



Full wwPDB X-ray Structure Validation Report i

May 29, 2020 – 03:10 am BST

PDB ID : 3MKU
Title : Structure of a Cation-bound Multidrug and Toxin Compound Extrusion (MATE) transporter
Authors : He, X.; Szewczyk, P.; Karyakin, A.; Evin, M.; Hong, W.-X.; Zhang, Q.; Chang, G.
Deposited on : 2010-04-15
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the i symbol.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

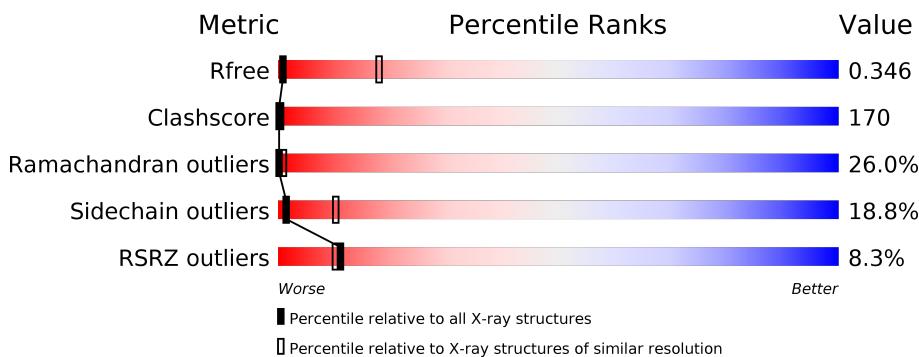
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

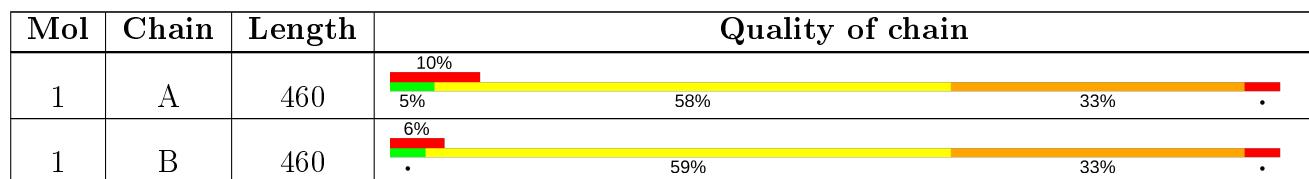
The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7013 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Multi antimicrobial extrusion protein (Na(+))/drug antiporter) MATE-like MDR efflux pump.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C 3505	N 2326	O 569	S 589	21	0	0
1	B	460	Total	C 3506	N 2326	O 569	S 590	21	0	0

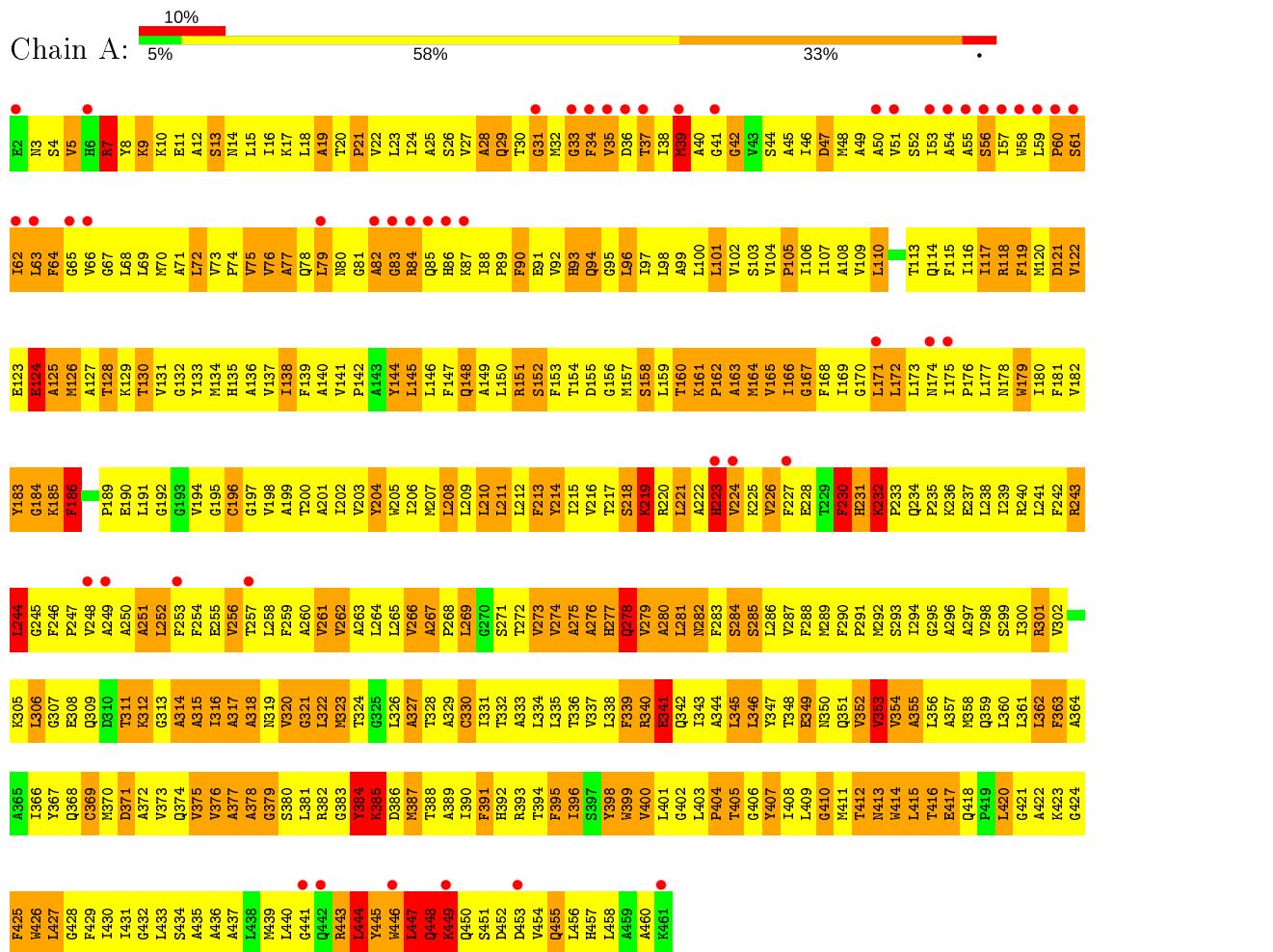
- Molecule 2 is RUBIDIUM ION (three-letter code: RB) (formula: Rb).

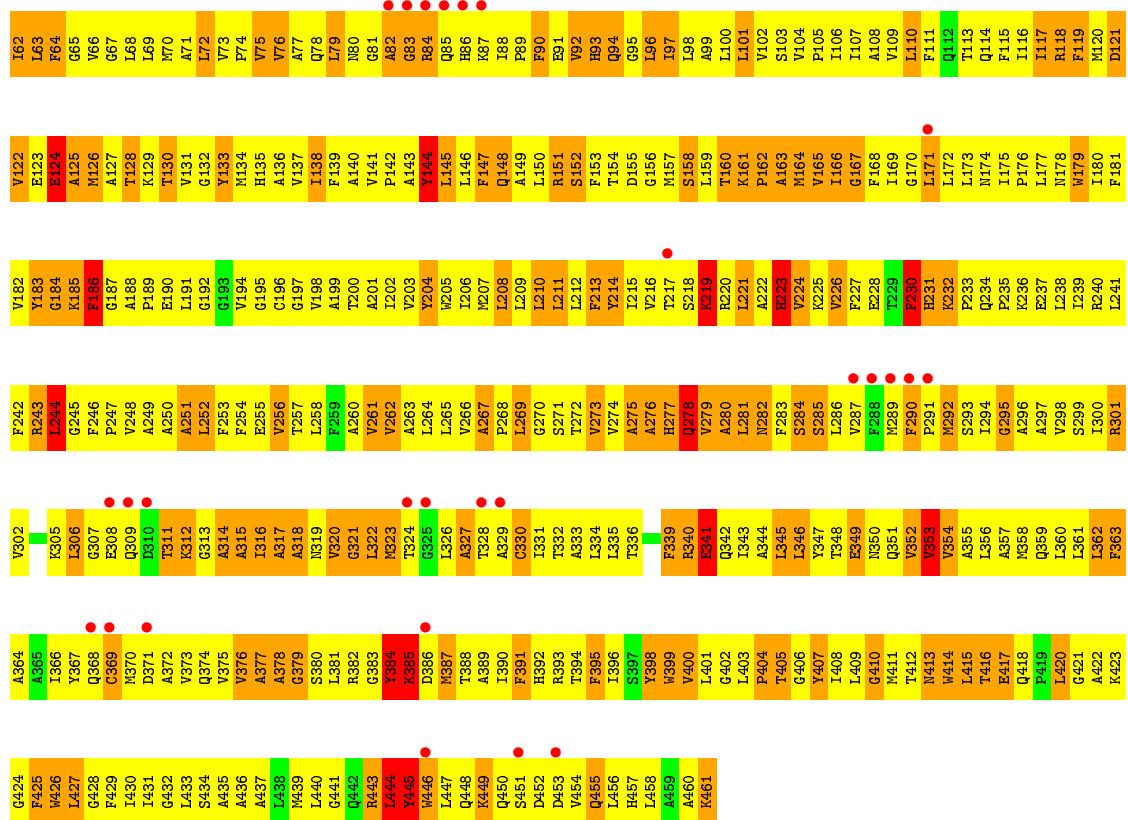
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Rb 1 1	0	0
2	A	1	Total Rb 1 1	0	0

3 Residue-property plots

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

- Molecule 1: Multi antimicrobial extrusion protein (Na(+)/drug antiporter) MATE-like MDR efflux pump





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.80 Å 241.85 Å 46.15 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.20 133.33 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-4.20) 99.0 (133.33-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	2.87 (at 4.01 Å)	Xtriage
Refinement program	CNS	Depositor
R , R_{free}	0.309 , 0.342 0.327 , 0.346	Depositor DCC
R_{free} test set	791 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	105.5	Xtriage
Anisotropy	1.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 145.2	EDS
L-test for twinning ²	$< L > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	7013	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.65	0/3585	0.97	13/4879 (0.3%)
1	B	0.64	0/3586	0.93	9/4879 (0.2%)
All	All	0.64	0/7171	0.95	22/9758 (0.2%)

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	B	0	2

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	VAL	CB-CA-C	-8.84	94.61	111.40
1	A	410	GLY	N-CA-C	-8.24	92.50	113.10
1	A	384	TYR	CB-CA-C	7.94	126.28	110.40
1	B	410	GLY	N-CA-C	-7.78	93.65	113.10
1	A	447	LEU	N-CA-C	-7.57	90.56	111.00
1	A	449	LYS	N-CA-CB	-7.45	97.19	110.60
1	B	353	VAL	CB-CA-C	-7.08	97.94	111.40
1	A	385	LYS	N-CA-CB	-6.88	98.22	110.60
1	A	448	GLN	N-CA-C	-6.42	93.66	111.00
1	B	444	LEU	CA-CB-CG	5.99	129.08	115.30
1	A	75	VAL	N-CA-C	-5.92	95.03	111.00
1	B	446	TRP	N-CA-C	-5.89	95.08	111.00
1	A	413	ASN	N-CA-C	-5.89	95.10	111.00
1	A	444	LEU	CA-CB-CG	5.86	128.78	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	413	ASN	N-CA-C	-5.65	95.75	111.00
1	A	385	LYS	N-CA-C	5.59	126.08	111.00
1	A	306	LEU	CA-CB-CG	5.56	128.09	115.30
1	B	420	LEU	CA-CB-CG	5.46	127.86	115.30
1	B	75	VAL	N-CA-C	-5.41	96.40	111.00
1	B	384	TYR	CA-CB-CG	5.38	123.62	113.40
1	B	306	LEU	CA-CB-CG	5.20	127.27	115.30
1	A	420	LEU	CA-CB-CG	5.10	127.02	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	133	TYR	Sidechain
1	B	144	TYR	Sidechain

5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3505	0	3676	1224	0
1	B	3506	0	3676	1223	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	7013	0	7352	2440	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 170.

All (2440) 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:A:447:LEU:CD1	1:A:450:GLN:HE21	1.27	1.48
1:A:447:LEU:CD1	1:A:450:GLN:NE2	1.96	1.27
1:A:447:LEU:HD13	1:A:450:GLN:NE2	1.50	1.24

