



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:42 PM BST

PDB ID : 3IZO
EMDB ID: : EMD-5172
Title : Model of the fiber tail and its interactions with the penton base of human adenovirus by cryo-electron microscopy
Authors : Liu, H.
Deposited on : 2010-11-05
Resolution : 3.60 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

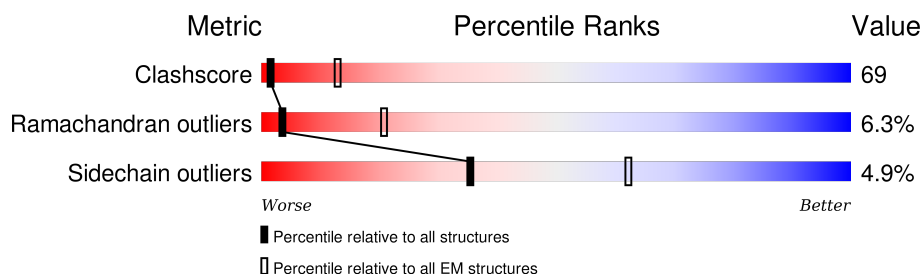
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	571	38% 36% 6% 20%
1	B	571	37% 37% 5% 20%
1	C	571	37% 37% 5% 20%
1	D	571	39% 36% 5% 20%
1	E	571	38% 36% 5% 20%
2	F	581	98%
2	G	581	98%
2	H	581	98%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18537 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.

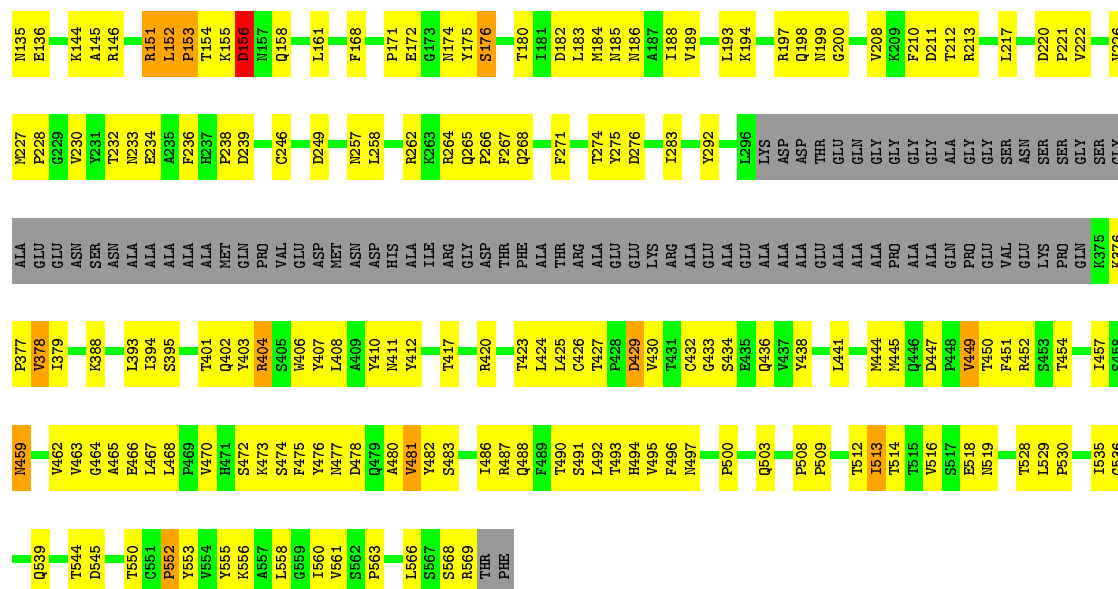
- Molecule 1 is a protein called Penton protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	455	Total	C	N	O	S	0	0
			3642	2308	632	690	12		
1	B	455	Total	C	N	O	S	0	0
			3642	2308	632	690	12		
1	C	455	Total	C	N	O	S	0	0
			3642	2308	632	690	12		
1	D	455	Total	C	N	O	S	0	0
			3642	2308	632	690	12		
1	E	455	Total	C	N	O	S	0	0
			3642	2308	632	690	12		

- Molecule 2 is a protein called Fiber.

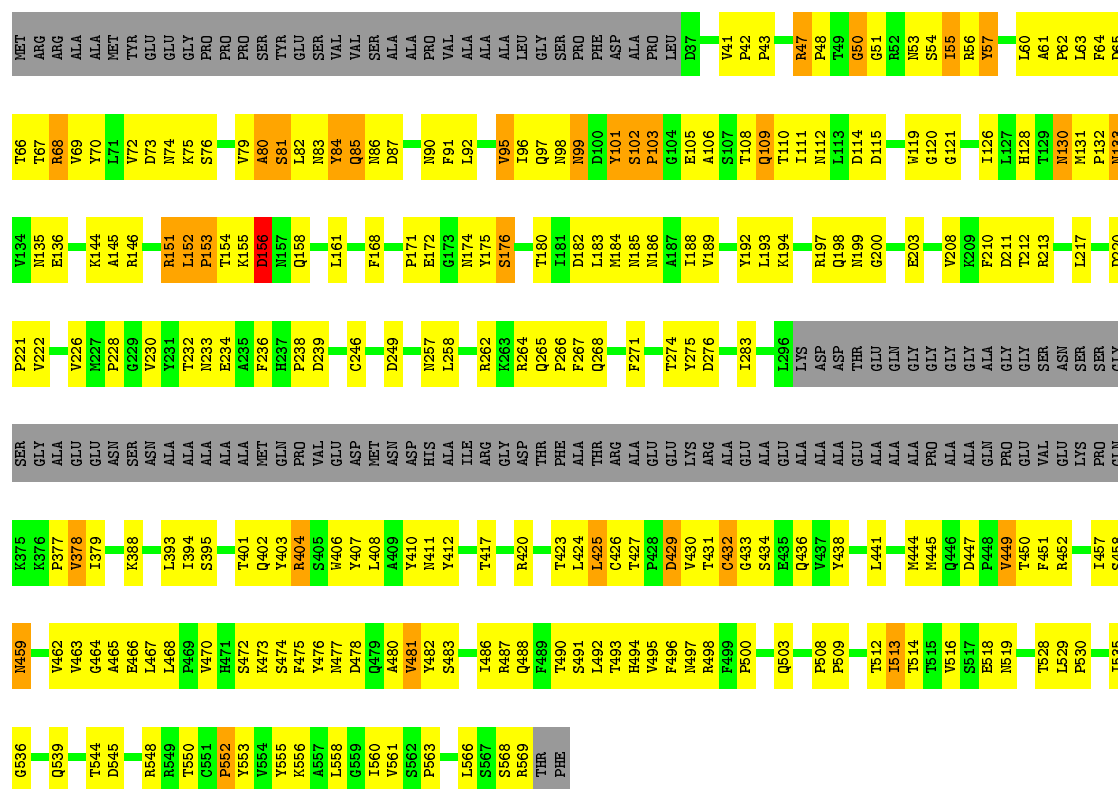
Mol	Chain	Residues	Atoms				AltConf	Trace
2	F	13	Total	C	N	O	0	0
			109	70	14	25		
2	G	13	Total	C	N	O	0	0
			109	70	14	25		
2	H	13	Total	C	N	O	0	0
			109	70	14	25		





• Molecule 1: Penton protein

Chain E: 38% 36% 5% 20%



• Molecule 2: Fiber

Chain F: 98%



[illegible]

- Molecule 2: Fiber

Chain G: .. 98%

[illegible]

- Molecule 2: Fiber

Chain H: 98%

GLU THR GLY ASP THR THR PRO SER SER TYR SER MET SER PHE SER TRP TRP TRP SER GLY HIS ASN TYR ILE ASN ASN GLU ILE PHE ALA THR SER SER TYR THR PHE SER TYR ILE ALA GLN GLU

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	Titan Krios	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	Not provided	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality

5.1 Standard geometry

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	0.33	0/3733	0.54	0/5088
1	B	0.33	0/3733	0.55	0/5088
1	C	0.33	0/3733	0.55	0/5088
1	D	0.33	0/3733	0.55	0/5088
1	E	0.33	0/3733	0.54	0/5088
2	F	0.22	0/113	0.39	0/156
2	G	0.22	0/113	0.39	0/156
2	H	0.22	0/113	0.39	0/156
All	All	0.33	0/19004	0.54	0/25908

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
All	All	0	10

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	47	ARG	Sidechain
1	A	68	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	47	ARG	Sidechain
1	B	68	ARG	Sidechain
1	C	47	ARG	Sidechain
1	C	68	ARG	Sidechain
1	D	47	ARG	Sidechain
1	D	68	ARG	Sidechain
1	E	47	ARG	Sidechain
1	E	68	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	3642	0	3571	777	0
1	B	3642	0	3571	780	0
1	C	3642	0	3571	757	0
1	D	3642	0	3571	735	0
1	E	3642	0	3571	742	0
2	F	109	0	88	55	0
2	G	109	0	88	52	0
2	H	109	0	88	55	0
All	All	18537	0	18119	2535	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 69.

All (2535) 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:D:410:TYR:CE2	1:D:425:LEU:HD12	1.34	1.62
1:D:425:LEU:HD13	1:E:172:GLU:CB	1.27	1.59
1:A:267:PHE:CZ	1:B:80:ALA:HA	1.34	1.58
1:C:450:THR:HG23	1:D:57:TYR:CE1	1.41	1.54
1:A:450:THR:HG23	1:B:57:TYR:CE1	1.45	1.51
1:A:57:TYR:CD1	1:E:450:THR:HG22	1.46	1.51
1:A:172:GLU:CB	1:E:425:LEU:HD13	1.41	1.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:TYR:CE2	1:D:60:LEU:HD13	1.47	1.48
1:A:60:LEU:CD2	1:E:452:ARG:HG2	1.41	1.47
1:D:450:THR:HG23	1:E:57:TYR:CE1	1.49	1.46
1:B:450:THR:HG23	1:C:57:TYR:CE1	1.48	1.43
1:A:60:LEU:HD21	1:E:452:ARG:CG	1.48	1.42
1:B:228:PRO:HG3	2:G:15:TYR:CE1	1.56	1.41
1:A:267:PHE:HZ	1:B:80:ALA:CA	1.32	1.40
1:A:228:PRO:HG3	2:F:15:TYR:CE1	1.56	1.40
1:A:57:TYR:HD1	1:E:450:THR:CG2	1.34	1.39
1:D:228:PRO:HG3	2:H:15:TYR:CE1	1.56	1.38
1:A:126:ILE:HD12	1:E:436:GLN:NE2	1.37	1.36
1:B:267:PHE:CE1	1:C:76:SER:HB2	1.59	1.35
1:D:436:GLN:NE2	1:E:126:ILE:HD12	1.37	1.33
1:D:292:TYR:CE1	1:D:376:LYS:HD3	1.63	1.33
1:B:267:PHE:HE1	1:C:76:SER:CB	1.41	1.33
1:A:450:THR:HG23	1:B:57:TYR:CD1	1.63	1.32
1:C:452:ARG:CG	1:D:60:LEU:HD21	1.57	1.32
1:C:425:LEU:HD13	1:D:172:GLU:CB	1.57	1.31
1:A:292:TYR:CE1	1:A:376:LYS:HD3	1.63	1.31
1:B:450:THR:HG23	1:C:57:TYR:CD1	1.63	1.31
1:B:292:TYR:CE1	1:B:376:LYS:HD3	1.63	1.31
1:D:425:LEU:CD1	1:E:172:GLU:HB2	1.62	1.30
1:C:228:PRO:HB3	1:D:493:THR:CG2	1.63	1.28
1:A:172:GLU:HB2	1:E:425:LEU:CD1	1.64	1.28
1:D:410:TYR:CD2	1:D:425:LEU:HD12	1.69	1.27
1:E:410:TYR:CD2	1:E:425:LEU:HD12	1.70	1.27
1:A:493:THR:CG2	1:E:228:PRO:HB3	1.64	1.26
1:C:436:GLN:NE2	1:D:126:ILE:HD12	1.51	1.25
1:C:452:ARG:CD	1:D:60:LEU:HD11	1.64	1.25
1:A:57:TYR:CE2	1:A:60:LEU:HG	1.72	1.25
1:A:60:LEU:HD21	1:E:452:ARG:CD	1.66	1.23
1:D:267:PHE:CE2	1:E:76:SER:HB3	1.73	1.23
1:C:267:PHE:CE2	1:D:76:SER:HB3	1.74	1.22
1:A:493:THR:HG21	1:E:228:PRO:CB	1.70	1.22
1:C:425:LEU:CD1	1:D:172:GLU:HB2	1.70	1.21
1:C:452:ARG:HG2	1:D:60:LEU:CG	1.71	1.21
1:B:410:TYR:CE2	1:C:172:GLU:HG3	1.76	1.20
1:C:228:PRO:CB	1:D:493:THR:HG21	1.70	1.20
1:C:267:PHE:CE2	1:D:76:SER:CB	2.24	1.20
1:C:410:TYR:CE2	1:D:172:GLU:HG3	1.76	1.19
1:A:172:GLU:HG3	1:E:410:TYR:CE2	1.77	1.19

