3	2.08	0.53
1:A:230:VAL:CG1	1:E:490:LEU:HB2	2.31	0.53
1:B:404:TRP:HE1	1:B:417:ILE:HG21	1.73	0.53
1:B:214:ASN:ND2	1:B:216:ARG:HB3	2.24	0.53
1:A:214:ASN:O	1:A:216:ARG:N	2.41	0.53
1:A:428:VAL:CG1	1:A:513:THR:HB	2.38	0.53
1:B:563:VAL:HG12	1:B:564:LEU:N	2.23	0.53
1:A:67:THR:HG21	1:B:447:VAL:CG2	2.37	0.53
1:D:495:ASN:O	1:D:498:PRO:HD3	2.08	0.53
1:A:486:GLN:HE22	1:A:495:ASN:ND2	2.07	0.53
1:C:243:LEU:HG	1:C:401:TYR:CE2	2.44	0.53
1:D:542:THR:HG22	1:D:543:ASP:H	1.74	0.53
1:A:542:THR:HG22	1:A:543:ASP:H	1.74	0.53
1:D:214:ASN:O	1:D:216:ARG:N	2.41	0.53
1:B:488:THR:CG2	1:C:479:VAL:CG1	2.86	0.53
1:B:542:THR:HG22	1:B:543:ASP:H	1.74	0.53
1:C:279:GLU:O	1:C:280:GLY:C	2.45	0.53
1:E:404:TRP:HE1	1:E:417:ILE:HG21	1.73	0.53
1:D:444:GLN:O	1:D:446:PRO:HD3	2.07	0.53
1:C:88:HIS:CD2	1:D:267:PHE:CZ	2.96	0.53
1:D:486:GLN:HE22	1:D:495:ASN:ND2	2.07	0.53
1:D:442:MET:HB2	1:D:537:GLN:OE1	2.09	0.53
1:C:542:THR:HG22	1:C:543:ASP:H	1.74	0.53
1:D:214:ASN:ND2	1:D:216:ARG:HB3	2.24	0.53
1:B:442:MET:HB2	1:B:537:GLN:OE1	2.09	0.53
1:A:442:MET:HB2	1:A:537:GLN:OE1	2.08	0.53
1:C:177:GLU:CG	1:C:178:THR:N	2.71	0.53
1:C:100:ASP:CG	1:D:450:ARG:HH12	2.10	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:THR:HG21	1:A:227:MET:SD	2.49	0.53
1:C:486:GLN:HE22	1:C:495:ASN:ND2	2.07	0.53
1:D:376:VAL:C	1:D:378:LYS:N	2.62	0.53
1:E:442:MET:HB2	1:E:537:GLN:OE1	2.08	0.53
1:C:52:ARG:N	1:C:116:ARG:NH1	2.56	0.53
1:B:57:TYR:OH	1:B:109:GLN:NE2	2.42	0.53
1:B:486:GLN:HE22	1:B:495:ASN:ND2	2.07	0.53
1:B:376:VAL:C	1:B:378:LYS:N	2.62	0.53
1:A:57:TYR:OH	1:A:109:GLN:NE2	2.42	0.53
1:D:392:ILE:HA	1:D:400:GLN:HE21	1.74	0.53
1:C:404:TRP:HE1	1:C:417:ILE:HG21	1.73	0.53
1:E:113:LEU:O	1:E:114:ASP:C	2.47	0.53
1:C:57:TYR:OH	1:C:109:GLN:NE2	2.42	0.52
1:E:486:GLN:HE22	1:E:495:ASN:ND2	2.07	0.52
1:D:223:THR:HG21	1:D:227:MET:SD	2.49	0.52
1:A:113:LEU:O	1:A:114:ASP:C	2.47	0.52
1:E:151:ARG:HB3	1:E:201:VAL:N	2.24	0.52
1:B:392:ILE:HA	1:B:400:GLN:HE21	1.74	0.52
1:D:68:ARG:NH1	1:D:68:ARG:CG	2.67	0.52
1:A:527:LEU:HD21	1:E:68:ARG:NE	2.25	0.52
1:D:491:THR:HG23	2:V:15:TYR:CE1	2.45	0.52
1:E:223:THR:HG21	1:E:227:MET:SD	2.49	0.52
1:E:376:VAL:C	1:E:378:LYS:N	2.62	0.52
1:E:455:ILE:HA	1:E:458:PHE:CE2	2.44	0.52
1:C:214:ASN:ND2	1:C:216:ARG:HB3	2.24	0.52
1:C:113:LEU:O	1:C:114:ASP:C	2.47	0.52
1:D:151:ARG:HB3	1:D:201:VAL:N	2.24	0.52
1:E:563:VAL:HG12	1:E:564:LEU:N	2.23	0.52
1:E:392:ILE:HA	1:E:400:GLN:HE21	1.74	0.52
1:E:126:ILE:HG12	1:E:521:LEU:HD23	1.91	0.52
1:D:57:TYR:OH	1:D:109:GLN:NE2	2.42	0.52
1:B:474:TYR:CD1	1:B:511:ILE:HD11	2.45	0.52
1:D:455:ILE:HA	1:D:458:PHE:CE2	2.45	0.52
1:A:88:HIS:CD2	1:B:267:PHE:CZ	2.97	0.52
1:A:474:TYR:CD1	1:A:511:ILE:HD11	2.45	0.52
1:A:491:THR:HG23	2:S:15:TYR:CE1	2.45	0.52
1:C:401:TYR:HD1	1:C:502:ILE:HG12	1.68	0.52
1:B:171:PRO:HG2	1:B:174:ASN:ND2	2.23	0.52
1:B:113:LEU:O	1:B:114:ASP:C	2.47	0.52
1:E:57:TYR:OH	1:E:109:GLN:NE2	2.42	0.52
1:A:243:LEU:HG	1:A:401:TYR:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ILE:HA	1:A:458:PHE:CE2	2.44	0.52
1:E:511:ILE:HD12	1:E:511:ILE:N	2.25	0.52
1:D:474:TYR:CD1	1:D:511:ILE:HD11	2.45	0.52
1:D:511:ILE:N	1:D:511:ILE:HD12	2.25	0.52
1:E:231:TYR:HD1	1:E:501:GLN:HB3	1.75	0.52
1:C:442:MET:HB2	1:C:537:GLN:OE1	2.08	0.52
1:B:128:HIS:CE1	1:C:432:SER:HG	2.27	0.52
1:C:392:ILE:HA	1:C:400:GLN:HE21	1.74	0.52
1:D:68:ARG:NE	1:E:527:LEU:HD21	2.25	0.52
1:B:491:THR:HG23	2:T:15:TYR:CE1	2.45	0.52
1:C:485:ARG:NH1	1:C:505:ARG:HH22	2.07	0.52
1:B:455:ILE:HA	1:B:458:PHE:CE2	2.44	0.52
1:C:455:ILE:HA	1:C:458:PHE:CE2	2.44	0.52
1:E:455:ILE:HD12	1:E:456:SER:N	2.25	0.52
1:A:455:ILE:HD12	1:A:456:SER:N	2.25	0.52
1:A:214:ASN:ND2	1:A:216:ARG:HB3	2.24	0.52
1:E:177:GLU:CG	1:E:178:THR:N	2.71	0.52
1:C:178:THR:OG1	1:C:509:PRO:HD2	2.10	0.52
1:A:418:ARG:HG2	1:A:418:ARG:O	2.10	0.52
1:E:214:ASN:ND2	1:E:216:ARG:HB3	2.24	0.52
1:C:556:LEU:HD12	1:C:556:LEU:C	2.30	0.52
1:A:177:GLU:CG	1:A:178:THR:N	2.71	0.52
1:D:177:GLU:CG	1:D:178:THR:N	2.72	0.52
1:A:151:ARG:HB3	1:A:201:VAL:N	2.24	0.52
1:C:151:ARG:HB3	1:C:201:VAL:N	2.24	0.52
1:A:126:ILE:HG12	1:A:521:LEU:HD23	1.91	0.52
1:A:448:THR:HG22	1:E:57:TYR:CD2	2.45	0.52
1:E:474:TYR:CD1	1:E:511:ILE:HD11	2.45	0.52
1:C:491:THR:HG23	2:U:15:TYR:CE1	2.45	0.52
1:D:490:LEU:HB2	1:E:230:VAL:CG1	2.29	0.52
1:A:231:TYR:HD1	1:A:501:GLN:HB3	1.75	0.52
1:C:74:ASN:OD1	1:D:434:GLN:OE1	2.28	0.52
1:E:491:THR:HG23	2:W:15:TYR:CE1	2.45	0.52
1:E:228:PRO:HG3	2:V:15:TYR:CE1	2.45	0.52
1:B:485:ARG:NH1	1:B:505:ARG:HH22	2.07	0.52
1:C:231:TYR:HD1	1:C:501:GLN:HB3	1.75	0.52
1:C:474:TYR:CD1	1:C:511:ILE:HD11	2.45	0.52
1:B:277:ASP:O	1:B:417:ILE:HD13	2.10	0.52
1:C:277:ASP:O	1:C:417:ILE:HD13	2.10	0.52
1:B:556:LEU:C	1:B:556:LEU:HD12	2.30	0.52
1:A:556:LEU:C	1:A:556:LEU:HD12	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ARG:HB3	1:B:201:VAL:N	2.24	0.52
1:B:228:PRO:HB3	2:S:15:TYR:HE1	1.75	0.51
1:B:231:TYR:HD1	1:B:501:GLN:HB3	1.75	0.51
1:E:277:ASP:O	1:E:417:ILE:HD13	2.10	0.51
1:E:154:THR:CG2	1:E:155:LYS:HG3	2.41	0.51
1:D:113:LEU:O	1:D:114:ASP:C	2.47	0.51
1:C:511:ILE:HD12	1:C:511:ILE:N	2.25	0.51
1:D:277:ASP:O	1:D:417:ILE:HD13	2.10	0.51
1:D:427:ASP:OD1	1:D:427:ASP:C	2.49	0.51
1:D:178:THR:OG1	1:D:509:PRO:HD2	2.10	0.51
1:A:88:HIS:HD2	1:B:267:PHE:CZ	2.28	0.51
1:C:128:HIS:CE1	1:D:432:SER:HG	2.28	0.51
1:E:132:PRO:HA	1:E:175:TYR:CZ	2.45	0.51
1:C:551:TYR:CZ	1:D:422:LEU:HD21	2.45	0.51
1:E:556:LEU:HD12	1:E:556:LEU:C	2.30	0.51
1:A:392:ILE:HA	1:A:400:GLN:HE21	1.74	0.51
1:D:418:ARG:O	1:D:418:ARG:HG2	2.10	0.51
1:B:126:ILE:HG12	1:B:521:LEU:HD23	1.91	0.51
1:A:497:PHE:CD1	1:A:503:LEU:HB3	2.44	0.51
1:E:427:ASP:C	1:E:427:ASP:OD1	2.49	0.51
1:A:427:ASP:OD1	1:A:427:ASP:C	2.49	0.51
1:E:387:ARG:NH1	1:E:387:ARG:HG2	2.26	0.51
1:E:418:ARG:O	1:E:418:ARG:HG2	2.10	0.51
1:D:485:ARG:NH1	1:D:505:ARG:HH22	2.07	0.51
1:C:427:ASP:C	1:C:427:ASP:OD1	2.49	0.51
1:B:178:THR:OG1	1:B:509:PRO:HD2	2.10	0.51
1:A:387:ARG:NH1	1:A:387:ARG:HG2	2.26	0.51
1:C:477:GLN:O	1:C:481:SER:HB3	2.07	0.51
1:A:484:ILE:HG23	1:B:480:TYR:HE1	1.75	0.51
1:E:542:THR:HG22	1:E:543:ASP:H	1.74	0.51
1:D:556:LEU:HD12	1:D:556:LEU:C	2.31	0.51
1:D:74:ASN:OD1	1:E:434:GLN:OE1	2.27	0.51
1:D:477:GLN:O	1:D:481:SER:HB3	2.07	0.51
1:D:227:MET:HB2	1:D:228:PRO:HD3	1.92	0.51
1:C:130:ASN:HD22	1:C:130:ASN:C	2.14	0.51
1:B:511:ILE:N	1:B:511:ILE:HD12	2.25	0.51
1:C:132:PRO:HA	1:C:175:TYR:CZ	2.45	0.51
1:E:130:ASN:HD22	1:E:130:ASN:C	2.14	0.51
1:A:178:THR:OG1	1:A:509:PRO:HD2	2.10	0.51
1:D:126:ILE:HG12	1:D:521:LEU:HD23	1.91	0.51