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:PRO:O	1:B:165:VAL:HG12	1.38	1.17
1:A:320:VAL:HG13	1:A:321:GLY:H	1.04	1.17
1:A:162:PRO:O	1:A:165:VAL:HG12	1.43	1.17
1:A:447:LEU:C	1:A:447:LEU:HD12	1.65	1.16
1:A:151:ARG:HG3	1:A:162:PRO:HG2	1.27	1.16
1:A:358:MET:HA	1:A:361:LEU:HD12	1.22	1.16
1:A:231:HIS:HB3	1:A:235:PRO:HD3	1.27	1.15
1:B:320:VAL:HG13	1:B:321:GLY:H	0.99	1.15
1:B:235:PRO:HA	1:B:238:LEU:HB2	1.26	1.15
1:B:398:TYR:HB3	1:B:436:ALA:HB2	1.18	1.14
1:B:73:VAL:HB	1:B:74:PRO:HD3	1.19	1.14
1:A:447:LEU:HD12	1:A:447:LEU:O	1.45	1.14
1:B:408:ILE:HA	1:B:411:MET:HB2	1.16	1.14
1:A:398:TYR:CB	1:A:436:ALA:HB2	1.77	1.13
1:B:151:ARG:HG3	1:B:162:PRO:HG2	1.23	1.13
1:B:165:VAL:HG13	1:B:166:ILE:H	1.09	1.13
1:A:447:LEU:O	1:A:447:LEU:CD1	1.97	1.12
1:A:398:TYR:HB3	1:A:436:ALA:HB2	1.11	1.11
1:A:266:VAL:HG12	1:A:269:LEU:HD11	1.33	1.11
1:A:117:ILE:HG22	1:A:118:ARG:H	1.15	1.10
1:B:398:TYR:CB	1:B:436:ALA:HB2	1.80	1.10
1:A:45:ALA:HB3	1:A:49:ALA:HB2	1.31	1.10
1:A:73:VAL:HB	1:A:74:PRO:HD3	1.20	1.10
1:A:165:VAL:HG13	1:A:166:ILE:H	1.13	1.09
1:A:447:LEU:HD11	1:A:450:GLN:HE21	0.94	1.08
1:A:235:PRO:HA	1:A:238:LEU:HB2	1.34	1.08
1:A:408:ILE:HA	1:A:411:MET:HB2	1.11	1.08
1:B:445:TYR:HB2	1:B:448:GLN:HA	1.31	1.07
1:B:118:ARG:HE	1:B:119:PHE:HB2	1.14	1.07
1:B:420:LEU:HD12	1:B:423:LYS:H	1.18	1.07
1:B:231:HIS:HB3	1:B:235:PRO:HD3	1.32	1.07
1:B:11:GLU:HA	1:B:301:ARG:HH22	1.13	1.07
1:A:118:ARG:HE	1:A:119:PHE:HB2	1.12	1.06
1:B:4:SER:O	1:B:8:TYR:CD2	2.08	1.06
1:B:266:VAL:HG12	1:B:269:LEU:HD11	1.30	1.06
1:B:147:PHE:HB2	1:B:211:LEU:HD13	1.39	1.05
1:B:45:ALA:HB3	1:B:49:ALA:HB2	1.34	1.05
1:B:340:ARG:HD2	1:B:358:MET:HG2	1.32	1.04
1:B:358:MET:HA	1:B:361:LEU:HD12	1.08	1.04
1:A:420:LEU:HD12	1:A:423:LYS:H	1.22	1.03
1:B:262:VAL:HG11	1:B:403:LEU:HD22	1.41	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:VAL:O	1:B:357:ALA:N	1.92	1.01
1:A:145:LEU:HD13	1:A:146:LEU:N	1.74	1.01
1:B:145:LEU:HD13	1:B:146:LEU:N	1.74	1.01
1:B:165:VAL:CG1	1:B:166:ILE:H	1.71	1.01
1:A:12:ALA:O	1:A:15:LEU:HG	1.58	1.01
1:A:165:VAL:CG1	1:A:166:ILE:H	1.73	1.00
1:A:11:GLU:HA	1:A:301:ARG:HH22	1.27	1.00
1:A:262:VAL:HG11	1:A:403:LEU:HD22	1.44	0.99
1:A:231:HIS:HB3	1:A:235:PRO:CD	1.90	0.99
1:B:12:ALA:O	1:B:15:LEU:HG	1.62	0.99
1:A:385:LYS:O	1:A:388:THR:OG1	1.80	0.98
1:B:231:HIS:HB3	1:B:235:PRO:CD	1.94	0.98
1:A:151:ARG:HA	1:A:155:ASP:HA	1.46	0.97
1:B:76:VAL:HA	1:B:78:GLN:HE21	1.28	0.97
1:B:165:VAL:HG13	1:B:166:ILE:N	1.78	0.97
1:B:376:VAL:HG13	1:B:377:ALA:H	1.27	0.97
1:A:287:VAL:HG11	1:A:368:GLN:OE1	1.64	0.97
1:A:312:LYS:O	1:A:316:ILE:HG12	1.65	0.97
1:A:244:LEU:HD23	1:A:385:LYS:O	1.65	0.97
1:A:340:ARG:HD2	1:A:358:MET:HG2	1.43	0.97
1:B:97:ILE:HG22	1:B:101:LEU:HD11	1.45	0.96
1:A:343:ILE:O	1:A:346:LEU:HB2	1.65	0.96
1:B:272:THR:HG23	1:B:275:ALA:HB3	1.47	0.96
1:A:272:THR:HG23	1:A:275:ALA:HB3	1.44	0.96
1:B:208:LEU:HD23	1:B:209:LEU:N	1.80	0.96
1:B:177:LEU:HD12	1:B:202:ILE:HD13	1.45	0.96
1:A:420:LEU:HB3	1:A:423:LYS:HG2	1.48	0.96
1:B:17:LYS:O	1:B:21:PRO:HG2	1.63	0.95
1:A:17:LYS:O	1:A:21:PRO:HG2	1.64	0.95
1:A:165:VAL:HG13	1:A:166:ILE:N	1.80	0.95
1:A:62:ILE:HG13	1:A:63:LEU:N	1.78	0.95
1:A:118:ARG:NE	1:A:119:PHE:HB2	1.80	0.95
1:A:28:ALA:O	1:A:32:MET:HG2	1.65	0.95
1:B:235:PRO:CA	1:B:238:LEU:HB2	1.97	0.95
1:A:262:VAL:HG21	1:A:403:LEU:HD13	1.46	0.95
1:A:177:LEU:HD12	1:A:202:ILE:HD13	1.47	0.95
1:B:343:ILE:O	1:B:346:LEU:HB2	1.66	0.95
1:A:445:TYR:CB	1:A:448:GLN:HA	1.97	0.95
1:A:203:VAL:O	1:A:206:ILE:HG12	1.67	0.94
1:A:147:PHE:HB2	1:A:211:LEU:HD13	1.46	0.94
1:B:358:MET:CA	1:B:361:LEU:HD12	1.98	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:VAL:HG13	1:B:321:GLY:N	1.80	0.94
1:B:177:LEU:HG	1:B:202:ILE:HG21	1.50	0.94
1:A:398:TYR:HB3	1:A:436:ALA:CB	1.99	0.93
1:B:203:VAL:O	1:B:206:ILE:HG12	1.67	0.93
1:A:180:ILE:HA	1:A:184:GLY:HA3	1.49	0.93
1:B:407:TYR:HA	1:B:425:PHE:HD2	1.34	0.93
1:B:118:ARG:NE	1:B:119:PHE:HB2	1.82	0.93
1:A:445:TYR:HB2	1:A:448:GLN:HA	1.51	0.93
1:B:16:ILE:HA	1:B:19:ALA:CB	1.99	0.93
1:B:353:VAL:HG12	1:B:357:ALA:N	1.83	0.92
1:A:208:LEU:HD23	1:A:209:LEU:N	1.83	0.92
1:A:222:ALA:O	1:A:224:VAL:HG13	1.68	0.92
1:A:94:GLN:NE2	1:A:231:HIS:HB2	1.85	0.92
1:B:62:ILE:HG13	1:B:63:LEU:N	1.80	0.92
1:B:16:ILE:HA	1:B:19:ALA:HB3	1.52	0.92
1:B:96:LEU:O	1:B:99:ALA:HB3	1.67	0.92
1:A:407:TYR:HA	1:A:425:PHE:HD2	1.35	0.92
1:B:88:ILE:HG12	1:B:89:PRO:HD3	1.52	0.92
1:B:4:SER:O	1:B:8:TYR:CE2	2.22	0.92
1:A:110:LEU:O	1:A:114:GLN:HG2	1.69	0.92
1:A:74:PRO:HB3	1:A:149:ALA:HB1	1.51	0.91
1:B:222:ALA:O	1:B:224:VAL:HG13	1.71	0.91
1:B:76:VAL:C	1:B:78:GLN:H	1.74	0.91
1:A:276:ALA:HB1	1:A:426:TRP:CZ2	2.04	0.91
1:A:63:LEU:HD23	1:A:64:PHE:H	1.33	0.91
1:B:315:ALA:O	1:B:319:ASN:HB2	1.71	0.91
1:B:73:VAL:CB	1:B:74:PRO:HD3	2.01	0.91
1:B:262:VAL:HG21	1:B:403:LEU:HD13	1.52	0.90
1:A:76:VAL:HA	1:A:78:GLN:HE21	1.33	0.90
1:A:320:VAL:HG13	1:A:321:GLY:N	1.85	0.90
1:B:287:VAL:HG11	1:B:368:GLN:OE1	1.71	0.90
1:B:391:PHE:HD2	1:B:392:HIS:N	1.70	0.90
1:A:11:GLU:HB3	1:A:320:VAL:CG2	2.02	0.90
1:A:88:ILE:HG12	1:A:89:PRO:HD3	1.50	0.90
1:A:382:ARG:NH2	1:A:445:TYR:H	1.68	0.90
1:A:177:LEU:HG	1:A:202:ILE:HG21	1.54	0.90
1:A:73:VAL:CB	1:A:74:PRO:HD3	2.02	0.90
1:A:418:GLN:NE2	1:A:421:GLY:HA2	1.87	0.90
1:B:385:LYS:O	1:B:388:THR:OG1	1.89	0.90
1:B:382:ARG:NH2	1:B:445:TYR:H	1.70	0.90
1:B:238:LEU:HA	1:B:241:LEU:HB2	1.52	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:VAL:C	1:A:78:GLN:H	1.74	0.89
1:A:97:ILE:HG22	1:A:101:LEU:HD11	1.53	0.89
1:A:123:GLU:O	1:A:124:GLU:O	1.88	0.89
1:A:59:LEU:HD12	1:A:59:LEU:H	1.37	0.89
1:B:11:GLU:HB3	1:B:320:VAL:CG2	2.02	0.89
1:A:206:ILE:O	1:A:210:LEU:HD22	1.72	0.89
1:A:253:PHE:HA	1:A:256:VAL:HB	1.53	0.89
1:A:353:VAL:O	1:A:357:ALA:N	2.06	0.89
1:B:232:LYS:HB3	1:B:233:PRO:HD3	1.55	0.88
1:B:398:TYR:HB3	1:B:436:ALA:CB	2.03	0.88
1:A:315:ALA:O	1:A:319:ASN:HB2	1.73	0.88
1:A:117:ILE:HG22	1:A:118:ARG:N	1.88	0.88
1:A:16:ILE:HA	1:A:19:ALA:HB3	1.56	0.88
1:B:320:VAL:CG1	1:B:321:GLY:H	1.82	0.88
1:B:327:ALA:O	1:B:331:ILE:HG22	1.72	0.88
1:A:391:PHE:HD2	1:A:392:HIS:N	1.71	0.88
1:A:16:ILE:HA	1:A:19:ALA:CB	2.04	0.88
1:B:276:ALA:HB1	1:B:426:TRP:CZ2	2.09	0.88
1:A:376:VAL:HG13	1:A:377:ALA:H	1.37	0.88
1:A:238:LEU:HA	1:A:241:LEU:HB2	1.54	0.87
1:A:113:THR:HA	1:A:116:ILE:HG22	1.56	0.87
1:B:15:LEU:HD12	1:B:16:ILE:N	1.89	0.87
1:A:231:HIS:O	1:A:235:PRO:HG2	1.73	0.87
1:A:4:SER:O	1:A:8:TYR:CD2	2.26	0.87
1:A:15:LEU:HD12	1:A:16:ILE:N	1.89	0.87
1:B:110:LEU:O	1:B:114:GLN:HG2	1.75	0.87
1:B:266:VAL:CG1	1:B:269:LEU:HD11	2.05	0.87
1:A:211:LEU:O	1:A:215:ILE:HG22	1.75	0.87
1:B:353:VAL:O	1:B:353:VAL:HG12	1.73	0.86
1:A:173:LEU:O	1:A:177:LEU:HD23	1.75	0.86
1:A:93:HIS:CE1	1:A:225:LYS:HB3	2.09	0.86
1:B:420:LEU:HB3	1:B:423:LYS:HG2	1.54	0.86
1:A:155:ASP:HB2	1:A:159:LEU:H	1.38	0.86
1:A:235:PRO:O	1:A:239:ILE:HG13	1.76	0.86
1:A:408:ILE:HA	1:A:411:MET:CB	2.02	0.86
1:B:94:GLN:NE2	1:B:231:HIS:HB2	1.89	0.86
1:B:28:ALA:O	1:B:32:MET:HG2	1.75	0.86
1:A:327:ALA:O	1:A:331:ILE:HG22	1.74	0.86
1:A:420:LEU:CD1	1:A:423:LYS:H	1.89	0.86
1:A:96:LEU:O	1:A:99:ALA:HB3	1.76	0.86
1:A:276:ALA:HA	1:A:426:TRP:HE1	1.38	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ILE:O	1:B:209:LEU:HB3	1.75	0.86
1:B:401:LEU:O	1:B:405:THR:HB	1.76	0.86
1:B:63:LEU:HD23	1:B:64:PHE:H	1.40	0.86
1:B:72:LEU:HD12	1:B:244:LEU:HD21	1.58	0.86
1:B:26:SER:HB2	1:B:289:MET:SD	2.14	0.86
1:A:231:HIS:C	1:A:235:PRO:HG2	1.96	0.86
1:B:395:PHE:O	1:B:398:TYR:HD1	1.58	0.86
1:A:265:LEU:O	1:A:268:PRO:HD3	1.75	0.86
1:A:353:VAL:HG12	1:A:357:ALA:N	1.91	0.86
1:B:235:PRO:HA	1:B:238:LEU:CB	2.05	0.85
1:B:72:LEU:O	1:B:75:VAL:HG22	1.76	0.85
1:B:107:ILE:HA	1:B:139:PHE:CZ	2.09	0.85
1:A:251:ALA:O	1:A:255:GLU:HB3	1.77	0.85
1:B:173:LEU:O	1:B:177:LEU:HD23	1.75	0.85
1:B:395:PHE:O	1:B:398:TYR:CD1	2.29	0.85
1:B:180:ILE:HA	1:B:184:GLY:HA3	1.59	0.85
1:B:231:HIS:O	1:B:235:PRO:HG2	1.77	0.85
1:A:235:PRO:CA	1:A:238:LEU:HB2	2.05	0.84
1:A:395:PHE:O	1:A:398:TYR:CD1	2.30	0.84
1:B:154:THR:O	1:B:158:SER:HA	1.77	0.84
1:A:206:ILE:O	1:A:209:LEU:HB3	1.78	0.84
1:A:320:VAL:CG1	1:A:321:GLY:H	1.88	0.84
1:B:211:LEU:O	1:B:215:ILE:HG22	1.77	0.84
1:B:93:HIS:CE1	1:B:225:LYS:HB3	2.12	0.84
1:A:401:LEU:O	1:A:405:THR:HB	1.74	0.84
1:B:312:LYS:O	1:B:316:ILE:HG12	1.76	0.84
1:A:232:LYS:HB3	1:A:233:PRO:HD3	1.59	0.84
1:A:408:ILE:CA	1:A:411:MET:HB2	2.03	0.83
1:B:445:TYR:HB2	1:B:448:GLN:CA	2.08	0.83
1:B:151:ARG:HA	1:B:155:ASP:HA	1.60	0.83
1:B:206:ILE:O	1:B:210:LEU:HD22	1.76	0.83
1:B:251:ALA:O	1:B:255:GLU:HB3	1.76	0.83
1:A:59:LEU:HB2	1:A:60:PRO:HD3	1.60	0.83
1:B:235:PRO:O	1:B:239:ILE:HG13	1.76	0.83
1:B:420:LEU:CD1	1:B:423:LYS:H	1.90	0.83
1:B:72:LEU:HA	1:B:75:VAL:HG13	1.60	0.83
1:B:46:ILE:C	1:B:48:MET:H	1.81	0.83
1:B:406:GLY:O	1:B:409:LEU:HB3	1.77	0.83
1:B:418:GLN:NE2	1:B:421:GLY:HA2	1.93	0.83
1:B:55:ALA:O	1:B:58:TRP:HB2	1.78	0.83
1:A:118:ARG:HE	1:A:119:PHE:CB	1.92	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ALA:C	1:A:74:PRO:HD2	1.99	0.83
1:B:74:PRO:HB3	1:B:149:ALA:HB1	1.60	0.83
1:A:74:PRO:CB	1:A:149:ALA:HB1	2.08	0.82
1:B:118:ARG:HE	1:B:119:PHE:CB	1.92	0.82
1:A:72:LEU:HA	1:A:75:VAL:HG13	1.59	0.82
1:A:142:PRO:HA	1:A:145:LEU:HB3	1.58	0.82
1:A:266:VAL:CG1	1:A:269:LEU:HD11	2.07	0.82
1:A:244:LEU:HB2	1:A:385:LYS:HZ3	1.44	0.82
1:A:72:LEU:O	1:A:75:VAL:HG22	1.78	0.82
1:A:137:VAL:CG1	1:A:201:ALA:HA	2.10	0.82
1:A:445:TYR:O	1:A:446:TRP:HB3	1.80	0.82
1:A:266:VAL:HG12	1:A:269:LEU:CD1	2.10	0.82
1:B:403:LEU:HD21	1:B:429:PHE:HD2	1.44	0.82
1:A:107:ILE:HA	1:A:139:PHE:CZ	2.15	0.82
1:A:151:ARG:CG	1:A:162:PRO:HG2	2.08	0.82
1:A:236:LYS:HA	1:A:239:ILE:HD12	1.61	0.82
1:A:353:VAL:HG12	1:A:353:VAL:O	1.79	0.82
1:B:71:ALA:CA	1:B:74:PRO:HD2	2.10	0.82
1:B:420:LEU:HD12	1:B:423:LYS:N	1.95	0.81
1:B:71:ALA:C	1:B:74:PRO:HD2	2.00	0.81
1:B:266:VAL:HG12	1:B:269:LEU:CD1	2.10	0.81
1:B:276:ALA:HB1	1:B:426:TRP:CE2	2.15	0.81
1:A:420:LEU:HD12	1:A:423:LYS:N	1.95	0.81
1:B:427:LEU:HD23	1:B:428:GLY:N	1.95	0.81
1:B:398:TYR:CG	1:B:436:ALA:HB2	2.16	0.81
1:A:72:LEU:HD12	1:A:244:LEU:HD21	1.61	0.81
1:A:77:ALA:CB	1:A:154:THR:HG23	2.11	0.81
1:B:58:TRP:O	1:B:61:SER:HB3	1.79	0.81
1:A:226:VAL:HG12	1:A:227:PHE:N	1.94	0.81
1:B:155:ASP:HB2	1:B:159:LEU:H	1.46	0.81
1:A:208:LEU:O	1:A:211:LEU:HB3	1.80	0.81
1:A:137:VAL:HG11	1:A:201:ALA:HA	1.62	0.81
1:A:252:LEU:O	1:A:255:GLU:HG2	1.81	0.80
1:B:137:VAL:CG1	1:B:201:ALA:HA	2.09	0.80
1:B:296:ALA:O	1:B:300:ILE:HG23	1.82	0.80
1:A:329:ALA:HB1	1:A:369:CYS:HA	1.63	0.80
1:A:395:PHE:O	1:A:398:TYR:HD1	1.62	0.80
1:A:57:ILE:HA	1:A:60:PRO:HG2	1.62	0.80
1:B:151:ARG:CG	1:B:162:PRO:HG2	2.08	0.80
1:A:63:LEU:HD12	1:A:106:ILE:HG21	1.61	0.80
1:A:74:PRO:CG	1:A:149:ALA:HB1	2.11	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:VAL:HG12	1:B:227:PHE:N	1.97	0.80
1:B:276:ALA:HA	1:B:426:TRP:HE1	1.47	0.80
1:B:73:VAL:HB	1:B:74:PRO:CD	2.07	0.80
1:B:407:TYR:HA	1:B:425:PHE:CD2	2.16	0.80
1:A:267:ALA:N	1:A:268:PRO:CD	2.45	0.80
1:B:266:VAL:HB	1:B:425:PHE:CZ	2.16	0.80
1:B:59:LEU:H	1:B:59:LEU:HD22	1.47	0.80
1:A:407:TYR:HA	1:A:425:PHE:CD2	2.16	0.80
1:A:447:LEU:HD11	1:A:450:GLN:NE2	1.76	0.80
1:A:87:LYS:HZ1	1:B:308:GLU:HG2	1.46	0.80
1:B:74:PRO:CG	1:B:149:ALA:HB1	2.12	0.80
1:A:53:ILE:O	1:A:56:SER:HB3	1.80	0.80
1:A:154:THR:O	1:A:158:SER:HA	1.82	0.80
1:B:211:LEU:HG	1:B:212:LEU:H	1.47	0.80
1:B:11:GLU:HA	1:B:301:ARG:NH2	1.95	0.79
1:A:398:TYR:CG	1:A:436:ALA:HB2	2.16	0.79
1:A:447:LEU:O	1:A:448:GLN:HB2	1.82	0.79
1:B:77:ALA:CB	1:B:154:THR:HG23	2.11	0.79
1:B:329:ALA:HB1	1:B:369:CYS:HA	1.63	0.79
1:A:272:THR:O	1:A:275:ALA:N	2.15	0.79
1:A:379:GLY:O	1:A:383:GLY:HA3	1.83	0.79
1:A:46:ILE:C	1:A:48:MET:H	1.85	0.79
1:B:98:LEU:HA	1:B:101:LEU:HD12	1.65	0.79
1:B:200:THR:HA	1:B:203:VAL:HG23	1.64	0.79
1:B:208:LEU:O	1:B:211:LEU:HB3	1.82	0.79
1:B:340:ARG:HD2	1:B:358:MET:CG	2.12	0.79
1:A:332:THR:O	1:A:335:LEU:HG	1.83	0.79
1:A:444:LEU:O	1:A:446:TRP:N	2.12	0.79
1:B:32:MET:HG3	1:B:33:GLY:N	1.98	0.79
1:A:276:ALA:HB1	1:A:426:TRP:CE2	2.16	0.79
1:A:84:ARG:HB3	1:A:87:LYS:HD2	1.65	0.79
1:A:98:LEU:HA	1:A:101:LEU:HD12	1.64	0.79
1:B:236:LYS:HA	1:B:239:ILE:HD12	1.64	0.79
1:B:353:VAL:HG12	1:B:357:ALA:CA	2.13	0.79
1:A:155:ASP:HB2	1:A:159:LEU:N	1.98	0.79
1:B:55:ALA:HB3	1:B:123:GLU:OE2	1.83	0.79
1:A:104:VAL:HA	1:A:107:ILE:HG13	1.63	0.78
1:A:445:TYR:HB2	1:A:448:GLN:CA	2.12	0.78
1:A:150:LEU:O	1:A:155:ASP:N	2.16	0.78
1:B:203:VAL:HG12	1:B:207:MET:SD	2.23	0.78
1:A:382:ARG:HH22	1:A:445:TYR:H	1.32	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:GLU:CD	1:A:342:GLN:H	1.87	0.78
1:A:358:MET:CA	1:A:361:LEU:HD12	2.10	0.78
1:A:63:LEU:HD23	1:A:64:PHE:N	1.98	0.78
1:B:420:LEU:HD11	1:B:422:ALA:HB3	1.66	0.78
1:A:124:GLU:O	1:A:125:ALA:C	2.22	0.78
1:B:341:GLU:O	1:B:344:ALA:HB3	1.84	0.78
1:A:235:PRO:HA	1:A:238:LEU:CB	2.12	0.78
1:A:327:ALA:C	1:A:331:ILE:HG22	2.02	0.78
1:B:231:HIS:C	1:B:235:PRO:HG2	2.03	0.78
1:A:11:GLU:HB3	1:A:320:VAL:HG21	1.64	0.78
1:A:272:THR:CG2	1:A:275:ALA:HB3	2.13	0.78
1:B:253:PHE:HA	1:B:256:VAL:HB	1.63	0.78
1:A:341:GLU:O	1:A:344:ALA:HB3	1.83	0.77
1:B:137:VAL:HG11	1:B:201:ALA:HA	1.64	0.77
1:B:379:GLY:O	1:B:383:GLY:HA3	1.85	0.77
1:A:403:LEU:HD21	1:A:429:PHE:HD2	1.49	0.77
1:B:267:ALA:N	1:B:268:PRO:CD	2.47	0.77
1:B:31:GLY:O	1:B:35:VAL:HG23	1.84	0.77
1:B:340:ARG:CB	1:B:361:LEU:HD13	2.14	0.77
1:A:161:LYS:H	1:A:162:PRO:CD	1.98	0.77
1:A:166:ILE:HB	1:A:210:LEU:CD2	2.12	0.77
1:B:104:VAL:HB	1:B:105:PRO:HD3	1.65	0.77
1:A:387:MET:HA	1:A:443:ARG:HH21	1.49	0.77
1:A:75:VAL:C	1:A:77:ALA:H	1.85	0.77
1:A:146:LEU:O	1:A:149:ALA:HB3	1.83	0.77
1:A:406:GLY:O	1:A:409:LEU:HB3	1.84	0.77
1:B:96:LEU:HD12	1:B:146:LEU:HD12	1.66	0.77
1:B:146:LEU:O	1:B:149:ALA:HB3	1.85	0.77
1:A:447:LEU:HD13	1:A:447:LEU:O	1.85	0.76
1:B:77:ALA:HB1	1:B:154:THR:HG23	1.65	0.76
1:B:116:ILE:HG23	1:B:117:ILE:O	1.85	0.76
1:B:161:LYS:H	1:B:162:PRO:CD	1.98	0.76
1:B:272:THR:O	1:B:275:ALA:N	2.17	0.76
1:B:411:MET:HA	1:B:414:TRP:CG	2.21	0.76
1:A:152:SER:O	1:A:160:THR:HA	1.85	0.76
1:A:272:THR:O	1:A:274:VAL:N	2.19	0.76
1:A:316:ILE:O	1:A:320:VAL:HG12	1.86	0.76
1:B:63:LEU:HD12	1:B:106:ILE:HG21	1.67	0.76
1:A:246:PHE:HB3	1:A:247:PRO:HD3	1.68	0.76
1:B:246:PHE:HB3	1:B:247:PRO:HD3	1.66	0.76
1:A:151:ARG:HD2	1:A:155:ASP:HA	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:THR:OG1	1:A:21:PRO:HD3	1.85	0.76
1:A:411:MET:HA	1:A:414:TRP:CG	2.21	0.76
1:B:142:PRO:HA	1:B:145:LEU:HB3	1.66	0.76
1:B:266:VAL:HG13	1:B:407:TYR:CE2	2.21	0.76
1:A:88:ILE:CG1	1:A:89:PRO:HD3	2.15	0.76
1:A:273:VAL:HG13	1:A:274:VAL:H	1.50	0.76
1:A:57:ILE:C	1:A:60:PRO:HD2	2.06	0.76
1:A:73:VAL:O	1:A:76:VAL:HB	1.85	0.76
1:B:24:ILE:HG21	1:B:164:MET:HG3	1.68	0.76
1:B:275:ALA:CB	1:B:353:VAL:HG11	2.15	0.76
1:B:327:ALA:C	1:B:331:ILE:HG22	2.05	0.76
1:B:90:PHE:HE2	1:B:228:GLU:HA	1.51	0.76
1:A:155:ASP:CB	1:A:159:LEU:H	1.98	0.75
1:A:90:PHE:CE2	1:A:228:GLU:HA	2.21	0.75
1:A:71:ALA:CA	1:A:74:PRO:HD2	2.17	0.75
1:B:182:VAL:HG22	1:B:195:GLY:HA3	1.68	0.75
1:A:447:LEU:C	1:A:447:LEU:CD1	2.36	0.75
1:B:74:PRO:CB	1:B:149:ALA:HB1	2.16	0.75
1:B:165:VAL:CG1	1:B:166:ILE:N	2.41	0.75
1:A:276:ALA:HA	1:A:426:TRP:NE1	2.00	0.75
1:A:445:TYR:CD2	1:A:448:GLN:HG2	2.22	0.75
1:B:46:ILE:O	1:B:48:MET:N	2.19	0.75
1:A:145:LEU:C	1:A:145:LEU:HD22	2.06	0.75
1:A:265:LEU:O	1:A:268:PRO:CD	2.35	0.75
1:A:407:TYR:O	1:A:411:MET:N	2.19	0.75
1:B:80:ASN:C	1:B:82:ALA:H	1.88	0.75
1:A:266:VAL:HG13	1:A:407:TYR:CE2	2.21	0.75
1:A:413:ASN:HB3	1:A:414:TRP:CE3	2.21	0.75
1:A:314:ALA:HB1	1:A:445:TYR:CE1	2.21	0.75
1:A:45:ALA:CB	1:A:49:ALA:HB2	2.13	0.75
1:A:76:VAL:HG23	1:A:78:GLN:NE2	2.02	0.75
1:B:252:LEU:O	1:B:255:GLU:HG2	1.87	0.75
1:B:358:MET:HA	1:B:361:LEU:CD1	2.04	0.75
1:A:191:LEU:HB3	1:A:194:VAL:HG23	1.67	0.75
1:B:117:ILE:HG22	1:B:118:ARG:N	2.02	0.75
1:B:123:GLU:O	1:B:124:GLU:O	2.04	0.75
1:A:142:PRO:O	1:A:145:LEU:HB3	1.86	0.75
1:A:326:LEU:O	1:A:330:CYS:CB	2.34	0.75
1:B:272:THR:CG2	1:B:275:ALA:HB3	2.15	0.75
1:A:117:ILE:CG2	1:A:118:ARG:H	1.90	0.74
1:A:272:THR:O	1:A:273:VAL:C	2.24	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:PHE:CE2	1:B:228:GLU:HA	2.22	0.74
1:B:185:LYS:HB2	1:B:189:PRO:HB3	1.68	0.74
1:B:216:VAL:HG22	1:B:225:LYS:HD3	1.68	0.74
1:B:273:VAL:HG13	1:B:274:VAL:H	1.52	0.74
1:A:211:LEU:HG	1:A:212:LEU:H	1.50	0.74
1:B:166:ILE:HB	1:B:210:LEU:CD2	2.18	0.74
1:B:141:VAL:HB	1:B:142:PRO:HD3	1.69	0.74
1:B:142:PRO:O	1:B:145:LEU:HB3	1.88	0.74
1:B:265:LEU:O	1:B:268:PRO:HD3	1.87	0.74
1:B:332:THR:O	1:B:335:LEU:HG	1.86	0.74
1:A:171:LEU:HD23	1:A:172:LEU:N	2.01	0.74
1:A:340:ARG:CA	1:A:361:LEU:HD13	2.18	0.74
1:B:210:LEU:HD22	1:B:210:LEU:H	1.51	0.74
1:A:36:ASP:HB2	1:A:178:ASN:ND2	2.03	0.73
1:B:113:THR:HA	1:B:116:ILE:HG22	1.69	0.73
1:B:93:HIS:HD2	1:B:228:GLU:HB3	1.51	0.73
1:B:391:PHE:CD2	1:B:391:PHE:C	2.60	0.73
1:B:123:GLU:HG2	1:B:127:ALA:HB3	1.70	0.73
1:A:267:ALA:H	1:A:268:PRO:CD	2.01	0.73
1:B:20:THR:OG1	1:B:21:PRO:HD3	1.88	0.73
1:A:202:ILE:O	1:A:205:TRP:HB3	1.88	0.73
1:B:211:LEU:HG	1:B:212:LEU:N	2.03	0.73
1:B:53:ILE:O	1:B:56:SER:HB3	1.89	0.73
1:A:93:HIS:HD2	1:A:228:GLU:HB3	1.52	0.73
1:A:409:LEU:HD12	1:A:424:GLY:O	1.88	0.73
1:B:416:THR:O	1:B:417:GLU:HB2	1.86	0.73
1:A:116:ILE:HG23	1:A:117:ILE:O	1.88	0.73
1:B:238:LEU:HD12	1:B:241:LEU:HD13	1.71	0.73
1:B:332:THR:HA	1:B:335:LEU:CD2	2.18	0.73
1:B:449:LYS:HG2	1:B:449:LYS:O	1.89	0.73
1:B:134:MET:O	1:B:137:VAL:HB	1.88	0.73
1:B:267:ALA:H	1:B:268:PRO:CD	2.00	0.73
1:B:423:LYS:HG3	1:B:424:GLY:N	2.04	0.73
1:A:113:THR:CA	1:A:116:ILE:HG22	2.18	0.73
1:A:275:ALA:CA	1:A:353:VAL:HG21	2.18	0.73
1:A:427:LEU:HD23	1:A:428:GLY:N	2.04	0.73
1:A:45:ALA:HB3	1:A:49:ALA:CB	2.15	0.73
1:B:117:ILE:HG22	1:B:118:ARG:H	1.54	0.73
1:B:200:THR:HA	1:B:203:VAL:CG2	2.18	0.73
1:B:300:ILE:HG13	1:B:301:ARG:N	2.04	0.73
1:B:44:SER:C	1:B:46:ILE:H	1.93	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ALA:HB3	1:B:49:ALA:CB	2.16	0.73
1:A:123:GLU:HG2	1:A:127:ALA:HB3	1.71	0.72
1:B:208:LEU:HD23	1:B:209:LEU:H	1.55	0.72
1:A:253:PHE:O	1:A:256:VAL:HG12	1.88	0.72
1:B:275:ALA:HA	1:B:353:VAL:HG11	1.71	0.72
1:A:141:VAL:HB	1:A:142:PRO:HD3	1.70	0.72
1:A:90:PHE:HE2	1:A:228:GLU:HA	1.55	0.72
1:A:244:LEU:HB2	1:A:385:LYS:NZ	2.04	0.72
1:A:26:SER:HB2	1:A:289:MET:SD	2.28	0.72
1:B:266:VAL:HG22	1:B:407:TYR:CE1	2.24	0.72
1:B:433:LEU:O	1:B:437:ALA:HB2	1.89	0.72
1:B:385:LYS:HD3	1:B:386:ASP:N	2.05	0.72
1:B:76:VAL:HG23	1:B:78:GLN:NE2	2.05	0.72
1:A:27:VAL:O	1:A:31:GLY:HA3	1.89	0.72
1:A:35:VAL:O	1:A:39:MET:HB3	1.89	0.72
1:B:215:ILE:HG23	1:B:216:VAL:H	1.54	0.72
1:B:75:VAL:C	1:B:77:ALA:H	1.91	0.72
1:A:250:ALA:O	1:A:254:PHE:HB3	1.88	0.72
1:B:213:PHE:O	1:B:217:THR:HG22	1.89	0.72
1:A:327:ALA:O	1:A:331:ILE:N	2.22	0.72
1:A:73:VAL:HB	1:A:74:PRO:CD	2.10	0.72
1:B:77:ALA:HB2	1:B:154:THR:OG1	1.89	0.72
1:A:340:ARG:CB	1:A:361:LEU:HD13	2.19	0.72
1:A:393:ARG:HG3	1:A:393:ARG:HH11	1.55	0.72
1:A:46:ILE:O	1:A:48:MET:N	2.23	0.72
1:B:132:GLY:O	1:B:135:HIS:HB2	1.89	0.72
1:B:171:LEU:HD23	1:B:172:LEU:N	2.04	0.72
1:B:326:LEU:O	1:B:330:CYS:CB	2.37	0.72
1:B:275:ALA:CA	1:B:353:VAL:HG21	2.19	0.72
1:B:46:ILE:O	1:B:46:ILE:HG22	1.88	0.72
1:B:316:ILE:O	1:B:320:VAL:HG12	1.90	0.72
1:A:145:LEU:HD22	1:A:145:LEU:O	1.90	0.71
1:A:234:GLN:N	1:A:235:PRO:CD	2.53	0.71
1:A:326:LEU:O	1:A:330:CYS:N	2.19	0.71
1:A:340:ARG:HA	1:A:361:LEU:HD13	1.72	0.71
1:A:353:VAL:HG12	1:A:357:ALA:CA	2.21	0.71
1:A:391:PHE:C	1:A:391:PHE:CD2	2.63	0.71
1:A:252:LEU:HD22	1:A:255:GLU:OE2	1.90	0.71
1:A:266:VAL:HB	1:A:425:PHE:CZ	2.25	0.71
1:A:272:THR:HG23	1:A:275:ALA:CB	2.20	0.71
1:A:299:SER:O	1:A:302:VAL:HG12	1.88	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ILE:CG1	1:B:89:PRO:HD3	2.19	0.71
1:A:151:ARG:O	1:A:155:ASP:N	2.23	0.71
1:B:63:LEU:HD23	1:B:64:PHE:N	2.03	0.71
1:A:104:VAL:HB	1:A:105:PRO:HD3	1.72	0.71
1:B:411:MET:O	1:B:414:TRP:HB2	1.90	0.71
1:B:24:ILE:O	1:B:27:VAL:HB	1.91	0.71
1:A:275:ALA:CB	1:A:353:VAL:HG11	2.20	0.71
1:A:148:GLN:O	1:A:152:SER:HB3	1.90	0.71
1:B:96:LEU:CA	1:B:146:LEU:HG	2.20	0.71
1:B:150:LEU:O	1:B:155:ASP:N	2.24	0.71
1:B:244:LEU:HB2	1:B:385:LYS:HZ3	1.55	0.71
1:B:409:LEU:HD12	1:B:424:GLY:O	1.91	0.71
1:A:130:THR:HG21	1:A:194:VAL:HG22	1.72	0.71
1:A:59:LEU:CD1	1:A:59:LEU:H	2.04	0.71
1:A:94:GLN:OE1	1:A:238:LEU:HD11	1.91	0.71
1:B:69:LEU:HG	1:B:245:GLY:HA3	1.72	0.71
1:A:433:LEU:O	1:A:437:ALA:HB2	1.91	0.71
1:A:77:ALA:HB1	1:A:154:THR:HG23	1.71	0.71
1:B:11:GLU:HB3	1:B:320:VAL:HG21	1.71	0.70
1:B:341:GLU:CD	1:B:342:GLN:H	1.94	0.70
1:B:251:ALA:HB1	1:B:395:PHE:CD1	2.26	0.70
1:B:104:VAL:HA	1:B:107:ILE:HG13	1.74	0.70
1:B:155:ASP:HB2	1:B:159:LEU:N	2.04	0.70
1:B:340:ARG:CA	1:B:361:LEU:HD13	2.21	0.70
1:B:420:LEU:CD1	1:B:422:ALA:HB3	2.21	0.70
1:A:173:LEU:O	1:A:176:PRO:HD2	1.91	0.70
1:A:423:LYS:HG3	1:A:424:GLY:N	2.04	0.70
1:B:408:ILE:HA	1:B:411:MET:CB	2.10	0.70
1:A:191:LEU:HB3	1:A:194:VAL:CG2	2.22	0.70
1:A:216:VAL:HG22	1:A:225:LYS:HD3	1.71	0.70
1:A:232:LYS:C	1:A:235:PRO:HD2	2.11	0.70
1:B:326:LEU:O	1:B:330:CYS:N	2.24	0.70
1:B:408:ILE:CA	1:B:411:MET:HB2	2.09	0.70
1:A:150:LEU:O	1:A:154:THR:HB	1.92	0.70
1:A:32:MET:HG3	1:A:33:GLY:N	2.07	0.70
1:A:68:LEU:HD13	1:A:68:LEU:O	1.91	0.70
1:B:40:ALA:O	1:B:44:SER:HB2	1.91	0.70
1:B:68:LEU:O	1:B:68:LEU:HD13	1.91	0.70
1:A:385:LYS:HD3	1:A:385:LYS:C	2.10	0.70
1:A:416:THR:O	1:A:417:GLU:HB2	1.92	0.70
1:A:132:GLY:O	1:A:135:HIS:HB2	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ARG:HD2	1:B:155:ASP:HA	1.73	0.70
1:B:155:ASP:CB	1:B:159:LEU:H	2.03	0.70
1:A:211:LEU:HG	1:A:212:LEU:N	2.06	0.70
1:A:215:ILE:HG23	1:A:216:VAL:N	2.07	0.70
1:A:215:ILE:HG23	1:A:216:VAL:H	1.57	0.70
1:A:244:LEU:HG	1:A:385:LYS:NZ	2.07	0.70
1:B:252:LEU:HD22	1:B:255:GLU:OE2	1.92	0.70
1:B:41:GLY:C	1:B:49:ALA:HB1	2.13	0.70
1:A:182:VAL:HG22	1:A:195:GLY:HA3	1.73	0.69
1:A:390:ILE:HG22	1:A:390:ILE:O	1.92	0.69
1:B:118:ARG:HH21	1:B:119:PHE:HB2	1.57	0.69
1:A:76:VAL:C	1:A:78:GLN:N	2.46	0.69
1:A:80:ASN:C	1:A:82:ALA:H	1.94	0.69
1:B:152:SER:O	1:B:160:THR:HA	1.92	0.69
1:B:173:LEU:O	1:B:176:PRO:HD2	1.92	0.69
1:B:423:LYS:HG3	1:B:424:GLY:H	1.57	0.69
1:A:266:VAL:HG22	1:A:407:TYR:CE1	2.27	0.69
1:A:412:THR:C	1:A:415:LEU:H	1.96	0.69
1:A:421:GLY:O	1:A:425:PHE:HB3	1.92	0.69
1:B:45:ALA:CB	1:B:49:ALA:HB2	2.15	0.69
1:A:203:VAL:HG12	1:A:207:MET:SD	2.33	0.69
1:A:236:LYS:HA	1:A:239:ILE:CD1	2.22	0.69
1:A:366:ILE:O	1:A:369:CYS:HB3	1.91	0.69
1:A:410:GLY:CA	1:A:425:PHE:HB2	2.22	0.69
1:A:75:VAL:O	1:A:77:ALA:N	2.26	0.69
1:A:300:ILE:HG13	1:A:301:ARG:N	2.05	0.69
1:A:118:ARG:HH21	1:A:119:PHE:HB2	1.58	0.69
1:A:74:PRO:HB3	1:A:149:ALA:CB	2.22	0.69
1:A:353:VAL:HG12	1:A:357:ALA:HB2	1.73	0.69
1:B:165:VAL:O	1:B:169:ILE:HB	1.92	0.69
1:B:403:LEU:HD21	1:B:429:PHE:CD2	2.27	0.69
1:A:131:VAL:HA	1:A:134:MET:HB2	1.74	0.69
1:A:174:ASN:HD21	1:A:203:VAL:HG22	1.58	0.69
1:A:449:LYS:O	1:A:449:LYS:HG2	1.93	0.69
1:A:314:ALA:HB2	1:A:449:LYS:NZ	2.07	0.69
1:B:215:ILE:HG23	1:B:216:VAL:N	2.07	0.69
1:B:236:LYS:HA	1:B:239:ILE:CD1	2.23	0.69
1:B:328:THR:HA	1:B:331:ILE:CG2	2.23	0.69
1:B:57:ILE:C	1:B:60:PRO:HD2	2.12	0.69
1:A:219:LYS:HD2	1:A:220:ARG:HG2	1.75	0.69
1:B:166:ILE:HD13	1:B:166:ILE:O	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ALA:HA	1:B:58:TRP:CD1	2.27	0.69
1:A:124:GLU:O	1:A:126:MET:N	2.26	0.69
1:A:353:VAL:CG1	1:A:357:ALA:HB2	2.23	0.69
1:A:411:MET:O	1:A:414:TRP:HB2	1.92	0.69
1:B:191:LEU:HB3	1:B:194:VAL:HG23	1.73	0.69
1:B:250:ALA:O	1:B:254:PHE:HB3	1.93	0.69
1:B:339:PHE:HB3	1:B:343:ILE:CG1	2.23	0.69
1:B:393:ARG:HH11	1:B:393:ARG:HG3	1.56	0.69
1:A:24:ILE:HG21	1:A:164:MET:HG3	1.75	0.69
1:A:92:VAL:HG12	1:A:93:HIS:N	2.08	0.69
1:A:410:GLY:HA3	1:A:425:PHE:HB2	1.75	0.69
1:B:13:SER:O	1:B:16:ILE:HG22	1.92	0.69
1:B:272:THR:HG23	1:B:275:ALA:CB	2.20	0.69
1:B:353:VAL:HG12	1:B:357:ALA:H	1.54	0.69
1:A:251:ALA:HB1	1:A:395:PHE:CD1	2.27	0.68
1:A:281:LEU:HD22	1:A:282:ASN:HD22	1.59	0.68
1:B:240:ARG:HD3	1:B:460:ALA:HA	1.75	0.68
1:A:232:LYS:H	1:A:233:PRO:CD	2.05	0.68
1:A:354:VAL:HA	1:A:357:ALA:HB3	1.74	0.68
1:A:441:GLY:O	1:A:444:LEU:HB2	1.93	0.68
1:B:144:TYR:CD1	1:B:145:LEU:N	2.62	0.68
1:B:362:LEU:HD23	1:B:363:PHE:N	2.08	0.68
1:B:86:HIS:CG	1:B:87:LYS:N	2.61	0.68
1:A:275:ALA:HA	1:A:353:VAL:HG11	1.75	0.68
1:A:4:SER:O	1:A:8:TYR:CE2	2.47	0.68
1:A:185:LYS:HB2	1:A:189:PRO:HB3	1.73	0.68
1:A:420:LEU:HB3	1:A:423:LYS:CG	2.20	0.68
1:B:244:LEU:HB2	1:B:385:LYS:NZ	2.09	0.68
1:B:247:PRO:O	1:B:251:ALA:HB2	1.93	0.68
1:A:130:THR:CG2	1:A:194:VAL:HG22	2.23	0.68
1:A:213:PHE:O	1:A:217:THR:HG22	1.93	0.68
1:A:295:GLY:O	1:A:299:SER:N	2.25	0.68
1:A:312:LYS:NZ	1:A:312:LYS:HA	2.08	0.68
1:B:93:HIS:CD2	1:B:228:GLU:HB3	2.28	0.68
1:B:370:MET:O	1:B:373:VAL:HG12	1.93	0.68
1:A:362:LEU:HD23	1:A:363:PHE:N	2.09	0.68
1:A:166:ILE:HD13	1:A:166:ILE:O	1.93	0.68
1:A:13:SER:O	1:A:16:ILE:HG22	1.94	0.68
1:A:457:HIS:HA	1:A:460:ALA:HB3	1.75	0.68
1:A:96:LEU:O	1:A:96:LEU:HD23	1.93	0.68
1:B:232:LYS:C	1:B:235:PRO:HD2	2.13	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:GLN:O	1:A:362:LEU:HB3	1.94	0.68
1:A:447:LEU:HD21	1:A:450:GLN:HG2	1.76	0.68
1:A:423:LYS:HG3	1:A:424:GLY:H	1.58	0.68
1:B:387:MET:HG3	1:B:446:TRP:HZ2	1.59	0.68
1:B:244:LEU:HG	1:B:385:LYS:NZ	2.09	0.68
1:B:443:ARG:O	1:B:445:TYR:N	2.26	0.67
1:B:72:LEU:CD1	1:B:244:LEU:HD21	2.24	0.67
1:A:387:MET:O	1:A:391:PHE:N	2.28	0.67
1:A:93:HIS:CD2	1:A:228:GLU:HB3	2.28	0.67
1:B:296:ALA:HA	1:B:299:SER:HB3	1.76	0.67
1:B:299:SER:O	1:B:302:VAL:HG12	1.95	0.67
1:A:238:LEU:HD12	1:A:241:LEU:HD13	1.77	0.67
1:B:124:GLU:O	1:B:125:ALA:C	2.31	0.67
1:B:272:THR:O	1:B:273:VAL:C	2.32	0.67
1:A:200:THR:HA	1:A:203:VAL:HG23	1.77	0.67
1:A:414:TRP:N	1:A:414:TRP:HE3	1.92	0.67
1:B:290:PHE:CB	1:B:291:PRO:HD3	2.24	0.67
1:A:413:ASN:HB2	1:A:418:GLN:HE21	1.57	0.67
1:A:46:ILE:HG22	1:A:46:ILE:O	1.93	0.67
1:B:185:LYS:C	1:B:185:LYS:HD3	2.15	0.67
1:B:275:ALA:N	1:B:353:VAL:HG21	2.10	0.67
1:B:445:TYR:CB	1:B:448:GLN:HA	2.17	0.67
1:B:76:VAL:HA	1:B:78:GLN:NE2	2.08	0.67
1:B:73:VAL:O	1:B:76:VAL:HB	1.95	0.67
1:A:225:LYS:O	1:A:226:VAL:HG23	1.95	0.67
1:A:238:LEU:HA	1:A:241:LEU:HD13	1.77	0.67
1:A:273:VAL:HG13	1:A:274:VAL:N	2.10	0.67
1:A:328:THR:HA	1:A:331:ILE:CG2	2.23	0.67
1:B:134:MET:HG3	1:B:197:GLY:HA3	1.75	0.67