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:TYR:HE2	1:E:172:GLU:HG3	1.06	1.19
1:D:267:PHE:CE2	1:E:76:SER:CB	2.24	1.18
1:A:410:TYR:CE2	1:B:172:GLU:HG3	1.78	1.18
1:D:57:TYR:CE2	1:D:60:LEU:CD1	2.27	1.18
1:E:410:TYR:CE2	1:E:425:LEU:HD12	1.77	1.18
1:A:436:GLN:HE21	1:A:465:ALA:HB1	1.07	1.18
1:D:410:TYR:CE2	1:E:172:GLU:HG3	1.79	1.17
1:B:63:LEU:HD22	1:B:67:THR:HG22	1.22	1.17
1:C:452:ARG:HG2	1:D:60:LEU:CD2	1.74	1.17
1:B:425:LEU:HD22	1:C:172:GLU:CB	1.73	1.17
1:B:436:GLN:HE21	1:B:465:ALA:HB1	1.08	1.17
1:A:425:LEU:HD22	1:B:172:GLU:CB	1.73	1.17
1:D:410:TYR:CD2	1:D:425:LEU:CD1	2.27	1.16
1:D:57:TYR:HE2	1:D:60:LEU:CD1	1.58	1.16
1:A:436:GLN:OE1	1:B:126:ILE:HD12	1.43	1.16
1:A:83:ASN:HB3	1:E:267:PHE:CD1	1.79	1.16
1:C:68:ARG:HD3	1:C:70:TYR:CE2	1.80	1.16
1:D:410:TYR:CE2	1:D:425:LEU:CD1	2.28	1.16
1:B:425:LEU:HD22	1:C:172:GLU:HB3	1.24	1.16
1:C:436:GLN:HE22	1:D:558:LEU:HD11	1.04	1.15
1:D:63:LEU:HD22	1:D:67:THR:HG22	1.22	1.15
1:B:410:TYR:HE2	1:C:172:GLU:HG3	1.05	1.15
1:A:60:LEU:HD11	1:E:452:ARG:CG	1.75	1.15
1:A:493:THR:HG21	1:E:228:PRO:HB3	1.15	1.14
1:C:68:ARG:CD	1:C:70:TYR:CE2	2.30	1.14
1:A:68:ARG:CD	1:A:70:TYR:CE2	2.31	1.14
1:C:233:ASN:HB3	1:D:491:SER:HA	1.29	1.14
1:A:410:TYR:HE2	1:B:172:GLU:HG3	1.04	1.14
1:E:68:ARG:CD	1:E:70:TYR:CE2	2.31	1.13
1:D:228:PRO:CG	2:H:15:TYR:HE1	1.62	1.13
1:B:68:ARG:CD	1:B:70:TYR:CE2	2.31	1.13
1:C:63:LEU:HD22	1:C:67:THR:HG22	1.22	1.13
1:B:436:GLN:OE1	1:C:126:ILE:HD12	1.44	1.13
1:A:83:ASN:ND2	1:A:91:PHE:HB2	1.63	1.12
1:A:228:PRO:CG	2:F:15:TYR:HE1	1.62	1.12
1:D:376:LYS:HD2	1:D:378:VAL:CG1	1.80	1.12
1:D:68:ARG:CD	1:D:70:TYR:CE2	2.31	1.12
1:B:433:GLY:HA2	1:C:555:TYR:CE2	1.84	1.12
1:A:433:GLY:HA2	1:B:555:TYR:CE2	1.84	1.12
1:C:436:GLN:NE2	1:D:558:LEU:HD11	1.64	1.12
1:E:83:ASN:ND2	1:E:91:PHE:HB2	1.63	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ASN:ND2	1:B:91:PHE:HB2	1.63	1.12
1:A:376:LYS:HD2	1:A:378:VAL:CG1	1.80	1.12
1:D:556:LYS:HE2	1:D:558:LEU:HD23	1.29	1.12
1:A:63:LEU:HD22	1:A:67:THR:HG22	1.22	1.11
1:A:172:GLU:HG3	1:E:410:TYR:HE2	1.06	1.11
1:B:480:ALA:O	1:B:481:VAL:HG22	1.50	1.11
1:C:83:ASN:ND2	1:C:91:PHE:HB2	1.63	1.11
1:B:267:PHE:CE1	1:C:76:SER:CB	2.25	1.11
1:E:556:LYS:HE2	1:E:558:LEU:HD23	1.29	1.11
1:A:47:ARG:HB2	1:E:569:ARG:CA	1.80	1.11
1:E:63:LEU:HD22	1:E:67:THR:HG22	1.22	1.11
1:B:228:PRO:CG	2:G:15:TYR:HE1	1.62	1.11
1:C:155:LYS:O	1:C:156:ASP:HB2	1.51	1.11
1:A:480:ALA:O	1:A:481:VAL:HG22	1.51	1.11
1:A:569:ARG:CA	1:B:47:ARG:HB2	1.81	1.11
1:D:433:GLY:HA2	1:E:555:TYR:CE2	1.86	1.11
1:C:452:ARG:HG3	1:D:60:LEU:HD21	1.29	1.10
1:C:450:THR:CG2	1:D:57:TYR:CE1	2.33	1.10
1:B:569:ARG:CA	1:C:47:ARG:HB2	1.80	1.10
1:B:376:LYS:HD2	1:B:378:VAL:CG1	1.80	1.10
1:D:83:ASN:ND2	1:D:91:PHE:HB2	1.63	1.10
1:A:486:ILE:CG2	1:E:482:TYR:CE1	2.35	1.10
1:C:410:TYR:HE2	1:D:172:GLU:HG3	1.03	1.10
1:B:155:LYS:O	1:B:156:ASP:HB2	1.51	1.10
1:A:68:ARG:HD3	1:A:70:TYR:CE2	1.83	1.10
1:A:227:MET:HB3	2:F:17:TYR:OH	1.51	1.09
1:D:227:MET:HB3	2:H:17:TYR:OH	1.51	1.09
1:A:556:LYS:HE2	1:A:558:LEU:HD23	1.18	1.09
1:D:569:ARG:CA	1:E:47:ARG:HB2	1.82	1.09
1:D:57:TYR:CE2	1:D:60:LEU:HD22	1.87	1.09
1:B:227:MET:HB3	2:G:17:TYR:OH	1.52	1.09
1:B:68:ARG:HD3	1:B:70:TYR:CE2	1.86	1.09
1:B:436:GLN:HE21	1:B:465:ALA:CB	1.65	1.09
1:A:491:SER:HA	1:E:233:ASN:HB3	1.33	1.09
1:E:473:LYS:HD2	1:E:475:PHE:HE1	1.13	1.09
1:A:60:LEU:HD11	1:E:452:ARG:HG3	1.20	1.08
1:A:473:LYS:HD2	1:A:475:PHE:HE1	1.13	1.08
1:B:459:ASN:HB2	1:C:99:ASN:HB3	1.34	1.08
1:E:68:ARG:HD3	1:E:70:TYR:CE2	1.86	1.08
1:D:473:LYS:HD2	1:D:475:PHE:HE1	1.13	1.08
1:D:155:LYS:O	1:D:156:ASP:HB2	1.51	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:LYS:HE2	1:B:558:LEU:HD23	1.29	1.08
1:A:155:LYS:O	1:A:156:ASP:HB2	1.51	1.08
1:D:47:ARG:HG3	1:D:48:PRO:HD2	1.35	1.08
1:E:473:LYS:HD2	1:E:475:PHE:CE1	1.89	1.07
1:D:376:LYS:HD2	1:D:378:VAL:HG13	1.26	1.07
1:D:233:ASN:HB3	1:E:491:SER:HA	1.33	1.07
1:A:233:ASN:HB3	1:B:491:SER:HA	1.30	1.07
1:B:376:LYS:HD2	1:B:378:VAL:HG13	1.26	1.07
1:C:569:ARG:CA	1:D:47:ARG:HB2	1.84	1.07
1:C:473:LYS:HD2	1:C:475:PHE:CE1	1.89	1.07
1:B:425:LEU:HD13	1:C:172:GLU:HB2	1.36	1.07
1:D:473:LYS:HD2	1:D:475:PHE:CE1	1.89	1.07
1:D:68:ARG:HD3	1:D:70:TYR:CE2	1.87	1.06
1:C:228:PRO:HB3	1:D:493:THR:HG21	1.17	1.06
1:C:473:LYS:HD2	1:C:475:PHE:HE1	1.13	1.06
1:A:376:LYS:HD2	1:A:378:VAL:HG13	1.26	1.06
1:A:425:LEU:HD22	1:B:172:GLU:HB3	1.33	1.06
1:B:473:LYS:HD2	1:B:475:PHE:CE1	1.90	1.06
2:H:8:GLU:O	2:H:9:ASP:HB2	1.52	1.06
1:B:473:LYS:HD2	1:B:475:PHE:HE1	1.13	1.06
1:A:473:LYS:HD2	1:A:475:PHE:CE1	1.89	1.06
1:A:558:LEU:HD11	1:E:436:GLN:HE22	1.17	1.05
1:B:436:GLN:OE1	1:C:558:LEU:HD11	1.56	1.05
1:B:57:TYR:CD2	1:B:60:LEU:HB3	1.90	1.05
1:A:450:THR:CG2	1:B:57:TYR:CE1	2.38	1.05
1:D:450:THR:HG23	1:E:57:TYR:CD1	1.91	1.05
1:C:57:TYR:CD2	1:C:60:LEU:HB3	1.90	1.05
1:A:436:GLN:HE21	1:A:465:ALA:CB	1.69	1.05
1:B:233:ASN:HB3	1:C:491:SER:HA	1.32	1.05
2:G:8:GLU:O	2:G:9:ASP:HB2	1.52	1.05
1:C:433:GLY:HA2	1:D:555:TYR:CE2	1.91	1.05
1:C:450:THR:HG23	1:D:57:TYR:CD1	1.90	1.05
1:C:482:TYR:CE1	1:D:486:ILE:CG2	2.40	1.05
2:G:8:GLU:HG3	2:G:9:ASP:H	1.22	1.05
2:F:8:GLU:O	2:F:9:ASP:HB2	1.52	1.05
1:C:452:ARG:HD2	1:D:60:LEU:HD11	1.06	1.04
1:C:436:GLN:HG3	1:C:466:GLU:O	1.57	1.04
1:B:450:THR:CG2	1:C:57:TYR:CE1	2.40	1.04
1:D:436:GLN:HG3	1:D:466:GLU:O	1.56	1.04
1:E:47:ARG:HG3	1:E:48:PRO:HD2	1.35	1.04
1:B:436:GLN:HG3	1:B:466:GLU:O	1.58	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:556:LYS:HE2	1:C:558:LEU:HD23	1.29	1.04
1:D:425:LEU:CD1	1:E:172:GLU:CB	2.24	1.03
1:A:410:TYR:CD2	1:A:425:LEU:CD1	2.41	1.03
1:A:47:ARG:HG3	1:A:48:PRO:HD2	1.35	1.03
1:E:436:GLN:HG3	1:E:466:GLU:O	1.58	1.03
1:B:47:ARG:HG3	1:B:48:PRO:HD2	1.36	1.03
2:F:8:GLU:HG3	2:F:9:ASP:H	1.22	1.03
1:A:558:LEU:HD11	1:E:436:GLN:NE2	1.71	1.03
1:D:459:ASN:HB2	1:E:99:ASN:HB3	1.37	1.03
2:G:14:VAL:HG13	1:C:203:GLU:OE2	1.59	1.03
1:C:481:VAL:HG12	1:D:490:THR:HB	1.41	1.03
1:A:436:GLN:HG3	1:A:466:GLU:O	1.57	1.03
1:A:433:GLY:HA2	1:B:555:TYR:HE2	1.21	1.03
1:D:47:ARG:CG	1:D:48:PRO:HD2	1.89	1.03
1:D:265:GLN:NE2	1:E:85:GLN:HA	1.72	1.03
1:C:265:GLN:NE2	1:D:85:GLN:HA	1.73	1.02
1:E:155:LYS:O	1:E:156:ASP:HB2	1.51	1.02
1:C:47:ARG:CG	1:C:48:PRO:HD2	1.89	1.02
1:E:47:ARG:CG	1:E:48:PRO:HD2	1.89	1.02
1:A:60:LEU:CG	1:E:452:ARG:HG2	1.90	1.02
1:D:436:GLN:HE22	1:E:126:ILE:HD12	0.88	1.02
1:A:292:TYR:HE1	1:A:376:LYS:CD	1.72	1.02
1:A:47:ARG:CG	1:A:48:PRO:HD2	1.89	1.02
1:A:476:TYR:HE2	1:B:477:ASN:HB3	1.23	1.02
1:D:482:TYR:CE1	1:E:486:ILE:CG2	2.42	1.02
1:B:292:TYR:HE1	1:B:376:LYS:CD	1.72	1.01
1:A:265:GLN:NE2	1:B:85:GLN:HA	1.73	1.01
1:A:60:LEU:CD1	1:E:452:ARG:HG2	1.89	1.01
1:A:556:LYS:NZ	1:E:436:GLN:HB2	1.75	1.01
1:D:292:TYR:HE1	1:D:376:LYS:CD	1.72	1.01
1:B:47:ARG:CG	1:B:48:PRO:HD2	1.89	1.01
1:A:490:THR:HB	1:E:481:VAL:HG12	1.41	1.01
1:A:57:TYR:CE2	1:A:60:LEU:CG	2.44	1.01
1:D:450:THR:CG2	1:E:57:TYR:CE1	2.42	1.01
2:F:14:VAL:HG13	1:B:203:GLU:OE2	1.60	1.01
1:D:436:GLN:NE2	1:E:126:ILE:CD1	2.23	1.01
1:B:174:ASN:ND2	1:B:183:LEU:CD1	2.23	1.01
1:A:85:GLN:HA	1:E:265:GLN:NE2	1.75	1.01
1:C:47:ARG:HG3	1:C:48:PRO:HD2	1.36	1.01
2:H:8:GLU:HG3	2:H:9:ASP:H	1.22	1.01
1:D:174:ASN:ND2	1:D:183:LEU:CD1	2.23	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ASN:ND2	1:C:183:LEU:CD1	2.23	1.01
1:A:174:ASN:ND2	1:A:183:LEU:CD1	2.23	1.01
2:H:13:PRO:HA	1:E:197:ARG:HH12	1.24	1.01
1:B:434:SER:HB2	1:C:128:HIS:ND1	1.75	1.01
1:A:47:ARG:HB2	1:E:569:ARG:O	1.61	1.01
1:D:436:GLN:HE22	1:E:558:LEU:HD11	1.25	1.00
1:D:292:TYR:HE1	1:D:376:LYS:HD3	0.84	1.00
1:A:57:TYR:HE2	1:A:60:LEU:HG	1.20	1.00
1:B:436:GLN:N	1:C:556:LYS:HZ1	1.59	1.00
1:E:410:TYR:CD2	1:E:425:LEU:CD1	2.43	1.00
2:H:14:VAL:HG13	1:E:203:GLU:OE2	1.61	1.00
2:H:12:ASN:O	2:H:14:VAL:HG23	1.62	1.00
1:D:481:VAL:HG12	1:E:490:THR:HB	1.44	1.00
1:E:174:ASN:ND2	1:E:183:LEU:CD1	2.23	1.00
1:C:459:ASN:HB2	1:D:99:ASN:HB3	1.38	1.00
2:G:12:ASN:O	2:G:14:VAL:HG23	1.62	0.99
1:C:267:PHE:HE2	1:D:76:SER:CB	1.69	0.99
1:B:265:GLN:NE2	1:C:85:GLN:HA	1.75	0.99
1:A:292:TYR:HE1	1:A:376:LYS:HD3	0.84	0.99
2:F:12:ASN:O	2:F:14:VAL:HG23	1.62	0.99
1:B:476:TYR:HE2	1:C:477:ASN:HB3	1.28	0.99
1:E:84:TYR:O	1:E:85:GLN:HG3	1.63	0.99
1:D:569:ARG:O	1:E:47:ARG:HB2	1.61	0.99
1:D:84:TYR:O	1:D:85:GLN:HG3	1.63	0.99
1:C:452:ARG:CG	1:D:60:LEU:CD2	2.35	0.99
1:C:452:ARG:CG	1:D:60:LEU:HD11	1.93	0.99
1:C:452:ARG:HG2	1:D:60:LEU:HD21	1.32	0.98
1:B:569:ARG:O	1:C:47:ARG:HB2	1.63	0.98
1:B:84:TYR:O	1:B:85:GLN:HG3	1.63	0.98
1:D:267:PHE:HE2	1:E:76:SER:CB	1.68	0.98
1:A:126:ILE:CD1	1:E:436:GLN:NE2	2.25	0.98
1:D:434:SER:HB3	1:E:556:LYS:HB2	1.45	0.98
1:C:569:ARG:O	1:D:47:ARG:HB2	1.64	0.98
1:A:267:PHE:HE2	1:B:84:TYR:CD1	1.81	0.98
2:G:13:PRO:HA	1:C:197:ARG:HH12	1.23	0.98
1:A:569:ARG:O	1:B:47:ARG:HB2	1.62	0.98
1:B:292:TYR:HE1	1:B:376:LYS:HD3	0.84	0.97
1:D:433:GLY:HA2	1:E:555:TYR:HE2	1.23	0.97
1:C:267:PHE:HE2	1:D:76:SER:HB2	1.29	0.97
1:D:434:SER:HB2	1:E:128:HIS:ND1	1.79	0.97
1:C:434:SER:HB2	1:D:128:HIS:ND1	1.78	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:GLN:HB2	1:E:556:LYS:NZ	1.80	0.97
1:A:82:LEU:HD13	1:A:92:LEU:HD13	1.46	0.97
1:A:60:LEU:CD1	1:E:452:ARG:CG	2.42	0.97
1:D:228:PRO:CG	2:H:15:TYR:CE1	2.42	0.97
1:D:267:PHE:HE2	1:E:76:SER:HB2	1.29	0.97
1:D:476:TYR:HE2	1:E:477:ASN:HB3	1.28	0.97
1:C:410:TYR:CD2	1:C:425:LEU:HD12	1.99	0.97
1:B:434:SER:HB3	1:C:556:LYS:HB2	1.43	0.97
1:A:228:PRO:CG	2:F:15:TYR:CE1	2.42	0.97
1:A:434:SER:HB2	1:B:128:HIS:ND1	1.78	0.97
1:D:425:LEU:HD13	1:E:172:GLU:CG	1.93	0.97
2:F:13:PRO:HA	1:B:197:ARG:HH12	1.27	0.97
1:E:82:LEU:HD13	1:E:92:LEU:HD13	1.46	0.96
1:A:436:GLN:HB2	1:B:556:LYS:NZ	1.80	0.96
1:C:82:LEU:HD13	1:C:92:LEU:HD13	1.46	0.96
1:B:433:GLY:CA	1:C:555:TYR:HE2	1.78	0.96
1:A:84:TYR:O	1:A:85:GLN:HG3	1.63	0.96
1:B:82:LEU:HD13	1:B:92:LEU:HD13	1.46	0.96
1:A:464:GLY:HA3	1:B:68:ARG:NH1	1.80	0.96
1:B:436:GLN:HB2	1:C:556:LYS:NZ	1.79	0.96
1:C:230:VAL:HG11	1:D:492:LEU:CB	1.96	0.96
1:A:436:GLN:OE1	1:B:558:LEU:HD11	1.66	0.96
1:A:569:ARG:HA	1:B:47:ARG:HB2	1.47	0.96
1:E:57:TYR:O	1:E:57:TYR:CD1	2.19	0.95
1:A:556:LYS:HZ1	1:E:436:GLN:N	1.63	0.95
1:D:436:GLN:NE2	1:E:558:LEU:HD11	1.80	0.95
1:A:476:TYR:CE2	1:B:477:ASN:HB3	2.01	0.95
1:D:57:TYR:O	1:D:57:TYR:CD1	2.19	0.95
1:C:433:GLY:HA2	1:D:555:TYR:HE2	1.29	0.95
1:C:434:SER:HB3	1:D:556:LYS:HB2	1.46	0.95
1:C:436:GLN:HE22	1:D:126:ILE:HD12	1.16	0.95
1:A:230:VAL:HG11	1:B:492:LEU:CB	1.97	0.95
1:C:569:ARG:HA	1:D:47:ARG:HB2	1.49	0.95
1:C:84:TYR:O	1:C:85:GLN:HG3	1.63	0.95
1:A:126:ILE:HD12	1:E:436:GLN:HE22	0.96	0.95
1:A:433:GLY:CA	1:B:555:TYR:HE2	1.78	0.95
1:C:228:PRO:CG	1:D:493:THR:HG21	1.96	0.95
1:B:434:SER:O	1:C:556:LYS:HD3	1.65	0.95
1:A:172:GLU:CG	1:E:425:LEU:HD13	1.95	0.94
1:B:450:THR:CG2	1:C:57:TYR:CD1	2.50	0.94
1:A:434:SER:HB3	1:B:556:LYS:HB2	1.45	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:LEU:CB	1:E:230:VAL:HG11	1.97	0.94
1:A:450:THR:CG2	1:B:57:TYR:CD1	2.50	0.94
1:C:425:LEU:HD13	1:D:172:GLU:HB2	0.95	0.94
1:B:433:GLY:HA2	1:C:555:TYR:HE2	1.24	0.94
1:B:376:LYS:CD	1:B:378:VAL:HG13	1.98	0.94
1:A:464:GLY:CA	1:B:68:ARG:NH1	2.30	0.94
1:D:569:ARG:HA	1:E:47:ARG:HB2	1.47	0.94
1:D:376:LYS:CD	1:D:378:VAL:HG13	1.98	0.94
1:C:436:GLN:HB2	1:D:556:LYS:NZ	1.82	0.94
1:D:433:GLY:CA	1:E:555:TYR:HE2	1.81	0.94
1:D:82:LEU:HD13	1:D:92:LEU:HD13	1.46	0.94
1:C:154:THR:O	1:C:155:LYS:HB2	1.68	0.94
1:B:230:VAL:HG11	1:C:492:LEU:CB	1.97	0.94
2:G:15:TYR:HB2	1:C:498:ARG:NH1	1.82	0.94
1:D:434:SER:O	1:E:556:LYS:HD3	1.67	0.94
1:A:555:TYR:CE2	1:E:433:GLY:HA2	2.03	0.94
1:C:452:ARG:HD2	1:D:60:LEU:CD1	1.96	0.94
1:D:57:TYR:HE2	1:D:60:LEU:CD2	1.81	0.94
1:E:174:ASN:ND2	1:E:183:LEU:HD11	1.84	0.93
1:B:57:TYR:CE2	1:B:60:LEU:CB	2.51	0.93
1:C:174:ASN:ND2	1:C:183:LEU:HD11	1.83	0.93
1:B:450:THR:HG23	1:C:57:TYR:HE1	1.23	0.93
1:A:556:LYS:HE2	1:A:558:LEU:CD2	1.97	0.93
1:C:436:GLN:N	1:D:556:LYS:HZ1	1.66	0.93
1:A:60:LEU:CD2	1:E:452:ARG:CG	2.23	0.93
1:C:57:TYR:CE2	1:C:60:LEU:CB	2.51	0.93
1:A:556:LYS:CE	1:A:558:LEU:HD23	1.97	0.93
1:A:63:LEU:HD22	1:A:67:THR:CG2	1.98	0.93
1:A:228:PRO:HG3	2:F:15:TYR:HE1	0.93	0.93
1:A:154:THR:O	1:A:155:LYS:HB2	1.68	0.93
1:A:172:GLU:CB	1:E:425:LEU:CD1	2.35	0.93
1:A:60:LEU:HD21	1:E:452:ARG:HG2	1.04	0.93
1:E:63:LEU:HD22	1:E:67:THR:CG2	1.98	0.93
1:B:569:ARG:HA	1:C:47:ARG:HB2	1.47	0.93
1:B:63:LEU:HD22	1:B:67:THR:CG2	1.98	0.92
1:A:86:ASN:O	1:E:267:PHE:CE1	2.22	0.92
1:C:63:LEU:HD22	1:C:67:THR:CG2	1.98	0.92
1:A:47:ARG:HB2	1:E:569:ARG:HA	1.46	0.92
1:A:556:LYS:HZ1	1:E:436:GLN:CB	1.82	0.92
1:A:436:GLN:N	1:B:556:LYS:HZ1	1.67	0.92
1:B:529:LEU:HD21	1:C:68:ARG:HH11	1.34	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ARG:HB2	1:E:569:ARG:C	1.90	0.92
1:D:174:ASN:ND2	1:D:183:LEU:HD11	1.84	0.92
1:B:154:THR:O	1:B:155:LYS:HB2	1.68	0.92
1:E:154:THR:O	1:E:155:LYS:HB2	1.68	0.92
1:A:376:LYS:CD	1:A:378:VAL:HG13	1.98	0.92
1:A:434:SER:O	1:B:556:LYS:HD3	1.68	0.92
1:E:68:ARG:HD2	1:E:70:TYR:CE2	2.04	0.92
1:B:144:LYS:HB2	1:B:249:ASP:HB3	1.52	0.92
1:C:434:SER:O	1:D:556:LYS:HD3	1.69	0.91
1:A:490:THR:HG21	1:E:482:TYR:HB2	1.50	0.91
2:G:13:PRO:HA	1:C:197:ARG:NH1	1.85	0.91
2:H:15:TYR:HB2	1:E:498:ARG:NH1	1.83	0.91
1:D:63:LEU:HD22	1:D:67:THR:CG2	1.98	0.91
1:D:476:TYR:CE2	1:E:477:ASN:HB3	2.05	0.91
1:C:144:LYS:HB2	1:C:249:ASP:HB3	1.52	0.91
1:A:68:ARG:NH1	1:E:464:GLY:HA3	1.86	0.91
1:A:144:LYS:HB2	1:A:249:ASP:HB3	1.52	0.91
1:B:267:PHE:CE2	1:C:86:ASN:O	2.24	0.91
1:C:450:THR:HG23	1:D:57:TYR:CZ	2.05	0.91
1:A:128:HIS:ND1	1:E:434:SER:HB2	1.85	0.91
1:C:410:TYR:HE2	1:D:172:GLU:CG	1.83	0.91
2:F:15:TYR:HB2	1:B:498:ARG:NH1	1.86	0.91
1:A:450:THR:HG23	1:B:57:TYR:HE1	1.21	0.91
1:D:230:VAL:HG11	1:E:492:LEU:CB	2.00	0.91
1:E:47:ARG:CZ	1:E:53:ASN:HD22	1.83	0.91
1:C:267:PHE:CD1	1:D:83:ASN:HB3	2.06	0.91
1:B:221:PRO:HG3	1:C:194:LYS:HB2	1.53	0.91
1:A:267:PHE:CE1	1:B:76:SER:O	2.23	0.91
1:B:174:ASN:ND2	1:B:183:LEU:HD11	1.84	0.91
1:B:47:ARG:CZ	1:B:53:ASN:HD22	1.84	0.91
1:A:569:ARG:C	1:B:47:ARG:HB2	1.92	0.91
2:H:15:TYR:OH	1:E:493:THR:HB	1.69	0.90
1:B:425:LEU:CD1	1:C:172:GLU:HB2	2.00	0.90
1:B:233:ASN:HB3	1:C:491:SER:CA	2.01	0.90
1:C:47:ARG:CZ	1:C:53:ASN:HD22	1.84	0.90
1:D:47:ARG:CZ	1:D:53:ASN:HD22	1.83	0.90
1:E:144:LYS:HB2	1:E:249:ASP:HB3	1.52	0.90
1:C:452:ARG:HG2	1:D:60:LEU:HG	1.52	0.90
1:B:68:ARG:HD2	1:B:70:TYR:CE2	2.04	0.90
1:A:57:TYR:CD1	1:E:450:THR:HA	2.07	0.90
1:A:493:THR:HG21	1:E:228:PRO:CG	2.01	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:PHE:CD1	1:E:83:ASN:HB3	2.05	0.90
1:B:410:TYR:HE2	1:C:172:GLU:CG	1.84	0.90
1:D:68:ARG:HD2	1:D:70:TYR:CE2	2.04	0.90
1:B:476:TYR:CE2	1:C:477:ASN:HB3	2.05	0.90
1:C:82:LEU:HB3	1:C:92:LEU:HD12	1.54	0.90
1:A:425:LEU:HD13	1:B:172:GLU:HB2	1.53	0.90
1:D:154:THR:O	1:D:155:LYS:HB2	1.68	0.90
1:E:174:ASN:HD21	1:E:183:LEU:HD13	1.36	0.90
1:B:228:PRO:CG	2:G:15:TYR:CE1	2.42	0.90
1:A:491:SER:CA	1:E:233:ASN:HB3	2.02	0.90
1:C:476:TYR:HE2	1:D:477:ASN:HB3	1.37	0.90
1:D:174:ASN:HD21	1:D:183:LEU:HD13	1.36	0.90
1:D:228:PRO:HG3	2:H:15:TYR:HE1	0.94	0.90
1:C:174:ASN:HD21	1:C:183:LEU:HD13	1.35	0.90
1:B:450:THR:HG21	1:C:96:ILE:HG23	1.54	0.90
1:B:425:LEU:HD13	1:C:172:GLU:CB	2.00	0.90
1:A:410:TYR:HE2	1:B:172:GLU:CG	1.85	0.90
1:A:47:ARG:CZ	1:A:53:ASN:HD22	1.84	0.89
1:B:556:LYS:CE	1:B:558:LEU:HD23	2.03	0.89
1:A:174:ASN:ND2	1:A:183:LEU:HD11	1.84	0.89
1:A:83:ASN:HB3	1:E:267:PHE:CE1	2.06	0.89
1:A:68:ARG:HD2	1:A:70:TYR:CE2	2.05	0.89
1:D:144:LYS:HB2	1:D:249:ASP:HB3	1.52	0.89
1:A:172:GLU:CG	1:E:410:TYR:HE2	1.85	0.89
1:A:194:LYS:HB2	1:E:221:PRO:HG3	1.51	0.89
1:D:57:TYR:CE2	1:D:60:LEU:CD2	2.54	0.89
1:B:434:SER:O	1:C:556:LYS:CD	2.20	0.89
1:D:482:TYR:HB2	1:E:490:THR:HG21	1.53	0.89
1:B:174:ASN:HD21	1:B:183:LEU:HD13	1.36	0.89
1:E:410:TYR:CE2	1:E:425:LEU:CD1	2.55	0.89
2:F:15:TYR:OH	1:B:493:THR:HB	1.70	0.89
1:C:68:ARG:HD2	1:C:70:TYR:CZ	2.08	0.89
1:D:569:ARG:C	1:E:47:ARG:HB2	1.92	0.89
1:B:267:PHE:CD1	1:C:76:SER:HB2	2.07	0.89
1:C:233:ASN:HB3	1:D:491:SER:CA	2.01	0.89
1:A:60:LEU:HD21	1:E:452:ARG:NE	1.85	0.89
1:C:57:TYR:CE2	1:C:60:LEU:HB2	2.08	0.89
1:B:57:TYR:CE2	1:B:60:LEU:HB2	2.08	0.88
1:A:99:ASN:HB3	1:E:459:ASN:HB3	1.55	0.88
1:D:436:GLN:HE22	1:E:126:ILE:CD1	1.82	0.88
1:D:436:GLN:N	1:E:556:LYS:HZ1	1.72	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:PHE:HE1	1:C:76:SER:HB2	0.98	0.88
1:C:556:LYS:CE	1:C:558:LEU:HD23	2.02	0.88
1:B:569:ARG:C	1:C:47:ARG:HB2	1.92	0.88
1:A:555:TYR:OH	1:E:257:ASN:CB	2.21	0.88
1:A:83:ASN:HD21	1:A:91:PHE:HB2	1.35	0.88
1:A:233:ASN:HB3	1:B:491:SER:CA	2.02	0.88
1:E:556:LYS:CE	1:E:558:LEU:HD23	2.03	0.88
1:A:482:TYR:CE1	1:B:486:ILE:CG2	2.55	0.88
1:A:82:LEU:HB3	1:A:92:LEU:HD12	1.54	0.88
1:A:174:ASN:HD21	1:A:183:LEU:HD13	1.36	0.88
1:D:82:LEU:HB3	1:D:92:LEU:HD12	1.54	0.88
1:D:425:LEU:HD13	1:E:172:GLU:HB3	1.54	0.88
1:A:68:ARG:NH1	1:E:464:GLY:CA	2.37	0.88
1:C:267:PHE:CE1	1:D:86:ASN:O	2.27	0.88
1:E:82:LEU:HB3	1:E:92:LEU:HD12	1.54	0.88
1:A:198:GLN:NE2	1:E:222:VAL:HG21	1.89	0.88
1:C:433:GLY:CA	1:D:555:TYR:HE2	1.85	0.88
2:H:13:PRO:HA	1:E:197:ARG:NH1	1.88	0.87
1:D:556:LYS:CE	1:D:558:LEU:HD23	2.03	0.87
1:E:83:ASN:HD21	1:E:91:PHE:HB2	1.35	0.87
1:C:68:ARG:HD2	1:C:70:TYR:CE2	2.07	0.87
1:C:221:PRO:HG3	1:D:194:LYS:HB2	1.55	0.87
1:D:221:PRO:HG3	1:E:194:LYS:HB2	1.56	0.87
1:A:556:LYS:HD3	1:E:434:SER:O	1.74	0.87
1:D:267:PHE:CE1	1:E:86:ASN:O	2.26	0.87
1:C:569:ARG:C	1:D:47:ARG:HB2	1.95	0.87
1:A:267:PHE:HE1	1:B:76:SER:O	1.58	0.87
1:B:82:LEU:HB3	1:B:92:LEU:HD12	1.54	0.87
1:C:83:ASN:HD21	1:C:91:PHE:HB2	1.36	0.87
1:A:57:TYR:CD1	1:E:450:THR:CB	2.57	0.87
1:B:228:PRO:HG3	2:G:15:TYR:CD1	2.10	0.87
1:C:482:TYR:HB2	1:D:490:THR:HG21	1.56	0.87
1:B:227:MET:O	2:G:17:TYR:CE2	2.28	0.87
1:C:233:ASN:CB	1:D:491:SER:HA	2.05	0.87
1:C:174:ASN:ND2	1:C:183:LEU:HD13	1.90	0.87
1:D:57:TYR:HE2	1:D:60:LEU:CG	1.88	0.86
1:A:172:GLU:HB2	1:E:425:LEU:HD13	0.88	0.86
1:B:230:VAL:HG13	1:B:503:GLN:HE22	1.40	0.86
2:G:15:TYR:OH	1:C:493:THR:HB	1.74	0.86
1:A:228:PRO:HG3	2:F:15:TYR:CD1	2.10	0.86
2:H:13:PRO:HB2	2:H:17:TYR:HE1	1.40	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ARG:HD3	1:B:70:TYR:HE2	1.40	0.86
1:A:68:ARG:HD3	1:A:70:TYR:HE2	1.39	0.86
1:A:477:ASN:HB3	1:E:476:TYR:HE2	1.39	0.86
1:A:174:ASN:ND2	1:A:183:LEU:HD13	1.90	0.86
1:A:230:VAL:HG13	1:A:503:GLN:HE22	1.40	0.86
1:A:76:SER:HB3	1:E:267:PHE:CE2	2.10	0.86
1:A:410:TYR:CE2	1:A:425:LEU:HD13	2.10	0.86
1:E:68:ARG:HD3	1:E:70:TYR:HE2	1.40	0.86
1:D:230:VAL:HG13	1:D:503:GLN:HE22	1.40	0.86
1:B:266:PRO:HD3	1:C:87:ASP:HB3	1.57	0.86
1:D:436:GLN:CB	1:E:556:LYS:HZ1	1.88	0.86
1:D:83:ASN:HD21	1:D:91:PHE:HB2	1.35	0.86
1:A:76:SER:CB	1:E:267:PHE:CE2	2.57	0.86
1:A:221:PRO:HG3	1:B:194:LYS:HB2	1.58	0.86
1:D:57:TYR:CZ	1:D:60:LEU:HD13	2.09	0.86
1:A:227:MET:O	2:F:17:TYR:HE2	1.57	0.86
2:F:13:PRO:HA	1:B:197:ARG:NH1	1.91	0.86
1:D:233:ASN:HB3	1:E:491:SER:CA	2.04	0.86
1:A:450:THR:HG21	1:B:96:ILE:HG23	1.56	0.86
1:B:434:SER:HB3	1:C:556:LYS:CB	2.04	0.86
1:B:227:MET:O	2:G:17:TYR:HE2	1.57	0.86
1:A:227:MET:O	2:F:17:TYR:CE2	2.28	0.86
1:D:227:MET:O	2:H:17:TYR:CE2	2.28	0.86
1:D:228:PRO:HG3	2:H:15:TYR:CD1	2.10	0.86
1:A:233:ASN:CB	1:B:491:SER:HA	2.06	0.86
1:E:230:VAL:HG13	1:E:503:GLN:HE22	1.40	0.86
1:D:410:TYR:HE2	1:E:172:GLU:CG	1.86	0.85
1:B:482:TYR:HB2	1:C:490:THR:HG21	1.55	0.85
1:D:434:SER:O	1:E:556:LYS:CD	2.23	0.85
1:B:222:VAL:HG21	1:C:198:GLN:NE2	1.91	0.85
1:E:60:LEU:HG	1:E:61:ALA:H	1.42	0.85
1:A:459:ASN:HB3	1:B:99:ASN:HB3	1.58	0.85
1:E:152:LEU:HB3	1:E:153:PRO:HD2	1.59	0.85
1:C:434:SER:O	1:D:556:LYS:CD	2.24	0.85
1:A:410:TYR:CD2	1:A:425:LEU:HD13	2.12	0.85
1:C:152:LEU:HB3	1:C:153:PRO:HD2	1.59	0.85
1:D:434:SER:HB3	1:E:556:LYS:CB	2.07	0.85
1:C:230:VAL:HG13	1:C:503:GLN:HE22	1.40	0.85
1:A:434:SER:O	1:B:556:LYS:CD	2.23	0.85
1:D:152:LEU:HB3	1:D:153:PRO:HD2	1.59	0.85
1:A:491:SER:HA	1:E:233:ASN:CB	2.06	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:TYR:CD2	1:D:425:LEU:HD11	2.10	0.85
2:G:13:PRO:HB2	2:G:17:TYR:HE1	1.40	0.85
1:B:152:LEU:HB3	1:B:153:PRO:HD2	1.59	0.85
1:B:60:LEU:HG	1:B:61:ALA:H	1.42	0.84
1:B:410:TYR:CD2	1:B:425:LEU:CD1	2.59	0.84
1:B:233:ASN:CB	1:C:491:SER:HA	2.05	0.84
1:C:436:GLN:NE2	1:D:126:ILE:CD1	2.40	0.84
1:A:57:TYR:HD1	1:E:450:THR:CB	1.90	0.84
1:D:450:THR:HG21	1:E:96:ILE:HG23	1.57	0.84
1:C:60:LEU:HG	1:C:61:ALA:H	1.42	0.84
1:D:227:MET:O	2:H:17:TYR:HE2	1.57	0.84
1:E:174:ASN:ND2	1:E:183:LEU:HD13	1.90	0.84
1:A:152:LEU:HB3	1:A:153:PRO:HD2	1.59	0.84
1:B:459:ASN:HB2	1:C:99:ASN:CB	2.07	0.84
1:C:425:LEU:O	1:D:132:PRO:HG2	1.77	0.84
1:C:436:GLN:CB	1:D:556:LYS:HZ1	1.90	0.84
1:C:556:LYS:HE2	1:C:558:LEU:CD2	2.07	0.84
1:B:449:VAL:HG13	1:C:55:ILE:HD13	1.58	0.84
1:B:482:TYR:CE1	1:C:486:ILE:CG2	2.60	0.84
1:A:87:ASP:HB3	1:E:266:PRO:HD3	1.57	0.84
2:F:13:PRO:HB2	2:F:17:TYR:HE1	1.40	0.84
1:B:425:LEU:O	1:C:132:PRO:HG2	1.77	0.84
1:A:68:ARG:HD2	1:A:70:TYR:CZ	2.12	0.84
1:C:268:GLN:HE21	1:D:84:TYR:HD2	1.26	0.84
1:A:555:TYR:HE2	1:E:433:GLY:CA	1.90	0.84
1:C:266:PRO:HD3	1:D:87:ASP:HB3	1.59	0.84
1:B:83:ASN:HD21	1:B:91:PHE:HB2	1.35	0.84
1:D:436:GLN:HB2	1:E:556:LYS:HZ1	1.39	0.84
1:C:450:THR:HG21	1:D:96:ILE:HG23	1.58	0.84
1:D:222:VAL:HG21	1:E:198:GLN:NE2	1.93	0.84
2:H:9:ASP:O	2:H:10:THR:HB	1.79	0.83
1:A:434:SER:HB3	1:B:556:LYS:CB	2.07	0.83
1:A:556:LYS:HZ1	1:E:436:GLN:HB2	1.36	0.83
1:B:174:ASN:ND2	1:B:183:LEU:HD13	1.90	0.83
1:E:556:LYS:HE2	1:E:558:LEU:CD2	2.08	0.83
1:C:434:SER:HB3	1:D:556:LYS:CB	2.07	0.83
1:B:425:LEU:CD2	1:C:172:GLU:HB3	2.08	0.83
1:A:486:ILE:HG23	1:E:482:TYR:CE1	2.11	0.83
1:D:266:PRO:HD3	1:E:87:ASP:HB3	1.60	0.83
1:D:556:LYS:HE2	1:D:558:LEU:CD2	2.08	0.83
1:B:436:GLN:NE2	1:B:465:ALA:CB	2.40	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ASN:CB	1:E:491:SER:HA	2.08	0.83
1:D:57:TYR:CD2	1:D:60:LEU:HB2	2.14	0.83
1:E:57:TYR:CD2	1:E:60:LEU:HB3	2.13	0.83