1:E:237:HIS:CD2	1:E:423:LEU:HD11	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:TYR:HD1	1:D:376:VAL:HG12	1.75	0.51
1:B:427:ASP:OD1	1:B:427:ASP:C	2.49	0.51
1:E:485:ARG:NH1	1:E:505:ARG:HH22	2.07	0.51
1:A:292:TYR:HD1	1:A:376:VAL:HG12	1.75	0.51
1:C:376:VAL:C	1:C:378:LYS:N	2.62	0.51
1:B:235:ALA:C	1:B:236:PHE:HD1	2.15	0.51
1:D:130:ASN:C	1:D:130:ASN:HD22	2.14	0.51
1:C:64:PHE:HD1	1:D:118:HIS:NE2	2.09	0.51
1:C:126:ILE:HG12	1:C:521:LEU:HD23	1.91	0.51
1:C:67:THR:CG2	1:D:447:VAL:CG2	2.89	0.50
1:E:477:GLN:O	1:E:481:SER:HB3	2.07	0.50
1:E:227:MET:HB2	1:E:228:PRO:HD3	1.92	0.50
1:D:237:HIS:CD2	1:D:423:LEU:HD11	2.46	0.50
1:C:292:TYR:HD1	1:C:376:VAL:HG12	1.75	0.50
1:A:277:ASP:O	1:A:417:ILE:HD13	2.10	0.50
1:C:171:PRO:CA	1:D:409:ASN:HD22	2.24	0.50
1:B:497:PHE:HD1	1:B:503:LEU:CB	2.25	0.50
1:B:228:PRO:HG3	2:S:15:TYR:CE1	2.46	0.50
1:E:422:LEU:HD23	1:E:423:LEU:H	1.76	0.50
1:B:551:TYR:CE2	1:C:422:LEU:HD21	2.47	0.50
1:E:235:ALA:C	1:E:236:PHE:HD1	2.15	0.50
1:C:497:PHE:HD1	1:C:503:LEU:CB	2.25	0.50
1:B:295:SER:CB	1:B:375:PRO:CG	2.90	0.50
1:D:154:THR:CG2	1:D:155:LYS:HG3	2.41	0.50
1:A:511:ILE:N	1:A:511:ILE:HD12	2.25	0.50
1:C:237:HIS:CD2	1:C:423:LEU:HD11	2.46	0.50
1:A:235:ALA:C	1:A:236:PHE:HD1	2.15	0.50
1:D:64:PHE:HD1	1:E:118:HIS:NE2	2.09	0.50
1:C:235:ALA:C	1:C:236:PHE:HD1	2.15	0.50
1:B:418:ARG:O	1:B:418:ARG:HG2	2.10	0.50
1:C:227:MET:HB2	1:C:228:PRO:HD3	1.92	0.50
2:T:15:TYR:HD2	2:T:16:PRO:HD2	1.77	0.50
1:B:179:MET:HE3	1:B:485:ARG:HH22	1.76	0.50
2:S:15:TYR:HD2	2:S:16:PRO:HD2	1.77	0.50
1:D:231:TYR:HD1	1:D:501:GLN:HB3	1.75	0.50
1:B:237:HIS:CD2	1:B:423:LEU:HD11	2.46	0.50
1:C:543:ASP:OD1	1:C:547:ARG:HG2	2.12	0.50
1:B:154:THR:CG2	1:B:155:LYS:HG3	2.40	0.50
1:A:130:ASN:C	1:A:130:ASN:HD22	2.14	0.50
1:E:178:THR:OG1	1:E:509:PRO:HD2	2.10	0.50
1:A:373:LYS:O	1:A:374:LYS:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:VAL:HA	1:E:63:LEU:HD12	1.93	0.50
2:U:15:TYR:HD2	2:U:16:PRO:HD2	1.76	0.50
1:D:132:PRO:HA	1:D:175:TYR:CZ	2.45	0.50
1:D:422:LEU:HD23	1:D:423:LEU:H	1.76	0.50
1:D:543:ASP:OD1	1:D:547:ARG:HG2	2.12	0.50
1:C:387:ARG:NH1	1:C:387:ARG:HG2	2.26	0.50
1:B:387:ARG:HG2	1:B:387:ARG:NH1	2.26	0.50
1:B:553:TYR:HE2	1:C:432:SER:N	2.09	0.50
1:C:418:ARG:O	1:C:418:ARG:HG2	2.10	0.50
1:A:485:ARG:NH1	1:A:505:ARG:HH22	2.07	0.50
1:D:228:PRO:CB	2:U:15:TYR:HE1	2.25	0.50
1:A:237:HIS:CD2	1:A:423:LEU:HD11	2.46	0.50
1:B:132:PRO:HA	1:B:175:TYR:CZ	2.45	0.50
1:B:542:THR:HG22	1:B:543:ASP:N	2.27	0.50
1:C:130:ASN:N	1:C:130:ASN:HD22	2.10	0.50
1:E:384:SER:O	1:E:386:LYS:N	2.45	0.50
1:D:243:LEU:CD2	1:D:244:PRO:HD3	2.42	0.50
2:V:15:TYR:HD2	2:V:16:PRO:HD2	1.77	0.50
1:A:497:PHE:HD1	1:A:503:LEU:CB	2.25	0.50
1:D:484:ILE:CG2	1:E:480:TYR:HE1	2.22	0.50
1:E:295:SER:CB	1:E:375:PRO:CG	2.90	0.50
1:D:373:LYS:O	1:D:374:LYS:HG3	2.12	0.50
1:B:68:ARG:CG	1:B:68:ARG:NH1	2.67	0.49
1:D:63:LEU:HD12	1:E:447:VAL:HA	1.93	0.49
1:D:243:LEU:CG	1:D:401:TYR:HE2	2.25	0.49
1:B:227:MET:HB2	1:B:228:PRO:HD3	1.92	0.49
1:E:131:MET:HA	1:E:551:TYR:CD2	2.47	0.49
1:E:173:GLY:O	1:E:175:TYR:CE1	2.65	0.49
1:C:173:GLY:O	1:C:175:TYR:CE1	2.65	0.49
1:A:376:VAL:C	1:A:378:LYS:N	2.62	0.49
1:B:292:TYR:HD1	1:B:376:VAL:HG12	1.76	0.49
1:D:384:SER:O	1:D:386:LYS:N	2.45	0.49
1:C:151:ARG:CB	1:C:201:VAL:H	2.25	0.49
1:A:227:MET:HB2	1:A:228:PRO:HD3	1.92	0.49
1:B:543:ASP:OD1	1:B:547:ARG:HG2	2.12	0.49
1:D:455:ILE:HD12	1:D:456:SER:N	2.25	0.49
1:E:542:THR:HG22	1:E:543:ASP:N	2.27	0.49
1:B:130:ASN:HD22	1:B:130:ASN:C	2.14	0.49
1:D:197:ARG:HG3	1:D:198:GLN:N	2.27	0.49
1:D:131:MET:HA	1:D:551:TYR:CD2	2.47	0.49
1:C:295:SER:CB	1:C:375:PRO:CG	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:542:THR:HG22	1:D:543:ASP:N	2.27	0.49
2:W:10:THR:CG2	2:W:10:THR:O	2.60	0.49
1:D:240:ILE:HD11	1:D:273:ILE:HG21	1.95	0.49
1:E:201:VAL:HG13	1:E:201:VAL:O	2.12	0.49
1:D:392:ILE:HD11	1:D:396:SER:OG	2.13	0.49
1:B:98:ASN:C	1:B:98:ASN:ND2	2.66	0.49
1:C:63:LEU:HD12	1:D:447:VAL:HA	1.95	0.49
1:C:98:ASN:C	1:C:98:ASN:ND2	2.66	0.49
1:B:243:LEU:CG	1:B:401:TYR:HE2	2.25	0.49
1:E:197:ARG:HG3	1:E:198:GLN:N	2.27	0.49
1:D:491:THR:HG22	1:D:492:HIS:N	2.27	0.49
1:A:243:LEU:CD2	1:A:244:PRO:HD3	2.42	0.49
1:A:243:LEU:CG	1:A:401:TYR:HE2	2.25	0.49
1:C:197:ARG:HG3	1:C:198:GLN:N	2.27	0.49
1:B:132:PRO:CA	1:B:175:TYR:OH	2.53	0.49
1:A:173:GLY:O	1:A:175:TYR:CE1	2.65	0.49
1:D:295:SER:CB	1:D:375:PRO:CG	2.90	0.49
1:A:74:ASN:OD1	1:B:434:GLN:OE1	2.30	0.49
1:C:392:ILE:HD11	1:C:396:SER:OG	2.13	0.49
1:B:243:LEU:CD2	1:B:244:PRO:HD3	2.42	0.49
1:B:491:THR:HG22	1:B:492:HIS:N	2.27	0.49
1:D:501:GLN:OE1	1:D:501:GLN:HA	2.12	0.49
1:D:173:GLY:O	1:D:175:TYR:CE1	2.65	0.49
1:C:501:GLN:HA	1:C:501:GLN:OE1	2.12	0.49
1:B:131:MET:HA	1:B:551:TYR:CD2	2.47	0.49
1:A:295:SER:CB	1:A:375:PRO:CG	2.90	0.49
1:A:542:THR:HG22	1:A:543:ASP:N	2.27	0.49
1:C:154:THR:CG2	1:C:155:LYS:HG3	2.41	0.49
1:A:130:ASN:N	1:A:130:ASN:HD22	2.10	0.49
1:C:240:ILE:HD11	1:C:273:ILE:HG21	1.95	0.49
1:D:387:ARG:NH1	1:D:387:ARG:HG2	2.26	0.49
1:D:235:ALA:C	1:D:236:PHE:HD1	2.15	0.49
1:B:384:SER:O	1:B:386:LYS:N	2.45	0.49
1:E:151:ARG:CB	1:E:201:VAL:H	2.26	0.49
1:D:518:VAL:CG2	1:D:519:PRO:HD2	2.42	0.49
1:D:151:ARG:CB	1:D:201:VAL:H	2.25	0.49
1:B:201:VAL:O	1:B:201:VAL:HG13	2.12	0.49
1:C:518:VAL:CG2	1:C:519:PRO:HD2	2.43	0.49
1:B:392:ILE:HD11	1:B:396:SER:OG	2.13	0.49
1:C:373:LYS:O	1:C:374:LYS:HG3	2.12	0.49
1:B:389:TYR:O	1:B:390:ASN:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:NH1	1:A:68:ARG:CG	2.67	0.49
1:E:68:ARG:NH1	1:E:68:ARG:CG	2.67	0.49
1:E:243:LEU:CG	1:E:401:TYR:HE2	2.25	0.49
1:A:495:ASN:ND2	1:A:498:PRO:HB3	2.28	0.49
1:C:243:LEU:CD2	1:C:244:PRO:HD3	2.43	0.49
1:A:131:MET:HA	1:A:551:TYR:CD2	2.47	0.49
1:A:384:SER:O	1:A:386:LYS:N	2.45	0.49
1:E:518:VAL:CG2	1:E:519:PRO:HD2	2.42	0.49
1:E:373:LYS:O	1:E:374:LYS:HG3	2.12	0.49
1:B:373:LYS:O	1:B:374:LYS:HG3	2.12	0.49
1:C:131:MET:HA	1:C:551:TYR:CD2	2.47	0.49
1:D:98:ASN:C	1:D:98:ASN:ND2	2.66	0.49
1:D:130:ASN:N	1:D:130:ASN:HD22	2.10	0.49
1:B:130:ASN:HD22	1:B:130:ASN:N	2.10	0.49
1:C:389:TYR:O	1:C:390:ASN:C	2.51	0.49
1:A:98:ASN:ND2	1:A:98:ASN:C	2.66	0.49
1:D:495:ASN:ND2	1:D:498:PRO:HB3	2.28	0.49
1:C:243:LEU:CG	1:C:401:TYR:HE2	2.25	0.49
1:C:491:THR:HG22	1:C:492:HIS:N	2.27	0.49
1:C:542:THR:HG22	1:C:543:ASP:N	2.27	0.49
1:A:240:ILE:HD11	1:A:273:ILE:HG21	1.95	0.49
1:A:151:ARG:CB	1:A:201:VAL:H	2.25	0.49
1:D:497:PHE:HD1	1:D:503:LEU:CB	2.25	0.49
1:A:501:GLN:HA	1:A:501:GLN:OE1	2.12	0.49
1:C:422:LEU:HD23	1:C:423:LEU:H	1.76	0.49
1:C:455:ILE:HD12	1:C:456:SER:N	2.25	0.49
2:U:10:THR:CG2	2:U:10:THR:O	2.60	0.49
1:E:130:ASN:HD22	1:E:130:ASN:N	2.10	0.49