1:A:231:HIS:HB3	1:A:235:PRO:CG	2.25	0.67
1:A:264:LEU:O	1:A:267:ALA:N	2.27	0.67
1:A:340:ARG:HD2	1:A:358:MET:CG	2.24	0.67
1:A:34:PHE:C	1:A:34:PHE:CD1	2.68	0.67
1:A:55:ALA:O	1:A:58:TRP:HB3	1.94	0.67
1:B:161:LYS:H	1:B:162:PRO:HD2	1.60	0.67
1:B:376:VAL:HG13	1:B:377:ALA:N	2.07	0.67
1:A:77:ALA:HB2	1:A:154:THR:OG1	1.94	0.67
1:A:86:HIS:CG	1:A:87:LYS:N	2.63	0.67
1:B:413:ASN:HB2	1:B:418:GLN:NE2	2.10	0.67
1:A:118:ARG:CZ	1:A:119:PHE:HB2	2.24	0.66
1:A:18:LEU:C	1:A:21:PRO:HD2	2.15	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:LEU:HA	1:B:241:LEU:HD13	1.76	0.66
1:B:279:VAL:HG21	1:B:357:ALA:HA	1.77	0.66
1:B:118:ARG:CZ	1:B:119:PHE:HB2	2.26	0.66
1:B:130:THR:HG21	1:B:194:VAL:HG22	1.77	0.66
1:B:247:PRO:CB	1:B:389:ALA:HA	2.25	0.66
1:B:316:ILE:C	1:B:320:VAL:HG12	2.16	0.66
1:B:340:ARG:HA	1:B:361:LEU:HD13	1.77	0.66
1:B:148:GLN:O	1:B:152:SER:HB3	1.95	0.66
1:B:234:GLN:O	1:B:238:LEU:N	2.29	0.66
1:B:281:LEU:HD22	1:B:282:ASN:HD22	1.59	0.66
1:A:353:VAL:HG12	1:A:357:ALA:H	1.59	0.66
1:A:262:VAL:CG2	1:A:403:LEU:HD13	2.23	0.66
1:A:417:GLU:HA	1:A:417:GLU:OE1	1.95	0.66
1:A:413:ASN:HB2	1:A:418:GLN:NE2	2.10	0.66
1:B:225:LYS:O	1:B:226:VAL:HG23	1.95	0.66
1:B:327:ALA:O	1:B:331:ILE:N	2.29	0.66
1:A:144:TYR:CD1	1:A:145:LEU:N	2.63	0.66
1:A:165:VAL:O	1:A:169:ILE:HB	1.96	0.66
1:A:210:LEU:H	1:A:210:LEU:HD22	1.59	0.66
1:B:234:GLN:N	1:B:235:PRO:CD	2.58	0.66
1:B:253:PHE:O	1:B:256:VAL:HG12	1.96	0.66
1:B:353:VAL:HG12	1:B:357:ALA:HB2	1.76	0.66
1:A:118:ARG:NH2	1:A:119:PHE:HB2	2.10	0.66
1:A:423:LYS:O	1:A:426:TRP:HB2	1.95	0.66
1:B:389:ALA:O	1:B:392:HIS:HB3	1.95	0.66
1:A:113:THR:HA	1:A:116:ILE:CG2	2.24	0.66
1:A:284:SER:O	1:A:286:LEU:N	2.29	0.66
1:A:290:PHE:CB	1:A:291:PRO:HD3	2.25	0.66
1:A:44:SER:C	1:A:46:ILE:H	1.97	0.66
1:B:298:VAL:HG21	1:B:321:GLY:HA3	1.77	0.66
1:A:183:TYR:O	1:A:185:LYS:N	2.28	0.66
1:B:118:ARG:NH2	1:B:119:PHE:HB2	2.11	0.66
1:B:145:LEU:HD22	1:B:145:LEU:C	2.16	0.66
1:B:276:ALA:HA	1:B:426:TRP:NE1	2.10	0.66
1:A:296:ALA:HA	1:A:299:SER:HB3	1.78	0.66
1:A:379:GLY:HA2	1:A:391:PHE:HE1	1.61	0.66
1:A:63:LEU:O	1:A:65:GLY:N	2.29	0.66
1:B:354:VAL:CA	1:B:357:ALA:HB3	2.26	0.66
1:A:208:LEU:HD23	1:A:209:LEU:H	1.57	0.66
1:A:87:LYS:NZ	1:B:308:GLU:HG2	2.10	0.66
1:A:96:LEU:CA	1:A:146:LEU:HG	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:LYS:O	1:B:239:ILE:HB	1.96	0.66
1:B:420:LEU:HB3	1:B:423:LYS:CG	2.25	0.66
1:A:161:LYS:H	1:A:162:PRO:HD2	1.60	0.65
1:A:391:PHE:CD2	1:A:392:HIS:N	2.61	0.65
1:B:12:ALA:HA	1:B:15:LEU:HD21	1.76	0.65
1:B:354:VAL:HA	1:B:357:ALA:HB3	1.78	0.65
1:B:382:ARG:O	1:B:387:MET:HB2	1.96	0.65
1:A:296:ALA:O	1:A:300:ILE:HG23	1.97	0.65
1:B:63:LEU:O	1:B:65:GLY:N	2.28	0.65
1:A:114:GLN:O	1:A:128:THR:HG23	1.95	0.65
1:A:378:ALA:HB2	1:A:440:LEU:HG	1.78	0.65
1:A:420:LEU:HD11	1:A:422:ALA:HB3	1.78	0.65
1:A:73:VAL:O	1:A:76:VAL:CB	2.44	0.65
1:B:11:GLU:CG	1:B:320:VAL:HB	2.26	0.65
1:B:262:VAL:CG2	1:B:403:LEU:HD13	2.25	0.65
1:A:240:ARG:HD3	1:A:460:ALA:HA	1.76	0.65
1:B:146:LEU:HD22	1:B:149:ALA:HB3	1.78	0.65
1:B:235:PRO:C	1:B:238:LEU:HB2	2.16	0.65
1:B:413:ASN:HB2	1:B:418:GLN:HE21	1.61	0.65
1:B:94:GLN:HE21	1:B:231:HIS:HB2	1.61	0.65
1:A:146:LEU:HD22	1:A:149:ALA:HB3	1.79	0.65
1:B:128:THR:HG22	1:B:129:LYS:N	2.11	0.65
1:B:130:THR:CG2	1:B:194:VAL:HG22	2.27	0.65
1:B:247:PRO:CG	1:B:389:ALA:HA	2.27	0.65
1:B:244:LEU:HD23	1:B:385:LYS:O	1.97	0.65
1:B:407:TYR:O	1:B:411:MET:N	2.23	0.65
1:A:444:LEU:C	1:A:446:TRP:H	1.98	0.65
1:B:135:HIS:HA	1:B:138:ILE:HG22	1.78	0.65
1:B:96:LEU:O	1:B:99:ALA:CB	2.44	0.65
1:A:301:ARG:O	1:A:301:ARG:HD3	1.95	0.65
1:A:332:THR:HA	1:A:335:LEU:CD2	2.27	0.65
1:A:275:ALA:N	1:A:353:VAL:HG21	2.11	0.65
1:B:428:GLY:O	1:B:431:ILE:HB	1.97	0.65
1:B:70:MET:CE	1:B:99:ALA:HB2	2.27	0.65
1:A:279:VAL:HG21	1:A:357:ALA:HA	1.79	0.65
1:B:290:PHE:HB3	1:B:291:PRO:HD3	1.79	0.65
1:B:247:PRO:HB3	1:B:389:ALA:HA	1.79	0.65
1:A:134:MET:HG3	1:A:197:GLY:HA3	1.79	0.65
1:A:290:PHE:HB3	1:A:291:PRO:HD3	1.79	0.65
1:A:326:LEU:O	1:A:330:CYS:HB2	1.96	0.65
1:A:339:PHE:HB3	1:A:343:ILE:CG1	2.27	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:O	1:A:261:VAL:HB	1.97	0.64
1:A:94:GLN:HE21	1:A:231:HIS:HB2	1.62	0.64
1:B:264:LEU:O	1:B:265:LEU:C	2.34	0.64
1:A:258:LEU:HD22	1:A:399:TRP:CZ2	2.32	0.64
1:A:96:LEU:HD12	1:A:146:LEU:HD12	1.79	0.64
1:B:134:MET:SD	1:B:198:VAL:HA	2.37	0.64
1:B:18:LEU:C	1:B:21:PRO:HD2	2.18	0.64
1:B:275:ALA:CA	1:B:353:VAL:HG11	2.27	0.64
1:A:131:VAL:HB	1:A:135:HIS:NE2	2.13	0.64
1:A:273:VAL:O	1:A:277:HIS:N	2.30	0.64
1:A:93:HIS:HE1	1:A:225:LYS:HB3	1.61	0.64
1:B:125:ALA:O	1:B:126:MET:O	2.16	0.64
1:B:301:ARG:NH2	1:B:316:ILE:HG22	2.11	0.64
1:B:353:VAL:CG1	1:B:357:ALA:HB2	2.28	0.64
1:B:382:ARG:HH22	1:B:445:TYR:H	1.44	0.64
1:A:137:VAL:HG11	1:A:201:ALA:CA	2.28	0.64
1:A:98:LEU:HA	1:A:101:LEU:CD1	2.27	0.64
1:B:36:ASP:HB2	1:B:178:ASN:ND2	2.11	0.64
1:B:359:GLN:O	1:B:362:LEU:HB3	1.98	0.64
1:B:96:LEU:HD23	1:B:96:LEU:O	1.98	0.64
1:A:251:ALA:HB2	1:A:392:HIS:ND1	2.13	0.64
1:A:354:VAL:CA	1:A:357:ALA:HB3	2.27	0.64
1:B:273:VAL:HG13	1:B:274:VAL:N	2.11	0.64
1:A:185:LYS:HD3	1:A:185:LYS:C	2.18	0.64
1:A:5:VAL:HA	1:A:8:TYR:CZ	2.32	0.64
1:B:145:LEU:HA	1:B:148:GLN:NE2	2.13	0.64
1:B:350:ASN:OD1	1:B:352:VAL:HB	1.98	0.64
1:B:275:ALA:CB	1:B:353:VAL:CG1	2.74	0.64
1:B:436:ALA:O	1:B:439:MET:N	2.31	0.64
1:A:177:LEU:CD1	1:A:202:ILE:HD13	2.25	0.64
1:A:144:TYR:CD2	1:A:207:MET:HB3	2.33	0.64
1:A:274:VAL:O	1:A:275:ALA:C	2.35	0.64
1:B:145:LEU:O	1:B:145:LEU:HD22	1.97	0.64
1:B:326:LEU:O	1:B:330:CYS:HB2	1.97	0.64
1:B:35:VAL:O	1:B:39:MET:HB3	1.98	0.64
1:B:51:VAL:O	1:B:54:ALA:HB3	1.97	0.64
1:A:207:MET:HA	1:A:210:LEU:HD23	1.80	0.64
1:B:102:VAL:C	1:B:105:PRO:HD2	2.19	0.64
1:B:353:VAL:HG12	1:B:357:ALA:CB	2.28	0.64
1:B:63:LEU:O	1:B:66:VAL:HG22	1.98	0.64
1:A:173:LEU:C	1:A:177:LEU:HD23	2.18	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ALA:CB	1:A:353:VAL:CG1	2.76	0.64
1:A:394:THR:HG23	1:A:439:MET:HB3	1.80	0.64
1:A:276:ALA:CA	1:A:426:TRP:HE1	2.09	0.64
1:B:302:VAL:O	1:B:306:LEU:HB2	1.98	0.64
1:B:366:ILE:O	1:B:369:CYS:HB3	1.97	0.64
1:B:390:ILE:O	1:B:390:ILE:HG22	1.97	0.64
1:B:45:ALA:HB1	1:B:126:MET:HE1	1.80	0.64
1:B:12:ALA:HA	1:B:15:LEU:CD2	2.27	0.63
1:B:173:LEU:C	1:B:177:LEU:HD23	2.17	0.63
1:B:236:LYS:HA	1:B:239:ILE:CG1	2.29	0.63
1:A:102:VAL:C	1:A:105:PRO:HD2	2.19	0.63
1:A:128:THR:HG22	1:A:129:LYS:N	2.12	0.63
1:A:148:GLN:HA	1:A:152:SER:HB2	1.80	0.63
1:A:17:LYS:O	1:A:21:PRO:CG	2.43	0.63
1:A:63:LEU:C	1:A:65:GLY:N	2.50	0.63
1:B:11:GLU:CD	1:B:320:VAL:HB	2.18	0.63
1:B:378:ALA:HB2	1:B:440:LEU:HG	1.80	0.63
1:B:441:GLY:O	1:B:444:LEU:HB2	1.97	0.63
1:A:125:ALA:O	1:A:126:MET:O	2.16	0.63
1:B:117:ILE:HG22	1:B:119:PHE:H	1.63	0.63
1:B:96:LEU:HA	1:B:146:LEU:HG	1.80	0.63
1:B:191:LEU:HB3	1:B:194:VAL:CG2	2.28	0.63
1:B:181:PHE:CD2	1:B:198:VAL:HG11	2.34	0.63
1:B:272:THR:O	1:B:274:VAL:N	2.31	0.63
1:B:373:VAL:HG13	1:B:437:ALA:HB1	1.80	0.63
1:A:12:ALA:HA	1:A:15:LEU:HD21	1.80	0.63
1:A:135:HIS:HA	1:A:138:ILE:HG22	1.79	0.63
1:A:72:LEU:CD1	1:A:244:LEU:HD21	2.26	0.63
1:A:342:GLN:O	1:A:345:LEU:HB2	1.99	0.63
1:A:352:VAL:HG13	1:A:352:VAL:O	1.99	0.63
1:B:231:HIS:HB3	1:B:235:PRO:CG	2.27	0.63
1:A:386:ASP:O	1:A:389:ALA:N	2.31	0.63
1:A:40:ALA:O	1:A:44:SER:HB2	1.99	0.63
1:A:45:ALA:O	1:A:48:MET:HB2	1.99	0.63
1:B:264:LEU:O	1:B:267:ALA:N	2.31	0.63
1:B:414:TRP:HE3	1:B:414:TRP:N	1.96	0.63
1:B:420:LEU:HD13	1:B:422:ALA:H	1.62	0.63
1:A:287:VAL:O	1:A:290:PHE:HB2	1.99	0.63
1:A:63:LEU:O	1:A:66:VAL:HG22	1.98	0.63
1:B:363:PHE:CE2	1:B:426:TRP:HB3	2.33	0.63
1:B:445:TYR:O	1:B:448:GLN:N	2.32	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ALA:O	1:A:28:ALA:HB3	1.99	0.63
1:A:264:LEU:O	1:A:265:LEU:C	2.36	0.63
1:A:52:SER:O	1:A:123:GLU:OE2	2.16	0.63
1:B:238:LEU:CA	1:B:241:LEU:HB2	2.27	0.63
1:A:267:ALA:N	1:A:268:PRO:HD2	2.13	0.63
1:A:408:ILE:HG22	1:A:408:ILE:O	1.99	0.63
1:A:373:VAL:HG13	1:A:437:ALA:HB1	1.81	0.63
1:A:55:ALA:HB3	1:A:123:GLU:OE2	1.99	0.63
1:A:89:PRO:O	1:A:93:HIS:ND1	2.32	0.63
1:B:16:ILE:HA	1:B:19:ALA:HB2	1.76	0.63
1:B:45:ALA:O	1:B:48:MET:HB2	1.99	0.63
1:A:120:MET:HG2	1:A:120:MET:O	1.99	0.63
1:B:113:THR:CA	1:B:116:ILE:HG22	2.29	0.63
1:B:25:ALA:O	1:B:28:ALA:HB3	1.98	0.63
1:A:149:ALA:O	1:A:154:THR:HB	1.98	0.62
1:A:299:SER:CB	1:A:380:SER:HA	2.28	0.62
1:A:117:ILE:HG22	1:A:119:PHE:H	1.64	0.62
1:A:147:PHE:HE2	1:A:215:ILE:HB	1.64	0.62
1:A:298:VAL:HG21	1:A:321:GLY:HA3	1.81	0.62
1:A:59:LEU:HD12	1:A:59:LEU:N	2.12	0.62
1:B:344:ALA:HB1	1:B:354:VAL:HG22	1.80	0.62
1:A:445:TYR:O	1:A:446:TRP:CB	2.47	0.62
1:B:333:ALA:O	1:B:336:THR:HB	1.99	0.62
1:B:63:LEU:C	1:B:65:GLY:N	2.50	0.62
1:B:7:ARG:HB3	1:B:11:GLU:OE1	1.98	0.62
1:A:284:SER:O	1:A:287:VAL:N	2.33	0.62
1:A:428:GLY:O	1:A:431:ILE:HB	1.98	0.62
1:B:147:PHE:HE2	1:B:215:ILE:HB	1.64	0.62
1:B:444:LEU:O	1:B:446:TRP:O	2.18	0.62
1:B:59:LEU:N	1:B:59:LEU:HD22	2.13	0.62
1:A:45:ALA:HB1	1:A:126:MET:HE1	1.82	0.62
1:B:219:LYS:HD2	1:B:220:ARG:HG2	1.81	0.62
1:B:339:PHE:HB3	1:B:343:ILE:HG13	1.79	0.62
1:B:423:LYS:O	1:B:426:TRP:HB2	1.99	0.62
1:A:215:ILE:HG23	1:A:216:VAL:HG23	1.81	0.62
1:A:314:ALA:O	1:A:318:ALA:HB3	1.99	0.62
1:A:40:ALA:HB1	1:A:182:VAL:HG11	1.81	0.62
1:B:265:LEU:O	1:B:268:PRO:CD	2.48	0.62
1:B:262:VAL:O	1:B:266:VAL:HG23	2.00	0.62
1:B:408:ILE:O	1:B:408:ILE:HG22	1.98	0.62
1:B:412:THR:C	1:B:415:LEU:H	2.02	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:VAL:HG22	1:A:204:TYR:HB3	1.81	0.62
1:A:84:ARG:C	1:A:86:HIS:H	2.02	0.62
1:B:284:SER:O	1:B:287:VAL:N	2.33	0.62
1:B:417:GLU:OE1	1:B:417:GLU:HA	1.99	0.62
1:A:15:LEU:O	1:A:19:ALA:N	2.30	0.62
1:A:316:ILE:C	1:A:320:VAL:HG12	2.20	0.62
1:B:52:SER:O	1:B:123:GLU:OE2	2.17	0.62
1:B:14:ASN:N	1:B:14:ASN:HD22	1.97	0.62
1:B:174:ASN:HD21	1:B:203:VAL:HG22	1.63	0.62
1:B:141:VAL:HG22	1:B:204:TYR:HB3	1.81	0.62
1:B:328:THR:O	1:B:332:THR:HG23	2.00	0.62
1:B:34:PHE:C	1:B:34:PHE:CD1	2.72	0.62
1:B:69:LEU:HD23	1:B:69:LEU:C	2.20	0.62
1:A:200:THR:HA	1:A:203:VAL:CG2	2.30	0.62
1:A:203:VAL:O	1:A:207:MET:HG3	2.00	0.62
1:A:398:TYR:HB2	1:A:432:GLY:O	2.00	0.62
1:B:238:LEU:HG	1:B:241:LEU:HD22	1.81	0.62
1:B:53:ILE:C	1:B:53:ILE:HD12	2.19	0.62
1:A:353:VAL:HG12	1:A:357:ALA:CB	2.29	0.62
1:B:40:ALA:HB1	1:B:182:VAL:HG11	1.82	0.62
1:B:421:GLY:O	1:B:425:PHE:HB3	2.00	0.62
1:B:60:PRO:O	1:B:63:LEU:HD23	2.00	0.62
1:B:92:VAL:HG12	1:B:93:HIS:N	2.15	0.62
1:A:171:LEU:HD23	1:A:172:LEU:H	1.63	0.61
1:B:100:LEU:HD12	1:B:100:LEU:N	2.15	0.61
1:B:137:VAL:HG11	1:B:201:ALA:CA	2.28	0.61
1:B:221:LEU:N	1:B:221:LEU:HD12	2.15	0.61
1:B:32:MET:CG	1:B:33:GLY:N	2.63	0.61
1:A:247:PRO:CG	1:A:389:ALA:HA	2.30	0.61
1:A:403:LEU:HD21	1:A:429:PHE:CD2	2.32	0.61
1:B:250:ALA:O	1:B:251:ALA:O	2.18	0.61
1:B:423:LYS:CG	1:B:424:GLY:H	2.13	0.61
1:B:74:PRO:HB3	1:B:149:ALA:CB	2.30	0.61
1:B:73:VAL:HG13	1:B:241:LEU:HG	1.83	0.61
1:B:342:GLN:O	1:B:345:LEU:HB2	2.00	0.61
1:B:340:ARG:HB2	1:B:361:LEU:HD13	1.83	0.61
1:B:98:LEU:HA	1:B:101:LEU:CD1	2.29	0.61
1:A:391:PHE:C	1:A:391:PHE:HD2	2.02	0.61
1:B:26:SER:HB2	1:B:289:MET:CG	2.30	0.61
1:B:284:SER:O	1:B:286:LEU:N	2.34	0.61
1:B:295:GLY:O	1:B:299:SER:N	2.27	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:VAL:O	1:B:93:HIS:C	2.38	0.61
1:A:126:MET:O	1:A:130:THR:HG23	2.01	0.61
1:A:144:TYR:CG	1:A:207:MET:HB3	2.35	0.61
1:A:339:PHE:HB3	1:A:343:ILE:HG12	1.81	0.61
1:A:57:ILE:HA	1:A:60:PRO:CG	2.29	0.61
1:B:202:ILE:O	1:B:205:TRP:HB3	2.00	0.61
1:B:94:GLN:OE1	1:B:238:LEU:HD11	2.00	0.61
1:B:74:PRO:HG3	1:B:149:ALA:HB1	1.82	0.61
1:A:423:LYS:CG	1:A:424:GLY:H	2.13	0.61
1:B:126:MET:O	1:B:130:THR:HG23	2.01	0.61
1:A:443:ARG:O	1:A:445:TYR:N	2.33	0.61
1:A:86:HIS:O	1:A:87:LYS:HB2	2.01	0.61
1:B:131:VAL:HB	1:B:135:HIS:NE2	2.16	0.61
1:B:251:ALA:HB2	1:B:392:HIS:ND1	2.16	0.61
1:B:276:ALA:CA	1:B:426:TRP:HE1	2.13	0.61
1:B:312:LYS:NZ	1:B:312:LYS:HA	2.15	0.61
1:B:385:LYS:HD3	1:B:385:LYS:C	2.21	0.61
1:B:84:ARG:HB3	1:B:87:LYS:HD2	1.81	0.61
1:A:245:GLY:HA2	1:A:248:VAL:HG22	1.83	0.61
1:A:252:LEU:HA	1:A:255:GLU:OE2	2.00	0.61
1:A:58:TRP:O	1:A:61:SER:HB3	2.00	0.61
1:B:153:PHE:O	1:B:155:ASP:OD1	2.19	0.61
1:B:21:PRO:CB	1:B:160:THR:HG23	2.31	0.61
1:B:33:GLY:O	1:B:37:THR:HB	2.00	0.61
1:A:220:ARG:HG3	1:A:221:LEU:HD12	1.83	0.61
1:A:238:LEU:CA	1:A:241:LEU:HB2	2.30	0.61
1:A:72:LEU:HD12	1:A:244:LEU:HD11	1.81	0.61
1:A:328:THR:O	1:A:332:THR:HG23	2.01	0.61
1:A:33:GLY:O	1:A:37:THR:HB	2.01	0.61
1:A:414:TRP:N	1:A:414:TRP:CE3	2.68	0.61
1:A:41:GLY:C	1:A:49:ALA:HB1	2.21	0.61
1:B:387:MET:HG3	1:B:446:TRP:CZ2	2.35	0.61
1:A:96:LEU:HA	1:A:146:LEU:HG	1.83	0.60
1:B:89:PRO:O	1:B:93:HIS:ND1	2.34	0.60
1:A:24:ILE:O	1:A:27:VAL:HB	2.01	0.60
1:A:406:GLY:HA2	1:A:428:GLY:HA3	1.81	0.60
1:A:7:ARG:HB3	1:A:11:GLU:OE1	2.02	0.60
1:B:181:PHE:CG	1:B:198:VAL:HG11	2.35	0.60
1:B:75:VAL:O	1:B:77:ALA:N	2.34	0.60
1:A:69:LEU:HG	1:A:245:GLY:HA3	1.82	0.60
1:A:53:ILE:C	1:A:53:ILE:HD12	2.22	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:VAL:HA	1:B:134:MET:HB2	1.84	0.60
1:B:314:ALA:HB2	1:B:449:LYS:NZ	2.15	0.60
1:B:353:VAL:O	1:B:353:VAL:CG1	2.46	0.60
1:A:31:GLY:O	1:A:35:VAL:HG23	2.02	0.60
1:A:431:ILE:O	1:A:435:ALA:HB2	2.01	0.60
1:B:114:GLN:O	1:B:128:THR:HG23	2.01	0.60
1:B:183:TYR:O	1:B:185:LYS:N	2.35	0.60
1:B:301:ARG:HH12	1:B:320:VAL:HG11	1.66	0.60
1:A:11:GLU:CD	1:A:320:VAL:HB	2.21	0.60
1:B:248:VAL:O	1:B:251:ALA:HB3	2.02	0.60
1:B:252:LEU:HA	1:B:255:GLU:OE2	2.02	0.60
1:B:250:ALA:HA	1:B:254:PHE:HB2	1.84	0.60
1:B:46:ILE:C	1:B:48:MET:N	2.47	0.60
1:A:166:ILE:O	1:A:170:GLY:HA3	2.01	0.60
1:B:147:PHE:CG	1:B:211:LEU:HA	2.37	0.60
1:B:166:ILE:O	1:B:170:GLY:N	2.35	0.60
1:B:273:VAL:O	1:B:277:HIS:N	2.33	0.60
1:B:398:TYR:HB2	1:B:432:GLY:O	2.02	0.60
1:B:72:LEU:HB3	1:B:244:LEU:HD13	1.83	0.60
1:A:129:LYS:HA	1:A:132:GLY:HA3	1.83	0.60
1:A:370:MET:O	1:A:373:VAL:HG12	2.01	0.60
1:B:5:VAL:HA	1:B:8:TYR:CZ	2.37	0.60
1:A:196:CYS:SG	1:A:197:GLY:N	2.74	0.60
1:A:239:ILE:HA	1:A:242:PHE:HB2	1.83	0.60
1:B:232:LYS:H	1:B:233:PRO:CD	2.15	0.60
1:B:267:ALA:N	1:B:268:PRO:HD2	2.15	0.60
1:B:314:ALA:O	1:B:315:ALA:C	2.40	0.60
1:B:59:LEU:CD2	1:B:59:LEU:H	2.14	0.60
1:A:221:LEU:HD12	1:A:221:LEU:N	2.17	0.60
1:B:211:LEU:CG	1:B:212:LEU:N	2.64	0.60
1:A:69:LEU:HD23	1:A:69:LEU:C	2.23	0.59
1:B:177:LEU:CD1	1:B:202:ILE:HD13	2.25	0.59
1:B:202:ILE:O	1:B:206:ILE:HG23	2.02	0.59
1:B:209:LEU:HD12	1:B:210:LEU:HD13	1.82	0.59
1:B:387:MET:HA	1:B:443:ARG:HH21	1.66	0.59
1:A:118:ARG:HH21	1:A:119:PHE:CB	2.15	0.59
1:A:235:PRO:C	1:A:238:LEU:HB2	2.23	0.59
1:A:250:ALA:O	1:A:251:ALA:O	2.20	0.59
1:A:420:LEU:CD1	1:A:422:ALA:HB3	2.32	0.59
1:A:420:LEU:CB	1:A:423:LYS:HG2	2.28	0.59
1:B:123:GLU:CG	1:B:127:ALA:HB3	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:PHE:CE2	1:B:215:ILE:HB	2.37	0.59
1:B:178:ASN:CG	1:B:199:ALA:HB2	2.23	0.59
1:B:207:MET:HA	1:B:210:LEU:HD23	1.84	0.59
1:B:367:TYR:HA	1:B:430:ILE:HG13	1.84	0.59
1:A:123:GLU:CG	1:A:127:ALA:HB3	2.32	0.59
1:A:166:ILE:HB	1:A:210:LEU:HD21	1.83	0.59
1:A:275:ALA:CA	1:A:353:VAL:HG11	2.31	0.59
1:A:299:SER:OG	1:A:380:SER:HA	2.02	0.59
1:A:81:GLY:HA3	1:A:307:GLY:O	2.02	0.59
1:A:354:VAL:O	1:A:358:MET:N	2.28	0.59
1:B:127:ALA:O	1:B:131:VAL:HG22	2.01	0.59
1:B:21:PRO:HB3	1:B:160:THR:O	2.03	0.59
1:B:65:GLY:HA2	1:B:253:PHE:CD2	2.37	0.59
1:A:191:LEU:O	1:A:195:GLY:N	2.34	0.59
1:B:147:PHE:CD2	1:B:211:LEU:HA	2.37	0.59
1:B:171:LEU:HD23	1:B:172:LEU:H	1.67	0.59
1:B:263:ALA:O	1:B:266:VAL:C	2.41	0.59
1:A:147:PHE:CD2	1:A:211:LEU:HA	2.38	0.59
1:A:16:ILE:HA	1:A:19:ALA:HB2	1.81	0.59
1:A:234:GLN:O	1:A:238:LEU:HD13	2.02	0.59
1:A:333:ALA:O	1:A:336:THR:HB	2.02	0.59
1:A:445:TYR:HD2	1:A:448:GLN:HG2	1.64	0.59
1:A:68:LEU:HD22	1:A:71:ALA:HB3	1.82	0.59
1:B:233:PRO:O	1:B:236:LYS:HB3	2.02	0.59
1:B:379:GLY:HA2	1:B:391:PHE:HE1	1.68	0.59
1:B:88:ILE:N	1:B:89:PRO:CD	2.65	0.59
1:A:202:ILE:O	1:A:206:ILE:HG23	2.03	0.59
1:A:234:GLN:O	1:A:238:LEU:N	2.36	0.59
1:B:277:HIS:HD2	1:B:278:GLN:OE1	1.86	0.59
1:A:235:PRO:HA	1:A:238:LEU:HD22	1.84	0.59
1:A:354:VAL:O	1:A:358:MET:CB	2.51	0.59
1:A:7:ARG:HH11	1:A:7:ARG:HB3	1.68	0.59
1:B:106:ILE:HG22	1:B:139:PHE:HE1	1.68	0.59
1:B:80:ASN:C	1:B:82:ALA:N	2.54	0.59
1:A:11:GLU:OE2	1:A:320:VAL:HB	2.03	0.59
1:B:443:ARG:CZ	1:B:446:TRP:NE1	2.66	0.59
1:B:452:ASP:O	1:B:456:LEU:HG	2.03	0.59
1:A:142:PRO:CA	1:A:145:LEU:HB3	2.30	0.59
1:A:151:ARG:HG3	1:A:152:SER:N	2.18	0.59
1:A:314:ALA:O	1:A:315:ALA:C	2.40	0.59
1:A:11:GLU:CG	1:A:320:VAL:HB	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ARG:HG3	1:B:152:SER:H	1.67	0.59
1:B:11:GLU:HG2	1:B:316:ILE:CG2	2.33	0.59
1:B:382:ARG:CD	1:B:382:ARG:N	2.65	0.59
1:B:86:HIS:CG	1:B:87:LYS:H	2.21	0.59
1:A:142:PRO:O	1:A:145:LEU:HD12	2.03	0.58
1:A:236:LYS:O	1:A:239:ILE:HB	2.02	0.58
1:A:351:GLN:O	1:A:354:VAL:HG23	2.03	0.58
1:B:151:ARG:O	1:B:155:ASP:N	2.35	0.58
1:B:17:LYS:O	1:B:21:PRO:CG	2.46	0.58
1:B:301:ARG:NH1	1:B:320:VAL:HG11	2.18	0.58
1:B:313:GLY:O	1:B:317:ALA:HB3	2.03	0.58
1:B:251:ALA:HB1	1:B:395:PHE:HD1	1.67	0.58
1:B:63:LEU:CG	1:B:64:PHE:N	2.66	0.58
1:A:355:ALA:O	1:A:358:MET:HB3	2.02	0.58
1:A:370:MET:HG3	1:A:434:SER:HB2	1.85	0.58
1:A:74:PRO:HG3	1:A:149:ALA:HB1	1.85	0.58
1:B:72:LEU:HD12	1:B:244:LEU:HD11	1.85	0.58
1:A:141:VAL:HA	1:A:204:TYR:HB2	1.86	0.58
1:A:250:ALA:O	1:A:254:PHE:N	2.36	0.58
1:A:281:LEU:HD22	1:A:282:ASN:ND2	2.17	0.58
1:A:363:PHE:CD1	1:A:364:ALA:N	2.71	0.58
1:A:407:TYR:C	1:A:409:LEU:H	2.06	0.58
1:A:408:ILE:HG12	1:A:411:MET:SD	2.44	0.58
1:A:426:TRP:HA	1:A:426:TRP:CE3	2.38	0.58
1:A:55:ALA:O	1:A:59:LEU:CD1	2.50	0.58
1:A:92:VAL:O	1:A:93:HIS:C	2.40	0.58
1:A:219:LYS:HD3	1:A:220:ARG:HE	1.68	0.58
1:A:65:GLY:HA2	1:A:253:PHE:CD2	2.38	0.58
1:A:302:VAL:O	1:A:306:LEU:HB2	2.03	0.58
1:B:178:ASN:ND2	1:B:199:ALA:CB	2.67	0.58
1:B:244:LEU:HG	1:B:385:LYS:HZ1	1.67	0.58
1:B:340:ARG:HG3	1:B:341:GLU:H	1.66	0.58
1:B:354:VAL:O	1:B:358:MET:CB	2.51	0.58
1:B:274:VAL:O	1:B:275:ALA:C	2.41	0.58
1:B:353:VAL:O	1:B:357:ALA:CB	2.52	0.58
1:A:70:MET:CE	1:A:99:ALA:HB2	2.34	0.58
1:B:151:ARG:HG3	1:B:152:SER:N	2.19	0.58
1:B:281:LEU:HD22	1:B:282:ASN:ND2	2.18	0.58
1:B:314:ALA:O	1:B:318:ALA:HB3	2.03	0.58
1:B:413:ASN:HB2	1:B:418:GLN:HG2	1.85	0.58
1:A:326:LEU:HD13	1:A:330:CYS:HB2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:LEU:CD1	1:B:16:ILE:N	2.66	0.58
1:B:245:GLY:HA2	1:B:248:VAL:HG22	1.86	0.58
1:B:53:ILE:C	1:B:56:SER:HB3	2.24	0.58
1:A:21:PRO:HB3	1:A:160:THR:O	2.03	0.58
1:A:247:PRO:CB	1:A:389:ALA:HA	2.34	0.58
1:A:251:ALA:HB1	1:A:395:PHE:HD1	1.67	0.58
1:A:367:TYR:HA	1:A:430:ILE:HG13	1.86	0.58
1:B:302:VAL:HG23	1:B:317:ALA:HB3	1.86	0.58
1:B:351:GLN:O	1:B:352:VAL:C	2.41	0.58
1:A:236:LYS:HA	1:A:239:ILE:CG1	2.34	0.58
1:A:312:LYS:HZ2	1:A:312:LYS:HA	1.68	0.58
1:A:72:LEU:HA	1:A:75:VAL:CG1	2.33	0.58
1:B:141:VAL:HA	1:B:204:TYR:HB2	1.86	0.58
1:B:398:TYR:CD1	1:B:399:TRP:N	2.71	0.58
1:B:461:LYS:OXT	1:B:461:LYS:HD2	2.04	0.58
1:B:86:HIS:O	1:B:87:LYS:HB2	2.04	0.58
1:A:12:ALA:HA	1:A:15:LEU:CD2	2.33	0.58
1:A:147:PHE:CE2	1:A:215:ILE:HB	2.39	0.58
1:A:367:TYR:HE2	1:A:429:PHE:CD1	2.21	0.58
1:B:410:GLY:HA3	1:B:425:PHE:HB2	1.86	0.58
1:A:379:GLY:HA2	1:A:391:PHE:CE1	2.39	0.57
1:B:353:VAL:C	1:B:357:ALA:HB2	2.25	0.57
1:B:455:GLN:HA	1:B:458:LEU:HB2	1.85	0.57
1:B:62:ILE:CG1	1:B:63:LEU:N	2.63	0.57
1:A:160:THR:HG23	1:A:160:THR:O	2.04	0.57
1:A:250:ALA:O	1:A:254:PHE:CB	2.52	0.57
1:A:363:PHE:CE2	1:A:426:TRP:HB3	2.40	0.57
1:A:447:LEU:O	1:A:448:GLN:CB	2.51	0.57
1:B:407:TYR:C	1:B:409:LEU:H	2.06	0.57
1:B:443:ARG:CZ	1:B:446:TRP:HE1	2.16	0.57
1:A:74:PRO:CG	1:A:149:ALA:CB	2.82	0.57
1:A:389:ALA:O	1:A:392:HIS:HB3	2.04	0.57
1:A:96:LEU:O	1:A:99:ALA:CB	2.52	0.57
1:B:144:TYR:CD2	1:B:207:MET:HB3	2.39	0.57
1:B:413:ASN:HB3	1:B:414:TRP:CE3	2.39	0.57
1:B:73:VAL:CB	1:B:74:PRO:CD	2.77	0.57
1:A:57:ILE:O	1:A:60:PRO:HB2	2.04	0.57
1:B:318:ALA:HA	1:B:381:LEU:HD11	1.86	0.57
1:B:406:GLY:HA2	1:B:428:GLY:HA3	1.86	0.57
1:B:57:ILE:HA	1:B:60:PRO:HG2	1.87	0.57
1:A:145:LEU:HA	1:A:148:GLN:NE2	2.18	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ALA:HA	1:A:353:VAL:HG21	1.85	0.57
1:A:63:LEU:CD2	1:A:64:PHE:N	2.65	0.57
1:B:149:ALA:O	1:B:154:THR:HB	2.04	0.57
1:B:172:LEU:O	1:B:176:PRO:HD2	2.04	0.57
1:B:324:THR:O	1:B:327:ALA:HB3	2.05	0.57
1:B:376:VAL:O	1:B:380:SER:HB3	2.04	0.57
1:A:106:ILE:HG22	1:A:139:PHE:HE1	1.70	0.57
1:A:19:ALA:O	1:A:22:VAL:HG22	2.03	0.57
1:B:211:LEU:O	1:B:212:LEU:C	2.43	0.57
1:B:460:ALA:O	1:B:461:LYS:O	2.23	0.57
1:B:97:ILE:HG22	1:B:101:LEU:CD1	2.29	0.57
1:A:350:ASN:ND2	1:A:352:VAL:H	2.02	0.57
1:B:314:ALA:HB2	1:B:449:LYS:HZ1	1.68	0.57
1:B:352:VAL:O	1:B:352:VAL:HG13	2.04	0.57
1:A:147:PHE:CG	1:A:211:LEU:HA	2.40	0.57
1:A:152:SER:O	1:A:155:ASP:OD1	2.23	0.57
1:A:420:LEU:HD13	1:A:422:ALA:H	1.69	0.57
1:B:107:ILE:O	1:B:110:LEU:HB3	2.05	0.57
1:B:215:ILE:HG23	1:B:216:VAL:HG23	1.85	0.57
1:B:235:PRO:HA	1:B:238:LEU:CG	2.35	0.57
1:B:237:GLU:O	1:B:241:LEU:HD12	2.05	0.57
1:A:191:LEU:HG	1:A:192:GLY:N	2.19	0.57
1:A:88:ILE:CG1	1:A:89:PRO:CD	2.82	0.57
1:B:239:ILE:HA	1:B:242:PHE:HB2	1.87	0.57
1:A:139:PHE:C	1:A:142:PRO:HD2	2.26	0.56
1:A:14:ASN:HD22	1:A:14:ASN:N	2.03	0.56
1:A:63:LEU:CG	1:A:64:PHE:N	2.67	0.56
1:A:72:LEU:HD13	1:A:75:VAL:HG21	1.86	0.56
1:B:299:SER:CB	1:B:380:SER:HA	2.35	0.56
1:A:178:ASN:CG	1:A:199:ALA:HB2	2.25	0.56
1:A:292:MET:HA	1:A:375:VAL:HG11	1.86	0.56
1:A:418:GLN:HE22	1:A:421:GLY:HA2	1.69	0.56
1:A:88:ILE:N	1:A:89:PRO:CD	2.68	0.56
1:B:136:ALA:HA	1:B:139:PHE:HD2	1.70	0.56
1:B:332:THR:HA	1:B:335:LEU:HG	1.87	0.56
1:B:426:TRP:CE3	1:B:426:TRP:HA	2.40	0.56
1:B:83:GLY:O	1:B:85:GLN:N	2.37	0.56
1:B:84:ARG:C	1:B:86:HIS:H	2.09	0.56
1:A:110:LEU:HD13	1:A:114:GLN:HG3	1.86	0.56
1:A:247:PRO:HB3	1:A:389:ALA:HA	1.88	0.56
1:B:118:ARG:HH21	1:B:119:PHE:CB	2.17	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:VAL:O	1:B:377:ALA:C	2.43	0.56
1:B:248:VAL:HG12	1:B:391:PHE:CZ	2.40	0.56
1:B:391:PHE:CD2	1:B:392:HIS:N	2.60	0.56
1:A:237:GLU:O	1:A:240:ARG:HB3	2.05	0.56
1:A:353:VAL:CG1	1:A:353:VAL:O	2.51	0.56
1:A:398:TYR:CD1	1:A:399:TRP:N	2.73	0.56
1:A:68:LEU:HD12	1:A:248:VAL:HB	1.87	0.56
1:B:146:LEU:O	1:B:149:ALA:CB	2.52	0.56
1:B:159:LEU:O	1:B:161:LYS:N	2.38	0.56
1:B:181:PHE:O	1:B:190:GLU:HG2	2.05	0.56
1:B:427:LEU:O	1:B:430:ILE:N	2.38	0.56
1:B:81:GLY:HA3	1:B:307:GLY:O	2.04	0.56
1:A:237:GLU:O	1:A:241:LEU:HD12	2.05	0.56
1:A:261:VAL:HG12	1:A:262:VAL:N	2.20	0.56
1:A:367:TYR:N	1:A:430:ILE:HD11	2.20	0.56
1:A:376:VAL:O	1:A:377:ALA:C	2.44	0.56
1:A:390:ILE:CG2	1:A:390:ILE:O	2.53	0.56
1:A:407:TYR:CD2	1:A:411:MET:HG3	2.41	0.56
1:B:100:LEU:C	1:B:102:VAL:H	2.08	0.56
1:B:15:LEU:O	1:B:19:ALA:N	2.32	0.56
1:B:199:ALA:O	1:B:203:VAL:HG23	2.06	0.56
1:B:235:PRO:HA	1:B:238:LEU:HD22	1.86	0.56
1:A:73:VAL:CB	1:A:74:PRO:CD	2.79	0.56
1:B:160:THR:HG23	1:B:160:THR:O	2.05	0.56
1:B:384:TYR:HE1	1:B:446:TRP:HH2	1.52	0.56
1:B:382:ARG:HA	1:B:387:MET:HG2	1.86	0.56
1:B:74:PRO:CG	1:B:149:ALA:CB	2.84	0.56
1:B:75:VAL:C	1:B:77:ALA:N	2.58	0.56
1:B:78:GLN:HG3	1:B:79:LEU:HD12	1.86	0.56
1:A:88:ILE:HG13	1:A:89:PRO:N	2.20	0.56
1:B:178:ASN:O	1:B:181:PHE:N	2.39	0.56
1:B:209:LEU:O	1:B:213:PHE:HB2	2.05	0.56
1:B:394:THR:HG23	1:B:439:MET:HB3	1.87	0.56
1:B:400:VAL:O	1:B:404:PRO:HD2	2.06	0.56
1:B:79:LEU:O	1:B:84:ARG:O	2.24	0.56
1:A:175:ILE:HG22	1:A:176:PRO:N	2.19	0.56
1:B:97:ILE:CG2	1:B:101:LEU:HD11	2.29	0.56
1:B:114:GLN:NE2	1:B:135:HIS:CE1	2.74	0.56
1:B:145:LEU:HD13	1:B:146:LEU:CA	2.35	0.56
1:B:150:LEU:O	1:B:154:THR:HB	2.06	0.56
1:B:320:VAL:O	1:B:322:LEU:N	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:VAL:O	1:B:321:GLY:C	2.44	0.56
1:B:63:LEU:CD2	1:B:64:PHE:N	2.69	0.56
1:A:77:ALA:HB2	1:A:154:THR:HG23	1.87	0.56
1:A:13:SER:O	1:A:16:ILE:CG2	2.53	0.56
1:A:220:ARG:HG3	1:A:221:LEU:CD1	2.35	0.56
1:A:423:LYS:CG	1:A:424:GLY:N	2.69	0.56
1:B:257:THR:O	1:B:261:VAL:HG23	2.06	0.56
1:B:414:TRP:CE3	1:B:414:TRP:N	2.74	0.56
1:B:457:HIS:HA	1:B:460:ALA:HB3	1.86	0.56
1:B:72:LEU:HD13	1:B:75:VAL:HG21	1.86	0.56
1:A:141:VAL:CG2	1:A:204:TYR:HB3	2.36	0.56
1:A:382:ARG:CD	1:A:382:ARG:N	2.69	0.56
1:B:219:LYS:HD3	1:B:220:ARG:HE	1.71	0.56
1:B:275:ALA:HA	1:B:353:VAL:HG21	1.87	0.56
1:B:350:ASN:ND2	1:B:352:VAL:H	2.04	0.56
1:B:387:MET:O	1:B:391:PHE:N	2.39	0.56
1:A:165:VAL:HG13	1:A:210:LEU:HG	1.87	0.56
1:A:356:LEU:O	1:A:360:LEU:N	2.27	0.56
1:A:400:VAL:O	1:A:404:PRO:HD2	2.06	0.56
1:B:146:LEU:HD13	1:B:146:LEU:C	2.27	0.56
1:B:151:ARG:O	1:B:153:PHE:N	2.39	0.56
1:B:166:ILE:O	1:B:170:GLY:HA3	2.06	0.56
1:B:343:ILE:O	1:B:344:ALA:C	2.45	0.56
1:B:70:MET:HE1	1:B:99:ALA:HB2	1.88	0.56
1:A:250:ALA:HA	1:A:254:PHE:HB2	1.88	0.55
1:B:387:MET:HE2	1:B:456:LEU:HD13	1.88	0.55
1:A:117:ILE:CG2	1:A:118:ARG:N	2.58	0.55
1:A:151:ARG:O	1:A:152:SER:C	2.45	0.55
1:A:166:ILE:O	1:A:170:GLY:N	2.38	0.55
1:A:98:LEU:HA	1:A:101:LEU:CG	2.36	0.55
1:B:138:ILE:HA	1:B:141:VAL:CG2	2.36	0.55
1:B:208:LEU:CD2	1:B:209:LEU:N	2.63	0.55
1:B:27:VAL:O	1:B:31:GLY:HA3	2.06	0.55
1:A:151:ARG:HG3	1:A:152:SER:H	1.70	0.55
1:A:213:PHE:O	1:A:215:ILE:N	2.40	0.55
1:A:262:VAL:O	1:A:266:VAL:HG23	2.05	0.55
1:B:151:ARG:O	1:B:152:SER:C	2.44	0.55
1:B:287:VAL:O	1:B:290:PHE:HB2	2.05	0.55
1:B:382:ARG:N	1:B:382:ARG:HD3	2.22	0.55
1:A:100:LEU:N	1:A:100:LEU:HD12	2.22	0.55
1:A:122:VAL:O	1:A:124:GLU:OE1	2.23	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LEU:CG	1:A:212:LEU:N	2.67	0.55
1:A:233:PRO:O	1:A:236:LYS:HB3	2.06	0.55
1:A:238:LEU:HG	1:A:241:LEU:HD22	1.88	0.55
1:A:286:LEU:O	1:A:289:MET:HB3	2.05	0.55
1:A:413:ASN:HB3	1:A:414:TRP:CZ3	2.40	0.55
1:B:145:LEU:HA	1:B:148:GLN:HE21	1.70	0.55
1:B:144:TYR:O	1:B:147:PHE:N	2.39	0.55
1:B:137:VAL:HG21	1:B:201:ALA:HB2	1.87	0.55
1:B:144:TYR:CG	1:B:207:MET:HB3	2.41	0.55
1:A:53:ILE:C	1:A:56:SER:HB3	2.26	0.55
1:B:129:LYS:HA	1:B:132:GLY:HA3	1.88	0.55
1:B:213:PHE:O	1:B:215:ILE:N	2.39	0.55
1:B:218:SER:O	1:B:220:ARG:N	2.40	0.55
1:B:220:ARG:HG3	1:B:221:LEU:HD12	1.88	0.55
1:B:242:PHE:O	1:B:244:LEU:N	2.35	0.55
1:A:134:MET:SD	1:A:198:VAL:HA	2.46	0.55
1:A:146:LEU:O	1:A:149:ALA:CB	2.52	0.55
1:A:165:VAL:CG1	1:A:166:ILE:N	2.42	0.55
1:B:180:ILE:HG23	1:B:181:PHE:HD1	1.71	0.55
1:A:134:MET:O	1:A:137:VAL:HB	2.06	0.55
1:A:146:LEU:C	1:A:146:LEU:HD13	2.27	0.55
1:A:324:THR:O	1:A:327:ALA:HB3	2.06	0.55
1:A:366:ILE:C	1:A:430:ILE:HD11	2.27	0.55