1:C:449:VAL:HG13	1:D:55:ILE:HD13	1.58	0.83
1:D:68:ARG:HD3	1:D:70:TYR:HE2	1.40	0.83
1:A:55:ILE:HD13	1:E:449:VAL:HG13	1.60	0.83
1:A:555:TYR:CE1	1:E:262:ARG:HD2	2.14	0.83
1:A:410:TYR:CD2	1:A:425:LEU:HD12	2.10	0.83
1:A:132:PRO:HG2	1:E:425:LEU:O	1.78	0.82
1:B:266:PRO:CD	1:C:87:ASP:CB	2.57	0.82
1:C:476:TYR:CE2	1:D:477:ASN:HB3	2.13	0.82
1:A:555:TYR:CE2	1:E:433:GLY:CA	2.62	0.82
1:E:82:LEU:HD13	1:E:92:LEU:CD1	2.09	0.82
1:A:436:GLN:NE2	1:A:465:ALA:CB	2.41	0.82
1:C:47:ARG:NH2	1:C:53:ASN:ND2	2.28	0.82
1:A:477:ASN:HB3	1:E:476:TYR:CE2	2.15	0.82
1:B:230:VAL:HG11	1:C:492:LEU:HB3	1.62	0.82
1:A:425:LEU:O	1:B:132:PRO:HG2	1.79	0.82
1:C:68:ARG:HD3	1:C:70:TYR:HE2	1.39	0.82
1:B:425:LEU:CD2	1:C:172:GLU:CB	2.56	0.82
1:D:174:ASN:ND2	1:D:183:LEU:HD13	1.90	0.82
1:C:436:GLN:HB2	1:D:556:LYS:HZ1	1.44	0.82
1:B:556:LYS:HE2	1:B:558:LEU:CD2	2.08	0.82
1:C:82:LEU:HD13	1:C:92:LEU:CD1	2.09	0.82
1:C:267:PHE:CD1	1:D:86:ASN:O	2.33	0.81
1:A:198:GLN:NE2	1:E:222:VAL:CG2	2.43	0.81
1:C:222:VAL:HG21	1:D:198:GLN:NE2	1.95	0.81
1:D:82:LEU:HD13	1:D:92:LEU:CD1	2.09	0.81
1:E:51:GLY:O	1:E:114:ASP:CB	2.28	0.81
1:B:82:LEU:HD13	1:B:92:LEU:CD1	2.09	0.81
1:B:264:ARG:NE	1:B:424:LEU:HD21	1.95	0.81
1:A:47:ARG:CB	1:E:569:ARG:O	2.29	0.81
1:A:492:LEU:HB3	1:E:230:VAL:HG11	1.62	0.81
1:A:222:VAL:HG21	1:B:198:GLN:NE2	1.96	0.81
1:C:51:GLY:O	1:C:114:ASP:CB	2.28	0.81
1:B:57:TYR:CE2	1:B:60:LEU:HB3	2.14	0.81
1:D:449:VAL:HG13	1:E:55:ILE:HD13	1.61	0.81
1:A:264:ARG:NE	1:A:424:LEU:HD21	1.96	0.81
2:F:9:ASP:O	2:F:10:THR:HB	1.79	0.81
1:A:82:LEU:HD13	1:A:92:LEU:CD1	2.09	0.81
1:D:264:ARG:NE	1:D:424:LEU:HD21	1.96	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:VAL:HG13	1:B:55:ILE:HD13	1.61	0.81
1:A:57:TYR:HD1	1:E:450:THR:HG22	0.65	0.81
1:A:51:GLY:O	1:A:114:ASP:CB	2.29	0.81
1:A:266:PRO:HD3	1:B:87:ASP:HB3	1.61	0.81
1:D:51:GLY:O	1:D:114:ASP:CB	2.28	0.81
1:B:51:GLY:O	1:B:114:ASP:CB	2.28	0.81
1:C:459:ASN:HB2	1:D:99:ASN:CB	2.10	0.81
1:A:450:THR:HG21	1:B:96:ILE:CG2	2.11	0.81
1:B:450:THR:HG21	1:C:96:ILE:CG2	2.10	0.81
1:D:459:ASN:HB2	1:E:99:ASN:CB	2.10	0.81
1:D:267:PHE:CD1	1:E:86:ASN:O	2.34	0.81
1:A:87:ASP:CB	1:E:266:PRO:CD	2.58	0.81
1:C:264:ARG:NE	1:C:424:LEU:HD21	1.96	0.81
1:E:264:ARG:NE	1:E:424:LEU:HD21	1.96	0.80
1:D:410:TYR:CZ	1:D:425:LEU:HD12	2.11	0.80
1:A:267:PHE:CE2	1:B:84:TYR:CD1	2.69	0.80
1:C:228:PRO:HB3	1:D:493:THR:HG23	1.60	0.80
1:A:425:LEU:CD2	1:B:172:GLU:CB	2.59	0.80
1:A:436:GLN:NE2	1:A:465:ALA:HB1	1.92	0.80
1:B:474:SER:HB3	1:C:473:LYS:HG3	1.63	0.80
1:A:475:PHE:HD2	1:E:476:TYR:CD1	1.99	0.80
1:C:57:TYR:CE2	1:C:60:LEU:HB3	2.13	0.80
1:C:257:ASN:CB	1:D:555:TYR:OH	2.29	0.80
1:B:222:VAL:CG2	1:C:198:GLN:NE2	2.45	0.80
1:D:569:ARG:O	1:E:47:ARG:CB	2.30	0.80
1:C:476:TYR:CD1	1:D:475:PHE:HD2	1.99	0.80
1:A:436:GLN:HB2	1:B:556:LYS:HZ1	1.46	0.80
1:C:234:GLU:HG3	1:D:487:ARG:HH21	1.46	0.80
1:C:425:LEU:HD22	1:D:172:GLU:HB3	1.64	0.80
1:A:410:TYR:CE2	1:A:425:LEU:CD1	2.65	0.80
1:D:425:LEU:O	1:E:132:PRO:HG2	1.80	0.80
1:D:268:GLN:HE21	1:E:84:TYR:HD2	1.26	0.80
1:C:411:ASN:ND2	1:D:172:GLU:H	1.79	0.80
1:A:493:THR:HG23	1:E:228:PRO:HB3	1.60	0.80
1:A:480:ALA:O	1:A:481:VAL:CG2	2.30	0.80
1:A:555:TYR:CD2	1:E:433:GLY:HA2	2.16	0.80
1:A:268:GLN:HE21	1:B:84:TYR:HD2	1.28	0.80
1:B:436:GLN:HG3	1:B:466:GLU:C	2.02	0.80
1:A:84:TYR:HD2	1:E:268:GLN:HE21	1.27	0.80
1:C:266:PRO:CD	1:D:87:ASP:CB	2.60	0.80
1:C:217:LEU:HD12	1:C:232:THR:HG21	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:GLN:HG3	1:D:466:GLU:C	2.02	0.80
1:C:436:GLN:HG3	1:C:466:GLU:C	2.02	0.80
1:A:425:LEU:HD22	1:B:172:GLU:HB2	1.63	0.80
1:A:436:GLN:CB	1:B:556:LYS:HZ1	1.94	0.80
1:B:68:ARG:HD2	1:B:70:TYR:CZ	2.17	0.80
1:B:480:ALA:O	1:B:481:VAL:CG2	2.30	0.80
1:C:452:ARG:CG	1:D:60:LEU:CD1	2.60	0.79
1:B:268:GLN:HE21	1:C:84:TYR:HD2	1.27	0.79
1:B:436:GLN:CB	1:C:556:LYS:HZ1	1.95	0.79
1:A:410:TYR:CG	1:A:425:LEU:HD12	2.16	0.79
1:A:86:ASN:O	1:E:267:PHE:CD1	2.34	0.79
1:B:476:TYR:HB2	1:C:475:PHE:CD2	2.18	0.79
1:C:482:TYR:CE1	1:D:486:ILE:HG23	2.16	0.79
1:B:217:LEU:HD12	1:B:232:THR:HG21	1.64	0.79
1:D:450:THR:HG21	1:E:96:ILE:CG2	2.11	0.79
1:D:217:LEU:HD12	1:D:232:THR:HG21	1.64	0.79
2:G:9:ASP:O	2:G:10:THR:HB	1.79	0.79
1:A:57:TYR:CD1	1:E:450:THR:CA	2.65	0.79
1:A:555:TYR:HE1	1:E:262:ARG:HD2	1.45	0.79
1:D:230:VAL:HG11	1:E:492:LEU:HB3	1.65	0.79
1:A:436:GLN:HG3	1:A:466:GLU:C	2.03	0.79
1:A:486:ILE:CG2	1:E:482:TYR:CD1	2.65	0.79
1:C:474:SER:HB3	1:D:473:LYS:HG3	1.65	0.79
1:A:87:ASP:HB3	1:E:266:PRO:CD	2.13	0.79
1:E:47:ARG:CZ	1:E:53:ASN:ND2	2.45	0.79
1:D:47:ARG:CZ	1:D:53:ASN:ND2	2.45	0.79
1:E:217:LEU:HD12	1:E:232:THR:HG21	1.64	0.79
1:A:57:TYR:CD2	1:A:60:LEU:HB2	2.17	0.79
1:A:464:GLY:HA2	1:B:68:ARG:NH1	1.98	0.79
1:A:569:ARG:O	1:B:47:ARG:CB	2.30	0.79
1:B:47:ARG:CZ	1:B:53:ASN:ND2	2.46	0.79
1:B:569:ARG:O	1:C:47:ARG:CB	2.31	0.79
1:B:266:PRO:CD	1:C:87:ASP:HB3	2.13	0.78
1:A:411:ASN:ND2	1:B:172:GLU:H	1.81	0.78
1:A:464:GLY:HA3	1:B:68:ARG:HH12	1.45	0.78
1:B:436:GLN:HB2	1:C:556:LYS:HZ3	1.46	0.78
1:E:68:ARG:HD2	1:E:70:TYR:CZ	2.17	0.78
1:A:486:ILE:HG22	1:E:482:TYR:CD1	2.18	0.78
1:D:266:PRO:CD	1:E:87:ASP:CB	2.62	0.78
1:B:234:GLU:HG3	1:C:487:ARG:HH21	1.48	0.78
1:C:450:THR:HG21	1:D:96:ILE:CG2	2.13	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:PRO:HG3	2:G:15:TYR:HE1	0.93	0.78
1:A:47:ARG:CZ	1:A:53:ASN:ND2	2.46	0.78
1:C:230:VAL:HG11	1:D:492:LEU:HB3	1.61	0.78
1:D:497:ASN:HD21	1:D:500:PRO:HB3	1.49	0.78
1:D:464:GLY:HA3	1:E:68:ARG:NH1	1.98	0.78
1:C:464:GLY:HA3	1:D:68:ARG:NH1	1.98	0.78
1:E:431:THR:O	1:E:432:CYS:HB2	1.81	0.78
1:A:217:LEU:HD12	1:A:232:THR:HG21	1.64	0.78
1:A:473:LYS:HG3	1:E:474:SER:HB3	1.64	0.78
1:B:266:PRO:HD3	1:C:87:ASP:CB	2.14	0.78
1:C:410:TYR:CD2	1:C:425:LEU:CD1	2.66	0.78
1:C:47:ARG:CZ	1:C:53:ASN:ND2	2.46	0.78
1:C:257:ASN:OD1	1:C:432:CYS:HA	1.83	0.78
1:D:425:LEU:CD1	1:E:172:GLU:CG	2.59	0.78
1:D:425:LEU:HD13	1:E:172:GLU:HB2	0.78	0.78
1:A:230:VAL:HG11	1:B:492:LEU:HB3	1.62	0.78
1:D:47:ARG:NH2	1:D:53:ASN:ND2	2.32	0.78
1:A:126:ILE:CD1	1:E:436:GLN:HE22	1.88	0.78
1:B:497:ASN:HD21	1:B:500:PRO:HB3	1.49	0.78
1:E:436:GLN:HG3	1:E:466:GLU:C	2.02	0.77
1:A:482:TYR:HB2	1:B:490:THR:HG21	1.65	0.77
2:F:8:GLU:O	2:F:9:ASP:CB	2.32	0.77
1:E:80:ALA:O	1:E:81:SER:HB3	1.84	0.77
1:A:172:GLU:CG	1:E:410:TYR:CE2	2.63	0.77
1:B:433:GLY:HA2	1:C:555:TYR:CD2	2.20	0.77
1:C:57:TYR:HE2	1:C:60:LEU:HB2	1.48	0.77
1:A:425:LEU:HD13	1:B:172:GLU:CB	2.13	0.77
1:A:482:TYR:CD1	1:B:486:ILE:CG2	2.68	0.77
1:A:475:PHE:CD2	1:E:476:TYR:HB2	2.19	0.77
1:D:482:TYR:CE1	1:E:486:ILE:HG23	2.18	0.77
1:A:234:GLU:HG3	1:B:487:ARG:HH21	1.47	0.77
1:E:497:ASN:HD21	1:E:500:PRO:HB3	1.49	0.77
1:D:68:ARG:HD2	1:D:70:TYR:CZ	2.19	0.77
1:D:257:ASN:CB	1:E:555:TYR:OH	2.33	0.77
2:G:10:THR:O	2:G:10:THR:HG22	1.84	0.77
1:D:411:ASN:ND2	1:E:172:GLU:H	1.82	0.77
1:D:474:SER:HG	1:E:475:PHE:HZ	1.33	0.77
1:A:87:ASP:CB	1:E:266:PRO:HD3	2.15	0.77
1:D:274:THR:HG22	1:D:275:TYR:H	1.50	0.77
1:A:474:SER:HB3	1:B:473:LYS:HG3	1.67	0.77
2:H:8:GLU:O	2:H:9:ASP:CB	2.32	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:THR:HG22	1:A:275:TYR:H	1.50	0.77
2:F:10:THR:HG22	2:F:10:THR:O	1.84	0.77
1:C:452:ARG:CG	1:D:60:LEU:CG	2.56	0.77
1:C:57:TYR:HD2	1:C:60:LEU:HB3	1.48	0.77
1:B:257:ASN:CB	1:C:555:TYR:OH	2.33	0.77
1:A:486:ILE:HG21	1:E:482:TYR:CE1	2.19	0.77
1:D:80:ALA:O	1:D:81:SER:HB3	1.84	0.77
1:A:266:PRO:CD	1:B:87:ASP:CB	2.62	0.77
1:A:497:ASN:HD21	1:A:500:PRO:HB3	1.49	0.77
1:A:425:LEU:CD1	1:B:172:GLU:HB2	2.15	0.77
1:D:222:VAL:CG2	1:E:198:GLN:NE2	2.48	0.77
1:B:80:ALA:O	1:B:81:SER:HB3	1.84	0.76
1:B:227:MET:CB	2:G:17:TYR:OH	2.32	0.76
1:A:410:TYR:CE2	1:B:172:GLU:CG	2.64	0.76
1:C:569:ARG:O	1:D:47:ARG:CB	2.32	0.76
2:H:10:THR:O	2:H:10:THR:HG22	1.84	0.76
1:C:497:ASN:HD21	1:C:500:PRO:HB3	1.49	0.76
1:C:425:LEU:HD13	1:D:172:GLU:CG	2.14	0.76
1:D:234:GLU:HG3	1:E:487:ARG:HH21	1.49	0.76
1:B:57:TYR:HD2	1:B:60:LEU:HB3	1.48	0.76
1:A:60:LEU:CD2	1:E:452:ARG:CD	2.59	0.76
1:D:227:MET:CB	2:H:17:TYR:OH	2.32	0.76
1:B:410:TYR:CD2	1:B:425:LEU:HD12	2.21	0.76
1:C:80:ALA:O	1:C:81:SER:HB3	1.84	0.76
1:A:172:GLU:H	1:E:411:ASN:ND2	1.84	0.76
1:A:227:MET:C	2:F:17:TYR:HE2	1.89	0.76
1:D:68:ARG:CD	1:D:70:TYR:HE2	1.94	0.76
1:E:274:THR:HG22	1:E:275:TYR:H	1.50	0.76
1:B:57:TYR:HE2	1:B:60:LEU:HB2	1.49	0.76
1:B:411:ASN:ND2	1:C:172:GLU:H	1.83	0.76
1:C:464:GLY:CA	1:D:68:ARG:NH1	2.49	0.76
1:A:47:ARG:CB	1:E:569:ARG:HA	2.14	0.76
1:D:57:TYR:CD2	1:D:60:LEU:HD22	2.20	0.76
1:E:68:ARG:CD	1:E:70:TYR:HE2	1.95	0.76
1:B:569:ARG:HA	1:C:47:ARG:HD2	1.68	0.76
1:C:262:ARG:HD2	1:D:555:TYR:CE1	2.21	0.76
1:B:463:VAL:C	1:C:70:TYR:OH	2.25	0.75
1:A:569:ARG:HA	1:B:47:ARG:CB	2.15	0.75
1:B:274:THR:HG22	1:B:275:TYR:H	1.49	0.75
1:C:436:GLN:NE2	1:D:558:LEU:HD21	2.00	0.75
2:H:9:ASP:O	2:H:10:THR:CB	2.34	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:TYR:CE2	1:E:432:CYS:O	2.39	0.75
1:A:227:MET:CB	2:F:17:TYR:OH	2.32	0.75
2:G:9:ASP:O	2:G:10:THR:CB	2.34	0.75
1:A:80:ALA:O	1:A:81:SER:HB3	1.84	0.75
1:C:266:PRO:HD3	1:D:87:ASP:CB	2.15	0.75
1:B:425:LEU:HD22	1:C:172:GLU:C	2.06	0.75
1:C:482:TYR:CD1	1:D:486:ILE:CG2	2.69	0.75
1:A:47:ARG:HD2	1:E:568:SER:O	1.87	0.75
1:C:265:GLN:NE2	1:D:85:GLN:CA	2.50	0.75
1:A:222:VAL:CG2	1:B:198:GLN:NE2	2.49	0.75
1:C:51:GLY:O	1:C:114:ASP:HB3	1.87	0.75
1:A:487:ARG:HH21	1:E:234:GLU:HG3	1.48	0.75
1:A:68:ARG:CD	1:A:70:TYR:HE2	1.97	0.75
1:A:476:TYR:HB2	1:B:475:PHE:CD2	2.21	0.75
2:H:8:GLU:HG3	2:H:9:ASP:N	2.01	0.75
2:F:8:GLU:HG3	2:F:9:ASP:N	2.01	0.75
1:C:222:VAL:CG2	1:D:198:GLN:NE2	2.49	0.75
1:B:227:MET:C	2:G:17:TYR:HE2	1.89	0.75
1:B:410:TYR:CE2	1:C:172:GLU:CG	2.62	0.75
1:D:464:GLY:CA	1:E:68:ARG:NH1	2.50	0.75
1:D:265:GLN:NE2	1:E:85:GLN:CA	2.50	0.75
1:A:60:LEU:HD22	1:E:452:ARG:HG2	1.64	0.75
1:C:267:PHE:CD2	1:D:76:SER:HB3	2.21	0.75
1:D:474:SER:HB3	1:E:473:LYS:HG3	1.69	0.75
2:F:9:ASP:O	2:F:10:THR:CB	2.34	0.75
1:B:530:PRO:HD3	1:C:66:THR:O	1.87	0.75
1:A:51:GLY:O	1:A:114:ASP:HB3	1.87	0.75
1:D:227:MET:C	2:H:17:TYR:HE2	1.89	0.74
1:A:556:LYS:HZ1	1:E:436:GLN:CA	1.99	0.74
1:A:490:THR:CG2	1:E:482:TYR:HD1	2.00	0.74
1:D:51:GLY:O	1:D:114:ASP:HB3	1.87	0.74
1:D:410:TYR:CE2	1:E:172:GLU:CG	2.65	0.74
1:B:476:TYR:CD1	1:C:475:PHE:HD2	2.05	0.74
1:B:569:ARG:HA	1:C:47:ARG:CB	2.15	0.74
1:D:155:LYS:HB2	1:D:158:GLN:HB2	1.69	0.74
1:E:434:SER:OG	1:E:467:LEU:HD11	1.87	0.74
1:C:266:PRO:CD	1:D:87:ASP:HB3	2.16	0.74
1:A:98:ASN:OD1	1:E:452:ARG:HD3	1.88	0.74
1:B:267:PHE:CD2	1:C:86:ASN:O	2.40	0.74
1:C:452:ARG:CD	1:D:60:LEU:CD1	2.56	0.74
1:B:452:ARG:HD3	1:C:98:ASN:OD1	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:PHE:CD2	1:E:76:SER:HB3	2.22	0.74
2:G:8:GLU:HG3	2:G:9:ASP:N	2.01	0.74
1:C:155:LYS:HB2	1:C:158:GLN:HB2	1.69	0.74
1:A:257:ASN:CB	1:B:555:TYR:OH	2.36	0.74
1:B:51:GLY:O	1:B:114:ASP:HB3	1.87	0.74
1:A:556:LYS:CD	1:E:434:SER:O	2.35	0.74
1:A:492:LEU:HB2	1:E:230:VAL:HG11	1.70	0.74
1:A:265:GLN:NE2	1:B:85:GLN:CA	2.51	0.73
1:C:452:ARG:HG2	1:D:60:LEU:CD1	2.18	0.73
1:C:410:TYR:CE2	1:D:172:GLU:CG	2.62	0.73
1:C:482:TYR:CD1	1:D:486:ILE:HG22	2.23	0.73
1:A:66:THR:O	1:E:530:PRO:HD3	1.88	0.73
1:A:474:SER:HG	1:B:475:PHE:HZ	1.35	0.73
2:H:10:THR:O	2:H:11:PHE:HB2	1.88	0.73
1:A:266:PRO:CD	1:B:87:ASP:HB3	2.18	0.73
1:C:482:TYR:CE1	1:D:486:ILE:HG21	2.23	0.73
1:B:155:LYS:HB2	1:B:158:GLN:HB2	1.69	0.73
1:D:84:TYR:O	1:D:85:GLN:CG	2.36	0.73
1:B:230:VAL:HG11	1:C:492:LEU:HB2	1.70	0.73
1:A:555:TYR:OH	1:E:257:ASN:ND2	2.21	0.73
1:D:433:GLY:HA2	1:E:555:TYR:CD2	2.24	0.73
1:B:568:SER:O	1:C:47:ARG:HD2	1.88	0.73
1:D:476:TYR:HB2	1:E:475:PHE:CD2	2.22	0.73
2:G:8:GLU:O	2:G:9:ASP:CB	2.32	0.73
1:D:266:PRO:CD	1:E:87:ASP:HB3	2.17	0.73
1:D:450:THR:HG23	1:E:57:TYR:CZ	2.22	0.73
1:D:569:ARG:HA	1:E:47:ARG:CB	2.16	0.73
1:A:475:PHE:CZ	1:E:475:PHE:O	2.42	0.73
1:E:51:GLY:O	1:E:114:ASP:HB3	1.87	0.73
1:A:47:ARG:HD2	1:E:569:ARG:HA	1.70	0.73
1:A:155:LYS:HB2	1:A:158:GLN:HB2	1.69	0.73
1:A:495:VAL:HG21	1:E:232:THR:OG1	1.88	0.73
1:A:516:VAL:HG21	1:E:513:ILE:HG12	1.70	0.73
1:B:233:ASN:ND2	1:C:490:THR:O	2.22	0.73
1:B:475:PHE:O	1:C:475:PHE:CZ	2.42	0.73
1:A:84:TYR:O	1:A:85:GLN:CG	2.36	0.73
1:C:436:GLN:NE2	1:D:558:LEU:CD1	2.49	0.73
1:C:274:THR:HG22	1:C:275:TYR:H	1.49	0.73
2:G:14:VAL:HG21	1:C:192:TYR:HE2	1.54	0.73
1:A:433:GLY:HA2	1:B:555:TYR:CD2	2.24	0.73
1:A:475:PHE:CD2	1:E:476:TYR:CD1	2.77	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:476:TYR:HB2	1:D:475:PHE:CD2	2.23	0.73
2:F:10:THR:O	2:F:11:PHE:HB2	1.88	0.73
1:D:266:PRO:HD3	1:E:87:ASP:CB	2.17	0.73
1:A:257:ASN:OD1	1:A:432:CYS:HA	1.89	0.73
1:B:513:ILE:HG12	1:C:516:VAL:HG21	1.71	0.73
1:D:257:ASN:ND2	1:D:432:CYS:O	2.22	0.72
1:E:84:TYR:O	1:E:85:GLN:CG	2.36	0.72
1:A:436:GLN:HB2	1:B:556:LYS:HZ3	1.51	0.72
1:D:57:TYR:CE2	1:D:60:LEU:CG	2.69	0.72
1:B:436:GLN:CB	1:C:558:LEU:HD21	2.19	0.72
1:A:568:SER:O	1:B:47:ARG:HD2	1.88	0.72
1:C:476:TYR:CD1	1:D:475:PHE:CD2	2.76	0.72
1:C:569:ARG:HA	1:D:47:ARG:CB	2.18	0.72
1:C:569:ARG:HA	1:D:47:ARG:HD2	1.72	0.72
1:D:482:TYR:HD1	1:E:490:THR:CG2	2.02	0.72
1:C:84:TYR:O	1:C:85:GLN:CG	2.37	0.72
1:B:376:LYS:HD2	1:B:378:VAL:HG11	1.70	0.72
1:A:475:PHE:CE2	1:E:475:PHE:O	2.43	0.72
1:C:230:VAL:HG11	1:D:492:LEU:HB2	1.70	0.72
1:C:529:LEU:HD21	1:D:68:ARG:HH21	1.55	0.72
1:D:482:TYR:CD1	1:E:486:ILE:CG2	2.72	0.72
1:A:99:ASN:HB3	1:E:459:ASN:CB	2.18	0.72
2:F:15:TYR:O	2:F:17:TYR:CD1	2.42	0.72
1:D:262:ARG:HD2	1:E:555:TYR:CE1	2.25	0.72
1:C:433:GLY:HA2	1:D:555:TYR:CD2	2.25	0.72
1:E:155:LYS:HB2	1:E:158:GLN:HB2	1.69	0.72
1:A:266:PRO:HD3	1:B:87:ASP:CB	2.18	0.72
1:E:83:ASN:OD1	1:E:91:PHE:HA	1.90	0.72
1:D:454:THR:HG21	1:D:459:ASN:OD1	1.90	0.72
1:C:452:ARG:HD3	1:D:98:ASN:OD1	1.89	0.71
1:A:450:THR:CG2	1:B:57:TYR:HE1	1.92	0.71
2:H:15:TYR:O	2:H:17:TYR:CD1	2.42	0.71
1:A:556:LYS:NZ	1:E:436:GLN:N	2.38	0.71
1:D:267:PHE:HE1	1:E:86:ASN:O	1.73	0.71
1:E:47:ARG:NH2	1:E:53:ASN:ND2	2.37	0.71
1:B:84:TYR:O	1:B:85:GLN:CG	2.36	0.71
1:B:454:THR:HG21	1:B:459:ASN:OD1	1.90	0.71
1:A:556:LYS:HB2	1:E:434:SER:HB3	1.71	0.71
1:A:556:LYS:NZ	1:E:434:SER:O	2.21	0.71
1:A:87:ASP:CB	1:E:266:PRO:HD2	2.20	0.71
2:G:10:THR:O	2:G:11:PHE:HB2	1.88	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:THR:OG1	1:C:495:VAL:HG21	1.90	0.71
1:A:376:LYS:HD2	1:A:378:VAL:HG11	1.70	0.71
1:C:83:ASN:OD1	1:C:91:PHE:HA	1.90	0.71
1:D:463:VAL:HB	1:D:529:LEU:HD13	1.72	0.71
1:D:482:TYR:CD1	1:E:486:ILE:HG22	2.25	0.71
1:B:265:GLN:NE2	1:C:85:GLN:CA	2.52	0.71
1:C:454:THR:HG21	1:C:459:ASN:OD1	1.90	0.71
2:G:15:TYR:O	2:G:17:TYR:CD1	2.42	0.71
1:C:463:VAL:HB	1:C:529:LEU:HD13	1.73	0.71
1:C:264:ARG:O	1:D:87:ASP:HB3	1.91	0.71
1:C:425:LEU:CD1	1:D:172:GLU:CB	2.46	0.71
1:B:463:VAL:HB	1:B:529:LEU:HD13	1.72	0.71
1:C:530:PRO:HD3	1:D:66:THR:O	1.91	0.71
1:A:68:ARG:HH12	1:E:464:GLY:HA3	1.53	0.71
1:A:569:ARG:HA	1:B:47:ARG:HD2	1.71	0.71
1:B:475:PHE:O	1:C:475:PHE:CE2	2.43	0.71
1:B:266:PRO:HD2	1:C:87:ASP:CB	2.19	0.71
1:B:266:PRO:CD	1:C:87:ASP:HB2	2.21	0.71
1:D:83:ASN:OD1	1:D:91:PHE:HA	1.90	0.71
1:C:449:VAL:CG1	1:D:55:ILE:HD13	2.20	0.71
1:D:568:SER:O	1:E:47:ARG:HD2	1.89	0.71
1:B:57:TYR:HE2	1:B:60:LEU:CB	2.00	0.71
1:A:530:PRO:HD3	1:B:66:THR:O	1.90	0.71
1:C:482:TYR:HD1	1:D:490:THR:CG2	2.04	0.71
1:B:83:ASN:OD1	1:B:91:PHE:HA	1.90	0.71
1:B:474:SER:HG	1:C:475:PHE:HZ	1.39	0.71
1:A:496:PHE:HE1	1:E:234:GLU:OE1	1.74	0.71
1:A:496:PHE:CE1	1:E:234:GLU:OE1	2.44	0.71
1:D:425:LEU:CD1	1:E:172:GLU:HG3	2.19	0.70
1:E:60:LEU:HG	1:E:61:ALA:N	2.06	0.70
1:A:230:VAL:HG11	1:B:492:LEU:HB2	1.72	0.70
1:A:558:LEU:HD21	1:E:436:GLN:CB	2.20	0.70
1:B:482:TYR:CD1	1:C:486:ILE:CG2	2.74	0.70
1:A:47:ARG:NH2	1:A:53:ASN:ND2	2.39	0.70
1:C:568:SER:O	1:D:47:ARG:HD2	1.91	0.70
1:E:57:TYR:HD2	1:E:60:LEU:HB3	1.52	0.70
1:B:450:THR:HG23	1:C:57:TYR:HD1	1.50	0.70
1:D:530:PRO:HD3	1:E:66:THR:O	1.91	0.70
1:A:482:TYR:CE1	1:B:486:ILE:HG23	2.25	0.70
1:C:425:LEU:HD22	1:D:172:GLU:CB	2.22	0.70
1:E:463:VAL:HB	1:E:529:LEU:HD13	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:569:ARG:HA	1:E:47:ARG:HD2	1.73	0.70
1:D:230:VAL:HG11	1:E:492:LEU:HB2	1.73	0.70
1:B:454:THR:CG2	1:B:459:ASN:OD1	2.40	0.70
1:B:459:ASN:CB	1:C:99:ASN:HB3	2.17	0.70
1:A:464:GLY:HA2	1:B:68:ARG:HH11	1.57	0.70
1:A:83:ASN:OD1	1:A:91:PHE:HA	1.90	0.70
1:A:70:TYR:OH	1:E:463:VAL:C	2.30	0.70
1:B:449:VAL:CG1	1:C:55:ILE:HD13	2.21	0.70
1:A:476:TYR:CD1	1:B:475:PHE:HD2	2.10	0.70
1:A:459:ASN:CB	1:B:99:ASN:HB3	2.20	0.70
1:A:87:ASP:HB2	1:E:266:PRO:CD	2.22	0.70
1:B:234:GLU:OE1	1:C:496:PHE:HE1	1.74	0.70
1:A:171:PRO:HA	1:E:411:ASN:ND2	2.06	0.70
1:B:411:ASN:ND2	1:C:171:PRO:HA	2.06	0.70
1:D:454:THR:CG2	1:D:459:ASN:OD1	2.40	0.70
2:H:13:PRO:CA	1:E:197:ARG:HH12	2.04	0.70
1:A:556:LYS:HZ3	1:E:436:GLN:HB2	1.54	0.70
1:A:425:LEU:HD22	1:B:172:GLU:C	2.11	0.70
1:A:463:VAL:HB	1:A:529:LEU:HD13	1.72	0.70
1:C:454:THR:CG2	1:C:459:ASN:OD1	2.40	0.70
1:D:452:ARG:HD3	1:E:98:ASN:OD1	1.90	0.70
1:C:233:ASN:ND2	1:D:490:THR:O	2.24	0.70
1:A:262:ARG:HD2	1:B:555:TYR:CE1	2.27	0.70
1:B:60:LEU:HG	1:B:61:ALA:N	2.06	0.70
1:C:267:PHE:CE2	1:D:76:SER:HB2	2.10	0.70
1:C:474:SER:HG	1:D:475:PHE:HZ	1.39	0.70
1:A:194:LYS:CB	1:E:221:PRO:HG3	2.19	0.70
1:B:234:GLU:OE1	1:C:496:PHE:CE1	2.45	0.70
1:B:436:GLN:CG	1:B:466:GLU:O	2.39	0.70
1:A:186:ASN:HD21	1:E:217:LEU:HD22	1.57	0.70
1:A:482:TYR:CD1	1:B:486:ILE:HG22	2.27	0.69
1:C:254:ARG:O	1:C:257:ASN:ND2	2.25	0.69
1:D:376:LYS:HD2	1:D:378:VAL:HG11	1.70	0.69
1:C:411:ASN:ND2	1:D:171:PRO:HA	2.06	0.69
1:D:476:TYR:CD1	1:E:475:PHE:HD2	2.09	0.69
1:C:266:PRO:CD	1:D:87:ASP:HB2	2.22	0.69
1:A:51:GLY:O	1:A:114:ASP:CG	2.31	0.69
1:B:410:TYR:CD2	1:B:425:LEU:HD13	2.27	0.69
1:B:434:SER:O	1:C:556:LYS:NZ	2.24	0.69
1:B:436:GLN:N	1:C:556:LYS:NZ	2.39	0.69
1:B:436:GLN:NE2	1:B:465:ALA:HB1	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLN:CA	1:E:265:GLN:NE2	2.52	0.69
1:C:266:PRO:HD2	1:D:87:ASP:CB	2.22	0.69
1:A:264:ARG:O	1:B:87:ASP:HB3	1.92	0.69
1:D:51:GLY:O	1:D:114:ASP:CG	2.31	0.69
1:A:228:PRO:HB2	1:B:493:THR:HG21	1.73	0.69
2:H:14:VAL:HG21	1:E:192:TYR:HE2	1.58	0.69
1:A:476:TYR:HE2	1:B:477:ASN:CB	2.03	0.69
1:B:221:PRO:CG	1:C:193:LEU:O	2.40	0.69
1:C:436:GLN:CG	1:C:466:GLU:O	2.39	0.69
1:A:436:GLN:OE1	1:B:126:ILE:CD1	2.33	0.69
1:A:475:PHE:O	1:B:475:PHE:CZ	2.46	0.69
1:A:193:LEU:O	1:E:221:PRO:CG	2.41	0.69
1:C:475:PHE:O	1:D:475:PHE:CZ	2.45	0.69
1:B:217:LEU:HD22	1:C:186:ASN:HD21	1.58	0.69
1:C:60:LEU:HG	1:C:61:ALA:N	2.06	0.69
1:B:529:LEU:HD11	1:C:68:ARG:NH1	2.07	0.69
1:B:262:ARG:HD2	1:C:555:TYR:CE1	2.28	0.69
1:C:436:GLN:CB	1:D:558:LEU:HD21	2.23	0.69
1:A:449:VAL:CG1	1:B:55:ILE:HD13	2.23	0.69
1:E:436:GLN:CG	1:E:466:GLU:O	2.39	0.69
1:C:410:TYR:CE2	1:C:425:LEU:HD12	2.27	0.69
1:C:436:GLN:HE22	1:D:558:LEU:CD1	1.95	0.69
1:A:434:SER:O	1:B:556:LYS:NZ	2.23	0.69
1:B:436:GLN:CD	1:C:558:LEU:HD11	2.12	0.69
1:C:68:ARG:CD	1:C:70:TYR:HE2	1.99	0.69
1:C:264:ARG:O	1:D:87:ASP:CG	2.31	0.69
1:C:51:GLY:O	1:C:114:ASP:CG	2.31	0.69
1:B:51:GLY:O	1:B:114:ASP:CG	2.31	0.69
1:A:267:PHE:CE2	1:B:80:ALA:HA	2.18	0.68
1:B:450:THR:CG2	1:C:57:TYR:HE1	1.95	0.68
1:D:152:LEU:HD21	1:D:199:ASN:O	1.94	0.68
1:E:51:GLY:O	1:E:114:ASP:CG	2.31	0.68
1:D:482:TYR:CE1	1:E:486:ILE:HG21	2.26	0.68
1:A:411:ASN:ND2	1:B:171:PRO:HA	2.08	0.68
1:A:68:ARG:NH1	1:E:464:GLY:HA2	2.05	0.68
1:D:449:VAL:CG1	1:E:55:ILE:HD13	2.23	0.68
1:C:513:ILE:HG12	1:D:516:VAL:HG21	1.75	0.68
1:B:221:PRO:HG3	1:C:194:LYS:CB	2.21	0.68
1:A:152:LEU:HD21	1:A:199:ASN:O	1.94	0.68
2:G:13:PRO:CA	1:C:197:ARG:NH1	2.57	0.68
1:A:228:PRO:CB	1:B:493:THR:HG21	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:482:TYR:HD1	1:E:490:THR:HG22	1.58	0.68
1:E:152:LEU:HD21	1:E:199:ASN:O	1.93	0.68
1:C:267:PHE:HE1	1:D:86:ASN:O	1.75	0.68
1:A:558:LEU:HD11	1:E:436:GLN:CD	2.13	0.68
1:D:436:GLN:HB2	1:E:556:LYS:HZ3	1.58	0.68
1:C:221:PRO:CG	1:D:193:LEU:O	2.41	0.68
1:D:264:ARG:O	1:E:87:ASP:HB3	1.92	0.68
1:C:234:GLU:OE1	1:D:496:PHE:HE1	1.77	0.68
1:B:267:PHE:HE2	1:C:87:ASP:HA	1.59	0.68
1:C:475:PHE:O	1:D:475:PHE:CE2	2.47	0.68
1:B:152:LEU:HD21	1:B:199:ASN:O	1.94	0.68
1:A:55:ILE:HD13	1:E:449:VAL:CG1	2.23	0.68
1:C:436:GLN:N	1:D:556:LYS:NZ	2.42	0.67
1:D:266:PRO:CD	1:E:87:ASP:HB2	2.24	0.67
1:D:436:GLN:CG	1:D:466:GLU:O	2.38	0.67
1:C:436:GLN:HB2	1:D:556:LYS:HZ3	1.57	0.67
1:B:135:ASN:HA	1:B:172:GLU:OE1	1.95	0.67
1:B:476:TYR:HE2	1:C:477:ASN:CB	2.06	0.67
1:C:152:LEU:HD21	1:C:199:ASN:O	1.94	0.67
1:A:135:ASN:HA	1:A:172:GLU:OE1	1.95	0.67
1:D:475:PHE:O	1:E:475:PHE:CZ	2.47	0.67
1:A:221:PRO:CG	1:B:193:LEU:O	2.42	0.67
1:D:411:ASN:ND2	1:E:171:PRO:HA	2.09	0.67
1:D:425:LEU:HD12	1:E:172:GLU:HG3	1.75	0.67
1:B:436:GLN:HB2	1:C:556:LYS:HZ1	1.50	0.67
1:B:436:GLN:CA	1:C:556:LYS:HZ1	2.06	0.67
1:B:482:TYR:CE1	1:C:486:ILE:HG23	2.29	0.67
1:A:266:PRO:CD	1:B:87:ASP:HB2	2.25	0.67
1:A:450:THR:HG23	1:B:57:TYR:HD1	1.53	0.67
1:A:99:ASN:CB	1:E:459:ASN:HB3	2.24	0.67
1:B:267:PHE:CE1	1:C:76:SER:OG	2.48	0.67
1:D:376:LYS:CD	1:D:378:VAL:CG1	2.66	0.67
1:B:410:TYR:CE2	1:B:425:LEU:HD13	2.29	0.67
1:A:234:GLU:OE1	1:B:496:PHE:HE1	1.78	0.67
1:D:101:TYR:CD2	1:D:105:GLU:HG2	2.29	0.67
1:E:101:TYR:CD2	1:E:105:GLU:HG2	2.29	0.67
1:B:230:VAL:O	1:C:493:THR:HG21	1.95	0.67
1:B:264:ARG:O	1:C:87:ASP:HB3	1.95	0.67
1:C:68:ARG:CD	1:C:70:TYR:CZ	2.73	0.67
1:E:135:ASN:HA	1:E:172:GLU:OE1	1.94	0.67
1:C:459:ASN:CB	1:D:99:ASN:HB3	2.20	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:PHE:CE1	1:E:83:ASN:HB3	2.29	0.67
1:D:513:ILE:HG12	1:E:516:VAL:HG21	1.76	0.67
1:A:513:ILE:HG12	1:B:516:VAL:HG21	1.76	0.67
1:C:434:SER:O	1:D:556:LYS:NZ	2.23	0.67
2:F:7:SER:O	2:F:8:GLU:C	2.33	0.67
1:D:266:PRO:HD2	1:E:87:ASP:CB	2.24	0.67
1:A:228:PRO:HB3	1:B:493:THR:CG2	2.25	0.67
1:A:556:LYS:CB	1:E:434:SER:HB3	2.24	0.67
1:B:410:TYR:CG	1:B:425:LEU:HD12	2.29	0.67
1:A:436:GLN:CG	1:A:466:GLU:O	2.38	0.67
1:D:232:THR:OG1	1:E:495:VAL:HG21	1.94	0.67
1:C:57:TYR:HE2	1:C:60:LEU:CB	2.00	0.67