1:A:518:VAL:CG2	1:A:519:PRO:HD2	2.43	0.49
1:D:201:VAL:HG13	1:D:201:VAL:O	2.12	0.49
1:B:249:ASP:C	1:B:249:ASP:OD1	2.51	0.49
1:A:540:THR:HG22	1:A:540:THR:O	2.13	0.49
1:D:57:TYR:CE2	1:E:448:THR:HG22	2.48	0.49
1:C:495:ASN:ND2	1:C:498:PRO:HB3	2.28	0.49
1:E:501:GLN:OE1	1:E:501:GLN:HA	2.12	0.49
1:D:237:HIS:HD2	1:D:238:PRO:O	1.96	0.49
1:B:237:HIS:HD2	1:B:238:PRO:O	1.96	0.49
1:C:201:VAL:O	1:C:201:VAL:HG13	2.12	0.49
1:E:540:THR:HG22	1:E:540:THR:O	2.13	0.49
1:D:249:ASP:C	1:D:249:ASP:OD1	2.51	0.49
1:B:197:ARG:HG3	1:B:198:GLN:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:15:TYR:HD2	2:W:16:PRO:HD2	1.76	0.48
1:B:173:GLY:O	1:B:175:TYR:CE1	2.65	0.48
1:E:543:ASP:OD1	1:E:547:ARG:HG2	2.12	0.48
1:A:447:VAL:HG23	1:E:67:THR:OG1	2.12	0.48
1:E:243:LEU:CD2	1:E:244:PRO:HD3	2.42	0.48
1:E:491:THR:HG22	1:E:492:HIS:N	2.27	0.48
1:A:132:PRO:HA	1:A:175:TYR:CZ	2.45	0.48
1:A:434:GLN:OE1	1:E:74:ASN:OD1	2.30	0.48
1:B:518:VAL:CG2	1:B:519:PRO:HD2	2.43	0.48
1:B:495:ASN:ND2	1:B:498:PRO:HB3	2.28	0.48
1:D:244:PRO:HA	1:D:275:TYR:CD2	2.49	0.48
1:A:154:THR:CG2	1:A:155:LYS:HG3	2.40	0.48
1:C:130:ASN:N	1:C:130:ASN:ND2	2.61	0.48
1:D:553:TYR:HE2	1:E:432:SER:N	2.11	0.48
1:A:201:VAL:O	1:A:201:VAL:HG13	2.12	0.48
1:B:151:ARG:CB	1:B:201:VAL:H	2.26	0.48
1:E:392:ILE:HD11	1:E:396:SER:OG	2.13	0.48
1:A:392:ILE:HD11	1:A:396:SER:OG	2.13	0.48
1:D:540:THR:O	1:D:540:THR:HG22	2.13	0.48
1:A:179:MET:HE3	1:A:485:ARG:NH2	2.28	0.48
1:E:497:PHE:O	1:E:499:GLU:N	2.45	0.48
1:E:495:ASN:ND2	1:E:498:PRO:HB3	2.28	0.48
1:A:197:ARG:HG3	1:A:198:GLN:N	2.27	0.48
1:B:228:PRO:HG3	2:S:15:TYR:CD1	2.48	0.48
1:E:237:HIS:HD2	1:E:238:PRO:O	1.96	0.48
1:A:237:HIS:HD2	1:A:238:PRO:O	1.96	0.48
1:E:292:TYR:HD1	1:E:376:VAL:HG12	1.75	0.48
1:D:130:ASN:ND2	1:D:130:ASN:N	2.61	0.48
1:A:389:TYR:O	1:A:390:ASN:C	2.51	0.48
1:A:477:GLN:O	1:A:481:SER:HB3	2.07	0.48
1:D:497:PHE:O	1:D:499:GLU:N	2.45	0.48
1:A:543:ASP:OD1	1:A:547:ARG:HG2	2.12	0.48
1:A:142:LYS:O	1:A:143:PHE:HB3	2.14	0.48
1:B:497:PHE:CD1	1:B:503:LEU:HB3	2.44	0.48
1:E:179:MET:CE	1:E:485:ARG:NH2	2.77	0.48
1:B:501:GLN:OE1	1:B:501:GLN:HA	2.12	0.48
2:V:10:THR:CG2	2:V:10:THR:O	2.60	0.48
1:D:74:ASN:O	1:D:75:LYS:C	2.52	0.48
1:B:142:LYS:O	1:B:143:PHE:HB3	2.14	0.48
1:B:142:LYS:HD3	1:B:167:GLU:OE2	2.14	0.48
1:C:142:LYS:O	1:C:143:PHE:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:LYS:O	1:D:143:PHE:HB3	2.14	0.48
1:B:491:THR:HG22	1:B:493:VAL:N	2.29	0.48
1:A:179:MET:CE	1:A:485:ARG:NH2	2.77	0.48
1:A:491:THR:HG22	1:A:492:HIS:N	2.27	0.48
1:C:244:PRO:HA	1:C:275:TYR:CD2	2.49	0.48
1:C:497:PHE:CD1	1:C:503:LEU:HB3	2.44	0.48
1:A:422:LEU:HD23	1:A:423:LEU:H	1.76	0.48
1:B:455:ILE:HD12	1:B:456:SER:N	2.25	0.48
1:C:74:ASN:O	1:C:75:LYS:C	2.52	0.48
1:A:130:ASN:ND2	1:A:130:ASN:N	2.61	0.48
1:A:142:LYS:HD3	1:A:167:GLU:OE2	2.14	0.48
1:C:249:ASP:OD1	1:C:249:ASP:C	2.52	0.48
1:D:179:MET:CE	1:D:485:ARG:NH2	2.77	0.48
1:E:491:THR:HG22	1:E:493:VAL:N	2.29	0.48
1:A:244:PRO:HA	1:A:275:TYR:CD2	2.49	0.48
1:C:193:LEU:HD22	1:C:197:ARG:NH1	2.29	0.48
1:B:211:ASP:HA	1:B:506:PRO:CG	2.44	0.48
1:B:75:LYS:O	1:B:78:ASP:OD1	2.32	0.48
1:C:384:SER:O	1:C:386:LYS:N	2.45	0.48
1:A:249:ASP:C	1:A:249:ASP:OD1	2.52	0.48
1:E:142:LYS:O	1:E:143:PHE:HB3	2.14	0.48
1:C:540:THR:HG22	1:C:540:THR:O	2.13	0.48
1:E:244:PRO:HA	1:E:275:TYR:CD2	2.49	0.48
1:C:179:MET:CE	1:C:485:ARG:NH2	2.77	0.48
1:D:454:GLN:O	1:D:456:SER:N	2.47	0.48
1:E:145:ALA:HA	1:E:248:VAL:HA	1.96	0.48
1:E:240:ILE:HD11	1:E:273:ILE:HG21	1.95	0.48
1:A:118:HIS:NE2	1:E:64:PHE:HD1	2.12	0.48
1:E:269:GLU:HG3	1:E:269:GLU:O	2.14	0.48
1:B:87:ASP:O	1:B:89:SER:N	2.46	0.48
1:B:193:LEU:HD22	1:B:197:ARG:NH1	2.29	0.48
1:D:228:PRO:HG3	2:U:15:TYR:CD1	2.49	0.48
1:B:542:THR:HG22	1:B:547:ARG:H	1.79	0.48
1:A:454:GLN:O	1:A:456:SER:N	2.47	0.48
1:C:171:PRO:HA	1:D:409:ASN:HD22	1.79	0.48
1:B:215:PHE:CE1	1:B:241:ILE:HD11	2.49	0.48
1:E:130:ASN:ND2	1:E:130:ASN:N	2.61	0.48
1:B:240:ILE:HD11	1:B:273:ILE:HG21	1.95	0.48
1:E:389:TYR:O	1:E:390:ASN:C	2.51	0.48
1:A:239:ASP:HB3	1:A:405:TYR:HB2	1.96	0.48
1:B:244:PRO:HA	1:B:275:TYR:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:491:THR:HG22	1:C:493:VAL:N	2.29	0.47
1:C:497:PHE:O	1:C:499:GLU:N	2.46	0.47
1:E:454:GLN:O	1:E:456:SER:N	2.47	0.47
1:B:145:ALA:HA	1:B:248:VAL:HA	1.96	0.47
1:D:215:PHE:CE1	1:D:241:ILE:HD11	2.49	0.47
1:B:74:ASN:O	1:B:75:LYS:C	2.52	0.47
1:E:75:LYS:O	1:E:78:ASP:OD1	2.32	0.47
1:B:183:LEU:HD21	1:C:236:PHE:HE2	1.78	0.47
1:D:461:VAL:HB	1:D:527:LEU:CD1	2.44	0.47
1:D:193:LEU:HD22	1:D:197:ARG:NH1	2.29	0.47
1:D:211:ASP:HA	1:D:506:PRO:CG	2.44	0.47
1:C:75:LYS:O	1:C:78:ASP:OD1	2.32	0.47
1:D:383:ASP:C	1:D:384:SER:O	2.52	0.47
1:E:142:LYS:HD3	1:E:167:GLU:OE2	2.14	0.47
1:B:540:THR:O	1:B:540:THR:HG22	2.13	0.47
1:E:249:ASP:OD1	1:E:249:ASP:C	2.51	0.47
1:E:497:PHE:CD1	1:E:503:LEU:HB3	2.44	0.47
1:B:179:MET:CE	1:B:485:ARG:NH2	2.77	0.47
1:A:491:THR:HG22	1:A:493:VAL:N	2.29	0.47
1:A:450:ARG:NH2	1:E:99:ASN:HB3	2.29	0.47
1:B:180:THR:HG21	1:B:258:LEU:CD2	2.44	0.47
1:C:180:THR:HG21	1:C:258:LEU:CD2	2.44	0.47
1:B:142:LYS:HG2	1:B:169:THR:HG22	1.97	0.47
1:A:269:GLU:O	1:A:269:GLU:HG3	2.14	0.47
1:B:422:LEU:HD23	1:B:423:LEU:H	1.76	0.47
1:A:74:ASN:O	1:A:75:LYS:C	2.52	0.47
1:E:179:MET:HE3	1:E:485:ARG:HH22	1.78	0.47
1:D:179:MET:HE3	1:D:485:ARG:NH2	2.29	0.47
1:C:131:MET:SD	1:C:138:MET:HG3	2.55	0.47
1:D:145:ALA:HA	1:D:248:VAL:HA	1.96	0.47
1:A:171:PRO:HA	1:B:409:ASN:HD22	1.80	0.47
1:A:277:ASP:O	1:A:279:GLU:N	2.46	0.47
1:A:211:ASP:HA	1:A:506:PRO:CG	2.44	0.47
1:E:211:ASP:HA	1:E:506:PRO:CG	2.44	0.47
1:E:74:ASN:O	1:E:75:LYS:C	2.52	0.47
1:D:180:THR:HG21	1:D:258:LEU:CD2	2.44	0.47
1:E:180:THR:HG21	1:E:258:LEU:CD2	2.44	0.47
1:D:142:LYS:HD3	1:D:167:GLU:OE2	2.14	0.47
1:D:389:TYR:O	1:D:390:ASN:C	2.51	0.47
1:B:269:GLU:HG3	1:B:269:GLU:O	2.14	0.47
1:C:102:SER:O	1:C:103:PRO:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:TYR:HD1	1:A:511:ILE:HD11	1.80	0.47
1:D:491:THR:HG22	1:D:493:VAL:N	2.29	0.47
1:B:488:THR:HG22	1:C:479:VAL:CG1	2.45	0.47
1:C:237:HIS:HD2	1:C:238:PRO:O	1.96	0.47
1:C:215:PHE:CE1	1:C:241:ILE:HD11	2.49	0.47
1:B:130:ASN:ND2	1:B:130:ASN:N	2.61	0.47
1:D:142:LYS:HG2	1:D:169:THR:HG22	1.97	0.47
1:B:96:ILE:O	1:C:448:THR:CB	2.63	0.47
1:C:454:GLN:O	1:C:456:SER:N	2.47	0.47
1:C:211:ASP:HA	1:C:506:PRO:CG	2.44	0.47
1:B:434:GLN:NE2	1:B:436:TYR:CE2	2.81	0.47
1:B:383:ASP:C	1:B:384:SER:O	2.52	0.47
1:C:553:TYR:HE2	1:D:432:SER:N	2.12	0.47
1:C:142:LYS:HD3	1:C:167:GLU:OE2	2.14	0.47
1:C:142:LYS:HG2	1:C:169:THR:HG22	1.97	0.47
1:E:142:LYS:HG2	1:E:169:THR:HG22	1.97	0.47