1:A:97:ILE:O	1:A:101:LEU:HG	2.07	0.55
1:B:166:ILE:HB	1:B:210:LEU:HD21	1.89	0.55
1:B:258:LEU:O	1:B:261:VAL:HB	2.06	0.55
1:B:72:LEU:HD13	1:B:75:VAL:CG2	2.36	0.55
1:A:217:THR:O	1:A:218:SER:C	2.44	0.55
1:A:84:ARG:HG2	1:B:309:GLN:HG2	1.89	0.55
1:A:83:GLY:O	1:A:85:GLN:N	2.40	0.55
1:B:13:SER:O	1:B:16:ILE:CG2	2.55	0.55
1:B:410:GLY:CA	1:B:425:PHE:HB2	2.37	0.55
1:A:159:LEU:O	1:A:161:LYS:N	2.40	0.55
1:A:197:GLY:O	1:A:200:THR:HB	2.06	0.55
1:A:207:MET:HA	1:A:210:LEU:CD2	2.37	0.55
1:A:343:ILE:O	1:A:344:ALA:C	2.46	0.55
1:B:120:MET:O	1:B:120:MET:HG2	2.06	0.55
1:B:122:VAL:O	1:B:124:GLU:OE1	2.25	0.55
1:B:162:PRO:HA	1:B:165:VAL:HB	1.87	0.55
1:B:299:SER:OG	1:B:380:SER:HA	2.07	0.55
1:A:114:GLN:NE2	1:A:135:HIS:CE1	2.75	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ARG:NH2	1:A:445:TYR:N	2.47	0.55
1:B:42:GLY:O	1:B:47:ASP:HA	2.07	0.55
1:A:178:ASN:ND2	1:A:199:ALA:CB	2.71	0.54
1:A:302:VAL:HG23	1:A:317:ALA:HB3	1.88	0.54
1:A:275:ALA:HB1	1:A:353:VAL:HG11	1.89	0.54
1:A:78:GLN:HG3	1:A:79:LEU:HD12	1.88	0.54
1:B:203:VAL:O	1:B:207:MET:HG3	2.07	0.54
1:A:23:LEU:HD13	1:A:23:LEU:C	2.27	0.54
1:A:276:ALA:CA	1:A:426:TRP:NE1	2.70	0.54
1:A:394:THR:HG21	1:A:440:LEU:HD13	1.89	0.54
1:B:23:LEU:C	1:B:23:LEU:HD13	2.28	0.54
1:B:367:TYR:HE2	1:B:429:PHE:CD1	2.24	0.54
1:B:73:VAL:O	1:B:76:VAL:CB	2.54	0.54
1:A:199:ALA:O	1:A:203:VAL:HG23	2.08	0.54
1:A:137:VAL:HG21	1:A:201:ALA:HB2	1.90	0.54
1:A:244:LEU:HG	1:A:385:LYS:CE	2.38	0.54
1:B:93:HIS:HE1	1:B:225:LYS:HB3	1.65	0.54
1:B:275:ALA:HB1	1:B:353:VAL:HG11	1.88	0.54
1:B:366:ILE:C	1:B:430:ILE:HD11	2.27	0.54
1:A:137:VAL:HG13	1:A:201:ALA:HA	1.89	0.54
1:A:209:LEU:O	1:A:213:PHE:HB2	2.08	0.54
1:A:328:THR:O	1:A:332:THR:OG1	2.21	0.54
1:A:86:HIS:CG	1:A:87:LYS:H	2.25	0.54
1:B:176:PRO:O	1:B:180:ILE:HG22	2.07	0.54
1:B:68:LEU:HD12	1:B:248:VAL:HB	1.89	0.54
1:B:367:TYR:N	1:B:430:ILE:HD11	2.23	0.54
1:B:76:VAL:C	1:B:78:GLN:N	2.47	0.54
1:A:155:ASP:O	1:A:157:MET:N	2.40	0.54
1:A:350:ASN:OD1	1:A:352:VAL:HB	2.08	0.54
1:A:72:LEU:HB3	1:A:244:LEU:HD13	1.88	0.54
1:A:382:ARG:HH21	1:A:443:ARG:C	2.11	0.54
1:A:398:TYR:CB	1:A:436:ALA:CB	2.68	0.54
1:B:113:THR:HA	1:B:116:ILE:CG2	2.38	0.54
1:B:191:LEU:HG	1:B:192:GLY:N	2.22	0.54
1:B:78:GLN:HG3	1:B:79:LEU:CD1	2.38	0.54
1:A:104:VAL:HA	1:A:107:ILE:CG1	2.37	0.54
1:A:151:ARG:O	1:A:153:PHE:N	2.41	0.54
1:A:345:LEU:O	1:A:347:TYR:O	2.25	0.54
1:B:266:VAL:CG1	1:B:407:TYR:CE2	2.89	0.54
1:A:116:ILE:O	1:A:117:ILE:C	2.46	0.54
1:A:181:PHE:CD2	1:A:198:VAL:HG11	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:SER:O	1:A:60:PRO:HD2	2.07	0.54
1:B:206:ILE:O	1:B:209:LEU:CB	2.52	0.54
1:B:226:VAL:CG1	1:B:227:PHE:N	2.68	0.54
1:B:237:GLU:O	1:B:241:LEU:N	2.41	0.54
1:B:250:ALA:O	1:B:254:PHE:N	2.40	0.54
1:A:235:PRO:HA	1:A:238:LEU:CG	2.37	0.54
1:A:345:LEU:O	1:A:347:TYR:N	2.41	0.54
1:B:273:VAL:O	1:B:277:HIS:CB	2.56	0.54
1:B:420:LEU:O	1:B:423:LYS:HG2	2.08	0.54
1:A:140:ALA:HB1	1:A:204:TYR:CE2	2.43	0.54
1:A:178:ASN:O	1:A:181:PHE:N	2.40	0.54
1:A:266:VAL:HG13	1:A:269:LEU:HD21	1.90	0.54
1:A:406:GLY:CA	1:A:428:GLY:HA3	2.38	0.54
1:A:410:GLY:HA2	1:A:421:GLY:O	2.08	0.54
1:A:426:TRP:HA	1:A:426:TRP:HE3	1.73	0.54
1:A:455:GLN:HA	1:A:458:LEU:HB2	1.90	0.54
1:A:72:LEU:HD13	1:A:75:VAL:CG2	2.37	0.54
1:B:144:TYR:O	1:B:145:LEU:C	2.46	0.54
1:B:137:VAL:HG13	1:B:201:ALA:HA	1.88	0.54
1:B:220:ARG:HG3	1:B:221:LEU:CD1	2.38	0.54
1:B:11:GLU:OE2	1:B:320:VAL:HB	2.08	0.54
1:B:418:GLN:HE22	1:B:421:GLY:HA2	1.71	0.54
1:B:436:ALA:HA	1:B:439:MET:CG	2.38	0.54
1:B:60:PRO:HA	1:B:63:LEU:HB3	1.90	0.54
1:A:142:PRO:O	1:A:145:LEU:CD1	2.56	0.53
1:A:191:LEU:HG	1:A:192:GLY:H	1.73	0.53
1:A:73:VAL:HG13	1:A:241:LEU:HG	1.90	0.53
1:B:100:LEU:H	1:B:100:LEU:CD1	2.20	0.53
1:B:197:GLY:O	1:B:200:THR:HB	2.08	0.53
1:B:301:ARG:HD3	1:B:301:ARG:O	2.08	0.53
1:B:423:LYS:CG	1:B:424:GLY:N	2.69	0.53
1:B:8:TYR:O	1:B:12:ALA:CB	2.56	0.53
1:A:218:SER:O	1:A:220:ARG:N	2.41	0.53
1:A:320:VAL:O	1:A:321:GLY:C	2.46	0.53
1:A:454:VAL:O	1:A:458:LEU:HD13	2.08	0.53
1:A:80:ASN:C	1:A:82:ALA:N	2.60	0.53
1:B:180:ILE:HG23	1:B:181:PHE:CD1	2.43	0.53
1:B:369:CYS:O	1:B:372:ALA:HB3	2.08	0.53
1:B:392:HIS:O	1:B:395:PHE:HB2	2.08	0.53
1:A:277:HIS:HD2	1:A:278:GLN:OE1	1.91	0.53
1:A:301:ARG:C	1:A:301:ARG:HD3	2.29	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:VAL:HG12	1:A:36:ASP:N	2.23	0.53
1:A:4:SER:HA	1:A:7:ARG:HB2	1.91	0.53
1:B:18:LEU:O	1:B:22:VAL:HG13	2.08	0.53
1:B:191:LEU:O	1:B:195:GLY:N	2.42	0.53
1:B:236:LYS:HG3	1:B:239:ILE:HD12	1.90	0.53
1:B:340:ARG:HB2	1:B:361:LEU:CD1	2.38	0.53
1:B:417:GLU:CD	1:B:418:GLN:H	2.12	0.53
1:B:454:VAL:O	1:B:458:LEU:HD13	2.07	0.53
1:A:107:ILE:O	1:A:110:LEU:HB3	2.07	0.53
1:A:318:ALA:HA	1:A:381:LEU:HD11	1.90	0.53
1:B:148:GLN:HA	1:B:152:SER:HB2	1.89	0.53
1:B:22:VAL:HG23	1:B:293:SER:HB3	1.89	0.53
1:A:136:ALA:HA	1:A:139:PHE:HD2	1.74	0.53
1:A:181:PHE:CG	1:A:198:VAL:HG11	2.43	0.53
1:A:340:ARG:HG3	1:A:341:GLU:H	1.72	0.53
1:A:432:GLY:O	1:A:435:ALA:HB3	2.08	0.53
1:A:72:LEU:CA	1:A:75:VAL:HG13	2.34	0.53
1:B:234:GLN:O	1:B:238:LEU:HD13	2.08	0.53
1:B:382:ARG:NH2	1:B:445:TYR:N	2.49	0.53
1:B:72:LEU:CA	1:B:75:VAL:HG13	2.36	0.53
1:A:123:GLU:HG2	1:A:123:GLU:O	2.07	0.53
1:A:178:ASN:O	1:A:179:TRP:C	2.46	0.53
1:A:279:VAL:HG12	1:A:280:ALA:N	2.23	0.53
1:A:351:GLN:C	1:A:351:GLN:CD	2.67	0.53
1:A:409:LEU:O	1:A:410:GLY:C	2.43	0.53
1:A:68:LEU:O	1:A:71:ALA:HB3	2.09	0.53
1:B:238:LEU:O	1:B:242:PHE:HD1	1.91	0.53
1:B:418:GLN:CD	1:B:421:GLY:HA2	2.29	0.53
1:B:93:HIS:O	1:B:97:ILE:HG13	2.08	0.53
1:A:244:LEU:HG	1:A:385:LYS:HE2	1.91	0.53
1:A:382:ARG:HA	1:A:387:MET:HG2	1.91	0.53
1:A:411:MET:HA	1:A:414:TRP:CD2	2.43	0.53
1:A:367:TYR:HE2	1:A:429:PHE:CE1	2.27	0.53
1:B:94:GLN:OE1	1:B:238:LEU:HD21	2.09	0.53
1:B:238:LEU:O	1:B:242:PHE:N	2.41	0.53
1:A:433:LEU:O	1:A:437:ALA:CB	2.55	0.53
1:A:7:ARG:HH11	1:A:7:ARG:CB	2.21	0.53
1:B:182:VAL:HG22	1:B:195:GLY:CA	2.37	0.53
1:B:200:THR:CA	1:B:203:VAL:HG23	2.38	0.53
1:B:35:VAL:HG12	1:B:36:ASP:N	2.23	0.53
1:A:239:ILE:CA	1:A:242:PHE:HB2	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:VAL:CG1	1:A:407:TYR:CE2	2.90	0.53
1:A:447:LEU:HD12	1:A:448:GLN:N	2.23	0.53
1:A:267:ALA:H	1:A:268:PRO:HD3	1.72	0.52
1:A:436:ALA:O	1:A:439:MET:N	2.43	0.52
1:A:387:MET:CE	1:A:456:LEU:HD13	2.39	0.52
1:B:326:LEU:HD13	1:B:330:CYS:HB2	1.92	0.52
1:B:411:MET:HA	1:B:414:TRP:CD2	2.45	0.52
1:B:413:ASN:HB2	1:B:418:GLN:CG	2.39	0.52
1:B:398:TYR:HD2	1:B:432:GLY:C	2.12	0.52
1:B:433:LEU:O	1:B:437:ALA:CB	2.56	0.52
1:A:18:LEU:O	1:A:21:PRO:HD2	2.09	0.52
1:A:263:ALA:O	1:A:266:VAL:C	2.46	0.52
1:A:287:VAL:HG11	1:A:368:GLN:CD	2.29	0.52
1:A:447:LEU:HD21	1:A:450:GLN:CG	2.39	0.52
1:B:353:VAL:CB	1:B:357:ALA:HB2	2.39	0.52
1:B:72:LEU:HA	1:B:75:VAL:CG1	2.36	0.52
1:A:101:LEU:O	1:A:105:PRO:HG2	2.09	0.52
1:A:120:MET:O	1:A:121:ASP:C	2.47	0.52
1:A:274:VAL:O	1:A:278:GLN:N	2.42	0.52
1:B:113:THR:O	1:B:116:ILE:HG22	2.09	0.52
1:B:45:ALA:HB1	1:B:126:MET:CE	2.39	0.52
1:B:398:TYR:CB	1:B:436:ALA:CB	2.72	0.52
1:B:63:LEU:C	1:B:65:GLY:H	2.12	0.52
1:A:130:THR:C	1:A:132:GLY:N	2.60	0.52
1:A:234:GLN:O	1:A:237:GLU:HB3	2.09	0.52
1:A:320:VAL:O	1:A:322:LEU:N	2.42	0.52
1:A:382:ARG:O	1:A:387:MET:HB2	2.09	0.52
1:B:101:LEU:O	1:B:105:PRO:HG2	2.09	0.52
1:B:155:ASP:O	1:B:157:MET:N	2.42	0.52
1:B:430:ILE:CG2	1:B:431:ILE:N	2.72	0.52
1:A:127:ALA:O	1:A:131:VAL:HG22	2.09	0.52
1:A:68:LEU:HD22	1:A:71:ALA:CB	2.40	0.52
1:B:141:VAL:CG2	1:B:204:TYR:HB3	2.39	0.52
1:B:154:THR:O	1:B:158:SER:CA	2.54	0.52
1:B:165:VAL:HG13	1:B:210:LEU:HG	1.91	0.52
1:B:298:VAL:HA	1:B:301:ARG:HB3	1.91	0.52
1:B:390:ILE:O	1:B:390:ILE:CG2	2.57	0.52
1:A:236:LYS:HG3	1:A:239:ILE:HD12	1.92	0.52
1:A:26:SER:HB2	1:A:289:MET:CG	2.39	0.52
1:A:32:MET:CG	1:A:33:GLY:N	2.72	0.52
1:A:360:LEU:O	1:A:361:LEU:C	2.46	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:VAL:HG13	1:A:377:ALA:N	2.17	0.52
1:A:430:ILE:CG2	1:A:431:ILE:N	2.72	0.52
1:A:394:THR:HG23	1:A:439:MET:CB	2.39	0.52
1:B:152:SER:O	1:B:155:ASP:OD1	2.28	0.52
1:A:145:LEU:HD13	1:A:146:LEU:CA	2.39	0.52
1:A:21:PRO:CB	1:A:160:THR:HG23	2.40	0.52
1:A:238:LEU:O	1:A:242:PHE:N	2.43	0.52
1:A:63:LEU:C	1:A:65:GLY:H	2.12	0.52
1:B:104:VAL:C	1:B:106:ILE:H	2.13	0.52
1:B:11:GLU:HG2	1:B:316:ILE:HG22	1.90	0.52
1:B:248:VAL:HG23	1:B:249:ALA:H	1.75	0.52
1:B:267:ALA:H	1:B:268:PRO:HD3	1.72	0.52
1:B:332:THR:HA	1:B:335:LEU:CG	2.39	0.52
1:B:351:GLN:O	1:B:354:VAL:HG23	2.08	0.52
1:B:379:GLY:HA2	1:B:391:PHE:CE1	2.45	0.52
1:A:123:GLU:C	1:A:124:GLU:O	2.47	0.52
1:A:212:LEU:O	1:A:215:ILE:HG22	2.10	0.52
1:A:420:LEU:HB3	1:A:423:LYS:CD	2.40	0.52
1:A:86:HIS:O	1:A:87:LYS:CB	2.57	0.52
1:B:142:PRO:O	1:B:145:LEU:HD12	2.09	0.52
1:B:312:LYS:HA	1:B:312:LYS:HZ2	1.72	0.52
1:A:113:THR:O	1:A:116:ILE:HG22	2.10	0.52
1:A:145:LEU:HA	1:A:148:GLN:HE21	1.75	0.52
1:A:159:LEU:HD21	1:A:220:ARG:HH11	1.75	0.52
1:A:226:VAL:HG12	1:A:227:PHE:H	1.71	0.52
1:A:394:THR:HG21	1:A:440:LEU:HD22	1.91	0.52
1:A:451:SER:HA	1:A:453:ASP:OD1	2.09	0.52
1:B:161:LYS:N	1:B:162:PRO:CD	2.68	0.52
1:B:11:GLU:HB3	1:B:320:VAL:CB	2.40	0.52
1:B:298:VAL:HG21	1:B:321:GLY:CA	2.40	0.52
1:B:339:PHE:HB3	1:B:343:ILE:HG12	1.91	0.52
1:B:387:MET:CE	1:B:456:LEU:HD13	2.40	0.52
1:B:42:GLY:CA	1:B:49:ALA:HB3	2.40	0.52
1:A:182:VAL:HG22	1:A:195:GLY:CA	2.40	0.52
1:A:69:LEU:HB2	1:A:249:ALA:HB2	1.92	0.52
1:A:340:ARG:HB2	1:A:361:LEU:HD13	1.91	0.52
1:A:367:TYR:HA	1:A:430:ILE:CG1	2.40	0.52
1:A:62:ILE:CG1	1:A:63:LEU:N	2.63	0.52
1:A:72:LEU:HD22	1:A:75:VAL:HG11	1.92	0.52
1:B:191:LEU:HG	1:B:192:GLY:H	1.75	0.52
1:B:431:ILE:O	1:B:435:ALA:HB2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ILE:HB	1:A:210:LEU:CG	2.40	0.51
1:A:181:PHE:O	1:A:190:GLU:HG2	2.09	0.51
1:A:166:ILE:HB	1:A:210:LEU:HG	1.90	0.51
1:A:436:ALA:HA	1:A:439:MET:CG	2.40	0.51
1:B:237:GLU:O	1:B:240:ARG:HB3	2.10	0.51
1:B:367:TYR:HE2	1:B:429:PHE:CE1	2.28	0.51
1:B:385:LYS:N	1:B:387:MET:SD	2.83	0.51
1:B:445:TYR:O	1:B:448:GLN:O	2.27	0.51
1:A:144:TYR:C	1:A:144:TYR:CD1	2.83	0.51
1:A:206:ILE:CG1	1:A:207:MET:N	2.72	0.51
1:A:51:VAL:O	1:A:54:ALA:HB3	2.10	0.51
1:A:127:ALA:O	1:A:128:THR:C	2.48	0.51
1:A:15:LEU:CD1	1:A:16:ILE:N	2.66	0.51
1:A:240:ARG:C	1:A:242:PHE:N	2.63	0.51
1:A:53:ILE:HD12	1:A:54:ALA:N	2.25	0.51
1:B:234:GLN:O	1:B:237:GLU:HB3	2.09	0.51
1:B:250:ALA:O	1:B:254:PHE:CB	2.59	0.51
1:B:314:ALA:O	1:B:318:ALA:N	2.42	0.51
1:B:258:LEU:HD22	1:B:399:TRP:CZ2	2.45	0.51
1:A:316:ILE:O	1:A:318:ALA:N	2.44	0.51
1:A:392:HIS:O	1:A:395:PHE:HB2	2.09	0.51
1:B:290:PHE:CB	1:B:291:PRO:CD	2.88	0.51
1:B:335:LEU:HD12	1:B:335:LEU:C	2.30	0.51
1:B:348:THR:C	1:B:349:GLU:HG3	2.30	0.51
1:B:420:LEU:CB	1:B:423:LYS:HG2	2.34	0.51
1:A:131:VAL:CA	1:A:134:MET:HB2	2.41	0.51
1:A:408:ILE:O	1:A:412:THR:N	2.44	0.51
1:B:212:LEU:O	1:B:215:ILE:HG22	2.10	0.51
1:B:386:ASP:O	1:B:389:ALA:N	2.43	0.51
1:A:222:ALA:O	1:A:223:HIS:C	2.49	0.51
1:A:242:PHE:O	1:A:244:LEU:N	2.42	0.51
1:A:273:VAL:CG1	1:A:274:VAL:H	2.23	0.51
1:A:81:GLY:HA3	1:A:307:GLY:C	2.30	0.51
1:A:353:VAL:CB	1:A:357:ALA:HB2	2.40	0.51
1:B:77:ALA:HB2	1:B:154:THR:CG2	2.41	0.51
1:B:32:MET:CG	1:B:33:GLY:H	2.23	0.51
1:B:96:LEU:CB	1:B:146:LEU:HG	2.40	0.51
1:A:209:LEU:HD12	1:A:210:LEU:HD13	1.92	0.51
1:A:226:VAL:CG1	1:A:227:PHE:N	2.66	0.51
1:A:301:ARG:NH2	1:A:316:ILE:HG22	2.26	0.51
1:A:332:THR:HA	1:A:335:LEU:HD21	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:CG	1:B:309:GLN:HG2	2.41	0.51
1:B:130:THR:C	1:B:132:GLY:N	2.61	0.51
1:B:222:ALA:O	1:B:223:HIS:C	2.49	0.51
1:B:332:THR:HA	1:B:335:LEU:HD21	1.90	0.51
1:B:393:ARG:CG	1:B:393:ARG:HH11	2.23	0.51
1:B:97:ILE:O	1:B:98:LEU:C	2.48	0.51
1:A:146:LEU:O	1:A:146:LEU:HD22	2.10	0.51
1:A:74:PRO:O	1:A:154:THR:OG1	2.29	0.51
1:A:166:ILE:O	1:A:170:GLY:CA	2.58	0.51
1:A:274:VAL:HG12	1:A:275:ALA:N	2.26	0.51
1:A:311:THR:C	1:A:312:LYS:HZ3	2.14	0.51
1:A:353:VAL:HB	1:A:357:ALA:HB2	1.93	0.51
1:A:371:ASP:O	1:A:375:VAL:HG23	2.10	0.51
1:A:433:LEU:HD12	1:A:433:LEU:N	2.26	0.51
1:B:353:VAL:HB	1:B:357:ALA:HB2	1.93	0.51
1:B:3:ASN:C	1:B:5:VAL:H	2.14	0.51
1:A:30:THR:O	1:A:31:GLY:C	2.49	0.51
1:B:98:LEU:HA	1:B:101:LEU:CG	2.41	0.51
1:B:313:GLY:O	1:B:317:ALA:N	2.44	0.51
1:B:363:PHE:CD1	1:B:364:ALA:N	2.79	0.51
1:B:436:ALA:O	1:B:439:MET:HB2	2.10	0.51
1:A:142:PRO:O	1:A:145:LEU:CB	2.55	0.51
1:A:145:LEU:O	1:A:148:GLN:HB3	2.11	0.51
1:A:290:PHE:CB	1:A:291:PRO:CD	2.89	0.51
1:A:348:THR:C	1:A:349:GLU:HG3	2.31	0.51
1:B:146:LEU:O	1:B:149:ALA:N	2.44	0.51
1:A:154:THR:O	1:A:158:SER:CA	2.56	0.50
1:A:176:PRO:O	1:A:180:ILE:HG22	2.09	0.50
1:A:238:LEU:O	1:A:242:PHE:HD1	1.93	0.50
1:A:244:LEU:CD2	1:A:385:LYS:O	2.49	0.50
1:A:73:VAL:O	1:A:76:VAL:CG1	2.59	0.50
1:A:76:VAL:HG23	1:A:78:GLN:HE21	1.76	0.50
1:B:142:PRO:CA	1:B:145:LEU:HB3	2.39	0.50
1:B:14:ASN:H	1:B:14:ASN:HD22	1.57	0.50
1:A:255:GLU:HG2	1:A:256:VAL:N	2.27	0.50
1:A:410:GLY:HA3	1:A:425:PHE:CB	2.41	0.50
1:A:73:VAL:O	1:A:76:VAL:HG12	2.11	0.50
1:B:386:ASP:O	1:B:389:ALA:HB3	2.12	0.50
1:B:88:ILE:CG1	1:B:89:PRO:CD	2.88	0.50
1:A:162:PRO:HA	1:A:165:VAL:HB	1.92	0.50
1:A:339:PHE:HB3	1:A:343:ILE:HG13	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LYS:HD3	1:A:386:ASP:N	2.26	0.50
1:A:398:TYR:HD2	1:A:432:GLY:C	2.15	0.50
1:B:127:ALA:O	1:B:128:THR:C	2.50	0.50
1:B:69:LEU:HG	1:B:245:GLY:CA	2.40	0.50
1:B:282:ASN:O	1:B:285:SER:HB3	2.11	0.50
1:B:398:TYR:HE2	1:B:433:LEU:HG	1.77	0.50
1:B:76:VAL:CA	1:B:78:GLN:HE21	2.11	0.50
1:A:28:ALA:O	1:A:29:GLN:C	2.50	0.50
1:A:387:MET:O	1:A:391:PHE:HB3	2.12	0.50
1:A:395:PHE:O	1:A:398:TYR:CE1	2.64	0.50
1:B:102:VAL:O	1:B:105:PRO:HD2	2.11	0.50
1:B:261:VAL:HG12	1:B:262:VAL:N	2.27	0.50
1:B:343:ILE:O	1:B:346:LEU:N	2.45	0.50
1:B:367:TYR:HA	1:B:430:ILE:CG1	2.41	0.50
1:B:369:CYS:SG	1:B:370:MET:HE1	2.52	0.50
1:B:299:SER:HA	1:B:380:SER:OG	2.12	0.50
1:B:394:THR:HG23	1:B:439:MET:CB	2.42	0.50
1:A:445:TYR:HB3	1:A:448:GLN:HA	1.88	0.50
1:B:100:LEU:HD12	1:B:100:LEU:H	1.74	0.50
1:B:18:LEU:HD13	1:B:300:ILE:HD11	1.92	0.50
1:B:345:LEU:O	1:B:347:TYR:O	2.30	0.50
1:A:232:LYS:N	1:A:235:PRO:HD2	2.26	0.50
1:A:233:PRO:N	1:A:235:PRO:HD2	2.27	0.50
1:A:445:TYR:CB	1:A:448:GLN:CA	2.76	0.50
1:A:76:VAL:HA	1:A:78:GLN:NE2	2.14	0.50
1:A:89:PRO:O	1:A:93:HIS:CE1	2.64	0.50
1:B:97:ILE:O	1:B:101:LEU:HG	2.12	0.50
1:B:104:VAL:C	1:B:106:ILE:N	2.65	0.50
1:B:185:LYS:HD3	1:B:186:PHE:N	2.26	0.50
1:B:239:ILE:CA	1:B:242:PHE:HB2	2.41	0.50
1:B:420:LEU:HB3	1:B:423:LYS:CD	2.41	0.50
1:B:443:ARG:O	1:B:444:LEU:C	2.50	0.50
1:A:151:ARG:CA	1:A:155:ASP:HA	2.31	0.50
1:A:208:LEU:CD2	1:A:209:LEU:N	2.66	0.50
1:A:344:ALA:O	1:A:345:LEU:C	2.49	0.50
1:A:58:TRP:HE3	1:A:59:LEU:HD12	1.76	0.50
1:B:110:LEU:HD13	1:B:114:GLN:HG3	1.94	0.50
1:B:283:PHE:O	1:B:284:SER:C	2.49	0.50
1:B:403:LEU:HB2	1:B:404:PRO:HD3	1.94	0.50
1:B:406:GLY:O	1:B:409:LEU:CB	2.53	0.50
1:B:81:GLY:HA3	1:B:307:GLY:C	2.33	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:MET:O	1:A:121:ASP:O	2.30	0.50
1:A:287:VAL:O	1:A:291:PRO:CD	2.60	0.50
1:A:382:ARG:HE	1:A:443:ARG:HB3	1.77	0.50
1:A:393:ARG:CG	1:A:393:ARG:HH11	2.23	0.50
1:A:413:ASN:HD22	1:A:421:GLY:H	1.59	0.50
1:B:100:LEU:CD1	1:B:100:LEU:N	2.75	0.50
1:B:178:ASN:ND2	1:B:199:ALA:HB2	2.27	0.50
1:B:137:VAL:HG11	1:B:201:ALA:N	2.27	0.50
1:B:20:THR:O	1:B:21:PRO:O	2.29	0.50
1:B:351:GLN:CD	1:B:351:GLN:C	2.70	0.50
1:B:33:GLY:O	1:B:37:THR:CB	2.60	0.50
1:B:406:GLY:CA	1:B:428:GLY:HA3	2.42	0.50
1:B:63:LEU:HG	1:B:64:PHE:N	2.27	0.50
1:A:409:LEU:HD12	1:A:424:GLY:C	2.31	0.50
1:B:173:LEU:O	1:B:176:PRO:CD	2.58	0.50
1:B:178:ASN:HD21	1:B:199:ALA:CB	2.25	0.50
1:B:207:MET:HA	1:B:210:LEU:CD2	2.42	0.50
1:B:215:ILE:CG2	1:B:216:VAL:H	2.23	0.50
1:B:22:VAL:O	1:B:25:ALA:HB3	2.12	0.50
1:B:398:TYR:HD2	1:B:432:GLY:O	1.94	0.50
1:A:386:ASP:O	1:A:389:ALA:HB3	2.12	0.49
1:B:120:MET:O	1:B:121:ASP:C	2.51	0.49
1:B:140:ALA:HB1	1:B:204:TYR:CE2	2.47	0.49
1:B:226:VAL:HG12	1:B:227:PHE:H	1.76	0.49
1:B:72:LEU:HB3	1:B:244:LEU:CD1	2.41	0.49
1:B:354:VAL:O	1:B:358:MET:N	2.40	0.49
1:A:313:GLY:O	1:A:317:ALA:N	2.45	0.49
1:A:244:LEU:HD23	1:A:388:THR:OG1	2.11	0.49
1:A:44:SER:C	1:A:46:ILE:N	2.66	0.49
1:A:447:LEU:HD11	1:A:450:GLN:HG2	1.93	0.49
1:A:60:PRO:O	1:A:63:LEU:HD23	2.13	0.49
1:B:145:LEU:CD1	1:B:146:LEU:N	2.64	0.49
1:B:217:THR:O	1:B:218:SER:C	2.48	0.49
1:B:276:ALA:CA	1:B:426:TRP:NE1	2.75	0.49
1:B:44:SER:C	1:B:46:ILE:N	2.61	0.49
1:A:72:LEU:HD12	1:A:244:LEU:CD2	2.37	0.49
1:A:84:ARG:C	1:A:86:HIS:N	2.64	0.49
1:A:5:VAL:HA	1:A:8:TYR:OH	2.12	0.49
1:B:21:PRO:HA	1:B:164:MET:CE	2.43	0.49
1:B:240:ARG:C	1:B:242:PHE:N	2.64	0.49
1:B:248:VAL:HG23	1:B:249:ALA:N	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:VAL:HG12	1:B:280:ALA:N	2.26	0.49
1:B:314:ALA:O	1:B:316:ILE:N	2.45	0.49
1:B:70:MET:HE2	1:B:99:ALA:HB2	1.95	0.49
1:A:314:ALA:O	1:A:318:ALA:N	2.44	0.49
1:A:354:VAL:O	1:A:358:MET:HB2	2.12	0.49
1:A:455:GLN:NE2	1:A:455:GLN:C	2.66	0.49
1:B:77:ALA:HB2	1:B:154:THR:HG23	1.90	0.49
1:B:175:ILE:HG22	1:B:176:PRO:N	2.27	0.49
1:B:126:MET:CE	1:B:191:LEU:HD21	2.42	0.49
1:B:328:THR:O	1:B:332:THR:OG1	2.22	0.49
1:B:3:ASN:O	1:B:4:SER:OG	2.21	0.49
1:B:72:LEU:HD12	1:B:244:LEU:CD2	2.36	0.49
1:B:7:ARG:HB3	1:B:7:ARG:HH11	1.77	0.49
1:A:206:ILE:HG13	1:A:207:MET:N	2.27	0.49
1:A:78:GLN:HG3	1:A:79:LEU:CD1	2.41	0.49
1:B:162:PRO:O	1:B:165:VAL:CG1	2.33	0.49
1:A:77:ALA:HB2	1:A:154:THR:CG2	2.43	0.49
1:A:279:VAL:HG13	1:A:361:LEU:HD23	1.94	0.49
1:A:244:LEU:CG	1:A:385:LYS:NZ	2.76	0.49
1:A:422:ALA:O	1:A:423:LYS:C	2.51	0.49
1:A:455:GLN:HE21	1:A:455:GLN:C	2.16	0.49
1:B:144:TYR:O	1:B:147:PHE:HB3	2.13	0.49
1:B:166:ILE:O	1:B:170:GLY:CA	2.61	0.49
1:B:279:VAL:HG13	1:B:361:LEU:HD23	1.94	0.49
1:A:102:VAL:CA	1:A:105:PRO:HD2	2.43	0.49
1:A:142:PRO:C	1:A:145:LEU:HB3	2.32	0.49
1:A:161:LYS:O	1:A:163:ALA:N	2.45	0.49
1:A:339:PHE:C	1:A:341:GLU:OE1	2.51	0.49
1:B:155:ASP:CB	1:B:159:LEU:N	2.71	0.49
1:B:176:PRO:HG2	1:B:177:LEU:HD22	1.95	0.49
1:B:274:VAL:O	1:B:278:GLN:N	2.45	0.49
1:A:45:ALA:HB1	1:A:126:MET:CE	2.42	0.49
1:A:145:LEU:HD13	1:A:146:LEU:H	1.70	0.49
1:A:339:PHE:O	1:A:340:ARG:O	2.30	0.49
1:B:28:ALA:O	1:B:29:GLN:C	2.50	0.49
1:A:106:ILE:HG22	1:A:139:PHE:CE1	2.48	0.49
1:A:338:LEU:O	1:A:340:ARG:HG2	2.12	0.49
1:B:271:SER:O	1:B:273:VAL:HG12	2.13	0.49
1:B:244:LEU:HG	1:B:385:LYS:CE	2.42	0.49
1:B:407:TYR:CD2	1:B:411:MET:HG3	2.47	0.49
1:A:124:GLU:C	1:A:124:GLU:OE1	2.50	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:O	1:A:22:VAL:HG13	2.13	0.49
1:A:257:THR:O	1:A:260:ALA:HB3	2.12	0.49
1:A:339:PHE:O	1:A:340:ARG:C	2.52	0.49
1:A:92:VAL:O	1:A:95:GLY:N	2.45	0.49
1:B:123:GLU:O	1:B:123:GLU:HG2	2.13	0.49
1:B:178:ASN:O	1:B:179:TRP:C	2.50	0.49
1:B:236:LYS:HA	1:B:239:ILE:HG13	1.94	0.49
1:B:292:MET:HA	1:B:375:VAL:HG11	1.95	0.49
1:A:118:ARG:HD2	1:A:118:ARG:O	2.12	0.48
1:A:407:TYR:C	1:A:409:LEU:N	2.66	0.48
1:A:420:LEU:HD12	1:A:423:LYS:HG2	1.95	0.48
1:A:427:LEU:O	1:A:430:ILE:N	2.46	0.48
1:A:76:VAL:CA	1:A:78:GLN:HE21	2.17	0.48
1:B:116:ILE:O	1:B:117:ILE:C	2.49	0.48
1:B:146:LEU:O	1:B:147:PHE:C	2.50	0.48
1:B:290:PHE:O	1:B:293:SER:HB2	2.13	0.48
1:B:248:VAL:HG12	1:B:391:PHE:HZ	1.77	0.48
1:B:76:VAL:HA	1:B:78:GLN:HG2	1.95	0.48
1:A:144:TYR:O	1:A:145:LEU:C	2.50	0.48
1:A:161:LYS:N	1:A:162:PRO:CD	2.67	0.48
1:A:345:LEU:HA	1:A:345:LEU:HD23	1.57	0.48
1:B:106:ILE:HG22	1:B:139:PHE:CE1	2.46	0.48
1:B:205:TRP:CE3	1:B:206:ILE:HG22	2.48	0.48
1:B:317:ALA:CA	1:B:320:VAL:HG12	2.42	0.48
1:B:387:MET:HE2	1:B:446:TRP:CH2	2.47	0.48
1:B:446:TRP:CH2	1:B:456:LEU:HD11	2.48	0.48
1:B:68:LEU:O	1:B:71:ALA:HB3	2.13	0.48
1:A:162:PRO:O	1:A:165:VAL:CG1	2.37	0.48
1:A:257:THR:O	1:A:261:VAL:HG23	2.12	0.48
1:A:272:THR:O	1:A:274:VAL:C	2.50	0.48
1:A:299:SER:HB2	1:A:380:SER:HA	1.94	0.48
1:A:376:VAL:O	1:A:380:SER:HB3	2.13	0.48
1:A:381:LEU:O	1:A:384:TYR:CD2	2.66	0.48
1:A:46:ILE:O	1:A:48:MET:HE2	2.13	0.48
1:B:314:ALA:C	1:B:318:ALA:HB3	2.33	0.48
1:B:353:VAL:C	1:B:357:ALA:CB	2.82	0.48
1:B:266:VAL:HG22	1:B:407:TYR:CZ	2.47	0.48
1:B:409:LEU:HD12	1:B:424:GLY:C	2.32	0.48
1:A:137:VAL:HG11	1:A:201:ALA:N	2.28	0.48
1:A:331:ILE:HG13	1:A:335:LEU:HD23	1.95	0.48
1:A:387:MET:HB3	1:A:443:ARG:HE	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:THR:HG21	1:A:440:LEU:CD1	2.43	0.48
1:B:316:ILE:O	1:B:318:ALA:N	2.46	0.48
1:B:369:CYS:SG	1:B:370:MET:CE	3.02	0.48
1:B:89:PRO:O	1:B:93:HIS:CE1	2.67	0.48
1:A:258:LEU:HA	1:A:261:VAL:CG2	2.43	0.48
1:A:370:MET:HA	1:A:373:VAL:HG12	1.96	0.48
1:B:139:PHE:C	1:B:142:PRO:HD2	2.33	0.48
1:B:161:LYS:O	1:B:163:ALA:N	2.46	0.48
1:B:215:ILE:CG2	1:B:216:VAL:N	2.76	0.48
1:A:146:LEU:O	1:A:147:PHE:C	2.51	0.48
1:A:163:ALA:HB3	1:A:164:MET:SD	2.54	0.48
1:A:271:SER:O	1:A:273:VAL:HG12	2.13	0.48
1:A:410:GLY:CA	1:A:425:PHE:CB	2.92	0.48
1:B:100:LEU:O	1:B:102:VAL:N	2.47	0.48
1:B:144:TYR:CD1	1:B:144:TYR:C	2.85	0.48
1:B:208:LEU:HD23	1:B:209:LEU:CA	2.44	0.48
1:B:344:ALA:O	1:B:345:LEU:C	2.50	0.48
1:B:426:TRP:HE3	1:B:426:TRP:HA	1.77	0.48
1:A:22:VAL:HG23	1:A:293:SER:HB3	1.95	0.48
1:A:276:ALA:O	1:A:277:HIS:C	2.51	0.48
1:A:287:VAL:O	1:A:291:PRO:HD2	2.13	0.48
1:A:314:ALA:HB2	1:A:449:LYS:HZ1	1.78	0.48
1:A:244:LEU:CB	1:A:385:LYS:HZ3	2.22	0.48
1:A:385:LYS:N	1:A:387:MET:SD	2.83	0.48
1:A:70:MET:HE1	1:A:99:ALA:HB2	1.95	0.48
1:B:218:SER:C	1:B:220:ARG:H	2.16	0.48
1:B:244:LEU:HG	1:B:385:LYS:HE2	1.96	0.48
1:B:96:LEU:HD23	1:B:96:LEU:C	2.34	0.48
1:A:192:GLY:O	1:A:195:GLY:N	2.47	0.48
1:A:284:SER:O	1:A:285:SER:C	2.52	0.48
1:A:314:ALA:O	1:A:316:ILE:N	2.46	0.48
1:A:326:LEU:O	1:A:330:CYS:HB3	2.11	0.48
1:A:345:LEU:O	1:A:346:LEU:C	2.51	0.48
1:A:360:LEU:CD2	1:A:423:LYS:CB	2.92	0.48
1:A:391:PHE:O	1:A:394:THR:HB	2.13	0.48
1:B:134:MET:SD	1:B:198:VAL:N	2.87	0.48
1:B:283:PHE:CE1	1:B:287:VAL:HG21	2.49	0.48
1:B:92:VAL:O	1:B:95:GLY:N	2.46	0.48
1:A:144:TYR:O	1:A:147:PHE:HB3	2.14	0.48
1:A:21:PRO:HA	1:A:164:MET:CE	2.44	0.48
1:A:273:VAL:O	1:A:277:HIS:CB	2.62	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ILE:CG2	1:B:117:ILE:N	2.76	0.48
1:B:12:ALA:O	1:B:13:SER:C	2.52	0.48
1:B:18:LEU:O	1:B:21:PRO:HD2	2.14	0.48
1:B:410:GLY:O	1:B:413:ASN:HB3	2.14	0.48
1:B:69:LEU:O	1:B:69:LEU:HD23	2.14	0.48
1:B:165:VAL:C	1:B:167:GLY:N	2.67	0.48
1:B:354:VAL:O	1:B:358:MET:HB2	2.13	0.48
1:B:408:ILE:O	1:B:408:ILE:CG2	2.61	0.48
1:B:81:GLY:O	1:B:82:ALA:CB	2.62	0.48
1:A:145:LEU:CD1	1:A:146:LEU:N	2.64	0.47
1:A:165:VAL:C	1:A:167:GLY:H	2.17	0.47
1:A:215:ILE:CG2	1:A:216:VAL:N	2.75	0.47
1:A:223:HIS:ND1	1:A:223:HIS:N	2.62	0.47
1:A:403:LEU:O	1:A:404:PRO:C	2.48	0.47
1:A:408:ILE:O	1:A:408:ILE:CG2	2.62	0.47
1:B:165:VAL:C	1:B:167:GLY:H	2.17	0.47
1:B:275:ALA:HB2	1:B:353:VAL:CG1	2.43	0.47
1:B:71:ALA:HA	1:B:74:PRO:HD2	1.94	0.47
1:A:141:VAL:HG22	1:A:204:TYR:CB	2.43	0.47
1:A:178:ASN:OD1	1:A:199:ALA:HB2	2.14	0.47
1:A:224:VAL:HB	1:A:225:LYS:H	1.43	0.47
1:A:374:GLN:HB2	1:A:437:ALA:HB2	1.96	0.47
1:A:418:GLN:CD	1:A:421:GLY:HA2	2.32	0.47
1:B:196:CYS:SG	1:B:197:GLY:N	2.87	0.47
1:B:409:LEU:O	1:B:410:GLY:C	2.49	0.47
1:B:94:GLN:O	1:B:97:ILE:HB	2.13	0.47
1:A:172:LEU:O	1:A:176:PRO:HD2	2.14	0.47
1:A:180:ILE:HG23	1:A:181:PHE:HD1	1.78	0.47
1:A:255:GLU:CG	1:A:256:VAL:N	2.76	0.47
1:A:328:THR:HA	1:A:331:ILE:HG23	1.96	0.47
1:A:60:PRO:O	1:A:61:SER:C	2.52	0.47
1:B:126:MET:HE3	1:B:191:LEU:HD21	1.97	0.47
1:B:61:SER:O	1:B:253:PHE:CE1	2.67	0.47
1:B:266:VAL:HG22	1:B:407:TYR:CD1	2.49	0.47
1:B:346:LEU:HB3	1:B:347:TYR:H	1.50	0.47
1:B:394:THR:HG21	1:B:440:LEU:HD22	1.96	0.47
1:B:451:SER:HA	1:B:453:ASP:OD1	2.14	0.47
1:B:77:ALA:CB	1:B:154:THR:CG2	2.90	0.47
1:A:178:ASN:ND2	1:A:199:ALA:HB2	2.29	0.47
1:A:335:LEU:HD12	1:A:335:LEU:C	2.34	0.47
1:A:403:LEU:HB2	1:A:404:PRO:HD3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:C	1:B:102:VAL:N	2.66	0.47
1:B:146:LEU:HD22	1:B:149:ALA:CB	2.45	0.47
1:B:273:VAL:CG1	1:B:274:VAL:H	2.24	0.47
1:B:287:VAL:O	1:B:291:PRO:CD	2.63	0.47
1:B:301:ARG:NH2	1:B:316:ILE:CG2	2.76	0.47
1:A:104:VAL:C	1:A:106:ILE:H	2.18	0.47
1:A:244:LEU:HG	1:A:385:LYS:HZ1	1.76	0.47
1:A:344:ALA:HB1	1:A:354:VAL:HG22	1.97	0.47
1:B:10:LYS:HA	1:B:13:SER:OG	2.14	0.47
1:B:332:THR:CA	1:B:335:LEU:HG	2.43	0.47
1:B:405:THR:HG22	1:B:406:GLY:N	2.30	0.47
1:B:394:THR:HG21	1:B:440:LEU:HD13	1.96	0.47
1:B:206:ILE:HG13	1:B:207:MET:N	2.30	0.47
1:B:345:LEU:O	1:B:346:LEU:C	2.53	0.47
1:B:314:ALA:HB1	1:B:445:TYR:CZ	2.49	0.47
1:B:445:TYR:O	1:B:446:TRP:C	2.53	0.47
1:A:178:ASN:HD21	1:A:199:ALA:CB	2.28	0.47
1:A:215:ILE:CG2	1:A:216:VAL:H	2.24	0.47
1:A:96:LEU:C	1:A:96:LEU:HD23	2.34	0.47
1:B:210:LEU:HD13	1:B:210:LEU:N	2.30	0.47
1:B:331:ILE:HG13	1:B:335:LEU:HD23	1.97	0.47
1:B:332:THR:C	1:B:335:LEU:HG	2.34	0.47
1:B:382:ARG:HH21	1:B:443:ARG:C	2.17	0.47
1:B:403:LEU:O	1:B:407:TYR:N	2.30	0.47
1:B:435:ALA:O	1:B:439:MET:HG2	2.15	0.47
1:B:53:ILE:HA	1:B:56:SER:HB3	1.97	0.47
1:B:68:LEU:HD22	1:B:71:ALA:HB3	1.96	0.47
1:B:69:LEU:O	1:B:73:VAL:HG23	2.14	0.47
1:A:74:PRO:HB3	1:A:149:ALA:CA	2.45	0.47
1:A:266:VAL:HG22	1:A:407:TYR:CZ	2.49	0.47
1:A:382:ARG:HB3	1:A:387:MET:HB2	1.96	0.47
1:A:72:LEU:HB3	1:A:244:LEU:CD1	2.45	0.47
1:B:161:LYS:C	1:B:163:ALA:H	2.17	0.47
1:B:18:LEU:HA	1:B:160:THR:CG2	2.45	0.47
1:B:206:ILE:CG1	1:B:207:MET:N	2.77	0.47
1:B:299:SER:CA	1:B:380:SER:OG	2.63	0.47
1:B:413:ASN:C	1:B:415:LEU:H	2.18	0.47
1:B:42:GLY:N	1:B:49:ALA:CB	2.78	0.47
1:B:86:HIS:O	1:B:87:LYS:CB	2.62	0.47
1:A:149:ALA:O	1:A:154:THR:CB	2.62	0.47
1:A:150:LEU:O	1:A:154:THR:CB	2.60	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:THR:OG1	1:A:312:LYS:N	2.47	0.47
1:A:436:ALA:O	1:A:439:MET:HB2	2.14	0.47
1:A:78:GLN:C	1:A:80:ASN:H	2.18	0.47
1:B:143:ALA:O	1:B:146:LEU:HB3	2.15	0.47
1:B:235:PRO:HA	1:B:238:LEU:CD2	2.45	0.47
1:B:376:VAL:CG1	1:B:377:ALA:H	2.10	0.47
1:B:71:ALA:N	1:B:74:PRO:HD2	2.30	0.47
1:A:181:PHE:C	1:A:183:TYR:N	2.66	0.47
1:A:191:LEU:H	1:A:194:VAL:HB	1.79	0.47
1:A:206:ILE:O	1:A:209:LEU:CB	2.55	0.47
1:A:275:ALA:HB2	1:A:353:VAL:CG2	2.45	0.47
1:A:10:LYS:NZ	1:A:305:LYS:NZ	2.62	0.47
1:A:244:LEU:CD2	1:A:388:THR:OG1	2.63	0.47
1:A:399:TRP:NE1	1:A:403:LEU:HD12	2.30	0.47
1:A:65:GLY:C	1:A:67:GLY:N	2.67	0.47
1:B:120:MET:O	1:B:121:ASP:O	2.32	0.47
1:B:42:GLY:N	1:B:49:ALA:HB3	2.30	0.47
1:A:210:LEU:N	1:A:210:LEU:HD13	2.30	0.47
1:A:211:LEU:O	1:A:212:LEU:C	2.52	0.47
1:A:218:SER:C	1:A:220:ARG:H	2.19	0.47