1:D:228:PRO:HB2	1:E:493:THR:HG21	1.76	0.67
1:D:434:SER:O	1:E:556:LYS:NZ	2.24	0.67
1:A:266:PRO:HD2	1:B:87:ASP:CB	2.24	0.67
1:A:232:THR:OG1	1:B:495:VAL:HG21	1.95	0.67
1:E:56:ARG:HB2	1:E:112:ASN:HB2	1.77	0.67
2:G:7:SER:O	2:G:8:GLU:C	2.33	0.66
1:C:234:GLU:OE1	1:D:496:PHE:CE1	2.48	0.66
1:A:101:TYR:CD2	1:A:105:GLU:HG2	2.29	0.66
1:C:101:TYR:CD2	1:C:105:GLU:HG2	2.29	0.66
1:B:264:ARG:O	1:C:87:ASP:CG	2.33	0.66
1:B:476:TYR:CD1	1:C:475:PHE:CD2	2.83	0.66
1:D:459:ASN:CB	1:E:99:ASN:HB3	2.20	0.66
2:G:13:PRO:HB2	2:G:17:TYR:CE1	2.29	0.66
1:D:135:ASN:HA	1:D:172:GLU:OE1	1.94	0.66
1:D:529:LEU:HD21	1:E:68:ARG:HH21	1.59	0.66
1:A:47:ARG:CB	1:E:569:ARG:CA	2.67	0.66
1:A:475:PHE:HZ	1:E:474:SER:HG	1.41	0.66
2:H:13:PRO:CA	1:E:197:ARG:NH1	2.58	0.66
1:D:221:PRO:HG3	1:E:194:LYS:CB	2.25	0.66
1:C:152:LEU:HB3	1:C:153:PRO:CD	2.26	0.66
1:D:264:ARG:O	1:E:87:ASP:CG	2.34	0.66
1:B:101:TYR:CD2	1:B:105:GLU:HG2	2.29	0.66
1:D:56:ARG:HB2	1:D:112:ASN:HB2	1.78	0.66
1:B:56:ARG:HB2	1:B:112:ASN:HB2	1.78	0.66
1:B:264:ARG:CZ	1:B:424:LEU:HD21	2.26	0.66
1:C:436:GLN:CA	1:D:556:LYS:HZ1	2.09	0.66
1:D:152:LEU:HB3	1:D:153:PRO:CD	2.26	0.66
1:A:264:ARG:O	1:B:87:ASP:CG	2.34	0.66
1:B:481:VAL:HG23	1:C:490:THR:CB	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:PRO:CG	1:E:193:LEU:O	2.44	0.66
1:D:234:GLU:OE1	1:E:496:PHE:HE1	1.78	0.66
1:B:393:LEU:HD23	1:B:401:THR:HG22	1.78	0.66
1:A:57:TYR:CD1	1:E:450:THR:CG2	2.26	0.66
2:F:14:VAL:HG21	1:B:192:TYR:HE2	1.60	0.66
1:A:425:LEU:CD2	1:B:172:GLU:HB2	2.22	0.66
2:H:7:SER:O	2:H:8:GLU:C	2.33	0.66
1:E:264:ARG:CZ	1:E:424:LEU:HD21	2.26	0.66
1:C:264:ARG:CZ	1:C:424:LEU:HD21	2.26	0.66
1:B:436:GLN:OE1	1:C:126:ILE:CD1	2.36	0.66
1:A:56:ARG:HB2	1:A:112:ASN:HB2	1.77	0.66
1:C:135:ASN:HA	1:C:172:GLU:OE1	1.95	0.66
1:A:475:PHE:O	1:B:475:PHE:CE2	2.48	0.66
1:A:155:LYS:HG3	1:A:158:GLN:OE1	1.96	0.66
1:A:264:ARG:CZ	1:A:424:LEU:HD21	2.26	0.66
1:B:230:VAL:CG1	1:C:492:LEU:HB2	2.26	0.66
1:D:228:PRO:CB	1:E:493:THR:HG21	2.25	0.66
1:D:234:GLU:OE1	1:E:496:PHE:CE1	2.49	0.66
1:D:57:TYR:OH	1:D:98:ASN:ND2	2.30	0.65
1:D:98:ASN:O	1:D:99:ASN:HB2	1.96	0.65
1:C:155:LYS:HG3	1:C:158:GLN:OE1	1.96	0.65
1:C:232:THR:OG1	1:D:495:VAL:HG21	1.95	0.65
1:C:56:ARG:HB2	1:C:112:ASN:HB2	1.78	0.65
1:B:482:TYR:CD1	1:C:486:ILE:HG22	2.30	0.65
1:B:152:LEU:HB3	1:B:153:PRO:CD	2.26	0.65
1:A:152:LEU:HB3	1:A:153:PRO:CD	2.26	0.65
1:D:264:ARG:CZ	1:D:424:LEU:HD21	2.26	0.65
1:B:228:PRO:HB2	1:C:493:THR:HG21	1.78	0.65
1:A:490:THR:O	1:E:233:ASN:ND2	2.29	0.65
1:C:230:VAL:CG1	1:D:492:LEU:HB2	2.25	0.65
1:A:172:GLU:HB3	1:E:425:LEU:HD13	1.70	0.65
1:B:257:ASN:OD1	1:B:432:CYS:HA	1.97	0.65
1:A:87:ASP:CG	1:E:264:ARG:O	2.34	0.65
1:C:450:THR:O	1:C:450:THR:HG22	1.97	0.65
1:B:292:TYR:CE1	1:B:376:LYS:CD	2.58	0.65
1:D:476:TYR:HE2	1:E:477:ASN:CB	2.07	0.65
1:D:475:PHE:O	1:E:475:PHE:CE2	2.49	0.65
1:C:221:PRO:HG3	1:D:194:LYS:CB	2.25	0.65
1:D:436:GLN:CB	1:E:558:LEU:HD21	2.27	0.65
1:A:425:LEU:CD2	1:B:172:GLU:HB3	2.18	0.65
1:A:490:THR:HG22	1:E:482:TYR:HD1	1.60	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ASN:HB3	1:B:99:ASN:CB	2.27	0.65
1:C:452:ARG:HG3	1:D:60:LEU:CD2	2.15	0.65
1:C:98:ASN:O	1:C:99:ASN:HB2	1.96	0.65
2:F:13:PRO:CA	1:B:197:ARG:HH12	2.07	0.65
1:C:267:PHE:CE1	1:D:83:ASN:HB3	2.32	0.65
1:C:482:TYR:HD1	1:D:490:THR:HG22	1.62	0.65
1:E:155:LYS:HG3	1:E:158:GLN:OE1	1.96	0.65
1:A:87:ASP:HB3	1:E:264:ARG:O	1.95	0.65
1:A:234:GLU:OE1	1:B:496:PHE:CE1	2.49	0.65
1:C:68:ARG:HD2	1:C:70:TYR:OH	1.96	0.65
1:E:154:THR:O	1:E:155:LYS:CB	2.45	0.65
2:F:12:ASN:O	2:F:14:VAL:N	2.30	0.65
1:A:514:THR:HB	1:E:476:TYR:CE1	2.31	0.65
1:A:492:LEU:HB2	1:E:230:VAL:CG1	2.27	0.65
1:C:154:THR:O	1:C:155:LYS:CB	2.45	0.65
1:A:393:LEU:HD23	1:A:401:THR:HG22	1.78	0.65
2:G:12:ASN:O	2:G:14:VAL:N	2.30	0.64
1:B:155:LYS:HG3	1:B:158:GLN:OE1	1.96	0.64
1:D:155:LYS:HG3	1:D:158:GLN:OE1	1.96	0.64
1:A:230:VAL:O	1:B:493:THR:HG21	1.97	0.64
1:D:228:PRO:HB3	1:E:493:THR:CG2	2.28	0.64
1:C:436:GLN:CD	1:D:558:LEU:HD11	2.16	0.64
1:A:436:GLN:CB	1:B:558:LEU:HD21	2.26	0.64
1:A:86:ASN:O	1:E:267:PHE:HE1	1.78	0.64
1:E:393:LEU:HD23	1:E:401:THR:HG22	1.78	0.64
1:A:450:THR:O	1:A:450:THR:HG22	1.97	0.64
1:C:217:LEU:HD22	1:D:186:ASN:HD21	1.61	0.64
1:A:98:ASN:O	1:A:99:ASN:HB2	1.96	0.64
1:E:90:ASN:HD22	1:E:457:ILE:HG21	1.63	0.64
1:E:98:ASN:O	1:E:99:ASN:HB2	1.96	0.64
1:A:376:LYS:CD	1:A:378:VAL:CG1	2.66	0.64
1:B:425:LEU:CD2	1:C:172:GLU:HB2	2.28	0.64
1:B:47:ARG:HG2	1:B:48:PRO:HD2	1.78	0.64
1:E:152:LEU:HB3	1:E:153:PRO:CD	2.26	0.64
1:C:90:ASN:HD22	1:C:457:ILE:HG21	1.63	0.64
1:B:63:LEU:HD23	1:B:64:PHE:O	1.98	0.64
1:D:393:LEU:HD23	1:D:401:THR:HG22	1.78	0.64
2:H:12:ASN:O	2:H:14:VAL:N	2.30	0.64
1:C:393:LEU:HD23	1:C:401:THR:HG22	1.78	0.64
1:A:230:VAL:CG1	1:B:492:LEU:HB2	2.27	0.64
2:H:13:PRO:HB2	2:H:17:TYR:CE1	2.29	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:PHE:CE2	1:E:76:SER:HB2	2.11	0.64
1:C:63:LEU:HD23	1:C:64:PHE:O	1.98	0.64
1:A:217:LEU:HD22	1:B:186:ASN:HD21	1.62	0.64
1:B:425:LEU:CD2	1:C:172:GLU:C	2.66	0.64
1:A:63:LEU:HD23	1:A:64:PHE:O	1.98	0.64
1:E:63:LEU:HD23	1:E:64:PHE:O	1.98	0.64
1:D:476:TYR:CD1	1:E:475:PHE:CD2	2.86	0.64
1:C:265:GLN:HE21	1:D:85:GLN:C	2.01	0.64
1:A:90:ASN:HD22	1:A:457:ILE:HG21	1.63	0.64
1:B:425:LEU:HD21	1:C:172:GLU:O	1.98	0.63
1:A:436:GLN:N	1:B:556:LYS:NZ	2.46	0.63
1:D:450:THR:O	1:D:450:THR:HG22	1.97	0.63
1:D:450:THR:CG2	1:E:57:TYR:CD1	2.77	0.63
1:A:230:VAL:HG11	1:B:492:LEU:CD1	2.28	0.63
1:B:426:CYS:SG	1:C:553:TYR:HD2	2.21	0.63
1:A:490:THR:CG2	1:E:482:TYR:CD1	2.81	0.63
1:C:262:ARG:HD2	1:D:555:TYR:HE1	1.60	0.63
1:A:50:GLY:HA2	1:A:54:SER:HB3	1.81	0.63
1:B:450:THR:O	1:B:450:THR:HG22	1.97	0.63
2:F:13:PRO:HB2	2:F:17:TYR:CE1	2.29	0.63
1:D:63:LEU:HD23	1:D:64:PHE:O	1.98	0.63
1:C:47:ARG:HG2	1:C:48:PRO:HD2	1.78	0.63
1:A:267:PHE:CZ	1:B:80:ALA:CA	2.24	0.63
1:B:98:ASN:O	1:B:99:ASN:HB2	1.96	0.63
1:C:425:LEU:HD22	1:D:172:GLU:C	2.18	0.63
1:A:555:TYR:OH	1:E:257:ASN:HB3	1.95	0.63
1:A:221:PRO:HG3	1:B:194:LYS:CB	2.27	0.63
1:B:378:VAL:HG23	1:B:379:ILE:H	1.64	0.63
1:C:476:TYR:CE1	1:D:514:THR:HB	2.34	0.63
1:E:378:VAL:HG23	1:E:379:ILE:H	1.64	0.63
1:D:57:TYR:HD2	1:D:60:LEU:HB2	1.63	0.63
1:A:254:ARG:O	1:A:257:ASN:ND2	2.32	0.63
1:D:217:LEU:HD22	1:E:186:ASN:HD21	1.63	0.63
1:D:90:ASN:HD22	1:D:457:ILE:HG21	1.63	0.63
1:D:436:GLN:CA	1:E:556:LYS:HZ1	2.10	0.63
1:B:425:LEU:HD22	1:C:172:GLU:HB2	1.75	0.63
1:B:480:ALA:O	1:B:482:TYR:N	2.30	0.63
1:A:553:TYR:HD2	1:E:426:CYS:SG	2.22	0.63
1:D:230:VAL:CG1	1:E:492:LEU:HB2	2.29	0.62
1:E:128:HIS:HB3	1:E:556:LYS:HB3	1.81	0.62
1:D:50:GLY:HA2	1:D:54:SER:HB3	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:TYR:OH	1:E:98:ASN:ND2	2.33	0.62
1:A:227:MET:HB3	2:F:17:TYR:CZ	2.34	0.62
1:D:378:VAL:HG23	1:D:379:ILE:H	1.64	0.62
1:B:68:ARG:CD	1:B:70:TYR:HE2	1.95	0.62
1:A:426:CYS:HG	1:B:553:TYR:HD2	1.43	0.62
1:C:50:GLY:HA2	1:C:54:SER:HB3	1.81	0.62
1:A:47:ARG:CD	1:E:569:ARG:HA	2.29	0.62
1:D:265:GLN:HE21	1:E:85:GLN:C	2.02	0.62
2:G:13:PRO:CA	1:C:197:ARG:HH12	2.04	0.62
2:H:15:TYR:HD2	2:H:16:PRO:HD2	1.65	0.62
1:A:436:GLN:CD	1:B:558:LEU:HD11	2.19	0.62
1:B:449:VAL:HG13	1:C:55:ILE:CD1	2.30	0.62
1:B:569:ARG:HA	1:C:47:ARG:CD	2.28	0.62
1:C:474:SER:O	1:D:473:LYS:NZ	2.32	0.62
1:D:426:CYS:HG	1:E:553:TYR:HD2	1.46	0.62
1:B:228:PRO:CB	1:C:493:THR:HG21	2.29	0.62
1:C:410:TYR:CG	1:C:425:LEU:HD12	2.34	0.62
1:A:463:VAL:C	1:B:70:TYR:OH	2.38	0.62
1:B:476:TYR:CE1	1:C:514:THR:HB	2.35	0.62
1:A:186:ASN:ND2	1:E:217:LEU:HD22	2.14	0.62
1:A:495:VAL:CG2	1:E:232:THR:OG1	2.47	0.62
1:A:476:TYR:CD1	1:B:475:PHE:CD2	2.87	0.62
1:B:227:MET:HB3	2:G:17:TYR:CZ	2.34	0.62
1:A:292:TYR:CE1	1:A:376:LYS:CD	2.57	0.62
1:E:47:ARG:HG2	1:E:48:PRO:HD2	1.78	0.62
1:A:473:LYS:NZ	1:E:474:SER:O	2.33	0.62
1:C:378:VAL:HG23	1:C:379:ILE:H	1.64	0.62
1:A:97:GLN:OE1	1:E:451:PHE:HZ	1.83	0.62
1:A:436:GLN:CA	1:B:556:LYS:HZ1	2.11	0.62
1:A:83:ASN:O	1:E:267:PHE:HD1	1.82	0.62
1:A:47:ARG:HG2	1:A:48:PRO:HD2	1.78	0.62
1:A:198:GLN:HE21	1:E:222:VAL:HG21	1.65	0.62
1:A:459:ASN:OD1	1:B:99:ASN:HB3	1.99	0.62
1:A:378:VAL:HG23	1:A:379:ILE:H	1.64	0.62
1:B:482:TYR:HD1	1:C:490:THR:CG2	2.11	0.62
1:D:482:TYR:CD1	1:E:490:THR:CG2	2.83	0.62
1:C:230:VAL:HG11	1:D:492:LEU:CD1	2.30	0.62
1:D:436:GLN:CD	1:E:558:LEU:HD11	2.20	0.62
1:B:128:HIS:HB3	1:B:556:LYS:HB3	1.81	0.62
1:B:90:ASN:HD22	1:B:457:ILE:HG21	1.63	0.62
1:E:57:TYR:CE2	1:E:60:LEU:HB2	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:PHE:CZ	1:C:97:GLN:OE1	2.52	0.61
2:H:14:VAL:HG12	2:H:14:VAL:O	2.00	0.61
1:B:50:GLY:HA2	1:B:54:SER:HB3	1.81	0.61
1:A:97:GLN:OE1	1:E:451:PHE:CZ	2.53	0.61
2:G:16:PRO:HD3	1:C:498:ARG:O	2.00	0.61
1:D:230:VAL:O	1:E:493:THR:HG21	1.99	0.61
1:A:76:SER:HB2	1:E:267:PHE:CE2	2.36	0.61
1:D:569:ARG:CA	1:E:47:ARG:CB	2.70	0.61
1:B:265:GLN:HE21	1:C:85:GLN:C	2.03	0.61
1:E:257:ASN:ND2	1:E:432:CYS:O	2.33	0.61
1:E:50:GLY:HA2	1:E:54:SER:HB3	1.81	0.61
1:A:99:ASN:HB3	1:E:459:ASN:CG	2.21	0.61
1:B:451:PHE:HZ	1:C:97:GLN:OE1	1.82	0.61
2:G:15:TYR:HD2	2:G:16:PRO:HD2	1.64	0.61
2:F:14:VAL:O	2:F:14:VAL:HG12	1.99	0.61
2:F:15:TYR:HD2	2:F:16:PRO:HD2	1.65	0.61
1:D:227:MET:HB3	2:H:17:TYR:CZ	2.34	0.61
1:D:463:VAL:C	1:E:70:TYR:OH	2.38	0.61
1:B:482:TYR:HB2	1:C:490:THR:CG2	2.29	0.61
1:B:232:THR:OG1	1:C:495:VAL:CG2	2.48	0.61
1:C:72:VAL:HG22	1:C:74:ASN:H	1.66	0.61
1:A:99:ASN:HB3	1:E:459:ASN:OD1	2.01	0.61
1:A:72:VAL:HG22	1:A:74:ASN:H	1.66	0.61
1:E:57:TYR:HE2	1:E:60:LEU:HB2	1.65	0.61
1:D:230:VAL:HG11	1:E:492:LEU:CD1	2.31	0.61
1:B:217:LEU:HD22	1:C:186:ASN:ND2	2.15	0.61
1:A:60:LEU:CD2	1:E:452:ARG:NE	2.62	0.61
1:E:410:TYR:CG	1:E:425:LEU:HD12	2.30	0.61
1:D:83:ASN:CG	1:D:91:PHE:HB2	2.21	0.61
1:E:72:VAL:HG22	1:E:74:ASN:H	1.66	0.61
1:A:265:GLN:HE21	1:B:85:GLN:C	2.03	0.61
1:B:410:TYR:CE2	1:B:425:LEU:CD1	2.83	0.61
1:C:426:CYS:SG	1:D:553:TYR:HD2	2.24	0.61
2:G:14:VAL:HG12	2:G:14:VAL:O	1.99	0.61
1:D:436:GLN:N	1:E:556:LYS:NZ	2.46	0.61
1:B:530:PRO:CD	1:C:66:THR:O	2.48	0.61
1:A:66:THR:O	1:E:530:PRO:CD	2.49	0.61
1:A:183:LEU:HD21	1:E:236:PHE:CE2	2.35	0.61
1:D:264:ARG:HG2	1:D:424:LEU:HD11	1.83	0.61
1:D:233:ASN:ND2	1:E:490:THR:O	2.34	0.61
1:B:267:PHE:CE2	1:C:87:ASP:HA	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ASN:CG	1:C:91:PHE:HB2	2.21	0.61
1:B:474:SER:O	1:C:473:LYS:NZ	2.32	0.61
1:C:450:THR:CG2	1:D:57:TYR:CD1	2.75	0.60
1:B:228:PRO:HB3	1:C:493:THR:CG2	2.31	0.60
1:D:128:HIS:HB3	1:D:556:LYS:HB3	1.82	0.60
1:C:410:TYR:CE2	1:C:425:LEU:CD1	2.84	0.60
1:C:128:HIS:HB3	1:C:556:LYS:HB3	1.81	0.60
1:C:464:GLY:HA3	1:D:68:ARG:HH12	1.66	0.60
1:A:459:ASN:CG	1:B:99:ASN:HB3	2.21	0.60
1:C:264:ARG:O	1:D:87:ASP:CB	2.49	0.60
2:F:13:PRO:CA	1:B:197:ARG:NH1	2.62	0.60
1:D:376:LYS:HG2	1:D:377:PRO:HD2	1.84	0.60
1:B:236:PHE:CE2	1:C:183:LEU:HD21	2.36	0.60
1:D:264:ARG:CG	1:D:424:LEU:HD21	2.32	0.60
1:D:411:ASN:HD21	1:E:172:GLU:H	1.49	0.60
1:A:558:LEU:HD21	1:E:436:GLN:HB2	1.83	0.60
1:B:436:GLN:HB2	1:C:558:LEU:HD21	1.82	0.60
1:A:63:LEU:HD21	1:E:530:PRO:HG2	1.83	0.60
1:C:80:ALA:O	1:C:81:SER:CB	2.50	0.60
1:A:495:VAL:HG21	1:E:232:THR:CB	2.31	0.60
1:B:257:ASN:ND2	1:B:432:CYS:O	2.35	0.60
1:A:569:ARG:HA	1:B:47:ARG:CD	2.31	0.60
1:B:80:ALA:O	1:B:81:SER:CB	2.50	0.60
1:B:459:ASN:O	1:C:99:ASN:ND2	2.34	0.60
1:B:436:GLN:NE2	1:B:465:ALA:HB3	2.15	0.60
1:A:474:SER:O	1:B:473:LYS:NZ	2.34	0.60
1:A:85:GLN:C	1:E:265:GLN:HE21	2.04	0.60
1:A:555:TYR:OH	1:E:257:ASN:CG	2.39	0.60
2:G:14:VAL:CG1	1:C:203:GLU:OE2	2.45	0.60
1:B:482:TYR:HD1	1:C:490:THR:HG22	1.66	0.60
1:D:47:ARG:HG2	1:D:48:PRO:HD2	1.78	0.60
1:A:264:ARG:CG	1:A:424:LEU:HD21	2.32	0.60
1:A:530:PRO:HG2	1:B:63:LEU:HD21	1.84	0.60
1:A:486:ILE:HG21	1:E:482:TYR:CZ	2.36	0.60
1:A:518:GLU:OE2	1:E:472:SER:O	2.20	0.60
1:D:72:VAL:HG22	1:D:74:ASN:H	1.66	0.60
1:B:436:GLN:OE1	1:C:558:LEU:CD1	2.43	0.60
1:C:464:GLY:HA2	1:D:68:ARG:NH1	2.15	0.60
1:B:264:ARG:CG	1:B:424:LEU:HD21	2.32	0.60
1:A:490:THR:HG22	1:E:482:TYR:CD1	2.37	0.60
1:A:451:PHE:O	1:B:60:LEU:CD2	2.50	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ASN:ND2	1:E:459:ASN:O	2.35	0.59
1:D:451:PHE:O	1:E:60:LEU:CD2	2.50	0.59
1:D:464:GLY:HA2	1:E:68:ARG:NH1	2.17	0.59
1:D:482:TYR:CD1	1:E:490:THR:HG22	2.36	0.59
1:B:72:VAL:HG22	1:B:74:ASN:H	1.66	0.59
1:B:154:THR:O	1:B:155:LYS:CB	2.45	0.59
1:C:569:ARG:HA	1:D:47:ARG:CD	2.33	0.59
1:B:222:VAL:HG21	1:C:198:GLN:HE21	1.66	0.59
1:A:496:PHE:HE1	1:E:234:GLU:CD	2.04	0.59
1:B:472:SER:O	1:C:518:GLU:OE2	2.20	0.59
1:C:57:TYR:O	1:C:57:TYR:CG	2.54	0.59
1:D:530:PRO:HG2	1:E:63:LEU:HD21	1.84	0.59
1:A:490:THR:HG22	1:E:482:TYR:HA	1.84	0.59
1:A:172:GLU:H	1:E:411:ASN:HD21	1.50	0.59
1:B:451:PHE:O	1:C:60:LEU:CD2	2.49	0.59
1:B:530:PRO:HG2	1:C:63:LEU:HD21	1.84	0.59
1:A:569:ARG:CA	1:B:47:ARG:CB	2.68	0.59
1:C:264:ARG:CG	1:C:424:LEU:HD21	2.32	0.59
1:B:232:THR:CB	1:C:495:VAL:HG21	2.32	0.59
1:D:262:ARG:HD2	1:E:555:TYR:HE1	1.63	0.59
1:D:569:ARG:HA	1:E:47:ARG:CD	2.33	0.59
1:E:80:ALA:O	1:E:81:SER:CB	2.50	0.59
1:E:264:ARG:HG2	1:E:424:LEU:HD11	1.83	0.59
1:A:436:GLN:NE2	1:A:465:ALA:HB3	2.16	0.59
1:A:68:ARG:HD2	1:A:70:TYR:OH	2.01	0.59
1:A:262:ARG:HD2	1:B:555:TYR:HE1	1.66	0.59
1:C:264:ARG:HG2	1:C:424:LEU:HD11	1.83	0.59
1:A:451:PHE:CZ	1:B:97:GLN:OE1	2.56	0.59
1:B:57:TYR:CG	1:B:57:TYR:O	2.54	0.59
1:C:411:ASN:HD21	1:D:172:GLU:H	1.47	0.59
1:B:433:GLY:CA	1:C:555:TYR:CE2	2.61	0.59
1:B:233:ASN:HB3	1:C:491:SER:CB	2.33	0.59
1:A:193:LEU:O	1:E:221:PRO:HG2	2.03	0.59
1:D:264:ARG:O	1:E:87:ASP:CB	2.51	0.59
1:B:234:GLU:CD	1:C:496:PHE:HE1	2.06	0.59
1:C:451:PHE:HZ	1:D:97:GLN:OE1	1.86	0.59
1:D:451:PHE:HZ	1:E:97:GLN:OE1	1.86	0.59
1:B:264:ARG:HG2	1:B:424:LEU:HD11	1.83	0.59
1:B:155:LYS:O	1:B:156:ASP:CB	2.37	0.59
1:C:221:PRO:HG2	1:D:193:LEU:O	2.02	0.59
1:E:264:ARG:CG	1:E:424:LEU:HD21	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:CYS:HG	1:C:553:TYR:HD2	1.47	0.59
1:B:411:ASN:HD21	1:C:172:GLU:H	1.50	0.59
1:A:480:ALA:O	1:A:482:TYR:N	2.30	0.59
1:A:482:TYR:CE1	1:B:486:ILE:HG21	2.38	0.59
1:B:569:ARG:CB	1:C:47:ARG:HB2	2.31	0.59
1:D:474:SER:O	1:E:473:LYS:NZ	2.36	0.59
1:C:79:VAL:HG12	1:C:79:VAL:O	2.03	0.59
1:A:555:TYR:HE2	1:E:433:GLY:HA3	1.65	0.59
1:B:376:LYS:HG2	1:B:377:PRO:HD2	1.84	0.59
1:A:411:ASN:HD21	1:B:172:GLU:H	1.49	0.59
1:A:55:ILE:CD1	1:E:449:VAL:HG13	2.32	0.59
1:A:490:THR:HG21	1:E:482:TYR:CB	2.28	0.59
1:D:80:ALA:O	1:D:81:SER:CB	2.50	0.59
1:A:555:TYR:HE2	1:E:432:CYS:O	1.82	0.59
1:A:264:ARG:O	1:B:87:ASP:CB	2.50	0.59
1:D:185:ASN:HD21	1:D:210:PHE:HB2	1.68	0.59
1:B:566:LEU:HB3	1:C:65:ASP:OD2	2.03	0.59
1:D:451:PHE:CZ	1:E:97:GLN:OE1	2.56	0.58
1:A:376:LYS:HG2	1:A:377:PRO:HD2	1.84	0.58
1:A:530:PRO:CD	1:B:66:THR:O	2.51	0.58
1:C:530:PRO:CD	1:D:66:THR:O	2.51	0.58
1:B:47:ARG:NH1	1:B:53:ASN:ND2	2.51	0.58
1:C:474:SER:OG	1:D:475:PHE:HZ	1.86	0.58
1:D:265:GLN:HE21	1:E:85:GLN:CA	2.16	0.58
1:D:426:CYS:SG	1:E:553:TYR:HD2	2.26	0.58
1:B:451:PHE:O	1:C:60:LEU:HD22	2.03	0.58
1:E:83:ASN:CG	1:E:91:PHE:HB2	2.21	0.58
1:B:425:LEU:HD22	1:C:172:GLU:CA	2.33	0.58
1:B:463:VAL:O	1:C:68:ARG:NH1	2.37	0.58
1:B:474:SER:OG	1:C:475:PHE:HZ	1.86	0.58
1:E:79:VAL:HG12	1:E:79:VAL:O	2.03	0.58
1:A:50:GLY:HA2	1:A:54:SER:CB	2.34	0.58
1:A:57:TYR:CG	1:A:57:TYR:O	2.56	0.58
1:A:154:THR:O	1:A:155:LYS:CB	2.45	0.58
1:D:47:ARG:NH2	1:D:53:ASN:HD22	1.98	0.58
1:A:264:ARG:HG2	1:A:424:LEU:HD11	1.83	0.58
1:C:50:GLY:HA2	1:C:54:SER:CB	2.34	0.58
1:E:50:GLY:HA2	1:E:54:SER:CB	2.34	0.58
1:E:185:ASN:HD21	1:E:210:PHE:HB2	1.68	0.58
1:A:482:TYR:HD1	1:B:490:THR:CG2	2.17	0.58
1:E:264:ARG:HG2	1:E:424:LEU:HD21	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:LEU:HD22	1:D:186:ASN:ND2	2.18	0.58
1:A:97:GLN:HB3	1:E:451:PHE:CE2	2.38	0.58
1:A:436:GLN:CB	1:B:556:LYS:NZ	2.56	0.58
1:A:491:SER:CB	1:E:233:ASN:HB3	2.32	0.58
1:A:553:TYR:HD2	1:E:426:CYS:HG	1.49	0.58
1:A:65:ASP:OD2	1:E:566:LEU:HB3	2.03	0.58
1:B:451:PHE:CE2	1:C:97:GLN:HB3	2.39	0.58
1:B:376:LYS:CD	1:B:378:VAL:CG1	2.66	0.58
1:A:83:ASN:CB	1:E:267:PHE:CD1	2.72	0.58
1:B:221:PRO:HG2	1:C:193:LEU:O	2.02	0.58
1:B:50:GLY:HA2	1:B:54:SER:CB	2.34	0.58
1:B:185:ASN:HD21	1:B:210:PHE:HB2	1.68	0.58
1:D:451:PHE:O	1:E:60:LEU:HD22	2.04	0.58
2:F:15:TYR:OH	1:B:493:THR:CB	2.48	0.58
1:A:558:LEU:HD21	1:E:436:GLN:NE2	2.18	0.58
1:A:75:LYS:O	1:A:79:VAL:HG23	2.04	0.58
1:D:79:VAL:HG12	1:D:79:VAL:O	2.03	0.58
1:A:221:PRO:HG2	1:B:193:LEU:O	2.04	0.58
1:D:264:ARG:HG2	1:D:424:LEU:HD21	1.86	0.58
1:D:50:GLY:HA2	1:D:54:SER:CB	2.34	0.58
1:E:57:TYR:O	1:E:57:TYR:CG	2.56	0.58
1:D:464:GLY:HA3	1:E:68:ARG:HH12	1.67	0.58
1:A:481:VAL:HG23	1:B:490:THR:CB	2.34	0.58
1:A:569:ARG:CB	1:B:47:ARG:HB2	2.34	0.58
1:A:79:VAL:HG12	1:A:79:VAL:O	2.03	0.58
1:C:426:CYS:HG	1:D:553:TYR:HD2	1.50	0.58
1:C:451:PHE:CZ	1:D:97:GLN:OE1	2.56	0.58
1:A:57:TYR:HD2	1:A:59:GLU:O	1.86	0.58
1:B:264:ARG:HG2	1:B:424:LEU:HD21	1.86	0.58
1:B:47:ARG:NH2	1:B:53:ASN:HB2	2.18	0.58
1:C:257:ASN:HB3	1:D:555:TYR:OH	2.03	0.58
1:D:232:THR:OG1	1:E:495:VAL:CG2	2.52	0.58
1:A:185:ASN:HD21	1:A:210:PHE:HB2	1.68	0.58
1:B:75:LYS:O	1:B:79:VAL:HG23	2.04	0.58
1:A:451:PHE:HZ	1:B:97:GLN:OE1	1.86	0.58
1:B:264:ARG:O	1:C:87:ASP:CB	2.52	0.58
1:C:449:VAL:HG13	1:D:55:ILE:CD1	2.31	0.58
1:A:68:ARG:CD	1:A:70:TYR:CZ	2.78	0.58
1:C:236:PHE:CE2	1:D:183:LEU:HD21	2.39	0.58
1:E:75:LYS:O	1:E:79:VAL:HG23	2.04	0.58
1:C:185:ASN:HD21	1:C:210:PHE:HB2	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ASN:CG	1:B:91:PHE:HB2	2.21	0.57
1:A:83:ASN:CG	1:A:91:PHE:HB2	2.21	0.57
1:B:481:VAL:HG23	1:C:490:THR:HB	1.85	0.57
1:B:47:ARG:NH2	1:B:53:ASN:ND2	2.52	0.57
1:C:47:ARG:CG	1:C:48:PRO:CD	2.76	0.57
1:A:426:CYS:SG	1:B:553:TYR:HD2	2.26	0.57
1:E:57:TYR:CD2	1:E:60:LEU:CB	2.87	0.57
2:H:16:PRO:HD3	1:E:498:ARG:O	2.04	0.57
1:B:463:VAL:O	1:C:70:TYR:OH	2.21	0.57
1:A:264:ARG:HG2	1:A:424:LEU:HD21	1.86	0.57
2:H:15:TYR:OH	1:E:493:THR:CB	2.49	0.57
1:C:436:GLN:HB2	1:D:558:LEU:HD21	1.85	0.57
1:B:434:SER:O	1:C:556:LYS:CG	2.52	0.57
1:C:530:PRO:HG2	1:D:63:LEU:HD21	1.87	0.57
1:A:66:THR:HG21	1:E:528:THR:HB	1.86	0.57
1:A:475:PHE:HZ	1:E:474:SER:OG	1.86	0.57
1:B:79:VAL:HG12	1:B:79:VAL:O	2.03	0.57
1:B:230:VAL:HG11	1:C:492:LEU:CD1	2.34	0.57
2:F:16:PRO:HD3	1:B:498:ARG:O	2.03	0.57
1:B:425:LEU:HD13	1:C:172:GLU:CG	2.34	0.57
1:A:528:THR:HB	1:B:66:THR:HG21	1.87	0.57
1:A:47:ARG:HB2	1:E:569:ARG:CB	2.33	0.57
2:G:15:TYR:CD2	2:G:15:TYR:C	2.78	0.57
1:D:47:ARG:CG	1:D:48:PRO:CD	2.75	0.57
2:H:8:GLU:CG	2:H:9:ASP:H	2.02	0.57
1:C:232:THR:OG1	1:D:495:VAL:CG2	2.52	0.57
1:A:450:THR:HA	1:B:57:TYR:CD1	2.39	0.57
1:C:75:LYS:O	1:C:79:VAL:HG23	2.04	0.57
1:C:230:VAL:HG13	1:C:503:GLN:NE2	2.17	0.57
1:C:264:ARG:HG2	1:C:424:LEU:HD21	1.86	0.57
1:A:145:ALA:HB3	1:A:168:PHE:HE1	1.70	0.57
1:D:434:SER:OG	1:D:467:LEU:HD11	2.05	0.57
1:A:434:SER:OG	1:A:467:LEU:HD11	2.05	0.57
1:D:530:PRO:CD	1:E:66:THR:O	2.53	0.57
1:A:267:PHE:HE2	1:B:84:TYR:HD1	1.47	0.57
1:C:434:SER:OG	1:C:467:LEU:HD11	2.05	0.57
1:B:434:SER:OG	1:B:467:LEU:HD11	2.05	0.57
1:A:555:TYR:OH	1:E:432:CYS:O	2.22	0.57
1:E:257:ASN:OD1	1:E:432:CYS:HA	2.05	0.57
1:C:106:ALA:HA	1:C:109:GLN:NE2	2.20	0.57
1:A:265:GLN:HE21	1:B:85:GLN:CA	2.17	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ARG:HD2	1:C:555:TYR:HE1	1.67	0.57
1:D:528:THR:HB	1:E:66:THR:HG21	1.87	0.57
1:C:476:TYR:HE2	1:D:477:ASN:CB	2.13	0.57
1:A:217:LEU:HD22	1:B:186:ASN:ND2	2.20	0.57
1:D:57:TYR:O	1:D:57:TYR:CG	2.58	0.57
1:A:410:TYR:CE2	1:A:425:LEU:HD12	2.37	0.57
1:B:436:GLN:CB	1:C:556:LYS:NZ	2.53	0.57
1:C:482:TYR:CD1	1:D:490:THR:CG2	2.86	0.57
1:B:449:VAL:HG22	1:C:55:ILE:HD13	1.87	0.57
1:D:257:ASN:OD1	1:D:258:LEU:N	2.38	0.57
1:A:490:THR:CG2	1:E:482:TYR:HB2	2.29	0.57
1:A:232:THR:OG1	1:B:495:VAL:CG2	2.53	0.57
1:C:145:ALA:HB3	1:C:168:PHE:HE1	1.70	0.57
1:B:450:THR:HA	1:C:57:TYR:CD1	2.39	0.56
1:A:558:LEU:HD21	1:E:436:GLN:CD	2.26	0.56
1:E:47:ARG:CG	1:E:48:PRO:CD	2.75	0.56
1:C:569:ARG:CB	1:D:47:ARG:HB2	2.35	0.56
1:A:106:ALA:HA	1:A:109:GLN:NE2	2.20	0.56
1:D:145:ALA:HB3	1:D:168:PHE:HE1	1.70	0.56
1:A:566:LEU:HB3	1:B:65:ASP:OD2	2.05	0.56
1:A:450:THR:CB	1:B:57:TYR:CD1	2.88	0.56
1:A:98:ASN:OD1	1:E:452:ARG:CD	2.53	0.56
1:A:449:VAL:HG13	1:B:55:ILE:CD1	2.33	0.56
1:C:233:ASN:HB3	1:D:491:SER:CB	2.35	0.56
1:C:463:VAL:C	1:D:70:TYR:OH	2.43	0.56
1:D:75:LYS:O	1:D:79:VAL:HG23	2.04	0.56
1:A:555:TYR:HH	1:E:257:ASN:HB3	1.70	0.56
1:D:217:LEU:HD22	1:E:186:ASN:ND2	2.20	0.56
1:E:145:ALA:HB3	1:E:168:PHE:HE1	1.70	0.56
1:C:459:ASN:O	1:D:99:ASN:ND2	2.38	0.56
1:A:558:LEU:CD1	1:E:436:GLN:NE2	2.60	0.56
1:C:482:TYR:CD1	1:D:490:THR:HG22	2.40	0.56
1:A:47:ARG:CA	1:E:569:ARG:O	2.54	0.56
1:C:47:ARG:NH2	1:C:53:ASN:HD22	1.94	0.56
1:C:257:ASN:HB2	1:D:555:TYR:OH	2.04	0.56
1:C:265:GLN:HE21	1:D:85:GLN:CA	2.17	0.56
1:C:232:THR:CB	1:D:495:VAL:HG21	2.36	0.56
1:C:472:SER:O	1:D:518:GLU:OE2	2.24	0.56
1:D:459:ASN:O	1:E:99:ASN:ND2	2.38	0.56
1:C:267:PHE:HD1	1:D:86:ASN:O	1.87	0.56
1:B:425:LEU:CD2	1:C:172:GLU:O	2.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:VAL:HG21	1:E:513:ILE:CG1	2.34	0.56
1:A:451:PHE:O	1:B:60:LEU:HD22	2.04	0.56
1:B:513:ILE:CG1	1:C:516:VAL:HG21	2.35	0.56
1:E:106:ALA:HA	1:E:109:GLN:NE2	2.20	0.56
1:E:410:TYR:CZ	1:E:425:LEU:HD12	2.39	0.56
1:B:452:ARG:CD	1:C:98:ASN:OD1	2.54	0.56
1:D:106:ALA:HA	1:D:109:GLN:NE2	2.21	0.56
1:A:55:ILE:HD13	1:E:449:VAL:HG22	1.88	0.56
1:B:145:ALA:HB3	1:B:168:PHE:HE1	1.70	0.56
1:A:60:LEU:CG	1:E:452:ARG:CG	2.67	0.56
2:H:15:TYR:CD2	2:H:15:TYR:C	2.78	0.56
1:D:236:PHE:CE2	1:E:183:LEU:HD21	2.41	0.56
1:E:57:TYR:CE2	1:E:60:LEU:CB	2.89	0.56
1:A:83:ASN:O	1:E:267:PHE:CD1	2.59	0.56
1:B:463:VAL:O	1:C:68:ARG:CZ	2.53	0.56
1:D:102:SER:HB3	1:D:103:PRO:HD2	1.88	0.56
1:A:60:LEU:HD21	1:E:452:ARG:HE	1.71	0.56
2:H:14:VAL:CG1	1:E:203:GLU:OE2	2.47	0.56
1:B:436:GLN:CD	1:C:558:LEU:HD21	2.27	0.56
1:B:528:THR:HB	1:C:66:THR:HG21	1.87	0.56
1:D:257:ASN:OD1	1:D:432:CYS:HA	2.06	0.56
1:A:474:SER:OG	1:B:475:PHE:HZ	1.88	0.56