1:B:497:PHE:O	1:B:499:GLU:N	2.46	0.47
1:C:83:ASN:CA	1:C:86:ASN:HD22	2.21	0.47
1:D:542:THR:CG2	1:D:547:ARG:H	2.28	0.47
1:E:98:ASN:C	1:E:98:ASN:ND2	2.66	0.47
1:A:215:PHE:CE1	1:A:241:ILE:HD11	2.50	0.47
1:A:75:LYS:O	1:A:78:ASP:OD1	2.32	0.47
1:D:289:VAL:HG13	1:D:290:ASP:N	2.30	0.47
1:A:497:PHE:O	1:A:499:GLU:N	2.46	0.47
1:B:131:MET:SD	1:B:138:MET:HG3	2.55	0.47
1:B:454:GLN:O	1:B:456:SER:N	2.47	0.47
1:C:269:GLU:HG3	1:C:269:GLU:O	2.14	0.47
1:A:461:VAL:HB	1:A:527:LEU:CD1	2.45	0.47
1:A:485:ARG:CZ	1:A:505:ARG:HH22	2.28	0.47
1:A:193:LEU:HD22	1:A:197:ARG:NH1	2.29	0.47
1:D:132:PRO:CA	1:D:175:TYR:OH	2.53	0.47
1:B:542:THR:CG2	1:B:547:ARG:H	2.28	0.47
1:D:542:THR:HG22	1:D:547:ARG:H	1.79	0.47
1:E:542:THR:HG22	1:E:547:ARG:H	1.79	0.47
1:D:78:ASP:HB2	1:D:82:LEU:HD12	1.97	0.47
1:E:78:ASP:HB2	1:E:82:LEU:HD12	1.97	0.47
1:A:78:ASP:HB2	1:A:82:LEU:HD12	1.97	0.47
1:A:180:THR:HG21	1:A:258:LEU:CD2	2.44	0.47
1:C:88:HIS:HD2	1:D:267:PHE:HZ	1.63	0.47
1:E:461:VAL:HB	1:E:527:LEU:CD1	2.44	0.46
1:B:447:VAL:HG12	1:B:448:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:MET:SD	1:D:138:MET:HG3	2.55	0.46
1:A:145:ALA:HA	1:A:248:VAL:HA	1.96	0.46
1:E:239:ASP:HB3	1:E:405:TYR:HB2	1.96	0.46
1:A:432:SER:HG	1:E:128:HIS:CE1	2.33	0.46
1:E:289:VAL:HG13	1:E:290:ASP:N	2.30	0.46
1:E:87:ASP:O	1:E:89:SER:N	2.46	0.46
1:C:67:THR:OG1	1:D:447:VAL:HG23	2.14	0.46
1:A:96:ILE:O	1:B:448:THR:HB	2.16	0.46
1:E:193:LEU:HD22	1:E:197:ARG:NH1	2.29	0.46
1:B:231:TYR:CD1	1:B:501:GLN:HB3	2.51	0.46
1:C:542:THR:HG22	1:C:547:ARG:H	1.79	0.46
1:D:239:ASP:HB3	1:D:405:TYR:HB2	1.96	0.46
1:D:75:LYS:O	1:D:78:ASP:OD1	2.32	0.46
1:D:269:GLU:HG3	1:D:269:GLU:O	2.14	0.46
1:A:485:ARG:HH21	1:B:234:GLU:CD	2.18	0.46
1:E:474:TYR:HD1	1:E:511:ILE:HD11	1.80	0.46
1:B:228:PRO:CB	2:S:15:TYR:HE1	2.28	0.46
1:C:179:MET:HE2	1:C:485:ARG:NH2	2.30	0.46
1:C:231:TYR:CD1	1:C:501:GLN:HB3	2.51	0.46
1:A:542:THR:CG2	1:A:547:ARG:H	2.28	0.46
1:A:542:THR:HG22	1:A:547:ARG:H	1.79	0.46
1:C:145:ALA:HA	1:C:248:VAL:HA	1.96	0.46
1:A:67:THR:CG2	1:B:447:VAL:CG2	2.94	0.46
1:B:474:TYR:HD1	1:B:511:ILE:HD11	1.80	0.46
1:E:542:THR:CG2	1:E:547:ARG:H	2.28	0.46
1:E:215:PHE:CE1	1:E:241:ILE:HD11	2.50	0.46
1:C:78:ASP:HB2	1:C:82:LEU:HD12	1.97	0.46
1:D:434:GLN:NE2	1:D:436:TYR:CE2	2.81	0.46
1:A:434:GLN:NE2	1:A:436:TYR:CE2	2.81	0.46
1:C:289:VAL:HG13	1:C:290:ASP:N	2.30	0.46
1:C:461:VAL:HB	1:C:527:LEU:CD1	2.45	0.46
1:B:461:VAL:HB	1:B:527:LEU:CD1	2.45	0.46
1:E:497:PHE:HD1	1:E:503:LEU:CB	2.25	0.46
1:A:295:SER:CB	1:A:375:PRO:HG2	2.46	0.46
1:C:295:SER:CB	1:C:375:PRO:HG2	2.46	0.46
1:E:295:SER:CB	1:E:375:PRO:HG2	2.46	0.46
1:D:123:LEU:HD13	1:D:559:VAL:HG22	1.98	0.46
1:C:542:THR:CG2	1:C:547:ARG:H	2.27	0.46
1:A:267:PHE:CZ	1:E:88:HIS:HD2	2.34	0.46
1:D:87:ASP:O	1:D:89:SER:N	2.46	0.46
1:B:452:THR:OG1	1:B:453:SER:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:ILE:HD11	1:C:463:ALA:HB3	1.97	0.46
1:B:477:GLN:OE1	1:B:477:GLN:HA	2.16	0.46
1:C:477:GLN:OE1	1:C:477:GLN:HA	2.16	0.46
2:U:15:TYR:CD2	2:U:16:PRO:HD2	2.51	0.46
1:E:123:LEU:HD13	1:E:559:VAL:HG22	1.98	0.46
1:A:267:PHE:CZ	1:E:88:HIS:CD2	3.04	0.46
1:C:87:ASP:O	1:C:89:SER:N	2.46	0.46
1:C:452:THR:OG1	1:C:453:SER:N	2.49	0.46
1:B:289:VAL:HG13	1:B:290:ASP:N	2.30	0.46
1:B:102:SER:O	1:B:103:PRO:C	2.52	0.46
1:E:447:VAL:HG12	1:E:448:THR:HG23	1.97	0.46
1:A:447:VAL:HG12	1:A:448:THR:HG23	1.97	0.46
1:E:485:ARG:CZ	1:E:505:ARG:HH22	2.28	0.46
1:B:477:GLN:O	1:B:481:SER:HB3	2.07	0.46
1:B:295:SER:CB	1:B:375:PRO:HG2	2.46	0.46
1:C:474:TYR:HD1	1:C:511:ILE:HD11	1.80	0.46
1:B:239:ASP:HB3	1:B:405:TYR:HB2	1.96	0.46
1:A:142:LYS:HG2	1:A:169:THR:HG22	1.97	0.46
1:D:485:ARG:CZ	1:D:505:ARG:HH22	2.29	0.46
1:C:485:ARG:CZ	1:C:505:ARG:HH22	2.28	0.46
1:A:376:VAL:C	1:A:378:LYS:H	2.19	0.46
1:C:242:LEU:HD22	1:C:247:GLY:HA2	1.98	0.46
1:C:239:ASP:HB3	1:C:405:TYR:HB2	1.96	0.46
1:A:553:TYR:HE2	1:B:432:SER:N	2.14	0.46
1:B:243:LEU:HA	1:B:243:LEU:HD23	1.82	0.46
1:E:477:GLN:HA	1:E:477:GLN:OE1	2.16	0.46
1:D:477:GLN:HA	1:D:477:GLN:OE1	2.15	0.46
2:W:15:TYR:CD2	2:W:16:PRO:HD2	2.50	0.46
1:B:485:ARG:CZ	1:B:505:ARG:HH22	2.28	0.46
1:E:131:MET:SD	1:E:138:MET:HG3	2.55	0.46
1:D:217:LEU:HA	1:D:217:LEU:HD23	1.74	0.46
1:E:452:THR:OG1	1:E:453:SER:N	2.49	0.46
1:B:243:LEU:HD21	1:B:401:TYR:CE2	2.51	0.46
1:A:132:PRO:CA	1:A:175:TYR:OH	2.53	0.46
1:D:295:SER:CB	1:D:375:PRO:HG2	2.46	0.46
1:E:135:ASN:OD1	1:E:135:ASN:C	2.55	0.46
1:E:242:LEU:HD22	1:E:247:GLY:HA2	1.98	0.46
1:E:102:SER:O	1:E:103:PRO:C	2.52	0.46
1:E:250:PHE:O	1:E:252:HIS:N	2.49	0.46
1:E:231:TYR:CD1	1:E:501:GLN:HB3	2.51	0.45
1:D:231:TYR:CD1	1:D:501:GLN:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:MET:SD	1:A:138:MET:HG3	2.55	0.45
1:D:545:ARG:O	1:D:546:ARG:HB2	2.16	0.45
1:B:242:LEU:HD22	1:B:247:GLY:HA2	1.98	0.45
1:B:277:ASP:O	1:B:279:GLU:N	2.46	0.45
1:C:123:LEU:HD13	1:C:559:VAL:HG22	1.98	0.45
1:D:102:SER:O	1:D:103:PRO:C	2.52	0.45
1:A:102:SER:O	1:A:103:PRO:C	2.53	0.45
1:A:63:LEU:HD12	1:B:447:VAL:HA	1.98	0.45
2:T:15:TYR:CD2	2:T:16:PRO:HD2	2.51	0.45
1:A:225:LEU:CD2	1:A:397:THR:HB	2.47	0.45
1:E:243:LEU:HD21	1:E:401:TYR:CE2	2.51	0.45
1:D:497:PHE:CD1	1:D:503:LEU:HB3	2.44	0.45
1:A:385:LYS:HZ2	2:S:16:PRO:HB3	1.82	0.45
2:S:15:TYR:CD2	2:S:16:PRO:HD2	2.51	0.45
1:C:243:LEU:HD21	1:C:401:TYR:CE2	2.51	0.45
1:C:237:HIS:HE1	1:C:424:CYS:O	2.00	0.45
1:D:135:ASN:OD1	1:D:135:ASN:C	2.55	0.45
1:C:556:LEU:CD2	1:D:434:GLN:HG2	2.44	0.45
1:B:491:THR:HG23	2:T:15:TYR:CZ	2.52	0.45
1:C:223:THR:HG22	1:C:225:LEU:HB2	1.99	0.45
1:A:477:GLN:HA	1:A:477:GLN:OE1	2.16	0.45
1:D:474:TYR:HD1	1:D:511:ILE:HD11	1.80	0.45
1:B:207:GLY:O	1:B:208:VAL:CB	2.64	0.45
1:A:432:SER:N	1:E:553:TYR:HE2	2.14	0.45
1:A:64:PHE:O	1:A:65:ASP:HB2	2.17	0.45
1:D:243:LEU:HD21	1:D:401:TYR:CE2	2.51	0.45
1:C:243:LEU:HD23	1:C:243:LEU:HA	1.82	0.45
1:D:223:THR:HG22	1:D:225:LEU:HB2	1.99	0.45
1:C:295:SER:HB3	1:C:375:PRO:HG2	1.98	0.45
1:C:545:ARG:O	1:C:546:ARG:HB2	2.16	0.45
1:B:135:ASN:OD1	1:B:135:ASN:C	2.55	0.45
1:A:123:LEU:HD13	1:A:559:VAL:HG22	1.98	0.45
1:E:177:GLU:HG3	1:E:178:THR:H	1.82	0.45
1:D:79:VAL:HG13	1:E:267:PHE:HD2	1.82	0.45
1:C:250:PHE:O	1:C:252:HIS:N	2.49	0.45
1:A:289:VAL:HG13	1:A:290:ASP:N	2.30	0.45
1:D:250:PHE:O	1:D:252:HIS:N	2.49	0.45
1:D:452:THR:OG1	1:D:453:SER:N	2.49	0.45
1:D:485:ARG:NH2	1:E:234:GLU:OE1	2.50	0.45
1:A:243:LEU:HD21	1:A:401:TYR:CE2	2.51	0.45
1:D:242:LEU:HD22	1:D:247:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:PHE:O	1:B:65:ASP:HB2	2.17	0.45
1:B:78:ASP:HB2	1:B:82:LEU:HD12	1.97	0.45
1:C:447:VAL:HG12	1:C:448:THR:HG23	1.97	0.45