1:A:235:PRO:HA	1:A:238:LEU:CD2	2.45	0.47
1:A:316:ILE:O	1:A:317:ALA:C	2.53	0.47
1:A:42:GLY:O	1:A:47:ASP:HA	2.14	0.47
1:A:61:SER:O	1:A:253:PHE:CE1	2.68	0.47
1:B:412:THR:HG23	1:B:416:THR:HB	1.96	0.47
1:A:153:PHE:O	1:A:155:ASP:OD1	2.32	0.46
1:A:3:ASN:C	1:A:5:VAL:H	2.18	0.46
1:B:102:VAL:CA	1:B:105:PRO:HD2	2.45	0.46
1:B:104:VAL:O	1:B:106:ILE:N	2.48	0.46
1:B:178:ASN:HD21	1:B:199:ALA:HB1	1.80	0.46
1:B:300:ILE:CG1	1:B:301:ARG:N	2.77	0.46
1:B:387:MET:O	1:B:391:PHE:HB3	2.15	0.46
1:B:433:LEU:HD12	1:B:433:LEU:N	2.30	0.46
1:A:155:ASP:CG	1:A:159:LEU:H	2.17	0.46
1:A:173:LEU:O	1:A:177:LEU:CD2	2.57	0.46
1:A:382:ARG:C	1:A:384:TYR:N	2.67	0.46
1:A:5:VAL:O	1:A:9:LYS:HB2	2.15	0.46
1:B:219:LYS:HD3	1:B:220:ARG:NE	2.30	0.46
1:B:339:PHE:O	1:B:343:ILE:HB	2.15	0.46
1:B:348:THR:O	1:B:349:GLU:HG3	2.15	0.46
1:B:355:ALA:O	1:B:358:MET:HB3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:VAL:C	1:A:106:ILE:N	2.68	0.46
1:A:11:GLU:HA	1:A:301:ARG:NH2	2.11	0.46
1:A:233:PRO:HA	1:A:236:LYS:HB2	1.96	0.46
1:A:340:ARG:HB2	1:A:361:LEU:CD1	2.44	0.46
1:B:173:LEU:O	1:B:174:ASN:C	2.53	0.46
1:B:191:LEU:CG	1:B:192:GLY:H	2.29	0.46
1:B:16:ILE:CA	1:B:19:ALA:HB3	2.35	0.46
1:B:232:LYS:CB	1:B:233:PRO:HD3	2.30	0.46
1:B:268:PRO:C	1:B:270:GLY:H	2.19	0.46
1:B:360:LEU:O	1:B:361:LEU:C	2.53	0.46
1:A:100:LEU:CD1	1:A:100:LEU:H	2.28	0.46
1:A:206:ILE:O	1:A:210:LEU:CD2	2.55	0.46
1:A:230:PHE:CG	1:A:231:HIS:N	2.81	0.46
1:A:381:LEU:O	1:A:384:TYR:CG	2.68	0.46
1:A:59:LEU:HB2	1:A:60:PRO:CD	2.40	0.46
1:A:75:VAL:C	1:A:77:ALA:N	2.53	0.46
1:B:118:ARG:O	1:B:118:ARG:HD2	2.15	0.46
1:B:178:ASN:OD1	1:B:199:ALA:HB2	2.14	0.46
1:B:30:THR:O	1:B:31:GLY:C	2.53	0.46
1:B:413:ASN:C	1:B:415:LEU:N	2.68	0.46
1:A:232:LYS:N	1:A:233:PRO:CD	2.70	0.46
1:A:298:VAL:HA	1:A:301:ARG:HB3	1.97	0.46
1:B:166:ILE:HB	1:B:210:LEU:HG	1.96	0.46
1:B:311:THR:OG1	1:B:312:LYS:N	2.47	0.46
1:B:316:ILE:O	1:B:317:ALA:C	2.54	0.46
1:B:455:GLN:HE21	1:B:455:GLN:C	2.18	0.46
1:A:100:LEU:C	1:A:102:VAL:H	2.18	0.46
1:A:139:PHE:O	1:A:142:PRO:HD2	2.16	0.46
1:A:237:GLU:O	1:A:241:LEU:N	2.48	0.46
1:A:410:GLY:O	1:A:413:ASN:HB3	2.16	0.46
1:B:131:VAL:O	1:B:134:MET:HB2	2.16	0.46
1:B:14:ASN:H	1:B:14:ASN:ND2	2.14	0.46
1:B:21:PRO:HA	1:B:164:MET:HE1	1.97	0.46
1:B:19:ALA:O	1:B:22:VAL:HG22	2.15	0.46
1:B:274:VAL:HG13	1:B:278:GLN:NE2	2.31	0.46
1:B:318:ALA:HA	1:B:381:LEU:CD1	2.45	0.46
1:B:328:THR:CA	1:B:331:ILE:CG2	2.94	0.46
1:B:409:LEU:HD13	1:B:409:LEU:C	2.36	0.46
1:B:443:ARG:NH2	1:B:446:TRP:HE1	2.13	0.46
1:A:231:HIS:C	1:A:235:PRO:CG	2.77	0.46
1:A:232:LYS:CB	1:A:233:PRO:HD3	2.32	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:HA	1:A:241:LEU:CB	2.37	0.46
1:A:260:ALA:O	1:A:261:VAL:C	2.54	0.46
1:A:290:PHE:HB3	1:A:291:PRO:CD	2.46	0.46
1:A:317:ALA:CA	1:A:320:VAL:HG12	2.46	0.46
1:A:445:TYR:HD2	1:A:448:GLN:CG	2.29	0.46
1:B:388:THR:O	1:B:391:PHE:CD2	2.69	0.46
1:A:131:VAL:HB	1:A:135:HIS:HE2	1.80	0.46
1:A:173:LEU:O	1:A:174:ASN:C	2.52	0.46
1:A:238:LEU:HA	1:A:241:LEU:CD1	2.45	0.46
1:A:301:ARG:C	1:A:301:ARG:CD	2.84	0.46
1:A:300:ILE:CG1	1:A:301:ARG:N	2.75	0.46
1:A:431:ILE:O	1:A:435:ALA:CB	2.63	0.46
1:A:63:LEU:HG	1:A:64:PHE:N	2.28	0.46
1:B:116:ILE:HG23	1:B:117:ILE:N	2.31	0.46
1:B:166:ILE:HB	1:B:210:LEU:CG	2.46	0.46
1:B:238:LEU:CA	1:B:241:LEU:HD13	2.46	0.46
1:B:88:ILE:HG13	1:B:89:PRO:N	2.30	0.46
1:A:299:SER:N	1:A:380:SER:OG	2.49	0.46
1:A:335:LEU:HD12	1:A:336:THR:N	2.31	0.46
1:B:178:ASN:ND2	1:B:199:ALA:HB1	2.31	0.46
1:B:213:PHE:O	1:B:217:THR:CG2	2.63	0.46
1:B:232:LYS:N	1:B:235:PRO:HD2	2.31	0.46
1:B:32:MET:HG3	1:B:33:GLY:H	1.74	0.46
1:B:65:GLY:CA	1:B:253:PHE:CG	2.99	0.46
1:B:76:VAL:C	1:B:78:GLN:HG2	2.36	0.46
1:A:135:HIS:C	1:A:137:VAL:N	2.67	0.46
1:A:135:HIS:O	1:A:138:ILE:HG22	2.16	0.46
1:A:205:TRP:CE3	1:A:206:ILE:HG22	2.50	0.46
1:A:299:SER:CA	1:A:380:SER:OG	2.64	0.46
1:A:81:GLY:O	1:A:82:ALA:CB	2.63	0.46
1:B:191:LEU:H	1:B:194:VAL:HB	1.81	0.46
1:B:19:ALA:O	1:B:20:THR:C	2.55	0.46
1:B:329:ALA:O	1:B:333:ALA:CB	2.64	0.46
1:B:76:VAL:CA	1:B:78:GLN:HG2	2.46	0.46
1:B:7:ARG:CB	1:B:7:ARG:HH11	2.29	0.46
1:A:86:HIS:NE2	1:B:83:GLY:HA2	2.31	0.46
1:A:180:ILE:HG23	1:A:181:PHE:CD1	2.51	0.45
1:A:94:GLN:OE1	1:A:238:LEU:HD21	2.16	0.45
1:A:339:PHE:O	1:A:343:ILE:HB	2.16	0.45
1:A:353:VAL:C	1:A:357:ALA:HB2	2.36	0.45
1:A:369:CYS:O	1:A:372:ALA:HB3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ASP:OD1	1:A:387:MET:N	2.50	0.45
1:A:69:LEU:HG	1:A:245:GLY:CA	2.46	0.45
1:B:145:LEU:O	1:B:148:GLN:HB3	2.15	0.45
1:B:238:LEU:HA	1:B:241:LEU:CB	2.35	0.45
1:B:381:LEU:O	1:B:384:TYR:CD2	2.69	0.45
1:B:247:PRO:HG2	1:B:389:ALA:HA	1.98	0.45
1:B:3:ASN:O	1:B:5:VAL:HG23	2.15	0.45
1:A:20:THR:O	1:A:21:PRO:C	2.51	0.45
1:A:18:LEU:HD13	1:A:300:ILE:HD11	1.98	0.45
1:A:328:THR:O	1:A:332:THR:CG2	2.64	0.45
1:A:358:MET:O	1:A:361:LEU:HB2	2.17	0.45
1:A:407:TYR:O	1:A:410:GLY:N	2.49	0.45
1:A:447:LEU:HD12	1:A:448:GLN:C	2.36	0.45
1:A:46:ILE:C	1:A:48:MET:N	2.51	0.45
1:A:87:LYS:HZ1	1:B:308:GLU:C	2.19	0.45
1:B:262:VAL:HG12	1:B:263:ALA:N	2.29	0.45
1:B:399:TRP:NE1	1:B:403:LEU:HD12	2.30	0.45
1:A:124:GLU:HB2	1:A:125:ALA:H	1.59	0.45
1:A:244:LEU:CB	1:A:385:LYS:NZ	2.76	0.45
1:A:409:LEU:O	1:A:410:GLY:O	2.34	0.45
1:A:69:LEU:C	1:A:71:ALA:H	2.20	0.45
1:A:73:VAL:N	1:A:74:PRO:CD	2.79	0.45
1:A:76:VAL:O	1:A:78:GLN:N	2.46	0.45
1:B:81:GLY:O	1:B:308:GLU:HA	2.16	0.45
1:B:31:GLY:O	1:B:35:VAL:CG2	2.59	0.45
1:B:46:ILE:O	1:B:48:MET:HE2	2.17	0.45
1:B:77:ALA:HB2	1:B:154:THR:CB	2.46	0.45
1:B:88:ILE:O	1:B:91:GLU:HB3	2.17	0.45
1:A:148:GLN:HA	1:A:152:SER:CB	2.45	0.45
1:A:180:ILE:HD11	1:A:186:PHE:HB2	1.98	0.45
1:A:319:ASN:O	1:A:323:MET:HB2	2.16	0.45
1:A:58:TRP:O	1:A:61:SER:N	2.49	0.45
1:B:341:GLU:CD	1:B:342:GLN:N	2.68	0.45
1:B:407:TYR:C	1:B:409:LEU:N	2.68	0.45
1:B:429:PHE:CE1	1:B:433:LEU:HD11	2.52	0.45
1:A:195:GLY:C	1:A:197:GLY:N	2.68	0.45
1:A:413:ASN:HB3	1:A:414:TRP:HE3	1.74	0.45
1:A:445:TYR:CG	1:A:448:GLN:HA	2.49	0.45
1:A:79:LEU:O	1:A:84:ARG:O	2.34	0.45
1:A:93:HIS:N	1:A:93:HIS:ND1	2.65	0.45
1:B:185:LYS:HG2	1:B:189:PRO:HD3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:LEU:HD12	1:B:336:THR:N	2.31	0.45
1:B:63:LEU:O	1:B:64:PHE:C	2.55	0.45
1:A:183:TYR:O	1:A:184:GLY:C	2.55	0.45
1:A:286:LEU:CD1	1:A:286:LEU:N	2.80	0.45
1:A:266:VAL:HG22	1:A:407:TYR:CD1	2.51	0.45
1:B:204:TYR:HA	1:B:207:MET:SD	2.57	0.45
1:B:275:ALA:H	1:B:353:VAL:HG21	1.82	0.45
1:B:53:ILE:HD12	1:B:54:ALA:N	2.31	0.45
1:A:8:TYR:O	1:A:12:ALA:CB	2.65	0.45
1:A:281:LEU:CD2	1:A:282:ASN:HD22	2.27	0.45
1:A:275:ALA:HB2	1:A:353:VAL:CG1	2.45	0.45
1:A:409:LEU:C	1:A:412:THR:H	2.20	0.45
1:A:394:THR:HG21	1:A:440:LEU:CD2	2.46	0.45
1:A:97:ILE:O	1:A:98:LEU:C	2.55	0.45
1:B:172:LEU:HD13	1:B:173:LEU:N	2.32	0.45
1:B:218:SER:C	1:B:220:ARG:N	2.70	0.45
1:B:18:LEU:HB2	1:B:297:ALA:HB1	1.99	0.45
1:B:403:LEU:O	1:B:404:PRO:C	2.54	0.45
1:B:78:GLN:C	1:B:80:ASN:H	2.20	0.45
1:B:95:GLY:O	1:B:96:LEU:C	2.55	0.45
1:A:20:THR:O	1:A:21:PRO:O	2.34	0.45
1:A:21:PRO:HA	1:A:164:MET:HE1	1.98	0.45
1:A:332:THR:C	1:A:335:LEU:HG	2.37	0.45
1:A:346:LEU:HB3	1:A:347:TYR:H	1.57	0.45
1:A:413:ASN:C	1:A:415:LEU:N	2.69	0.45
1:B:93:HIS:CD2	1:B:228:GLU:OE2	2.70	0.45
1:B:281:LEU:CD2	1:B:282:ASN:HD22	2.28	0.45
1:B:328:THR:HA	1:B:331:ILE:HG23	1.96	0.45
1:B:370:MET:HG3	1:B:434:SER:HB2	1.97	0.45
1:B:244:LEU:CG	1:B:385:LYS:NZ	2.79	0.45
1:A:128:THR:HG22	1:A:129:LYS:HG2	1.99	0.45
1:A:165:VAL:C	1:A:167:GLY:N	2.69	0.45
1:A:88:ILE:HG13	1:A:89:PRO:CD	2.46	0.45
1:B:142:PRO:O	1:B:145:LEU:CD1	2.65	0.45
1:B:290:PHE:HB3	1:B:291:PRO:CD	2.46	0.45
1:B:326:LEU:O	1:B:330:CYS:HB3	2.16	0.45
1:B:447:LEU:HG	1:B:447:LEU:H	1.56	0.45
1:B:455:GLN:NE2	1:B:455:GLN:C	2.70	0.45
1:A:218:SER:C	1:A:220:ARG:N	2.70	0.45
1:A:299:SER:HA	1:A:380:SER:OG	2.16	0.45
1:A:39:MET:CG	1:A:40:ALA:N	2.78	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:TYR:C	1:B:135:HIS:H	2.20	0.45
1:B:148:GLN:HB3	1:B:148:GLN:HE21	1.56	0.45
1:B:262:VAL:HG21	1:B:403:LEU:CD1	2.35	0.45
1:B:65:GLY:C	1:B:67:GLY:N	2.69	0.45
1:A:118:ARG:CD	1:A:118:ARG:C	2.86	0.44
1:A:266:VAL:HG12	1:A:269:LEU:CG	2.46	0.44
1:A:313:GLY:O	1:A:317:ALA:HB3	2.17	0.44
1:A:314:ALA:C	1:A:318:ALA:HB3	2.36	0.44
1:A:33:GLY:O	1:A:37:THR:CB	2.65	0.44
1:B:15:LEU:HD12	1:B:16:ILE:CA	2.47	0.44
1:B:210:LEU:O	1:B:211:LEU:O	2.35	0.44
1:A:87:LYS:NZ	1:B:308:GLU:C	2.70	0.44
1:A:103:SER:HB2	1:A:139:PHE:HD1	1.82	0.44
1:A:19:ALA:O	1:A:20:THR:C	2.53	0.44
1:B:124:GLU:HB2	1:B:125:ALA:H	1.62	0.44
1:B:14:ASN:ND2	1:B:14:ASN:N	2.64	0.44
1:B:250:ALA:O	1:B:251:ALA:C	2.54	0.44
1:B:358:MET:SD	1:B:358:MET:C	2.96	0.44
1:B:422:ALA:O	1:B:423:LYS:C	2.55	0.44
1:A:116:ILE:CG2	1:A:117:ILE:N	2.80	0.44
1:A:274:VAL:HG13	1:A:278:GLN:CD	2.37	0.44
1:A:294:ILE:O	1:A:297:ALA:HB3	2.17	0.44
1:A:429:PHE:CE1	1:A:433:LEU:HD11	2.52	0.44
1:B:141:VAL:CB	1:B:142:PRO:HD3	2.44	0.44
1:B:275:ALA:O	1:B:279:VAL:HB	2.17	0.44
1:B:299:SER:N	1:B:380:SER:OG	2.51	0.44
1:B:409:LEU:C	1:B:412:THR:H	2.20	0.44
1:B:84:ARG:C	1:B:86:HIS:N	2.70	0.44
1:A:417:GLU:CD	1:A:418:GLN:H	2.21	0.44
1:A:444:LEU:HD22	1:A:445:TYR:CD2	2.52	0.44
1:A:72:LEU:HD13	1:A:75:VAL:HG11	2.00	0.44
1:B:11:GLU:CG	1:B:316:ILE:HG23	2.47	0.44
1:B:328:THR:O	1:B:332:THR:CG2	2.64	0.44
1:B:59:LEU:O	1:B:60:PRO:C	2.55	0.44
1:B:7:ARG:O	1:B:11:GLU:HG3	2.18	0.44
1:B:80:ASN:ND2	1:B:157:MET:HG2	2.33	0.44
1:A:10:LYS:HA	1:A:13:SER:OG	2.17	0.44
1:A:151:ARG:HA	1:A:155:ASP:CA	2.31	0.44
1:A:185:LYS:HG2	1:A:189:PRO:HD3	1.99	0.44
1:A:242:PHE:O	1:A:246:PHE:N	2.31	0.44
1:A:362:LEU:HD23	1:A:362:LEU:C	2.37	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ASP:CG	1:B:159:LEU:H	2.21	0.44
1:B:181:PHE:O	1:B:183:TYR:N	2.51	0.44
1:B:382:ARG:C	1:B:384:TYR:N	2.67	0.44
1:B:93:HIS:N	1:B:93:HIS:ND1	2.62	0.44
1:A:11:GLU:HB3	1:A:320:VAL:HG23	1.93	0.44
1:A:279:VAL:O	1:A:280:ALA:C	2.55	0.44
1:A:329:ALA:O	1:A:333:ALA:CB	2.66	0.44
1:A:420:LEU:O	1:A:423:LYS:HG2	2.18	0.44
1:A:444:LEU:C	1:A:446:TRP:N	2.63	0.44
1:A:80:ASN:O	1:A:80:ASN:OD1	2.35	0.44
1:A:219:LYS:HD3	1:A:220:ARG:NE	2.32	0.44
1:A:328:THR:CA	1:A:331:ILE:CG2	2.92	0.44
1:A:63:LEU:O	1:A:64:PHE:C	2.55	0.44
1:B:103:SER:HB2	1:B:139:PHE:HD1	1.81	0.44
1:B:179:TRP:O	1:B:184:GLY:N	2.51	0.44
1:B:181:PHE:C	1:B:183:TYR:N	2.70	0.44
1:B:452:ASP:HA	1:B:455:GLN:HB2	2.00	0.44
1:A:100:LEU:HD12	1:A:100:LEU:H	1.81	0.44
1:A:133:TYR:C	1:A:135:HIS:H	2.21	0.44
1:A:146:LEU:HD22	1:A:149:ALA:CB	2.46	0.44
1:A:14:ASN:HD22	1:A:14:ASN:H	1.65	0.44
1:A:15:LEU:HD12	1:A:16:ILE:CA	2.48	0.44
1:A:452:ASP:O	1:A:456:LEU:HG	2.18	0.44
1:B:11:GLU:HB3	1:B:320:VAL:HG23	1.93	0.44
1:B:69:LEU:HB2	1:B:249:ALA:HB2	1.98	0.44
1:B:320:VAL:CG1	1:B:321:GLY:N	2.53	0.44
1:B:86:HIS:CD2	1:B:87:LYS:HG3	2.53	0.44
1:A:20:THR:OG1	1:A:21:PRO:CD	2.61	0.44
1:A:234:GLN:O	1:A:238:LEU:CD1	2.65	0.44
1:A:273:VAL:CG1	1:A:274:VAL:N	2.78	0.44
1:A:367:TYR:O	1:A:371:ASP:HB3	2.18	0.44
1:A:413:ASN:C	1:A:415:LEU:H	2.20	0.44
1:A:70:MET:HE2	1:A:99:ALA:HB2	1.98	0.44
1:A:97:ILE:HG22	1:A:101:LEU:CD1	2.37	0.44
1:B:183:TYR:O	1:B:184:GLY:C	2.57	0.44
1:B:20:THR:OG1	1:B:21:PRO:CD	2.63	0.44
1:B:238:LEU:HA	1:B:241:LEU:CD1	2.45	0.44
1:B:308:GLU:HB3	1:B:309:GLN:H	1.63	0.44
1:B:298:VAL:HG11	1:B:317:ALA:O	2.18	0.44
1:B:322:LEU:O	1:B:323:MET:C	2.56	0.44
1:B:360:LEU:HD21	1:B:423:LYS:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LEU:HG	1:B:388:THR:HG21	1.99	0.44
1:B:443:ARG:NH1	1:B:446:TRP:CD1	2.85	0.44
1:A:144:TYR:O	1:A:147:PHE:N	2.51	0.43
1:A:178:ASN:HD21	1:A:199:ALA:HB1	1.83	0.43
1:A:250:ALA:O	1:A:251:ALA:C	2.56	0.43
1:B:151:ARG:CG	1:B:152:SER:N	2.78	0.43
1:B:20:THR:O	1:B:21:PRO:C	2.56	0.43
1:B:223:HIS:N	1:B:223:HIS:ND1	2.65	0.43
1:B:374:GLN:HB2	1:B:437:ALA:HB2	2.00	0.43
1:A:135:HIS:CA	1:A:138:ILE:HG22	2.45	0.43
1:A:155:ASP:CB	1:A:159:LEU:N	2.69	0.43
1:A:161:LYS:C	1:A:163:ALA:H	2.20	0.43
1:A:322:LEU:O	1:A:324:THR:N	2.51	0.43
1:A:332:THR:HA	1:A:335:LEU:HG	1.98	0.43
1:A:357:ALA:O	1:A:358:MET:C	2.56	0.43
1:A:318:ALA:HA	1:A:381:LEU:CD1	2.48	0.43
1:A:386:ASP:C	1:A:386:ASP:OD1	2.56	0.43
1:A:3:ASN:O	1:A:4:SER:OG	2.23	0.43
1:A:410:GLY:N	1:A:425:PHE:HB2	2.32	0.43
1:B:159:LEU:O	1:B:160:THR:C	2.56	0.43
1:B:404:PRO:O	1:B:408:ILE:HB	2.18	0.43
1:B:4:SER:HA	1:B:7:ARG:HB2	2.00	0.43
1:A:151:ARG:HD2	1:A:155:ASP:CA	2.44	0.43
1:A:77:ALA:HB2	1:A:154:THR:CB	2.48	0.43
1:A:185:LYS:HD3	1:A:186:PHE:N	2.32	0.43
1:A:208:LEU:HD23	1:A:209:LEU:CA	2.47	0.43
1:A:234:GLN:HB3	1:A:235:PRO:HD3	2.00	0.43
1:A:72:LEU:HD11	1:A:383:GLY:O	2.18	0.43
1:B:135:HIS:CA	1:B:138:ILE:HG22	2.47	0.43
1:B:195:GLY:C	1:B:197:GLY:N	2.70	0.43
1:B:260:ALA:O	1:B:261:VAL:C	2.56	0.43
1:B:382:ARG:C	1:B:384:TYR:H	2.22	0.43
1:B:44:SER:O	1:B:46:ILE:N	2.51	0.43
1:B:60:PRO:O	1:B:61:SER:C	2.55	0.43
1:B:72:LEU:HD22	1:B:75:VAL:HG11	2.00	0.43
1:A:146:LEU:O	1:A:149:ALA:N	2.52	0.43
1:A:195:GLY:O	1:A:196:CYS:C	2.57	0.43
1:A:247:PRO:O	1:A:251:ALA:HB2	2.18	0.43
1:A:276:ALA:O	1:A:277:HIS:O	2.36	0.43
1:A:327:ALA:O	1:A:330:CYS:HB3	2.18	0.43
1:A:412:THR:O	1:A:416:THR:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:TYR:C	1:B:135:HIS:N	2.71	0.43
1:B:284:SER:O	1:B:285:SER:C	2.57	0.43
1:B:400:VAL:CG1	1:B:401:LEU:N	2.81	0.43
1:B:53:ILE:CA	1:B:56:SER:HB3	2.49	0.43
1:A:173:LEU:O	1:A:176:PRO:CD	2.64	0.43
1:A:130:THR:HB	1:A:194:VAL:HA	2.00	0.43
1:A:353:VAL:O	1:A:357:ALA:CB	2.66	0.43
1:A:386:ASP:O	1:A:387:MET:C	2.54	0.43
1:A:388:THR:O	1:A:391:PHE:CD2	2.71	0.43
1:B:128:THR:HG22	1:B:129:LYS:HG2	2.00	0.43
1:B:130:THR:O	1:B:131:VAL:C	2.56	0.43
1:B:145:LEU:HD13	1:B:145:LEU:C	2.35	0.43
1:B:238:LEU:O	1:B:242:PHE:CD1	2.71	0.43
1:B:316:ILE:HB	1:B:317:ALA:H	1.53	0.43
1:B:412:THR:O	1:B:416:THR:N	2.52	0.43
1:B:420:LEU:HD12	1:B:423:LYS:HG2	2.01	0.43
1:B:427:LEU:C	1:B:429:PHE:N	2.70	0.43
1:A:18:LEU:HB2	1:A:297:ALA:HB1	1.99	0.43
1:A:191:LEU:CG	1:A:192:GLY:H	2.30	0.43
1:A:191:LEU:CG	1:A:192:GLY:N	2.81	0.43
1:A:343:ILE:O	1:A:346:LEU:N	2.52	0.43
1:A:363:PHE:CD2	1:A:426:TRP:HB3	2.53	0.43
1:B:109:VAL:O	1:B:113:THR:HG22	2.17	0.43
1:B:118:ARG:CD	1:B:118:ARG:C	2.87	0.43
1:B:141:VAL:HG22	1:B:204:TYR:CB	2.47	0.43
1:B:212:LEU:O	1:B:213:PHE:O	2.36	0.43
1:B:247:PRO:HB3	1:B:388:THR:O	2.18	0.43
1:B:273:VAL:CG1	1:B:274:VAL:N	2.79	0.43
1:B:378:ALA:O	1:B:380:SER:N	2.51	0.43
1:A:131:VAL:O	1:A:135:HIS:CG	2.72	0.43
1:A:288:PHE:O	1:A:289:MET:C	2.57	0.43
1:B:131:VAL:HB	1:B:135:HIS:HE2	1.84	0.43
1:B:173:LEU:O	1:B:177:LEU:CD2	2.56	0.43
1:B:230:PHE:CG	1:B:231:HIS:N	2.83	0.43
1:B:345:LEU:HA	1:B:345:LEU:HD23	1.54	0.43
1:B:420:LEU:HB3	1:B:423:LYS:HE2	2.01	0.43
1:B:56:SER:O	1:B:60:PRO:HD2	2.18	0.43
1:A:179:TRP:O	1:A:184:GLY:N	2.50	0.43
1:A:27:VAL:O	1:A:31:GLY:CA	2.64	0.43
1:A:298:VAL:HG21	1:A:321:GLY:CA	2.46	0.43
1:A:275:ALA:HB1	1:A:353:VAL:CG1	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:HD13	1:A:75:VAL:CG1	2.49	0.43
1:A:8:TYR:CD1	1:A:9:LYS:N	2.87	0.43
1:B:11:GLU:HG2	1:B:316:ILE:HG23	1.99	0.43
1:B:147:PHE:CD1	1:B:211:LEU:HA	2.54	0.43
1:B:65:GLY:HA2	1:B:253:PHE:CG	2.54	0.43
1:B:294:ILE:O	1:B:297:ALA:HB3	2.19	0.43
1:B:60:PRO:O	1:B:63:LEU:HB3	2.18	0.43
1:B:60:PRO:O	1:B:63:LEU:CD2	2.66	0.43
1:A:212:LEU:O	1:A:213:PHE:O	2.37	0.43
1:A:271:SER:C	1:A:273:VAL:HG12	2.39	0.43
1:A:314:ALA:HB2	1:A:449:LYS:HZ3	1.82	0.43
1:A:287:VAL:HB	1:A:368:GLN:HG2	2.00	0.43
1:A:86:HIS:CE1	1:A:87:LYS:H	2.35	0.43
1:B:129:LYS:O	1:B:132:GLY:HA3	2.19	0.43
1:B:366:ILE:HG22	1:B:430:ILE:HD11	2.01	0.43
1:B:60:PRO:HA	1:B:63:LEU:HD22	2.01	0.43
1:A:109:VAL:O	1:A:113:THR:HG22	2.19	0.43
1:A:113:THR:O	1:A:116:ILE:N	2.48	0.43
1:A:218:SER:HB3	1:A:221:LEU:O	2.19	0.43
1:A:382:ARG:CA	1:A:387:MET:HB2	2.49	0.43
1:A:47:ASP:C	1:A:49:ALA:H	2.14	0.43
1:A:93:HIS:O	1:A:97:ILE:HG13	2.19	0.43
1:B:104:VAL:HA	1:B:107:ILE:CG1	2.47	0.43
1:B:266:VAL:HG21	1:B:407:TYR:CG	2.54	0.43
1:A:181:PHE:O	1:A:183:TYR:N	2.52	0.42
1:A:235:PRO:HA	1:A:238:LEU:HD13	2.01	0.42
1:A:427:LEU:C	1:A:429:PHE:N	2.72	0.42
1:B:24:ILE:HB	1:B:164:MET:SD	2.59	0.42
1:B:317:ALA:HA	1:B:320:VAL:CG1	2.49	0.42
1:B:416:THR:HB	1:B:417:GLU:H	1.54	0.42
1:B:413:ASN:HD22	1:B:421:GLY:H	1.67	0.42
1:A:122:VAL:C	1:A:124:GLU:N	2.72	0.42
1:A:134:MET:SD	1:A:198:VAL:N	2.92	0.42
1:A:180:ILE:CA	1:A:184:GLY:HA3	2.35	0.42
1:A:396:ILE:O	1:A:399:TRP:HB3	2.19	0.42
1:A:58:TRP:CE3	1:A:59:LEU:N	2.87	0.42
1:A:58:TRP:O	1:A:59:LEU:C	2.55	0.42
1:A:66:VAL:O	1:A:69:LEU:HB3	2.19	0.42
1:B:237:GLU:O	1:B:241:LEU:CD1	2.66	0.42
1:B:432:GLY:O	1:B:435:ALA:HB3	2.20	0.42
1:B:447:LEU:O	1:B:447:LEU:HD12	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:GLY:O	1:B:97:ILE:N	2.52	0.42
1:A:104:VAL:O	1:A:106:ILE:N	2.52	0.42
1:A:116:ILE:HG23	1:A:117:ILE:N	2.35	0.42
1:A:236:LYS:HA	1:A:239:ILE:HG13	2.02	0.42
1:A:298:VAL:HG11	1:A:317:ALA:O	2.20	0.42
1:A:393:ARG:NH1	1:A:393:ARG:CG	2.82	0.42
1:A:360:LEU:HD21	1:A:423:LYS:HB3	1.99	0.42
1:B:134:MET:SD	1:B:198:VAL:CA	3.05	0.42
1:B:187:GLY:O	1:B:188:ALA:HB2	2.19	0.42
1:B:191:LEU:CG	1:B:192:GLY:N	2.82	0.42
1:A:138:ILE:HA	1:A:141:VAL:CG2	2.49	0.42
1:A:176:PRO:HG2	1:A:177:LEU:HD22	2.00	0.42
1:A:203:VAL:C	1:A:205:TRP:N	2.71	0.42
1:A:200:THR:CA	1:A:203:VAL:HG23	2.48	0.42
1:A:234:GLN:C	1:A:238:LEU:HD13	2.40	0.42
1:A:272:THR:C	1:A:274:VAL:N	2.71	0.42
1:A:283:PHE:O	1:A:284:SER:C	2.58	0.42
1:A:413:ASN:HD22	1:A:421:GLY:N	2.17	0.42
1:B:142:PRO:O	1:B:143:ALA:C	2.56	0.42
1:B:266:VAL:HG13	1:B:269:LEU:HD21	2.02	0.42
1:B:281:LEU:HD23	1:B:281:LEU:C	2.40	0.42
1:B:11:GLU:HB3	1:B:320:VAL:HB	2.00	0.42
1:B:358:MET:O	1:B:361:LEU:HB2	2.19	0.42
1:B:244:LEU:HD23	1:B:388:THR:OG1	2.20	0.42
1:B:393:ARG:CG	1:B:393:ARG:NH1	2.82	0.42
1:A:259:PHE:O	1:A:260:ALA:C	2.58	0.42
1:A:290:PHE:O	1:A:293:SER:HB2	2.19	0.42
1:A:358:MET:SD	1:A:358:MET:C	2.98	0.42
1:B:163:ALA:HB3	1:B:164:MET:SD	2.60	0.42
1:B:206:ILE:O	1:B:210:LEU:CD2	2.58	0.42
1:B:403:LEU:HD23	1:B:403:LEU:HA	1.78	0.42
1:B:73:VAL:N	1:B:74:PRO:CD	2.82	0.42
1:B:73:VAL:O	1:B:76:VAL:HG12	2.20	0.42
1:B:96:LEU:HB2	1:B:146:LEU:HG	2.01	0.42
1:A:180:ILE:CD1	1:A:186:PHE:HB2	2.50	0.42
1:A:274:VAL:HA	1:A:277:HIS:HB3	2.01	0.42
1:A:332:THR:HA	1:A:335:LEU:CG	2.49	0.42
1:B:142:PRO:O	1:B:145:LEU:CB	2.61	0.42
1:B:294:ILE:O	1:B:295:GLY:C	2.57	0.42
1:B:339:PHE:O	1:B:343:ILE:HG12	2.20	0.42
1:B:395:PHE:O	1:B:398:TYR:CE1	2.71	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:VAL:HG23	1:A:135:HIS:CE1	2.54	0.42
1:A:161:LYS:C	1:A:163:ALA:N	2.72	0.42
1:A:266:VAL:CG1	1:A:269:LEU:HD21	2.49	0.42
1:A:436:ALA:HA	1:A:439:MET:HG2	2.00	0.42
1:B:142:PRO:C	1:B:145:LEU:HB3	2.38	0.42
1:B:161:LYS:C	1:B:163:ALA:N	2.73	0.42
1:B:185:LYS:C	1:B:185:LYS:CD	2.82	0.42
1:B:159:LEU:HD21	1:B:220:ARG:HH11	1.83	0.42
1:B:287:VAL:O	1:B:291:PRO:HD2	2.18	0.42
1:B:318:ALA:CB	1:B:381:LEU:HD13	2.50	0.42
1:B:399:TRP:HE1	1:B:403:LEU:HD12	1.85	0.42
1:A:216:VAL:CG2	1:A:225:LYS:HD3	2.47	0.42
1:A:392:HIS:O	1:A:395:PHE:CB	2.67	0.42
1:A:69:LEU:HG	1:A:245:GLY:C	2.40	0.42
1:A:88:ILE:O	1:A:91:GLU:HB3	2.20	0.42
1:B:34:PHE:O	1:B:35:VAL:O	2.37	0.42
1:B:72:LEU:HD11	1:B:383:GLY:O	2.19	0.42
1:B:452:ASP:O	1:B:455:GLN:HB3	2.19	0.42
1:A:238:LEU:CA	1:A:241:LEU:HD13	2.48	0.42
1:A:348:THR:O	1:A:349:GLU:HG3	2.20	0.42
1:A:351:GLN:O	1:A:352:VAL:C	2.58	0.42
1:A:247:PRO:HG2	1:A:389:ALA:HA	1.99	0.42
1:A:443:ARG:O	1:A:444:LEU:C	2.57	0.42
1:A:49:ALA:O	1:A:53:ILE:HG13	2.20	0.42
1:B:138:ILE:HA	1:B:141:VAL:HG23	2.02	0.42
1:B:244:LEU:CB	1:B:385:LYS:NZ	2.81	0.42
1:B:427:LEU:C	1:B:427:LEU:HD23	2.40	0.42
1:B:47:ASP:C	1:B:49:ALA:H	2.14	0.42
1:B:71:ALA:O	1:B:74:PRO:HB2	2.19	0.42
1:A:382:ARG:N	1:A:382:ARG:HD3	2.34	0.42
1:A:387:MET:HE1	1:A:456:LEU:HD13	2.01	0.42
1:A:98:LEU:HA	1:A:101:LEU:HG	2.01	0.42
1:B:96:LEU:CD1	1:B:146:LEU:HD12	2.46	0.42
1:B:276:ALA:O	1:B:277:HIS:C	2.57	0.42
1:B:339:PHE:O	1:B:340:ARG:O	2.38	0.42
1:B:381:LEU:O	1:B:384:TYR:CG	2.73	0.42
1:B:38:ILE:O	1:B:39:MET:C	2.58	0.42
1:B:392:HIS:O	1:B:395:PHE:CB	2.68	0.42
1:B:413:ASN:HB3	1:B:414:TRP:CZ3	2.55	0.42
1:B:415:LEU:HB3	1:B:416:THR:H	1.54	0.42
1:B:86:HIS:CE1	1:B:87:LYS:H	2.38	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LEU:O	1:B:99:ALA:C	2.57	0.42
1:A:97:ILE:CG2	1:A:101:LEU:HD11	2.39	0.41
1:A:308:GLU:HB3	1:A:309:GLN:H	1.67	0.41
1:A:357:ALA:O	1:A:360:LEU:N	2.53	0.41
1:B:122:VAL:C	1:B:124:GLU:N	2.73	0.41
1:B:23:LEU:O	1:B:24:ILE:C	2.57	0.41
1:B:427:LEU:HD23	1:B:428:GLY:CA	2.50	0.41
1:B:69:LEU:C	1:B:71:ALA:H	2.23	0.41
1:A:100:LEU:N	1:A:100:LEU:CD1	2.82	0.41
1:A:275:ALA:O	1:A:279:VAL:HB	2.20	0.41
1:A:367:TYR:O	1:A:368:GLN:C	2.57	0.41
1:A:386:ASP:C	1:A:389:ALA:H	2.23	0.41
1:A:388:THR:HA	1:A:391:PHE:CG	2.55	0.41
1:A:39:MET:SD	1:A:40:ALA:HB2	2.60	0.41
1:B:135:HIS:C	1:B:137:VAL:N	2.66	0.41
1:B:146:LEU:HD13	1:B:147:PHE:N	2.35	0.41
1:B:147:PHE:CE2	1:B:211:LEU:HA	2.55	0.41
1:B:287:VAL:O	1:B:291:PRO:HD3	2.20	0.41
1:B:72:LEU:HD13	1:B:75:VAL:CG1	2.50	0.41
1:B:97:ILE:O	1:B:99:ALA:N	2.53	0.41
1:A:145:LEU:C	1:A:145:LEU:HD13	2.37	0.41
1:A:219:LYS:CD	1:A:220:ARG:NE	2.83	0.41
1:A:454:VAL:O	1:A:458:LEU:HB2	2.20	0.41
1:A:76:VAL:C	1:A:78:GLN:HG2	2.41	0.41
1:B:18:LEU:HA	1:B:160:THR:HG21	2.02	0.41
1:B:276:ALA:O	1:B:277:HIS:O	2.38	0.41
1:B:408:ILE:HG12	1:B:411:MET:SD	2.60	0.41
1:A:248:VAL:HG12	1:A:391:PHE:CZ	2.55	0.41
1:A:363:PHE:HD1	1:A:364:ALA:N	2.16	0.41
1:B:185:LYS:O	1:B:186:PHE:CD2	2.73	0.41
1:B:219:LYS:CD	1:B:220:ARG:NE	2.84	0.41
1:B:408:ILE:O	1:B:412:THR:N	2.53	0.41
1:B:74:PRO:HB3	1:B:149:ALA:CA	2.50	0.41
1:B:8:TYR:O	1:B:12:ALA:HB2	2.21	0.41
1:B:97:ILE:C	1:B:99:ALA:N	2.72	0.41
1:A:102:VAL:O	1:A:105:PRO:HD2	2.21	0.41
1:A:178:ASN:ND2	1:A:199:ALA:HB1	2.35	0.41
1:A:322:LEU:O	1:A:323:MET:C	2.58	0.41
1:A:275:ALA:H	1:A:353:VAL:HG21	1.83	0.41
1:A:409:LEU:HA	1:A:412:THR:HB	2.01	0.41
1:A:7:ARG:O	1:A:11:GLU:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLN:O	1:A:95:GLY:C	2.57	0.41
1:B:117:ILE:CG2	1:B:118:ARG:H	2.18	0.41
1:B:266:VAL:CG2	1:B:407:TYR:CD1	3.03	0.41
1:B:275:ALA:HB2	1:B:353:VAL:CG2	2.49	0.41
1:B:276:ALA:HB1	1:B:426:TRP:NE1	2.34	0.41
1:B:363:PHE:CD2	1:B:426:TRP:HB3	2.55	0.41
1:B:80:ASN:OD1	1:B:80:ASN:O	2.39	0.41
1:A:235:PRO:CA	1:A:238:LEU:HD22	2.50	0.41
1:A:248:VAL:HG23	1:A:249:ALA:N	2.35	0.41
1:A:317:ALA:HA	1:A:320:VAL:CG1	2.50	0.41
1:A:38:ILE:O	1:A:39:MET:C	2.57	0.41
1:B:110:LEU:O	1:B:111:PHE:C	2.59	0.41
1:B:380:SER:O	1:B:383:GLY:N	2.53	0.41
1:B:42:GLY:HA2	1:B:49:ALA:HB3	2.01	0.41
1:A:131:VAL:O	1:A:134:MET:HB2	2.20	0.41
1:A:15:LEU:CG	1:A:16:ILE:N	2.84	0.41
1:B:296:ALA:O	1:B:300:ILE:HG12	2.20	0.41
1:A:262:VAL:HG12	1:A:263:ALA:N	2.36	0.41
1:A:287:VAL:O	1:A:291:PRO:HD3	2.21	0.41
1:A:34:PHE:CD1	1:A:35:VAL:N	2.88	0.41
1:A:360:LEU:CD2	1:A:423:LYS:HB2	2.51	0.41
1:A:81:GLY:O	1:A:308:GLU:HG3	2.20	0.41
1:B:127:ALA:C	1:B:130:THR:HG1	2.24	0.41
1:B:137:VAL:O	1:B:141:VAL:HG23	2.21	0.41
1:B:21:PRO:HB2	1:B:160:THR:HG23	2.03	0.41
1:B:273:VAL:O	1:B:277:HIS:HB2	2.20	0.41
1:B:286:LEU:O	1:B:289:MET:HB3	2.21	0.41
1:B:312:LYS:HZ1	1:B:449:LYS:CD	2.33	0.41
1:A:15:LEU:HD12	1:A:15:LEU:C	2.39	0.41
1:A:238:LEU:O	1:A:242:PHE:CD1	2.73	0.41
1:A:73:VAL:HG11	1:A:241:LEU:HD23	2.02	0.41
1:A:251:ALA:O	1:A:255:GLU:CB	2.58	0.41
1:A:314:ALA:O	1:A:318:ALA:CB	2.66	0.41
1:A:11:GLU:HG2	1:A:316:ILE:CG2	2.50	0.41
1:A:382:ARG:HB3	1:A:387:MET:CB	2.51	0.41
1:A:58:TRP:CE3	1:A:59:LEU:HA	2.56	0.41
1:A:63:LEU:O	1:A:66:VAL:N	2.53	0.41
1:B:131:VAL:CA	1:B:134:MET:HB2	2.50	0.41
1:B:225:LYS:O	1:B:226:VAL:CG2	2.68	0.41
1:B:356:LEU:O	1:B:360:LEU:N	2.34	0.41
1:A:195:GLY:O	1:A:198:VAL:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PRO:HB3	1:A:388:THR:O	2.21	0.41
1:A:382:ARG:C	1:A:384:TYR:H	2.24	0.41
1:B:107:ILE:CA	1:B:139:PHE:CZ	2.94	0.41
1:B:172:LEU:HD13	1:B:172:LEU:C	2.41	0.41
1:B:180:ILE:HD11	1:B:186:PHE:HB2	2.01	0.41
1:B:231:HIS:C	1:B:235:PRO:CG	2.84	0.41
1:B:272:THR:O	1:B:274:VAL:C	2.59	0.41
1:B:311:THR:HG23	1:B:312:LYS:N	2.36	0.41
1:B:339:PHE:O	1:B:343:ILE:CG1	2.69	0.41
1:B:388:THR:HA	1:B:391:PHE:CG	2.56	0.41
1:B:384:TYR:CE1	1:B:446:TRP:HH2	2.36	0.41
1:B:72:LEU:CD1	1:B:75:VAL:HG21	2.51	0.41
1:B:8:TYR:O	1:B:12:ALA:HB3	2.21	0.41
1:A:130:THR:O	1:A:134:MET:HG2	2.21	0.41
1:A:88:ILE:CG1	1:A:89:PRO:N	2.84	0.41
1:B:461:LYS:C	1:B:461:LYS:HD2	2.41	0.41
1:A:125:ALA:O	1:A:126:MET:C	2.60	0.40
1:A:195:GLY:O	1:A:197:GLY:N	2.54	0.40
1:A:277:HIS:O	1:A:278:GLN:C	2.59	0.40
1:B:65:GLY:HA3	1:B:253:PHE:CG	2.56	0.40
1:B:277:HIS:O	1:B:278:GLN:C	2.59	0.40
1:B:341:GLU:OE1	1:B:341:GLU:N	2.53	0.40
1:B:34:PHE:CD1	1:B:35:VAL:N	2.90	0.40
1:B:41:GLY:C	1:B:49:ALA:CB	2.85	0.40
1:B:447:LEU:O	1:B:450:GLN:NE2	2.53	0.40
1:A:172:LEU:HD13	1:A:173:LEU:N	2.36	0.40
1:A:281:LEU:HD23	1:A:281:LEU:C	2.42	0.40
1:A:3:ASN:O	1:A:5:VAL:HG23	2.21	0.40
1:A:60:PRO:HA	1:A:63:LEU:HB3	2.02	0.40
1:A:95:GLY:O	1:A:96:LEU:C	2.59	0.40
1:B:447:LEU:HD13	1:B:450:GLN:HG2	2.04	0.40
1:A:96:LEU:CB	1:A:146:LEU:HG	2.51	0.40
1:A:185:LYS:CD	1:A:185:LYS:C	2.86	0.40
1:A:232:LYS:H	1:A:233:PRO:HD3	1.85	0.40
1:A:282:ASN:O	1:A:283:PHE:C	2.60	0.40
1:A:360:LEU:HD13	1:A:426:TRP:CD1	2.56	0.40
1:A:57:ILE:HG22	1:A:57:ILE:O	2.22	0.40
1:B:195:GLY:O	1:B:196:CYS:C	2.60	0.40
1:B:233:PRO:N	1:B:235:PRO:HD2	2.37	0.40
1:B:66:VAL:O	1:B:69:LEU:HB3	2.21	0.40
1:B:70:MET:SD	1:B:99:ALA:N	2.94	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LYS:O	1:A:132:GLY:HA3	2.22	0.40
1:A:412:THR:HA	1:A:415:LEU:HB2	2.03	0.40
1:A:71:ALA:HA	1:A:74:PRO:HD2	1.98	0.40
1:B:239:ILE:C	1:B:242:PHE:HB2	2.42	0.40
1:B:257:THR:O	1:B:260:ALA:HB3	2.21	0.40
1:B:72:LEU:HD13	1:B:75:VAL:HG11	2.03	0.40
1:A:398:TYR:HD2	1:A:432:GLY:O	2.04	0.40
1:A:98:LEU:O	1:A:99:ALA:C	2.59	0.40
1:B:10:LYS:NZ	1:B:305:LYS:NZ	2.70	0.40
1:B:186:PHE:HA	1:B:186:PHE:HD2	1.83	0.40
1:B:209:LEU:CD1	1:B:210:LEU:HD13	2.49	0.40
1:B:218:SER:HB3	1:B:221:LEU:O	2.21	0.40
1:B:234:GLN:C	1:B:237:GLU:H	2.24	0.40
1:B:24:ILE:HD13	1:B:24:ILE:HA	1.99	0.40
1:B:353:VAL:O	1:B:357:ALA:CA	2.68	0.40
1:B:461:LYS:HE3	1:B:461:LYS:HB3	1.88	0.40
1:B:69:LEU:C	1:B:69:LEU:CD2	2.89	0.40
1:B:76:VAL:HG23	1:B:78:GLN:HE21	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	458/460 (100%)	218 (48%)	118 (26%)	122 (27%)	0 1
1	B	458/460 (100%)	221 (48%)	121 (26%)	116 (25%)	0 1
All	All	916/920 (100%)	439 (48%)	239 (26%)	238 (26%)	0 1