1:A:57:TYR:CE2	1:A:60:LEU:CD1	2.89	0.55
1:D:451:PHE:CE2	1:E:97:GLN:HB3	2.41	0.55
1:A:80:ALA:O	1:A:81:SER:CB	2.50	0.55
1:B:151:ARG:HG3	1:B:161:LEU:CD2	2.37	0.55
1:D:566:LEU:HB3	1:E:65:ASP:OD2	2.06	0.55
1:D:221:PRO:HG2	1:E:193:LEU:O	2.05	0.55
1:E:239:ASP:HB2	1:E:406:TRP:HB3	1.88	0.55
1:A:57:TYR:CE2	1:A:60:LEU:CB	2.89	0.55
1:B:569:ARG:CA	1:C:47:ARG:CB	2.68	0.55
1:D:476:TYR:CE1	1:E:514:THR:HB	2.41	0.55
1:A:459:ASN:O	1:B:99:ASN:ND2	2.38	0.55
1:D:267:PHE:HD1	1:E:86:ASN:O	1.89	0.55
1:C:463:VAL:O	1:D:68:ARG:CZ	2.55	0.55
1:D:449:VAL:HG13	1:E:55:ILE:CD1	2.33	0.55
1:A:477:ASN:CB	1:E:476:TYR:HE2	2.14	0.55
1:C:566:LEU:HB3	1:D:65:ASP:OD2	2.07	0.55
1:C:239:ASP:HB2	1:C:406:TRP:HB3	1.88	0.55
1:E:102:SER:HB3	1:E:103:PRO:HD2	1.88	0.55
1:A:451:PHE:CE2	1:B:97:GLN:HB3	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASN:HB3	1:B:491:SER:CB	2.37	0.55
1:A:87:ASP:CB	1:E:264:ARG:O	2.53	0.55
1:C:264:ARG:O	1:D:87:ASP:OD2	2.23	0.55
1:C:72:VAL:HG22	1:C:73:ASP:N	2.22	0.55
2:F:15:TYR:O	2:F:17:TYR:N	2.40	0.55
1:D:436:GLN:CD	1:E:558:LEU:HD21	2.27	0.55
1:B:465:ALA:O	1:C:560:ILE:HD11	2.06	0.55
1:B:482:TYR:HA	1:C:490:THR:HG22	1.89	0.55
1:D:569:ARG:CB	1:E:47:ARG:HB2	2.36	0.55
1:D:105:GLU:HG3	1:D:106:ALA:H	1.72	0.55
1:E:72:VAL:HG22	1:E:73:ASP:N	2.22	0.55
1:A:197:ARG:NH2	1:E:220:ASP:OD2	2.39	0.55
1:E:151:ARG:HG3	1:E:161:LEU:CD2	2.37	0.55
1:C:451:PHE:O	1:D:60:LEU:CD2	2.55	0.55
1:B:434:SER:OG	1:C:556:LYS:HG2	2.07	0.55
1:C:528:THR:HB	1:D:66:THR:HG21	1.89	0.55
1:A:47:ARG:CG	1:A:48:PRO:CD	2.75	0.55
1:A:476:TYR:CE1	1:B:514:THR:HB	2.41	0.55
1:B:72:VAL:HG22	1:B:73:ASP:N	2.22	0.55
2:G:18:ASP:HB2	2:G:19:THR:HA	1.88	0.55
2:F:15:TYR:C	2:F:15:TYR:CD2	2.78	0.55
1:B:264:ARG:O	1:C:87:ASP:OD2	2.25	0.55
1:A:449:VAL:HG22	1:B:55:ILE:HD13	1.89	0.55
1:C:222:VAL:HG21	1:D:198:GLN:HE21	1.70	0.55
2:H:18:ASP:HB2	2:H:19:THR:HA	1.89	0.55
1:B:84:TYR:C	1:B:85:GLN:HG3	2.27	0.55
1:A:425:LEU:CD2	1:B:172:GLU:O	2.55	0.55
1:A:434:SER:OG	1:B:556:LYS:HG2	2.07	0.55
1:A:436:GLN:CD	1:B:558:LEU:HD21	2.28	0.55
1:D:154:THR:O	1:D:155:LYS:CB	2.45	0.55
1:A:236:PHE:CE2	1:B:183:LEU:HD21	2.41	0.55
1:C:234:GLU:CD	1:D:496:PHE:HE1	2.10	0.55
1:A:151:ARG:HG3	1:A:161:LEU:CD2	2.36	0.55
1:B:146:ARG:O	1:B:246:CYS:HB2	2.07	0.55
1:D:239:ASP:HB2	1:D:406:TRP:HB3	1.88	0.55
1:A:102:SER:HB3	1:A:103:PRO:HD2	1.88	0.55
1:D:472:SER:O	1:E:518:GLU:OE2	2.25	0.55
1:B:57:TYR:HD2	1:B:59:GLU:O	1.90	0.54
1:B:226:VAL:HG12	1:B:228:PRO:HD2	1.89	0.54
1:B:220:ASP:OD2	1:C:197:ARG:NH2	2.40	0.54
1:A:558:LEU:CD1	1:E:436:GLN:OE1	2.55	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:ILE:HD11	1:E:465:ALA:O	2.07	0.54
1:D:434:SER:OG	1:E:556:LYS:HG2	2.07	0.54
1:A:84:TYR:C	1:A:85:GLN:HG3	2.28	0.54
2:G:15:TYR:CD2	2:G:16:PRO:HD2	2.42	0.54
2:H:15:TYR:O	2:H:17:TYR:N	2.40	0.54
1:C:63:LEU:CD2	1:C:67:THR:HG22	2.16	0.54
1:A:492:LEU:CD1	1:E:230:VAL:HG11	2.36	0.54
1:E:105:GLU:HG3	1:E:106:ALA:H	1.72	0.54
1:B:106:ALA:HA	1:B:109:GLN:NE2	2.21	0.54
1:A:72:VAL:HG22	1:A:73:ASP:N	2.22	0.54
1:E:146:ARG:O	1:E:246:CYS:HB2	2.07	0.54
1:C:57:TYR:CD2	1:C:59:GLU:O	2.61	0.54
2:F:15:TYR:CD2	2:F:16:PRO:HD2	2.42	0.54
1:C:482:TYR:CZ	1:D:486:ILE:HG21	2.42	0.54
1:A:264:ARG:O	1:B:87:ASP:OD2	2.25	0.54
1:B:239:ASP:HB2	1:B:406:TRP:HB3	1.88	0.54
1:A:472:SER:O	1:B:518:GLU:OE2	2.25	0.54
1:C:146:ARG:O	1:C:246:CYS:HB2	2.07	0.54
1:C:444:MET:HB2	1:C:539:GLN:HE22	1.72	0.54
1:C:102:SER:HB3	1:C:103:PRO:HD2	1.88	0.54
2:F:18:ASP:HB2	2:F:19:THR:HA	1.88	0.54
1:A:267:PHE:HZ	1:B:80:ALA:N	2.00	0.54
1:C:436:GLN:OE1	1:C:465:ALA:CB	2.55	0.54
1:A:436:GLN:HB2	1:B:558:LEU:HD21	1.88	0.54
1:B:482:TYR:CD1	1:C:490:THR:HG22	2.43	0.54
1:A:480:ALA:C	1:A:482:TYR:H	2.11	0.54
1:A:569:ARG:O	1:B:47:ARG:CA	2.55	0.54
1:D:482:TYR:HA	1:E:490:THR:HG22	1.90	0.54
1:D:234:GLU:CD	1:E:496:PHE:HE1	2.10	0.54
1:A:146:ARG:O	1:A:246:CYS:HB2	2.07	0.54
1:B:102:SER:HB3	1:B:103:PRO:HD2	1.88	0.54
1:C:151:ARG:HG3	1:C:161:LEU:CD2	2.37	0.54
1:C:451:PHE:CE2	1:D:97:GLN:HB3	2.43	0.54
2:G:15:TYR:O	2:G:17:TYR:N	2.40	0.54
1:C:84:TYR:C	1:C:85:GLN:HG3	2.28	0.54
1:D:232:THR:CB	1:E:495:VAL:HG21	2.37	0.54
1:D:72:VAL:HG22	1:D:73:ASP:N	2.22	0.54
1:D:180:THR:O	1:D:184:MET:HG3	2.08	0.54
1:B:450:THR:CB	1:C:57:TYR:CD1	2.90	0.54
1:A:226:VAL:HG12	1:A:228:PRO:HD2	1.89	0.54
1:B:264:ARG:HG3	1:B:424:LEU:HG	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:GLN:HB2	1:E:558:LEU:HD21	1.89	0.54
1:C:226:VAL:HG12	1:C:228:PRO:HD2	1.89	0.54
1:A:68:ARG:HH21	1:E:529:LEU:HD21	1.73	0.54
1:D:474:SER:OG	1:E:475:PHE:HZ	1.89	0.54
1:A:87:ASP:OD2	1:E:264:ARG:O	2.26	0.54
1:A:234:GLU:CD	1:B:496:PHE:HE1	2.11	0.54
1:C:105:GLU:HG3	1:C:106:ALA:H	1.72	0.54
1:B:105:GLU:HG3	1:B:106:ALA:H	1.72	0.54
1:A:239:ASP:HB2	1:A:406:TRP:HB3	1.88	0.54
1:C:434:SER:O	1:D:556:LYS:CG	2.56	0.54
1:A:425:LEU:HD13	1:B:172:GLU:CG	2.38	0.54
1:C:569:ARG:CA	1:D:47:ARG:CB	2.72	0.54
1:B:222:VAL:HG22	1:C:198:GLN:NE2	2.23	0.54
1:C:102:SER:HB3	1:C:103:PRO:CD	2.38	0.54
1:B:102:SER:HB3	1:B:103:PRO:CD	2.38	0.54
1:A:180:THR:O	1:A:184:MET:HG3	2.08	0.54
1:D:151:ARG:HG3	1:D:161:LEU:CD2	2.37	0.54
1:D:292:TYR:CE1	1:D:376:LYS:CD	2.57	0.54
1:C:436:GLN:OE1	1:C:465:ALA:HB1	2.08	0.54
1:A:410:TYR:CD1	1:A:425:LEU:HD12	2.43	0.54
1:D:569:ARG:O	1:E:47:ARG:CA	2.55	0.54
1:D:482:TYR:HB2	1:E:490:THR:CG2	2.31	0.54
1:C:236:PHE:CD2	1:D:174:ASN:HB3	2.43	0.54
1:C:264:ARG:HG3	1:C:424:LEU:HG	1.90	0.54
1:D:264:ARG:HG3	1:D:424:LEU:HG	1.90	0.54
1:D:146:ARG:O	1:D:246:CYS:HB2	2.07	0.54
1:B:57:TYR:CD2	1:B:59:GLU:O	2.61	0.54
1:C:57:TYR:HD2	1:C:59:GLU:O	1.90	0.54
1:A:228:PRO:CB	1:B:493:THR:CG2	2.86	0.54
1:C:482:TYR:HA	1:D:490:THR:HG22	1.89	0.54
1:C:262:ARG:HD2	1:D:555:TYR:CD1	2.43	0.54
1:A:85:GLN:CA	1:E:265:GLN:HE21	2.18	0.54
1:B:265:GLN:HE21	1:C:85:GLN:CA	2.18	0.54
1:E:264:ARG:HG3	1:E:424:LEU:HG	1.90	0.54
1:A:264:ARG:HG3	1:A:424:LEU:HG	1.90	0.54
1:B:444:MET:HB2	1:B:539:GLN:HE22	1.72	0.54
1:A:550:THR:O	1:A:552:PRO:HD3	2.08	0.54
1:B:550:THR:O	1:B:552:PRO:HD3	2.08	0.54
1:C:550:THR:O	1:C:552:PRO:HD3	2.08	0.54
1:A:556:LYS:NZ	1:E:436:GLN:CB	2.49	0.54
1:E:226:VAL:HG12	1:E:228:PRO:HD2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:ARG:O	1:C:47:ARG:CA	2.56	0.54
1:A:232:THR:CB	1:B:495:VAL:HG21	2.37	0.54
1:A:516:VAL:HG21	1:E:513:ILE:CD1	2.37	0.54
1:C:450:THR:CG2	1:C:450:THR:O	2.56	0.53
1:C:452:ARG:CD	1:D:98:ASN:OD1	2.56	0.53
1:C:449:VAL:HG22	1:D:55:ILE:HD13	1.90	0.53
1:B:513:ILE:CD1	1:C:516:VAL:HG21	2.37	0.53
1:D:444:MET:HB2	1:D:539:GLN:HE22	1.73	0.53
1:E:68:ARG:HD2	1:E:70:TYR:OH	2.08	0.53
1:D:220:ASP:OD2	1:E:197:ARG:NH2	2.42	0.53
1:D:482:TYR:CB	1:E:490:THR:HG21	2.33	0.53
1:C:230:VAL:CG1	1:D:492:LEU:CB	2.78	0.53
1:A:105:GLU:HG3	1:A:106:ALA:H	1.72	0.53
1:A:444:MET:HB2	1:A:539:GLN:HE22	1.72	0.53
1:D:450:THR:O	1:D:450:THR:CG2	2.56	0.53
1:C:411:ASN:ND2	1:D:172:GLU:N	2.54	0.53
1:A:463:VAL:O	1:B:68:ARG:CZ	2.57	0.53
1:A:68:ARG:HH11	1:E:464:GLY:HA2	1.71	0.53
1:A:555:TYR:CZ	1:E:432:CYS:O	2.61	0.53
1:D:222:VAL:HG21	1:E:198:GLN:HE21	1.69	0.53
1:E:102:SER:HB3	1:E:103:PRO:CD	2.38	0.53
1:A:102:SER:HB3	1:A:103:PRO:CD	2.38	0.53
1:E:444:MET:HB2	1:E:539:GLN:HE22	1.73	0.53
1:C:450:THR:HA	1:D:57:TYR:CG	2.44	0.53
1:B:436:GLN:OE1	1:C:558:LEU:HD21	2.09	0.53
1:A:68:ARG:CZ	1:E:463:VAL:O	2.55	0.53
1:D:482:TYR:CZ	1:E:486:ILE:HG21	2.44	0.53
1:B:180:THR:O	1:B:184:MET:HG3	2.08	0.53
1:A:57:TYR:CE1	1:E:450:THR:HB	2.43	0.53
1:B:450:THR:O	1:B:450:THR:CG2	2.57	0.53
1:C:434:SER:OG	1:D:556:LYS:HG2	2.09	0.53
1:C:436:GLN:CB	1:D:556:LYS:NZ	2.56	0.53
1:B:482:TYR:CD1	1:C:490:THR:CG2	2.92	0.53
1:D:449:VAL:HG22	1:E:55:ILE:HD13	1.90	0.53
1:A:481:VAL:HG23	1:B:490:THR:HG21	1.91	0.53
1:A:555:TYR:OH	1:E:257:ASN:HB2	2.08	0.53
1:E:180:THR:O	1:E:184:MET:HG3	2.08	0.53
1:A:220:ASP:OD2	1:B:197:ARG:NH2	2.42	0.53
2:H:15:TYR:CD2	2:H:16:PRO:HD2	2.42	0.53
1:B:529:LEU:CD2	1:C:68:ARG:HH11	2.14	0.53
1:D:233:ASN:HB3	1:E:491:SER:CB	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:VAL:HG21	1:B:198:GLN:HE21	1.70	0.53
1:A:57:TYR:OH	1:A:98:ASN:ND2	2.41	0.53
2:F:15:TYR:OH	1:B:494:HIS:N	2.41	0.53
1:D:436:GLN:OE1	1:E:558:LEU:CD1	2.57	0.53
1:B:68:ARG:HD2	1:B:70:TYR:OH	2.08	0.53
1:B:47:ARG:CG	1:B:48:PRO:CD	2.75	0.53
1:D:264:ARG:O	1:E:87:ASP:OD2	2.26	0.53
1:C:513:ILE:CG1	1:D:516:VAL:HG21	2.38	0.53
1:A:450:THR:O	1:A:450:THR:CG2	2.57	0.53
2:G:15:TYR:OH	1:C:494:HIS:N	2.42	0.53
1:D:102:SER:HB3	1:D:103:PRO:CD	2.38	0.53
1:C:180:THR:O	1:C:184:MET:HG3	2.08	0.53
1:D:257:ASN:HB3	1:E:555:TYR:OH	2.09	0.53
1:D:550:THR:O	1:D:552:PRO:HD3	2.08	0.53
1:D:226:VAL:HG12	1:D:228:PRO:HD2	1.89	0.52
1:C:465:ALA:O	1:D:560:ILE:HD11	2.09	0.52
1:B:436:GLN:H	1:C:556:LYS:HZ1	1.48	0.52
1:B:257:ASN:HB3	1:C:555:TYR:OH	2.08	0.52
1:B:480:ALA:C	1:B:482:TYR:H	2.12	0.52
1:A:70:TYR:OH	1:E:463:VAL:O	2.27	0.52
1:A:482:TYR:HD1	1:B:490:THR:HG22	1.73	0.52
1:C:220:ASP:OD2	1:D:197:ARG:NH2	2.42	0.52
1:C:436:GLN:CD	1:D:558:LEU:HD21	2.30	0.52
1:B:68:ARG:CD	1:B:70:TYR:CZ	2.83	0.52
2:F:10:THR:CG2	2:F:10:THR:O	2.57	0.52
1:A:274:THR:HG22	1:A:275:TYR:N	2.23	0.52
2:F:12:ASN:O	2:F:14:VAL:CG2	2.48	0.52
1:D:434:SER:O	1:E:556:LYS:CG	2.57	0.52
1:B:292:TYR:CD1	1:B:376:LYS:HD3	2.35	0.52
1:A:236:PHE:CD2	1:B:174:ASN:HB3	2.45	0.52
1:A:174:ASN:HB3	1:E:236:PHE:CD2	2.45	0.52
1:E:105:GLU:HG3	1:E:106:ALA:N	2.25	0.52
1:A:172:GLU:HG3	1:E:425:LEU:HD13	1.84	0.52
1:D:105:GLU:HG3	1:D:106:ALA:N	2.25	0.52
1:C:105:GLU:HG3	1:C:106:ALA:N	2.25	0.52
1:E:550:THR:O	1:E:552:PRO:HD3	2.08	0.52
1:C:441:LEU:HB2	1:C:445:MET:HG2	1.91	0.52
1:E:441:LEU:HB2	1:E:445:MET:HG2	1.92	0.52
1:A:267:PHE:CZ	1:B:80:ALA:N	2.78	0.52
1:A:76:SER:HB2	1:E:267:PHE:HE2	1.75	0.52
1:D:463:VAL:O	1:E:68:ARG:CZ	2.58	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ASN:HB2	1:C:555:TYR:OH	2.09	0.52
1:D:84:TYR:C	1:D:85:GLN:HG3	2.27	0.52
1:C:466:GLU:HG2	1:C:467:LEU:N	2.25	0.52
1:B:411:ASN:HD21	1:C:171:PRO:HA	1.74	0.52
1:A:68:ARG:HD2	1:E:463:VAL:O	2.10	0.52
1:A:66:THR:HG23	1:E:528:THR:OG1	2.10	0.52
1:D:257:ASN:HB2	1:E:555:TYR:OH	2.07	0.52
1:E:84:TYR:C	1:E:85:GLN:HG3	2.27	0.52
1:A:425:LEU:CD2	1:B:172:GLU:C	2.76	0.52
1:A:434:SER:O	1:B:556:LYS:CG	2.57	0.52
1:A:465:ALA:O	1:B:560:ILE:HD11	2.10	0.52
1:B:254:ARG:O	1:B:257:ASN:ND2	2.43	0.52
1:B:105:GLU:HG3	1:B:106:ALA:N	2.25	0.52
1:B:106:ALA:HA	1:B:109:GLN:HG3	1.92	0.52
1:A:441:LEU:HB2	1:A:445:MET:HG2	1.92	0.52
1:A:450:THR:CG2	1:B:57:TYR:HD1	2.15	0.52
1:D:452:ARG:CD	1:E:98:ASN:OD1	2.56	0.52
1:A:466:GLU:HG2	1:A:467:LEU:N	2.25	0.52
1:D:528:THR:OG1	1:E:66:THR:HG23	2.10	0.52
1:C:274:THR:HG22	1:C:275:TYR:N	2.22	0.52
1:C:513:ILE:CD1	1:D:516:VAL:HG21	2.39	0.52
1:D:69:VAL:HG23	1:D:561:VAL:HB	1.92	0.52
1:E:556:LYS:CE	1:E:558:LEU:CD2	2.81	0.52
1:A:292:TYR:CD1	1:A:376:LYS:HD3	2.35	0.52
1:C:482:TYR:CB	1:D:490:THR:HG21	2.34	0.52
1:D:68:ARG:CD	1:D:70:TYR:CZ	2.86	0.52
1:D:274:THR:HG22	1:D:275:TYR:N	2.23	0.52
1:D:441:LEU:HB2	1:D:445:MET:HG2	1.92	0.52
2:H:15:TYR:OH	1:E:494:HIS:N	2.43	0.51
1:E:466:GLU:HG2	1:E:467:LEU:N	2.25	0.51
1:A:410:TYR:CG	1:A:425:LEU:CD1	2.83	0.51
1:A:425:LEU:HD22	1:B:172:GLU:CA	2.37	0.51
1:A:528:THR:OG1	1:B:66:THR:HG23	2.10	0.51
1:B:466:GLU:HG2	1:B:467:LEU:N	2.25	0.51
1:C:433:GLY:CA	1:D:555:TYR:CE2	2.68	0.51
1:A:105:GLU:HG3	1:A:106:ALA:N	2.25	0.51
1:B:441:LEU:HB2	1:B:445:MET:HG2	1.92	0.51
1:C:79:VAL:O	1:C:80:ALA:C	2.48	0.51
1:B:274:THR:HG22	1:B:275:TYR:N	2.22	0.51
1:B:420:ARG:NH2	1:C:136:GLU:HB2	2.25	0.51
1:E:69:VAL:HG23	1:E:561:VAL:HB	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:14:VAL:HG22	1:C:203:GLU:CD	2.31	0.51
2:G:15:TYR:HD2	2:G:16:PRO:CD	2.23	0.51
1:A:228:PRO:HB3	1:B:493:THR:HB	1.92	0.51
1:A:490:THR:CG2	1:E:482:TYR:CB	2.87	0.51
1:E:79:VAL:O	1:E:80:ALA:C	2.48	0.51
1:A:198:GLN:NE2	1:E:222:VAL:HG22	2.22	0.51
1:C:420:ARG:NH2	1:D:136:GLU:HB2	2.25	0.51
1:E:95:VAL:HG12	1:E:95:VAL:O	2.11	0.51
1:A:136:GLU:HB2	1:E:420:ARG:NH2	2.26	0.51
2:H:12:ASN:O	2:H:14:VAL:CG2	2.48	0.51
2:H:15:TYR:HD2	2:H:16:PRO:CD	2.24	0.51
1:D:465:ALA:O	1:E:560:ILE:HD11	2.10	0.51
1:B:463:VAL:O	1:C:68:ARG:HD2	2.10	0.51
1:C:95:VAL:O	1:C:95:VAL:HG12	2.11	0.51
1:B:236:PHE:CD2	1:C:174:ASN:HB3	2.44	0.51
1:A:79:VAL:O	1:A:80:ALA:C	2.48	0.51
1:B:275:TYR:CE1	1:B:404:ARG:HD3	2.46	0.51
1:C:106:ALA:HA	1:C:109:GLN:HG3	1.92	0.51
1:B:95:VAL:O	1:B:95:VAL:HG12	2.11	0.51
1:D:63:LEU:CD2	1:D:67:THR:HG22	2.16	0.51
1:D:236:PHE:CD2	1:E:174:ASN:HB3	2.45	0.51
1:E:423:THR:O	1:E:424:LEU:HG	2.10	0.51
1:A:423:THR:O	1:A:424:LEU:HG	2.11	0.51
1:A:69:VAL:HG23	1:A:561:VAL:HB	1.91	0.51
1:B:212:THR:HG22	1:B:238:PRO:HG3	1.93	0.51
1:D:411:ASN:ND2	1:E:172:GLU:N	2.57	0.51
1:C:462:VAL:O	1:D:70:TYR:OH	2.21	0.51
1:A:183:LEU:HD21	1:E:236:PHE:HE2	1.76	0.51
1:A:275:TYR:CE1	1:A:404:ARG:HD3	2.46	0.51
1:A:513:ILE:CD1	1:B:516:VAL:HG21	2.41	0.51
1:D:212:THR:HG22	1:D:238:PRO:HG3	1.93	0.51
1:D:95:VAL:O	1:D:95:VAL:HG12	2.11	0.51
1:C:569:ARG:O	1:D:47:ARG:CA	2.58	0.51
1:B:236:PHE:HE2	1:C:183:LEU:HD21	1.76	0.51
1:E:230:VAL:HG13	1:E:503:GLN:NE2	2.17	0.51
1:D:79:VAL:O	1:D:80:ALA:C	2.48	0.51
2:G:15:TYR:OH	1:C:493:THR:CB	2.53	0.51
1:C:482:TYR:HB2	1:D:490:THR:CG2	2.33	0.51
1:A:433:GLY:CA	1:B:555:TYR:CE2	2.62	0.51
1:C:423:THR:O	1:C:424:LEU:HG	2.11	0.51
1:D:275:TYR:CE1	1:D:404:ARG:HD3	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:VAL:HG23	1:B:561:VAL:HB	1.92	0.51
1:C:449:VAL:CG1	1:D:55:ILE:CD1	2.87	0.51
1:B:528:THR:OG1	1:C:66:THR:HG23	2.11	0.51
1:A:55:ILE:CD1	1:E:449:VAL:CG1	2.89	0.51
1:C:222:VAL:HG22	1:D:198:GLN:NE2	2.26	0.51
1:B:79:VAL:O	1:B:80:ALA:C	2.48	0.51
1:D:466:GLU:HG2	1:D:467:LEU:N	2.25	0.51
1:E:212:THR:HG22	1:E:238:PRO:HG3	1.93	0.51
1:C:69:VAL:HG23	1:C:561:VAL:HB	1.92	0.51
1:A:96:ILE:O	1:E:450:THR:OG1	2.24	0.50
2:F:14:VAL:CG1	1:B:203:GLU:OE2	2.46	0.50
1:B:449:VAL:CG1	1:C:55:ILE:CD1	2.86	0.50
1:D:423:THR:O	1:D:424:LEU:HG	2.11	0.50
1:E:275:TYR:CE1	1:E:404:ARG:HD3	2.46	0.50
1:C:275:TYR:CE1	1:C:404:ARG:HD3	2.46	0.50
1:B:426:CYS:SG	1:C:553:TYR:CD2	2.99	0.50
1:D:228:PRO:CB	1:E:493:THR:CG2	2.89	0.50
1:B:267:PHE:HE1	1:C:76:SER:HB3	1.58	0.50
1:D:436:GLN:OE1	1:D:465:ALA:HB1	2.11	0.50
1:D:292:TYR:CD1	1:D:376:LYS:HD3	2.35	0.50
1:A:257:ASN:HB2	1:B:555:TYR:OH	2.11	0.50
1:C:57:TYR:CD2	1:C:60:LEU:CB	2.72	0.50
2:H:13:PRO:CB	2:H:17:TYR:HE1	2.19	0.50
1:E:436:GLN:OE1	1:E:465:ALA:CB	2.60	0.50
1:B:423:THR:O	1:B:424:LEU:HG	2.11	0.50
1:B:425:LEU:CD1	1:C:172:GLU:CB	2.75	0.50
1:E:106:ALA:HA	1:E:109:GLN:HG3	1.92	0.50
1:A:513:ILE:CG1	1:B:516:VAL:HG21	2.40	0.50
1:A:106:ALA:HA	1:A:109:GLN:HG3	1.92	0.50
1:B:427:THR:HG21	1:C:519:ASN:ND2	2.27	0.50
1:E:436:GLN:OE1	1:E:465:ALA:HB1	2.10	0.50
1:D:436:GLN:NE2	1:E:558:LEU:HD21	2.25	0.50
1:A:95:VAL:O	1:A:95:VAL:HG12	2.11	0.50
1:D:262:ARG:HD2	1:E:555:TYR:CD1	2.46	0.50
1:A:212:THR:HG22	1:A:238:PRO:HG3	1.93	0.50
1:C:451:PHE:O	1:D:60:LEU:HD23	2.11	0.50
1:A:60:LEU:HD13	1:E:451:PHE:O	2.12	0.50
1:D:257:ASN:HD21	1:D:432:CYS:HB3	1.76	0.50
1:D:106:ALA:HA	1:D:109:GLN:HG3	1.92	0.50
1:A:57:TYR:CE1	1:E:450:THR:O	2.65	0.50
1:D:449:VAL:CG1	1:E:55:ILE:CD1	2.90	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:15:TYR:HD2	2:F:16:PRO:CD	2.24	0.50
1:D:68:ARG:HD2	1:D:70:TYR:OH	2.11	0.50
1:A:480:ALA:C	1:A:481:VAL:HG22	2.29	0.50
1:A:230:VAL:HG13	1:A:503:GLN:NE2	2.17	0.50
1:A:558:LEU:HD11	1:E:436:GLN:OE1	2.10	0.50
1:D:529:LEU:HD21	1:E:68:ARG:NH2	2.27	0.50
1:B:47:ARG:NH2	1:B:53:ASN:CB	2.75	0.50
1:D:513:ILE:CG1	1:E:516:VAL:HG21	2.40	0.50
2:G:12:ASN:O	2:G:14:VAL:CG2	2.48	0.50
2:H:15:TYR:HD2	2:H:15:TYR:C	2.15	0.50
1:A:425:LEU:HD21	1:B:172:GLU:O	2.12	0.50
1:A:464:GLY:CA	1:B:68:ARG:HH11	2.15	0.50
1:D:155:LYS:O	1:D:156:ASP:CB	2.37	0.50
1:A:492:LEU:CB	1:E:230:VAL:CG1	2.80	0.50
1:B:228:PRO:HB3	1:C:493:THR:HB	1.93	0.49
1:C:425:LEU:CD2	1:D:172:GLU:HB3	2.39	0.49
1:E:274:THR:HG22	1:E:275:TYR:N	2.23	0.49
1:D:444:MET:HB2	1:D:539:GLN:NE2	2.27	0.49
2:F:15:TYR:C	2:F:15:TYR:HD2	2.15	0.49
1:C:444:MET:HB2	1:C:539:GLN:NE2	2.27	0.49
1:A:444:MET:HB2	1:A:539:GLN:NE2	2.27	0.49
1:C:212:THR:HG22	1:C:238:PRO:HG3	1.93	0.49
1:B:452:ARG:HD2	1:C:57:TYR:OH	2.12	0.49
2:G:15:TYR:C	2:G:15:TYR:HD2	2.15	0.49
2:F:14:VAL:HG22	1:B:203:GLU:CD	2.32	0.49
1:B:449:VAL:CG2	1:C:55:ILE:HD13	2.42	0.49
1:A:106:ALA:HA	1:A:109:GLN:HE21	1.77	0.49
1:B:106:ALA:HA	1:B:109:GLN:HE21	1.77	0.49
1:C:427:THR:HG21	1:D:519:ASN:ND2	2.27	0.49
1:A:519:ASN:ND2	1:E:427:THR:HG21	2.27	0.49
1:B:230:VAL:HG13	1:B:503:GLN:NE2	2.17	0.49
1:D:230:VAL:HG13	1:D:503:GLN:NE2	2.18	0.49
1:C:76:SER:HB2	1:C:83:ASN:HD22	1.76	0.49
1:B:482:TYR:CB	1:C:490:THR:CG2	2.90	0.49
1:D:433:GLY:CA	1:E:555:TYR:CE2	2.64	0.49
1:A:155:LYS:O	1:A:156:ASP:CB	2.37	0.49
1:E:106:ALA:HA	1:E:109:GLN:HE21	1.77	0.49
1:D:513:ILE:CD1	1:E:516:VAL:HG21	2.42	0.49
1:D:126:ILE:HD12	1:D:558:LEU:HD11	1.95	0.49
1:A:482:TYR:HA	1:B:490:THR:HG22	1.94	0.49
1:C:528:THR:OG1	1:D:66:THR:HG23	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ARG:HD2	1:C:555:TYR:CD1	2.47	0.49
1:E:110:THR:HG22	1:E:536:GLY:HA2	1.95	0.49
1:A:171:PRO:HA	1:E:411:ASN:HD21	1.74	0.49
1:D:450:THR:HA	1:E:57:TYR:CG	2.47	0.49
1:B:450:THR:CG2	1:C:57:TYR:HD1	2.14	0.49
1:D:257:ASN:ND2	1:E:555:TYR:HH	2.09	0.49
1:B:76:SER:HB2	1:B:83:ASN:HD22	1.77	0.49
1:D:228:PRO:HB3	1:E:493:THR:HB	1.95	0.49
1:B:556:LYS:CE	1:B:558:LEU:CD2	2.81	0.49
1:A:449:VAL:CG1	1:B:55:ILE:CD1	2.89	0.49
1:A:262:ARG:HD2	1:B:555:TYR:CD1	2.47	0.49
1:D:482:TYR:CB	1:E:490:THR:CG2	2.91	0.49
1:A:495:VAL:HG21	1:E:232:THR:HB	1.94	0.49
1:E:434:SER:OG	1:E:467:LEU:CD1	2.60	0.49
1:D:376:LYS:HG2	1:D:377:PRO:CD	2.43	0.49
1:B:135:ASN:CB	1:B:172:GLU:OE1	2.61	0.49
1:B:436:GLN:HB3	1:C:558:LEU:CD2	2.43	0.49
1:D:463:VAL:O	1:E:68:ARG:HD2	2.13	0.49
1:E:135:ASN:CB	1:E:172:GLU:OE1	2.61	0.48
1:D:450:THR:HG21	1:E:96:ILE:HG22	1.94	0.48
1:B:228:PRO:CB	1:C:493:THR:CG2	2.91	0.48
1:D:135:ASN:CB	1:D:172:GLU:OE1	2.61	0.48
1:B:434:SER:O	1:C:556:LYS:HG2	2.13	0.48
1:B:257:ASN:OD1	1:B:258:LEU:N	2.45	0.48
1:A:222:VAL:HG22	1:B:198:GLN:NE2	2.26	0.48
1:D:106:ALA:HA	1:D:109:GLN:HE21	1.77	0.48
1:E:444:MET:HB2	1:E:539:GLN:NE2	2.27	0.48
1:A:483:SER:CB	1:E:478:ASP:OD2	2.61	0.48
1:D:110:THR:HG22	1:D:536:GLY:HA2	1.95	0.48
1:B:230:VAL:CG1	1:C:492:LEU:CB	2.80	0.48
2:F:12:ASN:C	2:F:14:VAL:N	2.67	0.48
1:A:55:ILE:HD13	1:E:449:VAL:CG2	2.43	0.48
2:F:8:GLU:CG	2:F:9:ASP:H	2.02	0.48
1:B:232:THR:HB	1:C:495:VAL:HG21	1.95	0.48
2:G:18:ASP:CB	2:G:19:THR:HA	2.43	0.48
1:D:420:ARG:NH2	1:E:136:GLU:HB2	2.28	0.48
1:D:427:THR:HG21	1:E:519:ASN:ND2	2.28	0.48
1:A:420:ARG:NH2	1:B:136:GLU:HB2	2.28	0.48
1:B:464:GLY:HA2	1:C:70:TYR:HE2	1.77	0.48
1:C:529:LEU:HD21	1:D:68:ARG:NH2	2.25	0.48
1:C:283:ILE:HD12	1:C:403:TYR:HB3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:TYR:CD2	1:B:59:GLU:C	2.87	0.48
1:A:556:LYS:CE	1:A:558:LEU:CD2	2.74	0.48
1:A:376:LYS:HG2	1:A:377:PRO:CD	2.44	0.48
1:E:83:ASN:OD1	1:E:91:PHE:CA	2.61	0.48
1:B:444:MET:HB2	1:B:539:GLN:NE2	2.27	0.48
1:B:220:ASP:CG	1:C:197:ARG:NH2	2.67	0.48
1:C:126:ILE:HD12	1:C:558:LEU:HD11	1.95	0.48
1:C:463:VAL:O	1:D:68:ARG:HD2	2.14	0.48
1:A:197:ARG:NH2	1:E:220:ASP:CG	2.67	0.48
1:B:110:THR:HG22	1:B:536:GLY:HA2	1.95	0.48
2:H:12:ASN:C	2:H:14:VAL:N	2.67	0.48
1:B:411:ASN:ND2	1:C:172:GLU:N	2.57	0.48
1:B:126:ILE:HD12	1:B:558:LEU:HD11	1.95	0.48
1:B:63:LEU:CD2	1:B:67:THR:HG22	2.16	0.48
1:A:257:ASN:ND2	1:A:432:CYS:O	2.47	0.48
1:C:79:VAL:HG11	1:C:82:LEU:HD12	1.96	0.48
1:A:555:TYR:CE2	1:E:433:GLY:HA3	2.43	0.48
2:H:13:PRO:CB	2:H:17:TYR:CE1	2.96	0.48
2:H:14:VAL:HG22	1:E:203:GLU:CD	2.34	0.48
1:B:376:LYS:HG2	1:B:377:PRO:CD	2.44	0.48
1:B:482:TYR:CE1	1:C:486:ILE:HG21	2.46	0.48
1:B:482:TYR:CB	1:C:490:THR:HG21	2.35	0.48
1:A:482:TYR:HB2	1:B:490:THR:CG2	2.39	0.48
1:B:283:ILE:HD12	1:B:403:TYR:HB3	1.95	0.48
1:B:79:VAL:HG11	1:B:82:LEU:HD12	1.96	0.48
1:B:83:ASN:OD1	1:B:91:PHE:CA	2.61	0.48
1:D:436:GLN:OE1	1:E:558:LEU:HD11	2.13	0.48
1:C:411:ASN:HD21	1:D:171:PRO:HA	1.77	0.48
1:B:569:ARG:CB	1:C:47:ARG:CB	2.92	0.48
1:A:490:THR:CB	1:E:481:VAL:HG12	2.29	0.48
1:C:236:PHE:HE2	1:D:183:LEU:HD21	1.79	0.48
1:D:222:VAL:HG22	1:E:198:GLN:NE2	2.26	0.48
1:B:478:ASP:OD2	1:C:483:SER:CB	2.62	0.48
1:C:529:LEU:HD11	1:D:68:ARG:NH2	2.28	0.48
1:D:79:VAL:HG11	1:D:82:LEU:HD12	1.96	0.48
1:A:496:PHE:HE1	1:E:234:GLU:OE2	1.97	0.48
1:D:283:ILE:HD12	1:D:403:TYR:HB3	1.95	0.48
1:A:135:ASN:CB	1:A:172:GLU:OE1	2.61	0.48
1:A:463:VAL:O	1:B:68:ARG:HD2	2.13	0.48
1:C:106:ALA:HA	1:C:109:GLN:HE21	1.77	0.48
1:B:135:ASN:CA	1:B:172:GLU:OE1	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:ASP:O	1:D:63:LEU:CD1	2.62	0.47
1:E:79:VAL:HG11	1:E:82:LEU:HD12	1.95	0.47
1:E:130:ASN:HD22	1:E:130:ASN:C	2.18	0.47
1:B:60:LEU:CG	1:B:61:ALA:N	2.74	0.47
2:F:13:PRO:CB	2:F:17:TYR:CE1	2.96	0.47
1:A:411:ASN:ND2	1:B:172:GLU:N	2.56	0.47
1:A:194:LYS:HG3	1:E:221:PRO:HB2	1.95	0.47
1:A:57:TYR:HD2	1:A:60:LEU:HB2	1.76	0.47
1:A:427:THR:HG21	1:B:519:ASN:ND2	2.28	0.47
1:C:130:ASN:HD22	1:C:130:ASN:C	2.17	0.47
1:C:110:THR:HG22	1:C:536:GLY:HA2	1.95	0.47
1:C:57:TYR:CD2	1:C:59:GLU:C	2.87	0.47
1:C:425:LEU:CD2	1:D:172:GLU:CB	2.91	0.47
1:A:83:ASN:OD1	1:A:91:PHE:CA	2.61	0.47
1:D:268:GLN:HG2	1:E:84:TYR:CE2	2.49	0.47
1:A:72:VAL:HG22	1:A:73:ASP:H	1.80	0.47
1:A:110:THR:HG22	1:A:536:GLY:HA2	1.95	0.47
1:A:283:ILE:HD12	1:A:403:TYR:HB3	1.95	0.47
1:B:432:CYS:O	1:C:555:TYR:OH	2.28	0.47
1:E:72:VAL:HG22	1:E:73:ASP:H	1.80	0.47
1:E:283:ILE:HD12	1:E:403:TYR:HB3	1.95	0.47
1:A:57:TYR:CE1	1:E:450:THR:CB	2.98	0.47
1:A:558:LEU:CD2	1:E:436:GLN:HB3	2.44	0.47
1:D:436:GLN:OE1	1:D:465:ALA:CB	2.62	0.47
1:C:135:ASN:CB	1:C:172:GLU:OE1	2.61	0.47
1:D:497:ASN:ND2	1:D:500:PRO:HB3	2.25	0.47
1:D:72:VAL:HG22	1:D:73:ASP:H	1.80	0.47
1:B:72:VAL:HG22	1:B:73:ASP:H	1.79	0.47
1:A:57:TYR:CD2	1:A:60:LEU:CB	2.96	0.47
1:E:458:SER:O	1:E:459:ASN:CG	2.53	0.47