1:C:225:LEU:CD2	1:C:397:THR:HB	2.47	0.45
1:A:223:THR:HG22	1:A:225:LEU:HB2	1.99	0.45
1:D:502:ILE:C	1:D:504:ALA:H	2.20	0.45
1:E:225:LEU:CD2	1:E:397:THR:HB	2.47	0.45
1:A:439:LEU:N	1:A:440:PRO:CD	2.79	0.45
1:C:129:THR:HB	1:C:130:ASN:H	1.63	0.45
1:B:439:LEU:N	1:B:440:PRO:CD	2.79	0.45
1:E:382:GLU:HA	1:E:387:ARG:O	2.17	0.45
1:D:64:PHE:O	1:D:65:ASP:HB2	2.17	0.45
1:A:250:PHE:O	1:A:252:HIS:N	2.49	0.45
1:D:447:VAL:HG12	1:D:448:THR:HG23	1.97	0.45
1:A:228:PRO:CB	2:W:15:TYR:HE1	2.29	0.45
1:D:491:THR:HG23	2:V:15:TYR:CZ	2.52	0.45
2:V:15:TYR:CD2	2:V:16:PRO:HD2	2.51	0.45
1:A:502:ILE:C	1:A:504:ALA:H	2.20	0.45
1:A:491:THR:HG23	2:S:15:TYR:CZ	2.52	0.45
1:D:295:SER:HB3	1:D:375:PRO:HG2	1.99	0.45
1:E:376:VAL:O	1:E:377:ILE:C	2.55	0.45
1:B:223:THR:HG22	1:B:225:LEU:HB2	1.99	0.45
1:B:231:TYR:H	1:B:501:GLN:HE21	1.65	0.45
1:D:376:VAL:C	1:D:378:LYS:H	2.19	0.45
1:E:439:LEU:N	1:E:440:PRO:CD	2.79	0.45
1:D:100:ASP:CG	1:E:450:ARG:HH12	2.19	0.45
1:C:135:ASN:C	1:C:135:ASN:OD1	2.55	0.45
1:B:123:LEU:HD13	1:B:559:VAL:HG22	1.98	0.45
1:E:129:THR:HB	1:E:130:ASN:H	1.63	0.45
1:A:177:GLU:CG	1:A:178:THR:H	2.30	0.45
1:D:382:GLU:HA	1:D:387:ARG:O	2.17	0.45
1:D:225:LEU:CD2	1:D:397:THR:HB	2.47	0.45
1:D:237:HIS:HE1	1:D:424:CYS:O	2.00	0.45
1:B:295:SER:HB3	1:B:375:PRO:HG2	1.98	0.45
1:E:545:ARG:O	1:E:546:ARG:HB2	2.17	0.45
1:A:171:PRO:CA	1:B:409:ASN:HD22	2.30	0.45
1:A:417:ILE:HD12	1:A:417:ILE:HA	1.80	0.45
1:C:381:THR:CG2	1:C:381:THR:O	2.65	0.45
1:B:382:GLU:HA	1:B:387:ARG:O	2.17	0.45
1:A:64:PHE:HD1	1:B:118:HIS:NE2	2.15	0.45
1:A:474:TYR:CD1	1:A:511:ILE:CD1	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:LEU:CD2	1:B:397:THR:HB	2.47	0.45
1:A:480:TYR:HE1	1:E:484:ILE:CG2	2.24	0.45
1:A:295:SER:HB3	1:A:375:PRO:HG2	1.98	0.45
1:C:376:VAL:C	1:C:378:LYS:H	2.19	0.45
1:E:376:VAL:C	1:E:378:LYS:H	2.19	0.45
1:C:474:TYR:CD1	1:C:511:ILE:CD1	3.00	0.45
1:B:545:ARG:O	1:B:546:ARG:HB2	2.17	0.45
1:A:545:ARG:O	1:A:546:ARG:HB2	2.16	0.45
1:A:242:LEU:HD22	1:A:247:GLY:HA2	1.98	0.45
1:B:177:GLU:CG	1:B:178:THR:H	2.30	0.45
1:B:446:PRO:HG2	1:B:460:VAL:O	2.17	0.45
1:E:502:ILE:C	1:E:504:ALA:H	2.20	0.44
1:A:231:TYR:CD1	1:A:501:GLN:HB3	2.50	0.44
1:E:237:HIS:HE1	1:E:424:CYS:O	2.00	0.44
1:E:381:THR:HG22	1:E:382:GLU:HG3	1.99	0.44
1:A:237:HIS:HE1	1:A:424:CYS:O	2.00	0.44
1:B:237:HIS:HE1	1:B:424:CYS:O	1.99	0.44
1:D:171:PRO:O	1:D:172:GLU:O	2.36	0.44
1:B:171:PRO:O	1:B:172:GLU:O	2.36	0.44
1:A:381:THR:HG22	1:A:382:GLU:HG3	1.99	0.44
1:A:446:PRO:HG2	1:A:460:VAL:O	2.17	0.44
1:E:392:ILE:HG13	1:E:393:SER:N	2.32	0.44
1:A:452:THR:OG1	1:A:453:SER:N	2.49	0.44
1:C:202:LEU:HD23	1:C:202:LEU:N	2.33	0.44
1:B:502:ILE:C	1:B:504:ALA:H	2.20	0.44
1:C:485:ARG:NH2	1:D:234:GLU:OE1	2.49	0.44
1:B:376:VAL:O	1:B:377:ILE:C	2.55	0.44
1:E:458:PHE:O	1:E:546:ARG:NH2	2.50	0.44
1:E:506:PRO:HA	1:E:507:PRO:HD3	1.81	0.44
1:A:382:GLU:HA	1:A:387:ARG:O	2.17	0.44
1:A:88:HIS:HD2	1:B:267:PHE:HZ	1.63	0.44
1:D:392:ILE:HG13	1:D:393:SER:N	2.32	0.44
1:A:466:LEU:HA	1:A:467:PRO:HD3	1.78	0.44
1:E:231:TYR:H	1:E:501:GLN:HE21	1.65	0.44
1:B:458:PHE:O	1:B:546:ARG:NH2	2.50	0.44
1:C:171:PRO:O	1:C:172:GLU:O	2.36	0.44
1:A:383:ASP:C	1:A:384:SER:O	2.52	0.44
1:C:177:GLU:CG	1:C:178:THR:H	2.30	0.44
1:D:79:VAL:HG13	1:E:267:PHE:CD2	2.52	0.44
1:E:64:PHE:O	1:E:65:ASP:HB2	2.17	0.44
1:A:267:PHE:HB3	1:E:79:VAL:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:446:PRO:HG2	1:E:460:VAL:O	2.17	0.44
1:B:250:PHE:O	1:B:252:HIS:N	2.49	0.44
1:E:244:PRO:HA	1:E:275:TYR:CE2	2.53	0.44
1:A:244:PRO:HA	1:A:275:TYR:CE2	2.53	0.44
1:E:207:GLY:HA3	1:E:246:CYS:SG	2.58	0.44
1:A:69:VAL:HG22	1:A:559:VAL:HB	2.00	0.44
1:A:381:THR:CG2	1:A:381:THR:O	2.65	0.44
1:D:177:GLU:CG	1:D:178:THR:H	2.30	0.44
1:D:128:HIS:CE1	1:E:432:SER:HG	2.36	0.44
1:A:202:LEU:HD23	1:A:202:LEU:N	2.33	0.44
1:B:474:TYR:CD1	1:B:511:ILE:CD1	3.00	0.44
1:E:474:TYR:CD1	1:E:511:ILE:CD1	3.01	0.44
1:E:491:THR:HG23	2:W:15:TYR:CZ	2.52	0.44
1:C:502:ILE:C	1:C:504:ALA:H	2.20	0.44
1:B:376:VAL:C	1:B:378:LYS:H	2.19	0.44
1:E:295:SER:HB3	1:E:375:PRO:HG2	1.98	0.44
1:D:99:ASN:HB3	1:E:450:ARG:NH2	2.32	0.44
1:A:171:PRO:O	1:A:172:GLU:O	2.36	0.44
1:C:446:PRO:HG2	1:C:460:VAL:O	2.17	0.44
1:E:177:GLU:CG	1:E:178:THR:H	2.30	0.44
1:C:383:ASP:C	1:C:384:SER:O	2.52	0.44
1:D:79:VAL:HG13	1:E:267:PHE:HB3	1.99	0.44
1:C:64:PHE:O	1:C:65:ASP:HB2	2.17	0.44
1:D:202:LEU:N	1:D:202:LEU:HD23	2.33	0.44
1:B:244:PRO:HA	1:B:275:TYR:CE2	2.53	0.44
1:B:385:LYS:HZ2	2:T:16:PRO:HB3	1.82	0.44
1:C:385:LYS:HZ2	2:U:16:PRO:HB3	1.83	0.44
1:A:207:GLY:HA3	1:A:246:CYS:SG	2.58	0.44
1:B:113:LEU:HB3	1:B:119:TRP:CE2	2.53	0.44
1:C:57:TYR:CD2	1:D:448:THR:HG22	2.53	0.44
1:D:244:PRO:HA	1:D:275:TYR:CE2	2.53	0.44
1:C:491:THR:HG23	2:U:15:TYR:CZ	2.52	0.44
1:E:171:PRO:O	1:E:172:GLU:O	2.35	0.44
1:D:207:GLY:HA3	1:D:246:CYS:SG	2.58	0.44
1:C:382:GLU:HA	1:C:387:ARG:O	2.17	0.44
1:D:381:THR:HG22	1:D:382:GLU:HG3	1.99	0.44
1:A:113:LEU:HB3	1:A:119:TRP:CE2	2.53	0.44
1:A:189:VAL:O	1:A:192:TYR:N	2.51	0.44
1:E:202:LEU:HD23	1:E:202:LEU:N	2.33	0.44
1:E:69:VAL:HG22	1:E:559:VAL:HB	2.00	0.44
1:C:69:VAL:HG22	1:C:559:VAL:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:VAL:O	1:C:69:VAL:HG23	2.18	0.44
1:D:556:LEU:CD2	1:E:434:GLN:HG2	2.46	0.44
1:E:383:ASP:C	1:E:384:SER:O	2.52	0.44
1:B:381:THR:CG2	1:B:381:THR:O	2.65	0.44
1:D:67:THR:OG1	1:E:447:VAL:HG23	2.18	0.43
1:B:179:MET:HE3	1:B:485:ARG:NH2	2.33	0.43
1:C:466:LEU:HA	1:C:467:PRO:HD3	1.78	0.43
1:A:135:ASN:OD1	1:A:135:ASN:C	2.55	0.43
1:C:381:THR:HG22	1:C:382:GLU:HG3	1.99	0.43
1:D:381:THR:CG2	1:D:381:THR:O	2.65	0.43
1:B:189:VAL:O	1:B:192:TYR:N	2.51	0.43
1:E:223:THR:HG22	1:E:225:LEU:HB2	1.99	0.43
1:C:506:PRO:HA	1:C:507:PRO:HD3	1.81	0.43
1:E:189:VAL:O	1:E:192:TYR:N	2.51	0.43
1:B:392:ILE:HG13	1:B:393:SER:N	2.32	0.43
1:C:392:ILE:HG13	1:C:393:SER:N	2.32	0.43
1:D:474:TYR:CD1	1:D:511:ILE:CD1	3.00	0.43
1:D:458:PHE:O	1:D:546:ARG:NH2	2.50	0.43
1:D:446:PRO:HG2	1:D:460:VAL:O	2.17	0.43
1:D:113:LEU:HB3	1:D:119:TRP:CE2	2.53	0.43
1:B:202:LEU:HD23	1:B:202:LEU:N	2.33	0.43
1:D:192:TYR:CD1	1:D:196:GLY:HA3	2.54	0.43
1:C:179:MET:HE3	1:C:485:ARG:HH22	1.83	0.43
1:E:479:VAL:O	1:E:479:VAL:CG1	2.66	0.43
1:D:131:MET:HA	1:D:132:PRO:HD3	1.80	0.43
1:C:542:THR:HG23	1:C:547:ARG:N	2.34	0.43
1:A:564:LEU:O	1:A:565:SER:HB3	2.19	0.43
2:U:15:TYR:C	2:U:15:TYR:CD2	2.92	0.43
1:D:376:VAL:O	1:D:377:ILE:C	2.55	0.43
1:C:207:GLY:HA3	1:C:246:CYS:SG	2.58	0.43
1:E:96:ILE:HD13	1:E:96:ILE:HA	1.82	0.43
1:E:75:LYS:HB3	1:E:75:LYS:HE2	1.88	0.43
1:C:428:VAL:HG13	1:C:513:THR:HB	2.01	0.43
1:E:113:LEU:HB3	1:E:119:TRP:CE2	2.53	0.43