All (238) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ALA
1	A	35	VAL
1	A	56	SER
1	A	76	VAL
1	A	121	ASP
1	A	124	GLU
1	A	125	ALA
1	A	126	MET
1	A	128	THR
1	A	152	SER
1	A	165	VAL
1	A	184	GLY
1	A	211	LEU
1	A	213	PHE
1	A	226	VAL
1	A	251	ALA
1	A	261	VAL
1	A	273	VAL
1	A	277	HIS
1	A	279	VAL
1	A	280	ALA
1	A	282	ASN
1	A	285	SER
1	A	311	THR
1	A	314	ALA
1	A	316	ILE
1	A	340	ARG
1	A	346	LEU
1	A	352	VAL
1	A	353	VAL
1	A	376	VAL
1	A	378	ALA
1	A	416	THR
1	A	444	LEU
1	A	445	TYR
1	B	19	ALA
1	B	35	VAL
1	B	110	LEU
1	B	121	ASP
1	B	124	GLU
1	B	126	MET
1	B	128	THR
1	B	152	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	165	VAL
1	B	184	GLY
1	B	211	LEU
1	B	213	PHE
1	B	226	VAL
1	B	251	ALA
1	B	261	VAL
1	B	273	VAL
1	B	277	HIS
1	B	279	VAL
1	B	280	ALA
1	B	282	ASN
1	B	285	SER
1	B	311	THR
1	B	314	ALA
1	B	316	ILE
1	B	340	ARG
1	B	352	VAL
1	B	354	VAL
1	B	376	VAL
1	B	378	ALA
1	B	399	TRP
1	B	416	THR
1	B	444	LEU
1	A	7	ARG
1	A	9	LYS
1	A	33	GLY
1	A	47	ASP
1	A	50	ALA
1	A	110	LEU
1	A	160	THR
1	A	167	GLY
1	A	179	TRP
1	A	183	TYR
1	A	214	TYR
1	A	219	LYS
1	A	230	PHE
1	A	244	LEU
1	A	262	VAL
1	A	276	ALA
1	A	278	GLN
1	A	281	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	317	ALA
1	A	318	ALA
1	A	321	GLY
1	A	322	LEU
1	A	323	MET
1	A	399	TRP
1	A	402	GLY
1	A	417	GLU
1	A	446	TRP
1	A	448	GLN
1	B	7	ARG
1	B	21	PRO
1	B	33	GLY
1	B	47	ASP
1	B	50	ALA
1	B	56	SER
1	B	64	PHE
1	B	76	VAL
1	B	156	GLY
1	B	160	THR
1	B	167	GLY
1	B	183	TYR
1	B	214	TYR
1	B	219	LYS
1	B	230	PHE
1	B	244	LEU
1	B	262	VAL
1	B	269	LEU
1	B	278	GLN
1	B	317	ALA
1	B	318	ALA
1	B	321	GLY
1	B	323	MET
1	B	346	LEU
1	B	353	VAL
1	B	369	CYS
1	B	379	GLY
1	B	402	GLY
1	B	417	GLU
1	A	21	PRO
1	A	39	MET
1	A	64	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	82	ALA
1	A	84	ARG
1	A	158	SER
1	A	163	ALA
1	A	223	HIS
1	A	275	ALA
1	A	284	SER
1	A	327	ALA
1	A	334	LEU
1	A	339	PHE
1	B	9	LYS
1	B	39	MET
1	B	82	ALA
1	B	84	ARG
1	B	108	ALA
1	B	118	ARG
1	B	158	SER
1	B	179	TRP
1	B	186	PHE
1	B	243	ARG
1	B	275	ALA
1	B	276	ALA
1	B	281	LEU
1	B	284	SER
1	B	322	LEU
1	B	334	LEU
1	B	339	PHE
1	B	341	GLU
1	B	349	GLU
1	B	385	LYS
1	B	445	TYR
1	A	13	SER
1	A	29	GLN
1	A	31	GLY
1	A	37	THR
1	A	79	LEU
1	A	108	ALA
1	A	117	ILE
1	A	130	THR
1	A	151	ARG
1	A	156	GLY
1	A	186	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	218	SER
1	A	231	HIS
1	A	232	LYS
1	A	269	LEU
1	A	320	VAL
1	A	330	CYS
1	A	341	GLU
1	A	349	GLU
1	A	354	VAL
1	A	369	CYS
1	A	379	GLY
1	A	447	LEU
1	B	13	SER
1	B	37	THR
1	B	45	ALA
1	B	79	LEU
1	B	101	LEU
1	B	125	ALA
1	B	130	THR
1	B	163	ALA
1	B	223	HIS
1	B	231	HIS
1	B	232	LYS
1	B	320	VAL
1	A	28	ALA
1	A	42	GLY
1	A	77	ALA
1	A	122	VAL
1	A	161	LYS
1	A	162	PRO
1	A	172	LEU
1	A	185	LYS
1	A	243	ARG
1	A	315	ALA
1	A	355	ALA
1	B	29	GLN
1	B	42	GLY
1	B	96	LEU
1	B	117	ILE
1	B	122	VAL
1	B	161	LYS
1	B	315	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	327	ALA
1	B	330	CYS
1	B	377	ALA
1	A	96	LEU
1	A	101	LEU
1	A	375	VAL
1	A	377	ALA
1	A	385	LYS
1	B	28	ALA
1	B	31	GLY
1	B	83	GLY
1	B	138	ILE
1	B	151	ARG
1	B	162	PRO
1	A	83	GLY
1	A	138	ILE
1	B	5	VAL
1	B	267	ALA
1	B	295	GLY
1	B	92	VAL
1	A	5	VAL
1	A	224	VAL
1	A	266	VAL
1	A	267	ALA
1	B	97	ILE
1	A	274	VAL
1	B	224	VAL