1:E:60:LEU:CG	1:E:61:ALA:H	2.12	0.47
2:G:13:PRO:CB	2:G:17:TYR:CE1	2.96	0.47
1:A:558:LEU:CD1	1:E:436:GLN:CD	2.83	0.47
1:E:126:ILE:HD12	1:E:558:LEU:HD11	1.95	0.47
1:D:83:ASN:OD1	1:D:91:PHE:CA	2.61	0.47
1:A:449:VAL:CG2	1:B:55:ILE:HD13	2.44	0.47
1:C:449:VAL:CG2	1:D:55:ILE:HD13	2.45	0.47
1:D:449:VAL:CG2	1:E:55:ILE:HD13	2.45	0.47
1:B:221:PRO:HB2	1:C:194:LYS:HG3	1.96	0.47
1:A:458:SER:O	1:A:459:ASN:CG	2.53	0.47
1:A:553:TYR:CD2	1:E:426:CYS:SG	3.00	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ALA:HB2	1:B:109:GLN:NE2	2.30	0.47
1:D:478:ASP:OD2	1:E:483:SER:CB	2.63	0.47
1:A:130:ASN:C	1:A:130:ASN:HD22	2.18	0.47
1:C:482:TYR:CB	1:D:490:THR:CG2	2.93	0.47
1:A:555:TYR:CD1	1:E:262:ARG:HD2	2.50	0.47
1:C:213:ARG:HD3	1:C:509:PRO:HG2	1.97	0.47
1:E:213:ARG:HD3	1:E:509:PRO:HG2	1.98	0.47
1:D:98:ASN:O	1:D:99:ASN:CB	2.63	0.46
1:A:135:ASN:CA	1:A:172:GLU:OE1	2.62	0.46
1:D:230:VAL:CG1	1:E:492:LEU:CB	2.82	0.46
1:A:558:LEU:CD2	1:E:436:GLN:CB	2.93	0.46
1:B:528:THR:O	1:C:66:THR:CG2	2.63	0.46
1:B:480:ALA:C	1:B:481:VAL:HG22	2.30	0.46
1:A:491:SER:HA	1:E:233:ASN:CG	2.35	0.46
1:A:236:PHE:HE2	1:B:183:LEU:HD21	1.80	0.46
1:C:426:CYS:SG	1:D:553:TYR:CD2	3.02	0.46
1:B:213:ARG:HD3	1:B:509:PRO:HG2	1.98	0.46
1:A:76:SER:HB3	1:E:267:PHE:CD2	2.49	0.46
1:A:491:SER:HB2	1:E:233:ASN:HB3	1.97	0.46
1:B:98:ASN:O	1:B:99:ASN:CB	2.63	0.46
1:D:106:ALA:HB2	1:D:109:GLN:NE2	2.30	0.46
1:B:130:ASN:HD22	1:B:130:ASN:C	2.18	0.46
1:C:434:SER:O	1:D:556:LYS:HG2	2.16	0.46
1:A:70:TYR:HE2	1:E:464:GLY:HA2	1.80	0.46
1:B:528:THR:O	1:C:66:THR:HG22	2.16	0.46
1:C:232:THR:HB	1:D:495:VAL:HG21	1.97	0.46
1:E:497:ASN:ND2	1:E:500:PRO:HB3	2.25	0.46
1:D:130:ASN:C	1:D:130:ASN:HD22	2.18	0.46
1:C:478:ASP:OD2	1:D:483:SER:CB	2.64	0.46
1:A:172:GLU:HB3	1:E:425:LEU:HD22	1.98	0.46
2:G:12:ASN:C	2:G:14:VAL:N	2.67	0.46
1:B:464:GLY:HA3	1:C:68:ARG:NH2	2.30	0.46
1:B:257:ASN:HD21	1:B:432:CYS:HB3	1.81	0.46
1:A:63:LEU:CD2	1:A:67:THR:HG22	2.16	0.46
1:A:482:TYR:CD1	1:B:490:THR:CG2	2.98	0.46
1:A:183:LEU:HD21	1:E:236:PHE:CZ	2.50	0.46
1:A:106:ALA:HB2	1:A:109:GLN:NE2	2.31	0.46
1:A:213:ARG:HD3	1:A:509:PRO:HG2	1.97	0.46
1:A:228:PRO:HB3	1:B:493:THR:CB	2.46	0.46
1:C:83:ASN:OD1	1:C:91:PHE:CA	2.61	0.46
1:B:436:GLN:CD	1:C:558:LEU:CD1	2.82	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:ASP:O	1:C:63:LEU:CD1	2.64	0.46
1:B:234:GLU:OE2	1:C:496:PHE:HE1	1.99	0.46
1:D:106:ALA:CB	1:D:109:GLN:NE2	2.79	0.46
1:C:106:ALA:HB2	1:C:109:GLN:NE2	2.30	0.46
1:A:268:GLN:HG2	1:B:84:TYR:CE2	2.50	0.46
1:C:436:GLN:H	1:D:556:LYS:HZ1	1.53	0.46
1:A:436:GLN:H	1:B:556:LYS:HZ1	1.56	0.46
1:D:462:VAL:O	1:E:70:TYR:OH	2.27	0.46
1:E:258:LEU:HD13	1:E:430:VAL:HA	1.98	0.46
1:E:106:ALA:CB	1:E:109:GLN:NE2	2.79	0.46
1:E:106:ALA:HB2	1:E:109:GLN:NE2	2.30	0.46
1:A:79:VAL:HG11	1:A:82:LEU:HD12	1.96	0.46
1:B:106:ALA:CB	1:B:109:GLN:NE2	2.79	0.46
1:B:529:LEU:HD11	1:C:68:ARG:HH12	1.79	0.46
1:C:528:THR:O	1:D:66:THR:CG2	2.64	0.46
1:A:257:ASN:HB3	1:B:555:TYR:OH	2.12	0.46
1:A:47:ARG:CB	1:E:569:ARG:CB	2.93	0.46
1:A:482:TYR:CD1	1:B:490:THR:HG22	2.51	0.46
1:E:431:THR:O	1:E:432:CYS:CB	2.57	0.46
1:A:106:ALA:CB	1:A:109:GLN:NE2	2.79	0.46
1:A:230:VAL:CG1	1:B:492:LEU:HD12	2.46	0.46
1:C:436:GLN:NE2	1:D:558:LEU:CD2	2.74	0.46
1:A:47:ARG:NH1	1:A:53:ASN:HB2	2.31	0.46
1:C:220:ASP:CG	1:D:197:ARG:NH2	2.70	0.46
1:D:213:ARG:HD3	1:D:509:PRO:HG2	1.98	0.46
1:D:121:GLY:HA3	1:D:563:PRO:HA	1.98	0.46
1:E:121:GLY:HA3	1:E:563:PRO:HA	1.98	0.46
1:A:569:ARG:CB	1:B:47:ARG:CB	2.94	0.46
1:C:106:ALA:CB	1:C:109:GLN:NE2	2.79	0.46
1:C:450:THR:CG2	1:D:57:TYR:CZ	2.87	0.45
1:E:98:ASN:O	1:E:99:ASN:CB	2.63	0.45
1:A:411:ASN:HD21	1:B:171:PRO:HA	1.79	0.45
1:A:436:GLN:NE2	1:B:558:LEU:CD1	2.79	0.45
1:B:434:SER:O	1:C:556:LYS:CE	2.64	0.45
1:C:556:LYS:CE	1:C:558:LEU:CD2	2.80	0.45
1:D:529:LEU:HD11	1:E:68:ARG:NH2	2.30	0.45
1:A:66:THR:HG22	1:E:528:THR:O	2.16	0.45
1:A:47:ARG:NH1	1:A:53:ASN:ND2	2.64	0.45
1:D:257:ASN:ND2	1:E:555:TYR:OH	2.49	0.45
1:A:84:TYR:CE2	1:E:268:GLN:HG2	2.51	0.45
1:C:135:ASN:HA	1:C:172:GLU:CD	2.36	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ASN:CG	1:C:491:SER:HA	2.36	0.45
1:E:47:ARG:NH1	1:E:53:ASN:HB2	2.31	0.45
1:C:268:GLN:HG2	1:D:84:TYR:CE2	2.52	0.45
1:E:155:LYS:O	1:E:156:ASP:CB	2.37	0.45
1:B:236:PHE:CZ	1:C:183:LEU:HD21	2.51	0.45
1:A:450:THR:CB	1:B:57:TYR:HD1	2.29	0.45
1:A:135:ASN:HA	1:A:172:GLU:CD	2.36	0.45
1:A:172:GLU:N	1:E:411:ASN:ND2	2.58	0.45
1:B:135:ASN:HA	1:B:172:GLU:CD	2.36	0.45
1:A:528:THR:O	1:B:66:THR:CG2	2.65	0.45
1:B:121:GLY:HA3	1:B:563:PRO:HA	1.98	0.45
1:B:481:VAL:HG23	1:B:482:TYR:N	2.30	0.45
1:E:135:ASN:CA	1:E:172:GLU:OE1	2.63	0.45
1:E:135:ASN:HA	1:E:172:GLU:CD	2.36	0.45
1:E:488:GLN:HB3	1:E:494:HIS:NE2	2.32	0.45
1:C:528:THR:O	1:D:66:THR:HG22	2.17	0.45
1:B:268:GLN:HG2	1:C:84:TYR:CE2	2.51	0.45
1:A:128:HIS:HB3	1:A:556:LYS:HB3	1.98	0.45
1:C:436:GLN:HB3	1:D:558:LEU:CD2	2.46	0.45
1:A:66:THR:CG2	1:E:528:THR:O	2.65	0.45
1:B:569:ARG:HG2	1:C:47:ARG:HB3	1.99	0.45
1:D:135:ASN:HA	1:D:172:GLU:CD	2.36	0.45
1:C:476:TYR:HD1	1:D:475:PHE:CD2	2.33	0.45
1:A:79:VAL:O	1:A:81:SER:N	2.50	0.45
1:B:151:ARG:HG3	1:B:161:LEU:HD21	1.99	0.45
1:A:151:ARG:HG3	1:A:161:LEU:HD21	1.99	0.45
1:D:411:ASN:HD21	1:E:171:PRO:HA	1.79	0.45
1:A:230:VAL:CG1	1:B:492:LEU:CD1	2.94	0.45
1:A:434:SER:O	1:B:556:LYS:CE	2.65	0.45
1:A:436:GLN:OE1	1:B:558:LEU:HD21	2.16	0.45
1:E:438:TYR:CD1	1:E:462:VAL:HG11	2.52	0.45
1:A:70:TYR:OH	1:E:462:VAL:O	2.31	0.45
1:D:528:THR:O	1:E:66:THR:HG22	2.17	0.45
1:D:79:VAL:O	1:D:81:SER:N	2.50	0.45
1:C:72:VAL:HG22	1:C:73:ASP:H	1.80	0.45
1:A:478:ASP:OD2	1:B:483:SER:CB	2.64	0.45
1:A:528:THR:O	1:B:66:THR:HG22	2.16	0.45
1:A:47:ARG:NH2	1:A:53:ASN:HD22	2.05	0.45
1:A:481:VAL:HG23	1:B:490:THR:CG2	2.47	0.45
1:C:230:VAL:CG1	1:D:492:LEU:HD12	2.47	0.45
1:D:42:PRO:HA	1:D:43:PRO:HD3	1.87	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:TYR:CE1	1:C:172:GLU:O	2.70	0.45
1:B:436:GLN:NE2	1:C:558:LEU:CD1	2.80	0.45
1:A:514:THR:HB	1:E:476:TYR:CZ	2.52	0.45
1:B:90:ASN:ND2	1:B:457:ILE:HG21	2.32	0.45
1:C:151:ARG:HG3	1:C:161:LEU:HD21	1.99	0.45
1:B:79:VAL:O	1:B:81:SER:N	2.50	0.45
1:A:172:GLU:CB	1:E:425:LEU:HD22	2.46	0.45
1:B:467:LEU:HB2	1:C:126:ILE:HG21	1.99	0.45
1:A:481:VAL:HG23	1:B:490:THR:HB	1.98	0.45
1:E:47:ARG:NH1	1:E:53:ASN:ND2	2.64	0.45
1:C:497:ASN:ND2	1:C:500:PRO:HB3	2.25	0.45
1:D:151:ARG:HG3	1:D:161:LEU:HD21	1.99	0.45
1:B:479:GLN:O	1:B:483:SER:N	2.49	0.45
1:B:450:THR:CA	1:C:57:TYR:CD1	3.00	0.44
1:C:98:ASN:O	1:C:99:ASN:CB	2.63	0.44
1:A:220:ASP:CG	1:B:197:ARG:NH2	2.70	0.44
1:B:488:GLN:HB3	1:B:494:HIS:NE2	2.32	0.44
1:A:126:ILE:HD12	1:A:558:LEU:HD11	1.95	0.44
1:D:447:ASP:O	1:E:63:LEU:CD1	2.66	0.44
1:E:257:ASN:OD1	1:E:258:LEU:N	2.50	0.44
1:C:468:LEU:HG	1:C:470:VAL:HG23	1.99	0.44
1:A:450:THR:CA	1:B:57:TYR:CD1	3.00	0.44
1:B:436:GLN:NE2	1:C:558:LEU:HD11	2.32	0.44
1:D:463:VAL:O	1:E:70:TYR:OH	2.35	0.44
1:A:432:CYS:O	1:B:555:TYR:OH	2.28	0.44
1:B:481:VAL:HG23	1:C:490:THR:HG21	1.98	0.44
1:D:236:PHE:HE2	1:E:183:LEU:HD21	1.80	0.44
1:E:79:VAL:O	1:E:81:SER:N	2.50	0.44
1:C:221:PRO:HB2	1:D:194:LYS:HG3	1.99	0.44
1:A:57:TYR:CZ	1:A:60:LEU:HG	2.42	0.44
1:C:434:SER:O	1:D:556:LYS:CE	2.65	0.44
1:B:436:GLN:CB	1:C:558:LEU:CD2	2.92	0.44
1:A:232:THR:HB	1:B:495:VAL:HG21	1.99	0.44
1:B:237:HIS:HA	1:B:238:PRO:HD3	1.87	0.44
1:E:131:MET:HA	1:E:132:PRO:HD3	1.90	0.44
1:A:450:THR:HG21	1:B:96:ILE:HG22	1.93	0.44
1:A:172:GLU:CG	1:E:425:LEU:CD1	2.82	0.44
1:B:267:PHE:HE2	1:C:88:HIS:H	1.64	0.44
1:A:447:ASP:O	1:B:63:LEU:CD1	2.65	0.44
1:C:121:GLY:HA3	1:C:563:PRO:HA	1.98	0.44
1:A:121:GLY:HA3	1:A:563:PRO:HA	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:528:THR:O	1:E:66:THR:CG2	2.66	0.44
1:E:47:ARG:HG2	1:E:48:PRO:CD	2.45	0.44
1:A:497:ASN:ND2	1:A:500:PRO:HB3	2.25	0.44
1:A:101:TYR:CE2	1:A:105:GLU:HG2	2.53	0.44
1:C:101:TYR:CE2	1:C:105:GLU:HG2	2.53	0.44
1:D:488:GLN:HB3	1:D:494:HIS:NE2	2.32	0.44
1:A:438:TYR:CD1	1:A:462:VAL:HG11	2.52	0.44
1:A:544:THR:HG22	1:A:545:ASP:N	2.33	0.44
1:A:267:PHE:CD1	1:B:76:SER:O	2.70	0.44
1:A:172:GLU:HG3	1:E:425:LEU:CD1	2.47	0.44
1:B:267:PHE:HE2	1:C:86:ASN:O	1.92	0.44
1:D:438:TYR:CD1	1:D:462:VAL:HG11	2.52	0.44
1:C:438:TYR:CD1	1:C:462:VAL:HG11	2.52	0.44
1:A:481:VAL:HG23	1:A:482:TYR:N	2.32	0.44
1:C:79:VAL:O	1:C:81:SER:N	2.50	0.44
1:C:377:PRO:O	1:C:379:ILE:N	2.51	0.44
1:A:98:ASN:O	1:A:99:ASN:CB	2.63	0.44
1:D:434:SER:O	1:E:556:LYS:HG2	2.18	0.44
1:A:463:VAL:O	1:B:70:TYR:OH	2.35	0.44
2:H:8:GLU:CG	2:H:9:ASP:N	2.71	0.44
1:C:230:VAL:CG1	1:D:492:LEU:CD1	2.95	0.44
2:H:18:ASP:CB	2:H:19:THR:HA	2.43	0.44
1:E:508:PRO:HA	1:E:509:PRO:HD3	1.92	0.44
1:D:220:ASP:CG	1:E:197:ARG:NH2	2.70	0.44
1:C:135:ASN:CA	1:C:172:GLU:OE1	2.62	0.44
1:A:425:LEU:CD1	1:B:172:GLU:CB	2.87	0.44
1:A:63:LEU:CD1	1:E:447:ASP:O	2.66	0.44
1:B:481:VAL:HG23	1:C:490:THR:CG2	2.48	0.44
1:E:480:ALA:C	1:E:482:TYR:H	2.21	0.44
1:B:101:TYR:CE2	1:B:105:GLU:HG2	2.52	0.44
1:E:394:ILE:HG22	1:E:402:GLN:HG2	2.00	0.44
1:A:468:LEU:HG	1:A:470:VAL:HG23	1.99	0.44
1:C:544:THR:HG22	1:C:545:ASP:N	2.33	0.44
1:D:57:TYR:CE2	1:D:60:LEU:HB2	2.52	0.44
1:D:480:ALA:C	1:D:482:TYR:H	2.21	0.44
1:E:377:PRO:O	1:E:379:ILE:N	2.51	0.44
1:B:438:TYR:CD1	1:B:462:VAL:HG11	2.52	0.44
1:A:126:ILE:HG21	1:E:467:LEU:HB2	1.99	0.44
1:A:47:ARG:HB3	1:E:569:ARG:HG2	2.00	0.44
1:E:55:ILE:HG21	1:E:67:THR:HG21	2.00	0.44
1:D:232:THR:HB	1:E:495:VAL:HG21	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:TYR:CE2	1:D:105:GLU:HG2	2.53	0.44
1:E:101:TYR:CE2	1:E:105:GLU:HG2	2.53	0.44
1:B:394:ILE:HG22	1:B:402:GLN:HG2	2.00	0.44
1:C:133:ASN:HB2	1:C:175:TYR:CD2	2.53	0.44
1:B:468:LEU:HG	1:B:470:VAL:HG23	1.99	0.44
1:A:172:GLU:O	1:E:407:TYR:CE1	2.70	0.43
1:D:228:PRO:HB3	1:E:493:THR:CB	2.48	0.43
1:D:230:VAL:CG1	1:E:492:LEU:HD12	2.48	0.43
1:B:377:PRO:O	1:B:379:ILE:N	2.51	0.43
1:D:67:THR:O	1:D:563:PRO:HD2	2.18	0.43
1:C:233:ASN:CG	1:D:491:SER:HA	2.39	0.43
1:C:55:ILE:HG21	1:C:67:THR:HG21	2.00	0.43
1:C:67:THR:O	1:C:563:PRO:HD2	2.18	0.43
1:B:233:ASN:HB3	1:C:491:SER:HB2	1.99	0.43
1:A:569:ARG:HB3	1:B:47:ARG:H	1.83	0.43
1:E:264:ARG:NE	1:E:424:LEU:CD2	2.76	0.43
1:E:468:LEU:HG	1:E:470:VAL:HG23	1.99	0.43
1:D:544:THR:HG22	1:D:545:ASP:N	2.33	0.43
1:A:488:GLN:HB3	1:A:494:HIS:NE2	2.32	0.43
1:D:468:LEU:HG	1:D:470:VAL:HG23	1.99	0.43
1:E:544:THR:HG22	1:E:545:ASP:N	2.32	0.43
1:D:452:ARG:HG2	1:E:60:LEU:HD13	1.99	0.43
1:B:450:THR:HG21	1:C:96:ILE:HG22	1.94	0.43
1:C:57:TYR:O	1:C:57:TYR:CD1	2.71	0.43
1:B:228:PRO:CB	2:G:15:TYR:CE1	2.99	0.43
1:C:411:ASN:HD22	1:D:172:GLU:H	1.64	0.43
1:A:425:LEU:O	1:B:132:PRO:CG	2.60	0.43
1:B:55:ILE:HG21	1:B:67:THR:HG21	2.00	0.43
1:D:55:ILE:HG21	1:D:67:THR:HG21	2.00	0.43
1:A:55:ILE:HG21	1:A:67:THR:HG21	2.00	0.43
1:B:512:THR:HB	1:B:513:ILE:HD12	2.00	0.43
1:A:512:THR:HB	1:A:513:ILE:HD12	2.00	0.43
1:E:151:ARG:HG3	1:E:161:LEU:HD21	1.99	0.43
1:D:408:LEU:O	1:D:412:TYR:HB2	2.18	0.43
1:A:408:LEU:O	1:A:412:TYR:HB2	2.18	0.43
1:C:407:TYR:OH	1:D:172:GLU:O	2.35	0.43
1:A:377:PRO:O	1:A:379:ILE:N	2.51	0.43
1:C:480:ALA:C	1:C:482:TYR:H	2.21	0.43
1:E:67:THR:O	1:E:563:PRO:HD2	2.19	0.43
1:A:514:THR:CB	1:E:476:TYR:CE1	3.00	0.43
1:C:432:CYS:O	1:D:555:TYR:OH	2.36	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:ASN:HB2	1:E:175:TYR:CD2	2.53	0.43
1:A:450:THR:OG1	1:B:57:TYR:HD1	2.02	0.43
1:C:488:GLN:HB3	1:C:494:HIS:NE2	2.32	0.43
1:D:228:PRO:CB	2:H:15:TYR:CE1	2.99	0.43
1:A:556:LYS:HZ1	1:E:436:GLN:H	1.57	0.43
1:D:556:LYS:CE	1:D:558:LEU:CD2	2.81	0.43
1:A:425:LEU:HD13	1:B:172:GLU:HG3	2.00	0.43
1:A:47:ARG:H	1:E:569:ARG:HB3	1.83	0.43
1:B:569:ARG:HB3	1:C:47:ARG:H	1.83	0.43
1:D:221:PRO:HB2	1:E:194:LYS:HG3	2.00	0.43
1:D:512:THR:HB	1:D:513:ILE:HD12	2.00	0.43
1:A:133:ASN:HB2	1:A:175:TYR:CD2	2.53	0.43
1:D:133:ASN:HB2	1:D:175:TYR:CD2	2.53	0.43
1:E:408:LEU:O	1:E:412:TYR:HB2	2.18	0.43
1:C:394:ILE:HG22	1:C:402:GLN:HG2	2.00	0.43
2:G:12:ASN:O	2:G:13:PRO:C	2.57	0.43
1:D:434:SER:O	1:E:556:LYS:CE	2.65	0.43
1:A:257:ASN:OD1	1:A:258:LEU:N	2.51	0.43
1:B:544:THR:HG22	1:B:545:ASP:N	2.33	0.43
1:D:57:TYR:HH	1:D:98:ASN:ND2	2.17	0.43
1:C:436:GLN:CD	1:D:558:LEU:CD1	2.86	0.43
1:A:434:SER:O	1:B:556:LYS:HG2	2.17	0.43
1:B:155:LYS:CG	1:B:158:GLN:OE1	2.66	0.43
1:D:394:ILE:HG22	1:D:402:GLN:HG2	2.00	0.43
1:B:408:LEU:O	1:B:412:TYR:HB2	2.18	0.43
1:B:425:LEU:O	1:C:132:PRO:CG	2.59	0.43
1:A:264:ARG:NE	1:A:424:LEU:CD2	2.76	0.43
1:E:512:THR:HB	1:E:513:ILE:HD12	2.00	0.43
1:B:133:ASN:HB2	1:B:175:TYR:CD2	2.53	0.43
1:B:452:ARG:HG2	1:C:60:LEU:HD13	2.00	0.43
1:C:436:GLN:CB	1:D:558:LEU:CD2	2.96	0.43
1:A:436:GLN:OE1	1:B:558:LEU:CD1	2.54	0.43
1:D:569:ARG:CB	1:E:47:ARG:CB	2.96	0.43
1:A:394:ILE:HG22	1:A:402:GLN:HG2	2.00	0.43
1:A:267:PHE:O	1:A:267:PHE:CG	2.71	0.43
1:B:264:ARG:NE	1:B:424:LEU:CD2	2.76	0.43
1:D:135:ASN:CA	1:D:172:GLU:OE1	2.62	0.43
1:D:63:LEU:CD2	1:D:67:THR:CG2	2.86	0.43
1:C:512:THR:HB	1:C:513:ILE:HD12	2.00	0.43
1:A:197:ARG:HH21	1:E:220:ASP:CG	2.22	0.43
1:C:508:PRO:HA	1:C:509:PRO:HD3	1.92	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:PRO:O	1:D:379:ILE:N	2.51	0.43
1:C:407:TYR:CE1	1:D:172:GLU:O	2.72	0.43
1:B:480:ALA:C	1:B:482:TYR:N	2.72	0.43
1:A:47:ARG:HG2	1:A:48:PRO:CD	2.45	0.43
1:A:490:THR:HG23	1:E:482:TYR:HD1	1.83	0.43
1:C:569:ARG:CB	1:D:47:ARG:CB	2.96	0.43
1:D:234:GLU:OE2	1:E:496:PHE:HE1	2.02	0.43
1:A:237:HIS:HA	1:A:238:PRO:HD3	1.87	0.43
1:E:42:PRO:HA	1:E:43:PRO:HD3	1.87	0.43
1:A:67:THR:O	1:A:563:PRO:HD2	2.18	0.42
1:C:155:LYS:O	1:C:156:ASP:CB	2.37	0.42
1:E:47:ARG:NH2	1:E:53:ASN:HD22	2.03	0.42
1:B:476:TYR:OH	1:C:514:THR:OG1	2.36	0.42
1:A:90:ASN:ND2	1:A:457:ILE:HG21	2.32	0.42
1:D:184:MET:O	1:D:188:ILE:HG12	2.19	0.42
1:B:184:MET:O	1:B:188:ILE:HG12	2.19	0.42
1:A:468:LEU:HA	1:A:469:PRO:HD3	1.87	0.42
1:B:42:PRO:HA	1:B:43:PRO:HD3	1.87	0.42
1:A:172:GLU:C	1:E:425:LEU:HD22	2.39	0.42
1:B:228:PRO:HB3	1:C:493:THR:CB	2.49	0.42
1:C:131:MET:HA	1:C:132:PRO:HD3	1.90	0.42
1:C:408:LEU:O	1:C:412:TYR:HB2	2.18	0.42
1:B:450:THR:CB	1:C:57:TYR:HD1	2.29	0.42
1:A:230:VAL:CG1	1:B:492:LEU:CB	2.79	0.42
2:F:12:ASN:O	2:F:13:PRO:C	2.57	0.42
1:C:410:TYR:CZ	1:C:425:LEU:HB2	2.54	0.42
1:B:174:ASN:O	1:B:174:ASN:OD1	2.37	0.42
1:C:174:ASN:O	1:C:174:ASN:OD1	2.37	0.42
1:D:230:VAL:CG1	1:E:492:LEU:CD1	2.97	0.42
1:A:464:GLY:HA2	1:B:70:TYR:HE2	1.85	0.42
1:A:68:ARG:NH2	1:E:529:LEU:HD21	2.33	0.42
1:E:63:LEU:CD2	1:E:67:THR:HG22	2.16	0.42
1:D:508:PRO:HA	1:D:509:PRO:HD3	1.92	0.42
2:F:15:TYR:OH	1:B:493:THR:CA	2.68	0.42
1:B:67:THR:O	1:B:563:PRO:HD2	2.19	0.42
1:D:569:ARG:HB3	1:E:47:ARG:H	1.84	0.42
1:A:60:LEU:CD2	1:E:452:ARG:HE	2.30	0.42
2:H:12:ASN:O	2:H:13:PRO:C	2.57	0.42
1:B:410:TYR:CZ	1:B:425:LEU:HB2	2.54	0.42
1:A:436:GLN:HB3	1:B:558:LEU:CD2	2.50	0.42
1:A:569:ARG:HG2	1:B:47:ARG:HB3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:ASN:O	1:D:174:ASN:OD1	2.38	0.42
1:A:426:CYS:SG	1:B:553:TYR:CD2	3.04	0.42
1:C:425:LEU:O	1:D:132:PRO:CG	2.58	0.42
1:A:233:ASN:CG	1:B:491:SER:HA	2.40	0.42
1:C:184:MET:O	1:C:188:ILE:HG12	2.19	0.42
1:A:57:TYR:CG	1:E:450:THR:HA	2.51	0.42
1:B:530:PRO:CG	1:C:66:THR:O	2.68	0.42
1:C:155:LYS:CG	1:C:158:GLN:OE1	2.66	0.42
1:A:475:PHE:CD2	1:E:476:TYR:HD1	2.34	0.42
1:C:569:ARG:HG2	1:D:47:ARG:HB3	2.02	0.42
1:E:174:ASN:OD1	1:E:174:ASN:O	2.37	0.42
1:C:266:PRO:HD3	1:D:87:ASP:HB2	1.93	0.42
1:A:184:MET:O	1:A:188:ILE:HG12	2.19	0.42
1:A:378:VAL:HG23	1:A:379:ILE:N	2.34	0.42
1:B:425:LEU:CG	1:C:172:GLU:CB	2.98	0.42
1:A:482:TYR:CB	1:B:490:THR:HG21	2.43	0.42
1:A:174:ASN:OD1	1:A:174:ASN:O	2.38	0.42
1:C:234:GLU:OE2	1:D:496:PHE:HE1	2.03	0.42
1:B:497:ASN:ND2	1:B:500:PRO:HB3	2.25	0.42
1:B:457:ILE:H	1:B:457:ILE:HG13	1.60	0.42
1:E:184:MET:O	1:E:188:ILE:HG12	2.19	0.42
1:A:42:PRO:HA	1:A:43:PRO:HD3	1.87	0.42
1:B:57:TYR:CD1	1:B:57:TYR:O	2.72	0.42
1:B:220:ASP:CG	1:C:197:ARG:HH21	2.23	0.42
1:A:228:PRO:CB	2:F:15:TYR:CE1	2.99	0.42
1:A:528:THR:CB	1:B:66:THR:HG21	2.50	0.42
1:A:68:ARG:NH2	1:E:529:LEU:HD11	2.35	0.42
1:A:66:THR:HG21	1:E:528:THR:CB	2.50	0.42
1:A:221:PRO:HB2	1:B:194:LYS:HG3	2.02	0.42
1:A:57:TYR:CD2	1:A:59:GLU:C	2.93	0.41
1:E:155:LYS:CG	1:E:158:GLN:OE1	2.66	0.41
1:E:106:ALA:CB	1:E:109:GLN:CD	2.89	0.41
1:D:426:CYS:SG	1:E:553:TYR:CD2	3.04	0.41
1:C:237:HIS:HA	1:C:238:PRO:HD3	1.87	0.41
1:B:230:VAL:HB	1:C:493:THR:HG23	2.01	0.41
1:D:436:GLN:NE2	1:E:558:LEU:CD1	2.69	0.41
1:D:464:GLY:HA2	1:E:70:TYR:HE2	1.85	0.41
1:E:152:LEU:CB	1:E:153:PRO:CD	2.89	0.41
1:B:106:ALA:CB	1:B:109:GLN:CD	2.89	0.41
1:C:111:ILE:HB	1:C:535:ILE:HB	2.03	0.41
1:D:378:VAL:HG23	1:D:379:ILE:N	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:TYR:O	1:B:95:VAL:HG13	2.21	0.41
1:B:258:LEU:HD13	1:B:430:VAL:HA	2.03	0.41
1:B:481:VAL:CG2	1:B:482:TYR:N	2.83	0.41
1:C:106:ALA:CB	1:C:109:GLN:CD	2.89	0.41
1:C:258:LEU:HD13	1:C:430:VAL:HA	2.02	0.41
1:B:378:VAL:HG23	1:B:379:ILE:N	2.34	0.41
1:C:236:PHE:CZ	1:D:183:LEU:HD21	2.55	0.41
1:A:185:ASN:O	1:A:189:VAL:HG23	2.21	0.41
1:C:133:ASN:HB2	1:C:175:TYR:HD2	1.86	0.41
1:E:111:ILE:HB	1:E:535:ILE:HB	2.03	0.41
1:B:111:ILE:HB	1:B:535:ILE:HB	2.03	0.41
1:C:436:GLN:OE1	1:D:558:LEU:HD11	2.21	0.41
1:A:436:GLN:NE2	1:B:558:LEU:HD11	2.34	0.41
1:C:70:TYR:O	1:C:95:VAL:HG13	2.21	0.41
1:D:258:LEU:HD13	1:D:430:VAL:HA	2.03	0.41
1:D:569:ARG:HG2	1:E:47:ARG:HB3	2.02	0.41
1:B:454:THR:HG21	1:B:459:ASN:CG	2.40	0.41
1:A:70:TYR:O	1:A:95:VAL:HG13	2.21	0.41
1:E:68:ARG:CD	1:E:70:TYR:CZ	2.83	0.41
1:B:47:ARG:HG2	1:B:48:PRO:CD	2.45	0.41
1:C:264:ARG:NE	1:C:424:LEU:CD2	2.76	0.41
1:B:513:ILE:HD11	1:C:516:VAL:HG21	2.03	0.41
1:E:133:ASN:HB2	1:E:175:TYR:HD2	1.85	0.41
1:A:111:ILE:HB	1:A:535:ILE:HB	2.03	0.41
1:A:132:PRO:CG	1:E:425:LEU:O	2.60	0.41
1:D:436:GLN:HB3	1:E:558:LEU:CD2	2.50	0.41
1:C:425:LEU:HD21	1:D:172:GLU:O	2.21	0.41
1:A:66:THR:O	1:E:530:PRO:CG	2.69	0.41
1:A:47:ARG:HA	1:E:569:ARG:O	2.20	0.41
1:D:106:ALA:CB	1:D:109:GLN:CD	2.89	0.41
1:A:106:ALA:CB	1:A:109:GLN:CD	2.89	0.41
1:D:457:ILE:H	1:D:457:ILE:HG13	1.60	0.41
1:B:118:HIS:NE2	1:C:65:ASP:OD1	2.49	0.41
1:C:185:ASN:O	1:C:189:VAL:HG23	2.21	0.41
1:C:467:LEU:HB2	1:D:126:ILE:HG21	2.03	0.41
1:D:70:TYR:O	1:D:95:VAL:HG13	2.21	0.41
1:B:481:VAL:CG2	1:C:490:THR:CB	2.98	0.41
1:C:47:ARG:HG2	1:C:48:PRO:CD	2.45	0.41
1:D:111:ILE:HB	1:D:535:ILE:HB	2.03	0.41
1:A:267:PHE:HD2	1:B:84:TYR:HA	1.86	0.41
1:C:450:THR:HG21	1:D:96:ILE:HG22	1.95	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:THR:HG21	1:C:459:ASN:CG	2.41	0.41
1:A:99:ASN:CB	1:E:459:ASN:OD1	2.68	0.41
1:A:135:ASN:HA	1:A:172:GLU:OE2	2.21	0.41
1:A:556:LYS:HB3	1:E:434:SER:HB3	2.02	0.41
1:D:436:GLN:OE1	1:E:558:LEU:HD13	2.21	0.41
1:C:410:TYR:CE2	1:C:425:LEU:HD13	2.56	0.41
1:B:135:ASN:HA	1:B:172:GLU:OE2	2.21	0.41
1:B:434:SER:CB	1:C:556:LYS:CB	2.89	0.41
1:C:119:TRP:CE3	1:C:563:PRO:HB2	2.56	0.41
1:B:257:ASN:ND2	1:C:555:TYR:OH	2.54	0.41
1:B:257:ASN:CG	1:C:555:TYR:OH	2.59	0.41
1:A:257:ASN:HD21	1:A:432:CYS:HB3	1.85	0.41
1:A:119:TRP:CE3	1:A:563:PRO:HB2	2.56	0.41
1:E:119:TRP:CE3	1:E:563:PRO:HB2	2.56	0.41
1:A:479:GLN:O	1:A:480:ALA:O	2.39	0.41
1:D:47:ARG:HG2	1:D:48:PRO:CD	2.45	0.41
1:D:264:ARG:NE	1:D:424:LEU:CD2	2.75	0.41
1:E:185:ASN:O	1:E:189:VAL:HG23	2.21	0.41
1:B:185:ASN:O	1:B:189:VAL:HG23	2.21	0.41
1:A:151:ARG:O	1:A:151:ARG:HG2	2.21	0.41
1:A:558:LEU:HD13	1:E:436:GLN:OE1	2.20	0.41
1:C:135:ASN:HA	1:C:172:GLU:OE2	2.21	0.41
1:B:528:THR:CB	1:C:66:THR:HG21	2.51	0.41
1:A:480:ALA:C	1:A:482:TYR:N	2.72	0.41
1:B:155:LYS:CB	1:B:158:GLN:HB2	2.47	0.41
1:C:476:TYR:CE1	1:D:514:THR:CB	3.04	0.41
1:D:476:TYR:CE2	1:E:477:ASN:CB	2.91	0.41
1:C:569:ARG:HB3	1:D:47:ARG:H	1.86	0.41
1:D:482:TYR:CZ	1:E:486:ILE:CG2	3.00	0.41
1:C:236:PHE:HE2	1:D:174:ASN:HD22	1.66	0.41
1:B:414:ASP:HA	1:B:415:PRO:HD3	1.88	0.41
1:D:407:TYR:CE1	1:E:172:GLU:O	2.74	0.40
1:A:57:TYR:CE2	1:A:60:LEU:HD12	2.54	0.40
1:B:230:VAL:CG1	1:C:492:LEU:HD12	2.51	0.40
1:B:119:TRP:CE3	1:B:563:PRO:HB2	2.56	0.40
1:B:463:VAL:CA	1:C:70:TYR:OH	2.70	0.40
1:C:476:TYR:CZ	1:D:514:THR:HB	2.56	0.40
1:A:155:LYS:CB	1:A:158:GLN:HB2	2.47	0.40
1:B:273:ILE:O	1:B:273:ILE:HG23	2.22	0.40
1:A:475:PHE:CD2	1:E:476:TYR:CG	3.09	0.40
1:A:194:LYS:HG3	1:E:221:PRO:CB	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:ASN:ND2	1:E:457:ILE:HG21	2.32	0.40
1:B:230:VAL:CG1	1:C:492:LEU:CD1	2.99	0.40
1:D:119:TRP:CE3	1:D:563:PRO:HB2	2.56	0.40
1:D:47:ARG:NH1	1:D:53:ASN:HB2	2.36	0.40
1:D:233:ASN:CG	1:E:491:SER:HA	2.41	0.40
1:A:174:ASN:HD22	1:E:236:PHE:HE2	1.66	0.40
1:A:516:VAL:HG21	1:E:513:ILE:HD11	2.02	0.40
2:F:18:ASP:CB	2:F:19:THR:HA	2.43	0.40
1:C:151:ARG:O	1:C:151:ARG:HG2	2.21	0.40
1:B:450:THR:OG1	1:C:57:TYR:HD1	2.05	0.40
1:B:266:PRO:HD3	1:C:87:ASP:HB2	1.94	0.40
1:A:531:LEU:HD11	1:A:563:PRO:HB3	2.04	0.40
1:D:185:ASN:O	1:D:189:VAL:HG23	2.21	0.40
1:B:151:ARG:HG2	1:B:151:ARG:O	2.21	0.40
1:C:544:THR:CG2	1:C:548:ARG:HA	2.52	0.40
1:E:61:ALA:HA	1:E:62:PRO:HD3	1.96	0.40
1:A:529:LEU:HA	1:A:530:PRO:HD3	1.93	0.40
1:C:447:ASP:O	1:D:63:LEU:HD13	2.21	0.40
1:C:481:VAL:CG1	1:D:490:THR:HB	2.30	0.40
1:C:531:LEU:HD11	1:C:563:PRO:HB3	2.04	0.40
1:D:236:PHE:HE2	1:E:174:ASN:HD22	1.66	0.40
1:C:150:SER:HB3	1:C:199:ASN:HB3	2.04	0.40
1:D:266:PRO:HD2	1:E:87:ASP:HB2	1.97	0.40
1:E:151:ARG:O	1:E:151:ARG:HG2	2.20	0.40
1:A:544:THR:CG2	1:A:548:ARG:HA	2.52	0.40
1:E:544:THR:CG2	1:E:548:ARG:HA	2.52	0.40
1:C:273:ILE:HG23	1:C:273:ILE:O	2.22	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	451/571 (79%)	341 (76%)	84 (19%)	26 (6%)	2	25
1	B	451/571 (79%)	341 (76%)	85 (19%)	25 (6%)	2	26
1	C	451/571 (79%)	341 (76%)	85 (19%)	25 (6%)	2	26
1	D	451/571 (79%)	341 (76%)	85 (19%)	25 (6%)	2	26
1	E	451/571 (79%)	340 (75%)	85 (19%)	26 (6%)	2	25
2	F	11/581 (2%)	3 (27%)	2 (18%)	6 (54%)	0	0
2	G	11/581 (2%)	3 (27%)	2 (18%)	6 (54%)	0	0
2	H	11/581 (2%)	3 (27%)	2 (18%)	6 (54%)	0	0
All	All	2288/4598 (50%)	1713 (75%)	430 (19%)	145 (6%)	3	23