1:C:113:LEU:HB3	1:C:119:TRP:CE2	2.53	0.43
1:B:79:VAL:HG13	1:C:267:PHE:HD2	1.83	0.43
1:D:189:VAL:O	1:D:192:TYR:N	2.51	0.43
1:E:223:THR:CG2	1:E:225:LEU:HB2	2.49	0.43
1:A:376:VAL:O	1:A:377:ILE:C	2.55	0.43
1:D:428:VAL:HG13	1:D:513:THR:HB	2.01	0.43
1:B:88:HIS:CD2	1:C:267:PHE:CZ	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:TYR:CD1	1:B:196:GLY:HA3	2.54	0.43
1:D:564:LEU:O	1:D:565:SER:HB3	2.19	0.43
1:C:564:LEU:O	1:C:565:SER:HB3	2.19	0.43
1:C:181:ILE:O	1:C:184:MET:HB2	2.19	0.43
1:D:231:TYR:H	1:D:501:GLN:HE21	1.65	0.43
1:A:231:TYR:H	1:A:501:GLN:HE21	1.65	0.43
1:E:422:LEU:CD2	1:E:423:LEU:N	2.80	0.43
1:A:83:ASN:CA	1:A:86:ASN:HD22	2.21	0.43
1:B:69:VAL:HG23	1:B:69:VAL:O	2.18	0.43
1:E:428:VAL:HG13	1:E:513:THR:HB	2.00	0.43
1:D:64:PHE:CD1	1:E:118:HIS:NE2	2.86	0.43
1:A:392:ILE:HG13	1:A:393:SER:N	2.32	0.43
1:B:181:ILE:O	1:B:184:MET:HB2	2.19	0.43
1:E:474:TYR:HH	1:E:476:ASP:CG	2.21	0.43
1:E:132:PRO:CA	1:E:175:TYR:OH	2.53	0.43
1:C:458:PHE:O	1:C:546:ARG:NH2	2.50	0.43
1:B:69:VAL:HG22	1:B:559:VAL:HB	2.00	0.43
1:A:177:GLU:HG3	1:A:178:THR:H	1.82	0.43
1:B:381:THR:HG22	1:B:382:GLU:HG3	2.00	0.43
1:B:126:ILE:HG12	1:B:521:LEU:CD2	2.49	0.43
1:C:189:VAL:O	1:C:192:TYR:N	2.51	0.43
1:C:192:TYR:CD1	1:C:196:GLY:HA3	2.54	0.43
1:A:448:THR:HG22	1:E:57:TYR:CE2	2.54	0.43
1:D:385:LYS:HZ2	2:V:16:PRO:HB3	1.83	0.43
1:B:223:THR:CG2	1:B:225:LEU:HB2	2.49	0.43
2:S:15:TYR:CD2	2:S:15:TYR:C	2.92	0.43
1:A:422:LEU:HD21	1:E:551:TYR:CZ	2.53	0.43
1:C:231:TYR:H	1:C:501:GLN:HE21	1.65	0.43
1:B:207:GLY:HA3	1:B:246:CYS:SG	2.58	0.43
1:E:381:THR:CG2	1:E:381:THR:O	2.65	0.43
1:E:126:ILE:HG12	1:E:521:LEU:CD2	2.49	0.43
1:C:95:VAL:O	1:C:95:VAL:HG12	2.19	0.43
1:A:447:VAL:CG2	1:E:67:THR:CG2	2.97	0.43
1:A:234:GLU:OE1	1:E:485:ARG:NH2	2.52	0.43
1:A:223:THR:CG2	1:A:225:LEU:HB2	2.49	0.43
1:E:243:LEU:HD23	1:E:244:PRO:HD3	2.01	0.43
1:C:243:LEU:HD23	1:C:244:PRO:HD3	2.01	0.43
1:D:551:TYR:CZ	1:E:422:LEU:HD21	2.54	0.43
1:A:192:TYR:CD1	1:A:196:GLY:HA3	2.54	0.43
1:B:95:VAL:HG12	1:B:95:VAL:O	2.19	0.43
1:A:87:ASP:OD1	1:A:89:SER:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:TYR:CG	1:E:448:THR:HG22	2.55	0.42
1:C:58:SER:OG	1:C:59:GLU:N	2.52	0.42
1:C:96:ILE:O	1:D:448:THR:HB	2.19	0.42
1:A:96:ILE:HD13	1:A:96:ILE:HA	1.82	0.42
1:B:243:LEU:HD23	1:B:244:PRO:HD3	2.01	0.42
1:A:493:VAL:HG21	1:B:232:THR:HB	2.00	0.42
1:C:376:VAL:O	1:C:377:ILE:C	2.55	0.42
1:B:542:THR:HG23	1:B:547:ARG:N	2.34	0.42
1:B:58:SER:OG	1:B:59:GLU:N	2.52	0.42
1:A:96:ILE:HG22	1:A:98:ASN:N	2.28	0.42
1:E:179:MET:HE3	1:E:485:ARG:NH2	2.34	0.42
1:A:228:PRO:HB3	2:W:15:TYR:HE1	1.84	0.42
2:V:15:TYR:C	2:V:15:TYR:CD2	2.92	0.42
1:C:244:PRO:HA	1:C:275:TYR:CE2	2.53	0.42
1:D:223:THR:CG2	1:D:225:LEU:HB2	2.49	0.42
1:C:422:LEU:CD2	1:C:423:LEU:N	2.80	0.42
1:D:69:VAL:HG22	1:D:559:VAL:HB	2.00	0.42
1:E:277:ASP:O	1:E:279:GLU:N	2.46	0.42
1:E:192:TYR:CD1	1:E:196:GLY:HA3	2.54	0.42
1:E:87:ASP:OD1	1:E:89:SER:HB3	2.19	0.42
1:C:223:THR:CG2	1:C:225:LEU:HB2	2.49	0.42
1:E:228:PRO:CB	2:V:15:TYR:HE1	2.33	0.42
1:A:132:PRO:CD	1:A:551:TYR:CE2	3.02	0.42
2:T:10:THR:O	2:T:10:THR:CG2	2.60	0.42
1:A:479:VAL:O	1:A:479:VAL:CG1	2.66	0.42
1:D:69:VAL:HG23	1:D:69:VAL:O	2.18	0.42
1:E:542:THR:HG23	1:E:547:ARG:N	2.34	0.42
1:D:506:PRO:HA	1:D:507:PRO:HD3	1.81	0.42
1:B:177:GLU:HG3	1:B:178:THR:H	1.82	0.42
1:C:177:GLU:HG3	1:C:178:THR:H	1.82	0.42
1:B:564:LEU:O	1:B:565:SER:HB3	2.19	0.42
1:A:126:ILE:HG12	1:A:521:LEU:CD2	2.49	0.42
1:C:87:ASP:OD1	1:C:89:SER:HB3	2.19	0.42
1:E:549:CYS:HA	1:E:550:PRO:HD3	1.89	0.42
1:E:282:ASN:HA	1:E:402:ARG:HA	2.02	0.42
1:A:243:LEU:HD23	1:A:244:PRO:HD3	2.01	0.42
1:C:282:ASN:HA	1:C:402:ARG:HA	2.02	0.42
1:D:228:PRO:HB3	2:U:15:TYR:HE1	1.83	0.42
1:E:83:ASN:CA	1:E:86:ASN:HD22	2.21	0.42
1:E:69:VAL:HG23	1:E:69:VAL:O	2.18	0.42
1:B:129:THR:HB	1:B:130:ASN:H	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:VAL:HG13	1:A:513:THR:HB	2.00	0.42
1:B:428:VAL:HG13	1:B:513:THR:HB	2.00	0.42
1:B:87:ASP:OD1	1:B:89:SER:HB3	2.19	0.42
1:D:181:ILE:O	1:D:184:MET:HB2	2.19	0.42
2:W:15:TYR:CD2	2:W:15:TYR:C	2.92	0.42
1:B:132:PRO:CD	1:B:551:TYR:CE2	3.02	0.42
1:B:542:THR:HG21	1:B:546:ARG:HD2	2.01	0.42
1:B:75:LYS:HE2	1:B:75:LYS:HB3	1.88	0.42
1:A:58:SER:OG	1:A:59:GLU:N	2.52	0.42
1:D:95:VAL:O	1:D:95:VAL:HG12	2.19	0.42
1:A:422:LEU:CD2	1:A:423:LEU:N	2.80	0.42
1:E:132:PRO:CD	1:E:551:TYR:CE2	3.02	0.42
1:B:137:PHE:HE1	1:B:547:ARG:NE	2.18	0.42
1:A:458:PHE:O	1:A:546:ARG:NH2	2.50	0.42
1:C:207:GLY:O	1:C:208:VAL:CB	2.64	0.42
1:E:564:LEU:O	1:E:565:SER:HB3	2.19	0.42
1:E:181:ILE:O	1:E:184:MET:HB2	2.19	0.42
2:T:15:TYR:C	2:T:15:TYR:CD2	2.92	0.42
1:A:137:PHE:HE1	1:A:547:ARG:NE	2.18	0.42
1:A:450:ARG:HH12	1:E:100:ASP:CG	2.23	0.42
1:B:117:SER:HA	1:B:566:SER:HA	2.02	0.42
1:E:95:VAL:O	1:E:95:VAL:HG12	2.19	0.42
1:A:228:PRO:HG3	2:W:15:TYR:CD1	2.54	0.42
1:D:282:ASN:HA	1:D:402:ARG:HA	2.02	0.42
1:D:542:THR:HG21	1:D:546:ARG:HD2	2.02	0.42
1:C:277:ASP:O	1:C:279:GLU:N	2.46	0.42
2:S:10:THR:O	2:S:10:THR:CG2	2.60	0.42
1:B:88:HIS:HD2	1:C:267:PHE:CZ	2.38	0.42
1:C:126:ILE:HG12	1:C:521:LEU:CD2	2.49	0.42
1:A:95:VAL:O	1:A:95:VAL:HG12	2.19	0.42
1:E:243:LEU:HD23	1:E:243:LEU:HA	1.82	0.42
1:B:479:VAL:CG1	1:B:479:VAL:O	2.66	0.42
1:C:132:PRO:CD	1:C:551:TYR:CE2	3.02	0.42
1:A:69:VAL:HG23	1:A:69:VAL:O	2.18	0.42
1:B:426:PRO:O	1:B:427:ASP:CB	2.67	0.42
1:A:87:ASP:O	1:A:89:SER:N	2.46	0.42
1:D:117:SER:HA	1:D:566:SER:HA	2.02	0.42
1:E:58:SER:OG	1:E:59:GLU:N	2.52	0.41
1:A:243:LEU:HD23	1:A:243:LEU:HA	1.82	0.41
1:B:83:ASN:CA	1:B:86:ASN:HD22	2.21	0.41
1:D:542:THR:HG23	1:D:547:ARG:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:137:PHE:HE1	1:E:547:ARG:NE	2.18	0.41
1:A:207:GLY:O	1:A:208:VAL:CB	2.64	0.41
1:B:79:VAL:HG13	1:C:267:PHE:CD2	2.54	0.41
1:A:150:SER:OG	1:A:162:LYS:HB2	2.20	0.41
1:E:117:SER:HA	1:E:566:SER:HA	2.02	0.41
1:B:73:ASP:N	1:B:73:ASP:OD1	2.53	0.41
1:B:243:LEU:CG	1:B:401:TYR:CE2	3.03	0.41
1:B:224:GLY:O	1:B:397:THR:HB	2.21	0.41
1:D:132:PRO:CD	1:D:551:TYR:CE2	3.02	0.41
1:B:422:LEU:CD2	1:B:423:LEU:N	2.80	0.41
1:C:542:THR:HG21	1:C:546:ARG:HD2	2.02	0.41
1:C:137:PHE:HE1	1:C:547:ARG:NE	2.18	0.41
1:D:207:GLY:O	1:D:208:VAL:CB	2.64	0.41
1:D:126:ILE:HG12	1:D:521:LEU:CD2	2.49	0.41
1:D:87:ASP:OD1	1:D:89:SER:HB3	2.19	0.41
1:A:181:ILE:O	1:A:184:MET:HB2	2.19	0.41
1:C:224:GLY:O	1:C:397:THR:HB	2.20	0.41
1:D:224:GLY:O	1:D:397:THR:HB	2.21	0.41
1:A:542:THR:HG23	1:A:547:ARG:N	2.34	0.41
1:C:442:MET:HE2	1:C:443:MET:SD	2.60	0.41
1:C:117:SER:HA	1:C:566:SER:HA	2.02	0.41
1:A:474:TYR:HH	1:A:476:ASP:CG	2.24	0.41
1:A:442:MET:HE2	1:A:443:MET:SD	2.60	0.41