5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	364/364 (100%)	296 (81%)	68 (19%)	1 10
1	B	364/364 (100%)	295 (81%)	69 (19%)	1 10
All	All	728/728 (100%)	591 (81%)	137 (19%)	1 10

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	34	PHE
1	A	39	MET
1	A	60	PRO
1	A	61	SER
1	A	62	ILE
1	A	63	LEU
1	A	72	LEU
1	A	90	PHE
1	A	93	HIS
1	A	94	GLN
1	A	105	PRO
1	A	115	PHE
1	A	118	ARG
1	A	119	PHE
1	A	124	GLU
1	A	144	TYR
1	A	145	LEU
1	A	148	GLN
1	A	164	MET
1	A	166	ILE
1	A	168	PHE
1	A	171	LEU
1	A	186	PHE
1	A	196	CYS
1	A	204	TYR
1	A	208	LEU
1	A	210	LEU
1	A	214	TYR
1	A	219	LYS
1	A	221	LEU
1	A	223	HIS
1	A	230	PHE
1	A	232	LYS
1	A	243	ARG
1	A	244	LEU
1	A	252	LEU
1	A	256	VAL
1	A	278	GLN
1	A	301	ARG
1	A	312	LYS
1	A	337	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	341	GLU
1	A	345	LEU
1	A	362	LEU
1	A	363	PHE
1	A	371	ASP
1	A	384	TYR
1	A	385	LYS
1	A	387	MET
1	A	391	PHE
1	A	395	PHE
1	A	396	ILE
1	A	398	TYR
1	A	400	VAL
1	A	404	PRO
1	A	405	THR
1	A	407	TYR
1	A	412	THR
1	A	414	TRP
1	A	415	LEU
1	A	425	PHE
1	A	426	TRP
1	A	427	LEU
1	A	443	ARG
1	A	447	LEU
1	A	449	LYS
1	A	455	GLN
1	B	7	ARG
1	B	14	ASN
1	B	29	GLN
1	B	34	PHE
1	B	39	MET
1	B	57	ILE
1	B	61	SER
1	B	62	ILE
1	B	63	LEU
1	B	72	LEU
1	B	90	PHE
1	B	93	HIS
1	B	94	GLN
1	B	115	PHE
1	B	119	PHE
1	B	124	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	144	TYR
1	B	145	LEU
1	B	147	PHE
1	B	148	GLN
1	B	164	MET
1	B	166	ILE
1	B	168	PHE
1	B	171	LEU
1	B	185	LYS
1	B	186	PHE
1	B	204	TYR
1	B	208	LEU
1	B	210	LEU
1	B	214	TYR
1	B	219	LYS
1	B	221	LEU
1	B	223	HIS
1	B	230	PHE
1	B	243	ARG
1	B	244	LEU
1	B	252	LEU
1	B	256	VAL
1	B	278	GLN
1	B	290	PHE
1	B	292	MET
1	B	301	ARG
1	B	312	LYS
1	B	341	GLU
1	B	345	LEU
1	B	362	LEU
1	B	363	PHE
1	B	371	ASP
1	B	384	TYR
1	B	385	LYS
1	B	387	MET
1	B	391	PHE
1	B	395	PHE
1	B	396	ILE
1	B	398	TYR
1	B	400	VAL
1	B	404	PRO
1	B	405	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	407	TYR
1	B	414	TRP
1	B	415	LEU
1	B	425	PHE
1	B	426	TRP
1	B	427	LEU
1	B	443	ARG
1	B	445	TYR
1	B	449	LYS
1	B	455	GLN
1	B	461	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	78	GLN
1	A	85	GLN
1	A	148	GLN
1	A	174	ASN
1	A	277	HIS
1	A	282	ASN
1	A	350	ASN
1	A	413	ASN
1	A	418	GLN
1	A	442	GLN
1	A	450	GLN
1	A	455	GLN
1	A	457	HIS
1	B	14	ASN
1	B	78	GLN
1	B	85	GLN
1	B	114	GLN
1	B	148	GLN
1	B	174	ASN
1	B	277	HIS
1	B	282	ASN
1	B	418	GLN
1	B	442	GLN
1	B	455	GLN
1	B	457	HIS