All (145) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	SER
1	A	156	ASP
1	A	378	VAL
2	F	8	GLU
2	F	9	ASP
2	F	10	THR
2	F	11	PHE
1	B	81	SER
1	B	156	ASP
1	B	378	VAL
2	G	8	GLU
2	G	9	ASP
2	G	10	THR
2	G	11	PHE
1	C	81	SER
1	C	156	ASP
1	C	378	VAL
1	D	81	SER
1	D	156	ASP
1	D	378	VAL
2	H	8	GLU
2	H	9	ASP
2	H	10	THR
2	H	11	PHE
1	E	81	SER
1	E	156	ASP
1	E	378	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	80	ALA
1	A	85	GLN
1	A	99	ASN
1	A	103	PRO
1	A	153	PRO
1	A	449	VAL
1	A	480	ALA
2	F	16	PRO
1	B	80	ALA
1	B	85	GLN
1	B	99	ASN
1	B	103	PRO
1	B	153	PRO
1	B	449	VAL
2	G	16	PRO
1	C	80	ALA
1	C	85	GLN
1	C	99	ASN
1	C	103	PRO
1	C	153	PRO
1	C	449	VAL
1	D	80	ALA
1	D	85	GLN
1	D	99	ASN
1	D	103	PRO
1	D	153	PRO
1	D	449	VAL
2	H	16	PRO
1	E	80	ALA
1	E	85	GLN
1	E	99	ASN
1	E	103	PRO
1	E	153	PRO
1	E	449	VAL
1	A	208	VAL
1	A	429	ASP
1	B	208	VAL
1	B	429	ASP
1	C	208	VAL
1	C	429	ASP
1	D	208	VAL
1	D	429	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	208	VAL
1	E	429	ASP
1	A	151	ARG
1	A	552	PRO
2	F	13	PRO
1	B	151	ARG
1	B	552	PRO
2	G	13	PRO
1	C	151	ARG
1	C	552	PRO
1	D	151	ARG
1	D	552	PRO
2	H	13	PRO
1	E	151	ARG
1	E	552	PRO
1	A	41	VAL
1	A	102	SER
1	A	152	LEU
1	A	176	SER
1	A	388	LYS
1	B	41	VAL
1	B	102	SER
1	B	152	LEU
1	B	176	SER
1	B	388	LYS
1	B	459	ASN
1	C	41	VAL
1	C	102	SER
1	C	152	LEU
1	C	176	SER
1	C	388	LYS
1	C	459	ASN
1	D	41	VAL
1	D	102	SER
1	D	152	LEU
1	D	176	SER
1	D	388	LYS
1	E	41	VAL
1	E	102	SER
1	E	152	LEU
1	E	176	SER
1	E	388	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	432	CYS
1	E	459	ASN
1	A	120	GLY
1	A	200	GLY
1	A	459	ASN
1	A	513	ILE
1	B	120	GLY
1	B	200	GLY
1	B	513	ILE
1	C	120	GLY
1	C	200	GLY
1	C	513	ILE
1	D	120	GLY
1	D	200	GLY
1	D	459	ASN
1	D	513	ILE
1	E	120	GLY
1	E	200	GLY
1	E	513	ILE
1	A	481	VAL
1	C	481	VAL
1	B	481	VAL
1	D	481	VAL
1	E	481	VAL
1	A	50	GLY
1	A	95	VAL
1	B	50	GLY
1	B	95	VAL
1	C	50	GLY
1	C	95	VAL
1	D	50	GLY
1	D	95	VAL
1	E	50	GLY
1	E	95	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	412/489 (84%)	391 (95%)	21 (5%)	29	70
1	B	412/489 (84%)	392 (95%)	20 (5%)	31	71
1	C	412/489 (84%)	392 (95%)	20 (5%)	31	71
1	D	412/489 (84%)	393 (95%)	19 (5%)	33	73
1	E	412/489 (84%)	392 (95%)	20 (5%)	31	71
2	F	13/489 (3%)	12 (92%)	1 (8%)	16	56
2	G	13/489 (3%)	12 (92%)	1 (8%)	16	56
2	H	13/489 (3%)	12 (92%)	1 (8%)	16	56
All	All	2099/3912 (54%)	1996 (95%)	103 (5%)	35	71