1:A:117:SER:HA	1:A:566:SER:HA	2.01	0.41
1:D:73:ASP:OD1	1:D:73:ASP:N	2.53	0.41
1:C:228:PRO:HG3	2:T:15:TYR:CD1	2.55	0.41
1:A:224:GLY:O	1:A:397:THR:HB	2.20	0.41
1:A:491:THR:HG21	1:A:493:VAL:HG22	2.03	0.41
1:B:217:LEU:HA	1:B:217:LEU:HD23	1.74	0.41
1:C:479:VAL:O	1:C:479:VAL:CG1	2.66	0.41
1:A:217:LEU:HD23	1:A:217:LEU:HA	1.74	0.41
1:C:171:PRO:O	1:C:172:GLU:C	2.59	0.41
1:B:417:ILE:HD12	1:B:417:ILE:HA	1.80	0.41
1:C:439:LEU:O	1:C:441:ASP:N	2.54	0.41
1:A:183:LEU:HD21	1:B:236:PHE:CE2	2.47	0.41
1:A:549:CYS:HA	1:A:550:PRO:HD3	1.89	0.41
1:B:491:THR:HG21	1:B:493:VAL:HG22	2.02	0.41
1:E:179:MET:HE2	1:E:485:ARG:NH2	2.35	0.41
1:D:243:LEU:HD23	1:D:244:PRO:HD3	2.01	0.41
1:A:401:TYR:CE1	1:A:502:ILE:HG12	2.56	0.41
1:C:243:LEU:CG	1:C:401:TYR:CE2	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:LEU:CD2	1:D:423:LEU:N	2.80	0.41
1:E:217:LEU:HA	1:E:217:LEU:HD23	1.74	0.41
1:D:137:PHE:HE1	1:D:547:ARG:NE	2.18	0.41
1:D:154:THR:CG2	1:D:155:LYS:H	2.34	0.41
1:C:150:SER:OG	1:C:162:LYS:HB2	2.21	0.41
1:C:64:PHE:CD1	1:D:118:HIS:NE2	2.88	0.41
1:D:392:ILE:HD11	1:D:396:SER:CB	2.51	0.41
1:E:563:VAL:CG1	1:E:564:LEU:N	2.84	0.41
1:B:282:ASN:HA	1:B:402:ARG:HA	2.02	0.41
1:E:385:LYS:HZ2	2:W:16:PRO:HB3	1.85	0.41
1:C:481:SER:O	1:C:482:GLN:C	2.59	0.41
1:C:441:ASP:HB2	1:C:537:GLN:OE1	2.21	0.41
1:B:442:MET:HE2	1:B:443:MET:SD	2.60	0.41
1:B:114:ASP:OD2	1:B:116:ARG:NH1	2.54	0.41
1:C:405:TYR:O	1:C:409:ASN:OD1	2.39	0.41
1:A:196:GLY:O	1:A:201:VAL:HG12	2.21	0.41
1:C:563:VAL:CG1	1:C:564:LEU:N	2.84	0.41
1:A:282:ASN:HA	1:A:402:ARG:HA	2.02	0.41
1:E:231:TYR:OH	1:E:284:PRO:O	2.34	0.41
1:A:542:THR:HG21	1:A:546:ARG:HD2	2.02	0.41
1:C:434:GLN:NE2	1:C:436:TYR:CE2	2.81	0.41
1:C:114:ASP:OD2	1:C:116:ARG:NH1	2.54	0.41
1:E:405:TYR:O	1:E:409:ASN:OD1	2.39	0.41
1:D:150:SER:OG	1:D:162:LYS:HB2	2.21	0.41
1:A:563:VAL:CG1	1:A:564:LEU:N	2.84	0.41
1:D:58:SER:OG	1:D:59:GLU:N	2.52	0.41
1:D:479:VAL:O	1:D:479:VAL:CG1	2.66	0.41
1:E:224:GLY:O	1:E:397:THR:HB	2.20	0.41
1:C:491:THR:HG21	1:C:493:VAL:HG22	2.03	0.41
1:A:551:TYR:CZ	1:B:422:LEU:HD21	2.55	0.41
1:D:83:ASN:OD1	1:D:92:LEU:N	2.38	0.41
1:D:439:LEU:O	1:D:441:ASP:N	2.54	0.41
1:A:154:THR:CG2	1:A:155:LYS:H	2.34	0.41
1:C:75:LYS:HB3	1:C:75:LYS:HE2	1.88	0.41
2:V:18:ASP:O	2:V:19:THR:HB	2.21	0.41
1:E:434:GLN:NE2	1:E:436:TYR:CE2	2.81	0.41
1:A:114:ASP:OD2	1:A:116:ARG:NH1	2.54	0.41
1:D:114:ASP:OD2	1:D:116:ARG:NH1	2.54	0.41
1:B:196:GLY:O	1:B:201:VAL:HG12	2.21	0.41
1:A:267:PHE:HD2	1:E:79:VAL:HG13	1.86	0.41
1:B:563:VAL:CG1	1:B:564:LEU:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ASP:N	1:A:73:ASP:OD1	2.53	0.41
1:C:96:ILE:HD13	1:C:96:ILE:HA	1.82	0.41
1:E:491:THR:HG21	1:E:493:VAL:HG22	2.03	0.41
1:D:491:THR:HG21	1:D:493:VAL:HG22	2.03	0.41
1:E:542:THR:HG21	1:E:546:ARG:HD2	2.02	0.41
1:D:417:ILE:HA	1:D:417:ILE:HD12	1.79	0.41
1:C:154:THR:CG2	1:C:155:LYS:H	2.34	0.41
1:C:439:LEU:N	1:C:440:PRO:CD	2.79	0.41
1:B:441:ASP:HB2	1:B:537:GLN:OE1	2.21	0.41
1:A:441:ASP:HB2	1:A:537:GLN:OE1	2.21	0.41
1:E:114:ASP:OD2	1:E:116:ARG:NH1	2.54	0.41
1:D:88:HIS:CD2	1:E:267:PHE:CZ	3.09	0.41
1:E:150:SER:OG	1:E:162:LYS:HB2	2.21	0.41
1:E:243:LEU:CG	1:E:401:TYR:CE2	3.03	0.40
1:E:225:LEU:HD23	1:E:397:THR:HB	2.03	0.40
1:D:441:ASP:HB2	1:D:537:GLN:OE1	2.21	0.40
1:A:135:ASN:N	1:A:140:THR:OG1	2.54	0.40
1:A:439:LEU:O	1:A:441:ASP:N	2.54	0.40
2:S:18:ASP:O	2:S:19:THR:HB	2.21	0.40
1:A:267:PHE:CD2	1:E:79:VAL:HG13	2.56	0.40
1:B:149:VAL:HG13	1:B:195:VAL:HG11	2.04	0.40
1:C:53:ASN:ND2	1:C:53:ASN:O	2.54	0.40
1:C:225:LEU:HD23	1:C:397:THR:HB	2.04	0.40
1:A:481:SER:O	1:A:482:GLN:C	2.59	0.40
1:D:401:TYR:CE1	1:D:502:ILE:HG12	2.56	0.40
1:E:441:ASP:HB2	1:E:537:GLN:OE1	2.21	0.40
1:E:171:PRO:O	1:E:172:GLU:C	2.59	0.40
1:D:88:HIS:HD2	1:E:267:PHE:CZ	2.39	0.40
1:C:373:LYS:O	1:C:374:LYS:CG	2.70	0.40
1:B:373:LYS:O	1:B:374:LYS:CG	2.69	0.40
1:B:53:ASN:O	1:B:53:ASN:ND2	2.54	0.40
1:C:208:VAL:HG22	1:C:242:LEU:HD22	2.03	0.40
1:D:75:LYS:HB3	1:D:75:LYS:HE2	1.88	0.40
1:B:150:SER:OG	1:B:162:LYS:HB2	2.21	0.40
1:C:149:VAL:HG13	1:C:195:VAL:HG11	2.03	0.40
1:C:220:ASP:HB3	1:C:223:THR:HB	2.04	0.40
1:A:243:LEU:O	1:A:244:PRO:C	2.59	0.40
1:B:405:TYR:O	1:B:409:ASN:OD1	2.39	0.40
1:D:436:TYR:HD1	1:D:460:VAL:HG21	1.86	0.40
1:D:177:GLU:HG3	1:D:178:THR:H	1.82	0.40
1:E:196:GLY:O	1:E:201:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:LYS:O	1:E:374:LYS:CG	2.70	0.40
1:B:401:TYR:CE1	1:B:502:ILE:HG12	2.56	0.40
1:A:179:MET:CE	1:A:485:ARG:HH22	2.34	0.40
1:D:481:SER:O	1:D:482:GLN:C	2.59	0.40
1:A:220:ASP:HB3	1:A:223:THR:HB	2.04	0.40
1:D:243:LEU:O	1:D:244:PRO:C	2.59	0.40
1:B:179:MET:HE2	1:B:485:ARG:NH2	2.36	0.40
1:C:179:MET:CE	1:C:485:ARG:HH22	2.34	0.40
1:D:225:LEU:HD23	1:D:397:THR:HB	2.03	0.40
1:E:439:LEU:O	1:E:441:ASP:N	2.54	0.40
1:D:405:TYR:O	1:D:409:ASN:OD1	2.39	0.40
1:A:409:ASN:HD22	1:E:171:PRO:CA	2.35	0.40
2:U:18:ASP:O	2:U:19:THR:HB	2.21	0.40
1:C:436:TYR:HD1	1:C:460:VAL:HG21	1.86	0.40
1:E:434:GLN:HE21	1:E:436:TYR:HE2	1.69	0.40
1:E:536:VAL:CG2	1:E:536:VAL:O	2.69	0.40
1:B:392:ILE:HD11	1:B:396:SER:CB	2.51	0.40
1:C:392:ILE:HD11	1:C:396:SER:CB	2.51	0.40
1:A:373:LYS:O	1:A:374:LYS:CG	2.70	0.40
1:E:53:ASN:O	1:E:53:ASN:ND2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	436/523 (83%)	321 (74%)	69 (16%)	46 (11%)	0	11
1	B	436/523 (83%)	320 (73%)	70 (16%)	46 (11%)	0	11
1	C	436/523 (83%)	321 (74%)	69 (16%)	46 (11%)	0	11
1	D	436/523 (83%)	321 (74%)	69 (16%)	46 (11%)	0	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	436/523 (83%)	321 (74%)	69 (16%)	46 (11%)	0	11
2	S	8/19 (42%)	5 (62%)	3 (38%)	0	100	100
2	T	8/19 (42%)	5 (62%)	3 (38%)	0	100	100
2	U	8/19 (42%)	5 (62%)	3 (38%)	0	100	100
2	V	8/19 (42%)	5 (62%)	3 (38%)	0	100	100
2	W	8/19 (42%)	5 (62%)	3 (38%)	0	100	100
All	All	2220/2710 (82%)	1629 (73%)	361 (16%)	230 (10%)	1	12

All (230) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	LEU
1	A	130	ASN
1	A	172	GLU
1	A	174	ASN
1	A	201	VAL
1	A	216	ARG
1	A	280	GLY
1	A	376	VAL
1	A	447	VAL
1	A	455	ILE
1	A	467	PRO
1	A	479	VAL
1	A	496	ARG
1	B	82	LEU
1	B	130	ASN
1	B	172	GLU
1	B	174	ASN
1	B	201	VAL
1	B	216	ARG
1	B	280	GLY
1	B	376	VAL
1	B	447	VAL
1	B	467	PRO
1	B	479	VAL
1	B	496	ARG
1	C	82	LEU
1	C	130	ASN
1	C	172	GLU
1	C	174	ASN

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Mol	Chain	Res	Type
1	C	201	VAL
1	C	216	ARG
1	C	280	GLY
1	C	376	VAL
1	C	447	VAL
1	C	455	ILE
1	C	467	PRO
1	C	479	VAL
1	C	496	ARG
1	D	82	LEU
1	D	130	ASN
1	D	172	GLU
1	D	174	ASN
1	D	201	VAL
1	D	216	ARG
1	D	280	GLY
1	D	376	VAL
1	D	447	VAL
1	D	455	ILE