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	460/460 (100%)	0.13	48 (10%) 6 6	34, 111, 174, 267	0
1	B	460/460 (100%)	-0.03	28 (6%) 21 17	28, 117, 180, 253	0
All	All	920/920 (100%)	0.05	76 (8%) 11 10	28, 114, 180, 267	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	309	GLN	7.6
1	A	36	ASP	6.7
1	B	83	GLY	5.8
1	A	84	ARG	5.3
1	A	442	GLN	5.1
1	B	368	GLN	5.0
1	A	85	GLN	4.9
1	B	82	ALA	4.9
1	A	58	TRP	4.6
1	A	37	THR	4.6
1	B	84	ARG	4.6
1	A	57	ILE	4.5
1	B	85	GLN	4.4
1	B	386	ASP	4.1
1	A	2	GLU	4.1
1	A	62	ILE	4.1
1	A	60	PRO	4.0
1	A	86	HIS	4.0
1	A	249	ALA	3.9
1	A	56	SER	3.9
1	A	55	ALA	3.8
1	A	6	HIS	3.7
1	A	50	ALA	3.7
1	A	61	SER	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	461	LYS	3.4
1	A	446	TRP	3.4
1	B	371	ASP	3.3
1	A	253	PHE	3.2
1	A	54	ALA	3.2
1	A	441	GLY	3.2
1	B	289	MET	3.1
1	A	87	LYS	3.1
1	B	287	VAL	3.1
1	A	34	PHE	3.1
1	B	310	ASP	3.1
1	A	63	LEU	3.0
1	A	248	VAL	3.0
1	A	174	ASN	3.0
1	B	291	PRO	3.0
1	A	66	VAL	3.0
1	A	449	LYS	3.0
1	B	290	PHE	3.0
1	A	59	LEU	3.0
1	A	35	VAL	2.9
1	A	171	LEU	2.9
1	A	453	ASP	2.9
1	A	51	VAL	2.9
1	B	217	THR	2.8
1	B	288	PHE	2.7
1	A	175	ILE	2.7
1	B	308	GLU	2.7
1	B	451	SER	2.7
1	A	65	GLY	2.6
1	A	33	GLY	2.6
1	B	87	LYS	2.6
1	A	223	HIS	2.6
1	A	79	LEU	2.6
1	A	39	MET	2.5
1	A	41	GLY	2.5
1	A	83	GLY	2.5
1	B	324	THR	2.5
1	B	329	ALA	2.5
1	B	6	HIS	2.4
1	B	446	TRP	2.3
1	A	227	PHE	2.3
1	B	328	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	171	LEU	2.3
1	B	453	ASP	2.3
1	B	369	CYS	2.2
1	A	31	GLY	2.2
1	B	325	GLY	2.2
1	B	86	HIS	2.1
1	A	224	VAL	2.1
1	A	53	ILE	2.0
1	A	257	THR	2.0
1	A	82	ALA	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

There are no carbohydrates in this entry.

6.4 Ligands [\(i\)](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	RB	B	5002	1/1	0.66	0.20	186,186,186,186	0
2	RB	A	5001	1/1	0.80	0.10	182,182,182,182	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.