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ILE
1	A	57	TYR
1	A	84	TYR
1	A	101	TYR
1	A	108	THR
1	A	109	GLN
1	A	115	ASP
1	A	130	ASN
1	A	133	ASN
1	A	156	ASP
1	A	176	SER
1	A	182	ASP
1	A	211	ASP
1	A	271	PHE
1	A	276	ASP
1	A	395	SER
1	A	404	ARG
1	A	417	THR
1	A	425	LEU
1	A	429	ASP
1	A	555	TYR
2	F	15	TYR
1	B	55	ILE
1	B	57	TYR
1	B	84	TYR
1	B	101	TYR
1	B	108	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	109	GLN
1	B	115	ASP
1	B	130	ASN
1	B	133	ASN
1	B	156	ASP
1	B	176	SER
1	B	182	ASP
1	B	211	ASP
1	B	271	PHE
1	B	276	ASP
1	B	395	SER
1	B	404	ARG
1	B	417	THR
1	B	425	LEU
1	B	429	ASP
2	G	15	TYR
1	C	55	ILE
1	C	57	TYR
1	C	84	TYR
1	C	101	TYR
1	C	108	THR
1	C	109	GLN
1	C	115	ASP
1	C	130	ASN
1	C	133	ASN
1	C	156	ASP
1	C	176	SER
1	C	182	ASP
1	C	211	ASP
1	C	271	PHE
1	C	276	ASP
1	C	395	SER
1	C	404	ARG
1	C	417	THR
1	C	425	LEU
1	C	429	ASP
1	D	55	ILE
1	D	57	TYR
1	D	84	TYR
1	D	101	TYR
1	D	108	THR
1	D	109	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	115	ASP
1	D	130	ASN
1	D	133	ASN
1	D	156	ASP
1	D	176	SER
1	D	182	ASP
1	D	211	ASP
1	D	271	PHE
1	D	276	ASP
1	D	395	SER
1	D	404	ARG
1	D	417	THR
1	D	429	ASP
2	H	15	TYR
1	E	55	ILE
1	E	57	TYR
1	E	84	TYR
1	E	101	TYR
1	E	108	THR
1	E	109	GLN
1	E	115	ASP
1	E	130	ASN
1	E	133	ASN
1	E	156	ASP
1	E	176	SER
1	E	182	ASP
1	E	211	ASP
1	E	271	PHE
1	E	276	ASP
1	E	395	SER
1	E	404	ARG
1	E	417	THR
1	E	425	LEU
1	E	429	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	109	GLN
1	A	130	ASN
1	A	133	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	174	ASN
1	A	186	ASN
1	A	198	GLN
1	A	265	GLN
1	A	293	GLN
1	A	411	ASN
1	A	436	GLN
1	A	497	ASN
1	A	503	GLN
1	A	519	ASN
1	B	53	ASN
1	B	98	ASN
1	B	109	GLN
1	B	130	ASN
1	B	133	ASN
1	B	174	ASN
1	B	186	ASN
1	B	198	GLN
1	B	265	GLN
1	B	293	GLN
1	B	411	ASN
1	B	436	GLN
1	B	477	ASN
1	B	497	ASN
1	B	503	GLN
1	B	519	ASN
1	C	53	ASN
1	C	88	HIS
1	C	109	GLN
1	C	130	ASN
1	C	133	ASN
1	C	174	ASN
1	C	186	ASN
1	C	198	GLN
1	C	265	GLN
1	C	411	ASN
1	C	497	ASN
1	C	503	GLN
1	C	519	ASN
1	D	53	ASN
1	D	88	HIS
1	D	109	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	130	ASN
1	D	133	ASN
1	D	174	ASN
1	D	186	ASN
1	D	198	GLN
1	D	257	ASN
1	D	265	GLN
1	D	293	GLN
1	D	411	ASN
1	D	497	ASN
1	D	503	GLN
1	D	519	ASN
1	E	53	ASN
1	E	109	GLN
1	E	130	ASN
1	E	133	ASN
1	E	174	ASN
1	E	186	ASN
1	E	198	GLN
1	E	257	ASN
1	E	265	GLN
1	E	411	ASN
1	E	497	ASN
1	E	503	GLN
1	E	519	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [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.