1	D	467	PRO
1	D	479	VAL
1	D	496	ARG
1	E	82	LEU
1	E	130	ASN
1	E	172	GLU
1	E	174	ASN
1	E	201	VAL
1	E	216	ARG
1	E	280	GLY
1	E	376	VAL
1	E	447	VAL
1	E	455	ILE
1	E	467	PRO
1	E	479	VAL
1	E	496	ARG
1	A	58	SER
1	A	84	TYR
1	A	175	TYR
1	A	196	GLY
1	A	215	PHE
1	A	219	PHE
1	A	251	THR

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Mol	Chain	Res	Type
1	A	279	GLU
1	A	377	ILE
1	A	385	LYS
1	A	386	LYS
1	A	426	PRO
1	A	440	PRO
1	A	503	LEU
1	B	58	SER
1	B	84	TYR
1	B	175	TYR
1	B	196	GLY
1	B	215	PHE
1	B	219	PHE
1	B	251	THR
1	B	279	GLU
1	B	377	ILE
1	B	385	LYS
1	B	386	LYS
1	B	426	PRO
1	B	440	PRO
1	B	455	ILE
1	B	503	LEU
1	C	58	SER
1	C	84	TYR
1	C	175	TYR
1	C	196	GLY
1	C	215	PHE
1	C	219	PHE
1	C	251	THR
1	C	279	GLU
1	C	377	ILE
1	C	385	LYS
1	C	386	LYS
1	C	426	PRO
1	C	440	PRO
1	C	503	LEU
1	D	58	SER
1	D	84	TYR
1	D	175	TYR
1	D	196	GLY
1	D	215	PHE
1	D	219	PHE

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Mol	Chain	Res	Type
1	D	251	THR
1	D	279	GLU
1	D	377	ILE
1	D	385	LYS
1	D	386	LYS
1	D	426	PRO
1	D	440	PRO
1	D	503	LEU
1	E	58	SER
1	E	84	TYR
1	E	175	TYR
1	E	196	GLY
1	E	215	PHE
1	E	219	PHE
1	E	251	THR
1	E	279	GLU
1	E	377	ILE
1	E	385	LYS
1	E	386	LYS
1	E	426	PRO
1	E	440	PRO
1	E	503	LEU
1	A	75	LYS
1	A	81	SER
1	A	88	HIS
1	A	89	SER
1	A	101	TYR
1	A	114	ASP
1	A	176	SER
1	A	199	ASN
1	A	233	ASN
1	A	270	GLY
1	A	498	PRO
1	A	511	ILE
1	B	75	LYS
1	B	81	SER
1	B	88	HIS
1	B	89	SER
1	B	101	TYR
1	B	114	ASP
1	B	176	SER
1	B	199	ASN

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Mol	Chain	Res	Type
1	B	233	ASN
1	B	270	GLY
1	B	498	PRO
1	B	511	ILE
1	C	75	LYS
1	C	81	SER
1	C	88	HIS
1	C	89	SER
1	C	101	TYR
1	C	114	ASP
1	C	176	SER
1	C	199	ASN
1	C	233	ASN
1	C	270	GLY
1	C	498	PRO
1	C	511	ILE
1	D	75	LYS
1	D	81	SER
1	D	88	HIS
1	D	89	SER
1	D	101	TYR
1	D	114	ASP
1	D	176	SER
1	D	199	ASN
1	D	233	ASN
1	D	270	GLY
1	D	498	PRO
1	D	511	ILE
1	E	75	LYS
1	E	81	SER
1	E	88	HIS
1	E	89	SER
1	E	101	TYR
1	E	114	ASP
1	E	176	SER
1	E	199	ASN
1	E	233	ASN
1	E	270	GLY
1	E	498	PRO
1	E	511	ILE
1	A	55	ILE
1	A	67	THR

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Mol	Chain	Res	Type
1	A	208	VAL
1	A	380	LEU
1	B	55	ILE
1	B	67	THR
1	B	208	VAL
1	B	380	LEU
1	C	55	ILE
1	C	67	THR
1	C	208	VAL
1	C	380	LEU
1	D	55	ILE
1	D	67	THR
1	D	208	VAL
1	D	380	LEU
1	E	55	ILE
1	E	67	THR
1	E	208	VAL
1	E	380	LEU
1	A	390	ASN
1	B	390	ASN
1	C	390	ASN
1	D	390	ASN
1	E	390	ASN
1	D	416	GLY
1	A	379	PRO
1	A	416	GLY
1	B	379	PRO
1	B	416	GLY
1	C	379	PRO
1	C	416	GLY
1	D	379	PRO
1	E	379	PRO
1	E	416	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	399/451 (88%)	369 (92%)	30 (8%)	17	53
1	B	399/451 (88%)	370 (93%)	29 (7%)	17	54
1	C	399/451 (88%)	369 (92%)	30 (8%)	17	53
1	D	399/451 (88%)	369 (92%)	30 (8%)	17	53
1	E	399/451 (88%)	369 (92%)	30 (8%)	17	53
2	S	10/17 (59%)	9 (90%)	1 (10%)	9	38
2	T	10/17 (59%)	9 (90%)	1 (10%)	9	38
2	U	10/17 (59%)	9 (90%)	1 (10%)	9	38
2	V	10/17 (59%)	9 (90%)	1 (10%)	9	38
2	W	10/17 (59%)	9 (90%)	1 (10%)	9	38
All	All	2045/2340 (87%)	1891 (92%)	154 (8%)	21	53

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	98	ASN
1	A	107	SER
1	A	124	LYS
1	A	130	ASN
1	A	133	ASN
1	A	168	PHE
1	A	199	ASN
1	A	202	LEU
1	A	214	ASN
1	A	249	ASP
1	A	256	SER
1	A	271	PHE
1	A	276	ASP
1	A	279	GLU
1	A	399	THR
1	A	402	ARG
1	A	409	ASN
1	A	417	ILE
1	A	422	LEU
1	A	427	ASP
1	A	434	GLN
1	A	438	SER
1	A	448	THR

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Mol	Chain	Res	Type
1	A	457	ASN
1	A	476	ASP
1	A	482	GLN
1	A	510	THR
1	A	543	ASP
1	A	560	SER
1	B	83	ASN
1	B	98	ASN
1	B	107	SER
1	B	124	LYS
1	B	130	ASN
1	B	133	ASN
1	B	168	PHE
1	B	199	ASN
1	B	202	LEU
1	B	214	ASN
1	B	249	ASP
1	B	256	SER
1	B	271	PHE
1	B	276	ASP
1	B	399	THR
1	B	402	ARG
1	B	409	ASN
1	B	417	ILE
1	B	422	LEU
1	B	427	ASP
1	B	434	GLN
1	B	438	SER
1	B	448	THR
1	B	457	ASN
1	B	476	ASP
1	B	482	GLN
1	B	510	THR
1	B	543	ASP
1	B	560	SER
1	C	83	ASN
1	C	98	ASN
1	C	107	SER
1	C	124	LYS
1	C	130	ASN
1	C	133	ASN
1	C	168	PHE

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Mol	Chain	Res	Type
1	C	199	ASN
1	C	202	LEU
1	C	214	ASN
1	C	249	ASP
1	C	256	SER
1	C	271	PHE
1	C	276	ASP
1	C	279	GLU
1	C	399	THR
1	C	402	ARG
1	C	409	ASN
1	C	417	ILE
1	C	422	LEU
1	C	427	ASP
1	C	434	GLN
1	C	438	SER
1	C	448	THR
1	C	457	ASN
1	C	476	ASP
1	C	482	GLN
1	C	510	THR
1	C	543	ASP
1	C	560	SER
1	D	83	ASN
1	D	98	ASN
1	D	107	SER
1	D	124	LYS
1	D	130	ASN
1	D	133	ASN
1	D	168	PHE
1	D	199	ASN
1	D	202	LEU
1	D	214	ASN
1	D	249	ASP
1	D	256	SER
1	D	271	PHE
1	D	276	ASP
1	D	279	GLU
1	D	399	THR
1	D	402	ARG
1	D	409	ASN
1	D	417	ILE

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Mol	Chain	Res	Type
1	D	422	LEU
1	D	427	ASP
1	D	434	GLN
1	D	438	SER
1	D	448	THR
1	D	457	ASN
1	D	476	ASP
1	D	482	GLN
1	D	510	THR
1	D	543	ASP
1	D	560	SER
1	E	83	ASN
1	E	98	ASN
1	E	107	SER
1	E	124	LYS
1	E	130	ASN
1	E	133	ASN
1	E	168	PHE
1	E	199	ASN
1	E	202	LEU
1	E	214	ASN
1	E	249	ASP
1	E	256	SER
1	E	271	PHE
1	E	276	ASP
1	E	279	GLU
1	E	399	THR
1	E	402	ARG
1	E	409	ASN
1	E	417	ILE
1	E	422	LEU
1	E	427	ASP
1	E	434	GLN
1	E	438	SER
1	E	448	THR
1	E	457	ASN
1	E	476	ASP
1	E	482	GLN
1	E	510	THR
1	E	543	ASP
1	E	560	SER
2	S	15	TYR

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Mol	Chain	Res	Type
2	T	15	TYR
2	U	15	TYR
2	V	15	TYR
2	W	15	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	86	ASN
1	A	98	ASN
1	A	109	GLN
1	A	130	ASN
1	A	174	ASN
1	A	198	GLN
1	A	199	ASN
1	A	214	ASN
1	A	237	HIS
1	A	400	GLN
1	A	434	GLN
1	A	457	ASN
1	A	469	HIS
1	A	495	ASN
1	A	501	GLN
1	B	53	ASN
1	B	86	ASN
1	B	98	ASN
1	B	109	GLN
1	B	130	ASN
1	B	174	ASN
1	B	198	GLN
1	B	199	ASN
1	B	214	ASN
1	B	237	HIS
1	B	400	GLN
1	B	434	GLN
1	B	457	ASN
1	B	469	HIS
1	B	495	ASN
1	B	501	GLN
1	C	53	ASN
1	C	86	ASN

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Mol	Chain	Res	Type
1	C	98	ASN
1	C	109	GLN
1	C	130	ASN
1	C	174	ASN
1	C	198	GLN
1	C	199	ASN
1	C	214	ASN
1	C	237	HIS
1	C	400	GLN
1	C	434	GLN
1	C	457	ASN
1	C	469	HIS
1	C	495	ASN
1	C	501	GLN
1	D	53	ASN
1	D	86	ASN
1	D	98	ASN
1	D	109	GLN
1	D	130	ASN
1	D	174	ASN
1	D	198	GLN
1	D	199	ASN
1	D	214	ASN
1	D	237	HIS
1	D	400	GLN
1	D	434	GLN
1	D	457	ASN
1	D	469	HIS
1	D	495	ASN
1	D	501	GLN
1	E	53	ASN
1	E	86	ASN
1	E	98	ASN
1	E	109	GLN
1	E	130	ASN
1	E	174	ASN
1	E	198	GLN
1	E	199	ASN
1	E	214	ASN
1	E	237	HIS
1	E	400	GLN
1	E	457	ASN

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Mol	Chain	Res	Type
1	E	469	HIS
1	E	495	ASN
1	E	501	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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.