



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:45 am GMT

PDB ID : 4E3C
Title : X-ray crystal structure of human IKK2 in an active conformation
Authors : Polley, S.; Huang, D.B.; Hauenstein, A.V.; Ghosh, G.; Huxford, T.
Deposited on : 2012-03-09
Resolution : 3.98 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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

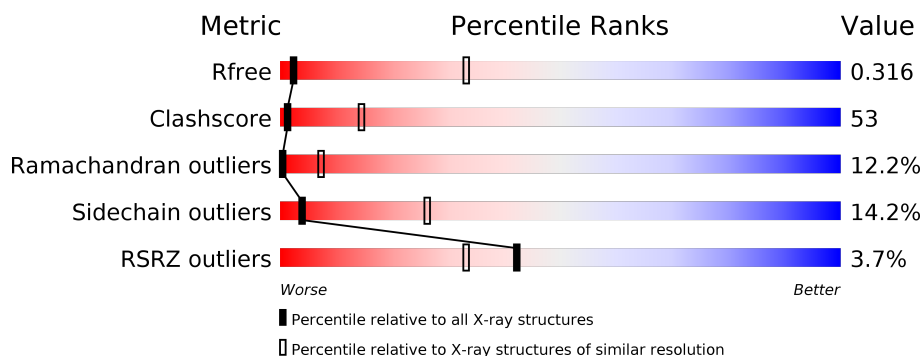
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.98 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}	100719	1066 (4.36-3.60)
Clashscore	112137	1163 (4.36-3.60)
Ramachandran outliers	110173	1119 (4.36-3.60)
Sidechain outliers	110143	1108 (4.36-3.60)
RSRZ outliers	101464	1078 (4.36-3.60)

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. 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.

Mol	Chain	Length	Quality of chain
1	A	669	<div> <div>4%</div> <div>28% 49% 14% 7%</div> </div>
1	B	669	<div> <div>3%</div> <div>28% 48% 17% 6%</div> </div>
1	C	669	<div> <div>2%</div> <div>28% 48% 16% 7%</div> </div>
1	D	669	<div> <div>3%</div> <div>28% 50% 14% 7%</div> </div>
1	E	669	<div> <div>4%</div> <div>27% 51% 14% 7%</div> </div>
1	F	669	<div> <div>5%</div> <div>26% 50% 15% 7%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 30416 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 Inhibitor of nuclear factor kappa-B kinase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			
1	B	632	Total	C	N	O	S	0	0	0
			5116	3219	904	959	34			
1	C	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			
1	D	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			
1	E	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			
1	F	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ASN	-	EXPRESSION TAG	UNP O14920
A	2	LEU	-	EXPRESSION TAG	UNP O14920
A	3	TYR	-	EXPRESSION TAG	UNP O14920
A	4	PHE	-	EXPRESSION TAG	UNP O14920
A	5	GLN	-	EXPRESSION TAG	UNP O14920
A	6	GLY	-	EXPRESSION TAG	UNP O14920
A	7	ALA	-	EXPRESSION TAG	UNP O14920
A	8	MET	-	EXPRESSION TAG	UNP O14920
A	9	GLY	-	EXPRESSION TAG	UNP O14920
A	10	SER	-	EXPRESSION TAG	UNP O14920
A	177	GLU	SER	ENGINEERED MUTATION	UNP O14920
A	181	GLU	SER	ENGINEERED MUTATION	UNP O14920
B	1	ASN	-	EXPRESSION TAG	UNP O14920
B	2	LEU	-	EXPRESSION TAG	UNP O14920
B	3	TYR	-	EXPRESSION TAG	UNP O14920
B	4	PHE	-	EXPRESSION TAG	UNP O14920
B	5	GLN	-	EXPRESSION TAG	UNP O14920

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	GLY	-	EXPRESSION TAG	UNP O14920
B	7	ALA	-	EXPRESSION TAG	UNP O14920
B	8	MET	-	EXPRESSION TAG	UNP O14920
B	9	GLY	-	EXPRESSION TAG	UNP O14920
B	10	SER	-	EXPRESSION TAG	UNP O14920
B	177	GLU	SER	ENGINEERED MUTATION	UNP O14920
B	181	GLU	SER	ENGINEERED MUTATION	UNP O14920
C	1	ASN	-	EXPRESSION TAG	UNP O14920
C	2	LEU	-	EXPRESSION TAG	UNP O14920
C	3	TYR	-	EXPRESSION TAG	UNP O14920
C	4	PHE	-	EXPRESSION TAG	UNP O14920
C	5	GLN	-	EXPRESSION TAG	UNP O14920
C	6	GLY	-	EXPRESSION TAG	UNP O14920
C	7	ALA	-	EXPRESSION TAG	UNP O14920
C	8	MET	-	EXPRESSION TAG	UNP O14920
C	9	GLY	-	EXPRESSION TAG	UNP O14920
C	10	SER	-	EXPRESSION TAG	UNP O14920
C	177	GLU	SER	ENGINEERED MUTATION	UNP O14920
C	181	GLU	SER	ENGINEERED MUTATION	UNP O14920
D	1	ASN	-	EXPRESSION TAG	UNP O14920
D	2	LEU	-	EXPRESSION TAG	UNP O14920
D	3	TYR	-	EXPRESSION TAG	UNP O14920
D	4	PHE	-	EXPRESSION TAG	UNP O14920
D	5	GLN	-	EXPRESSION TAG	UNP O14920
D	6	GLY	-	EXPRESSION TAG	UNP O14920
D	7	ALA	-	EXPRESSION TAG	UNP O14920
D	8	MET	-	EXPRESSION TAG	UNP O14920
D	9	GLY	-	EXPRESSION TAG	UNP O14920
D	10	SER	-	EXPRESSION TAG	UNP O14920
D	177	GLU	SER	ENGINEERED MUTATION	UNP O14920
D	181	GLU	SER	ENGINEERED MUTATION	UNP O14920
E	1	ASN	-	EXPRESSION TAG	UNP O14920
E	2	LEU	-	EXPRESSION TAG	UNP O14920
E	3	TYR	-	EXPRESSION TAG	UNP O14920
E	4	PHE	-	EXPRESSION TAG	UNP O14920
E	5	GLN	-	EXPRESSION TAG	UNP O14920
E	6	GLY	-	EXPRESSION TAG	UNP O14920
E	7	ALA	-	EXPRESSION TAG	UNP O14920
E	8	MET	-	EXPRESSION TAG	UNP O14920
E	9	GLY	-	EXPRESSION TAG	UNP O14920
E	10	SER	-	EXPRESSION TAG	UNP O14920
E	177	GLU	SER	ENGINEERED MUTATION	UNP O14920

Continued on next page...

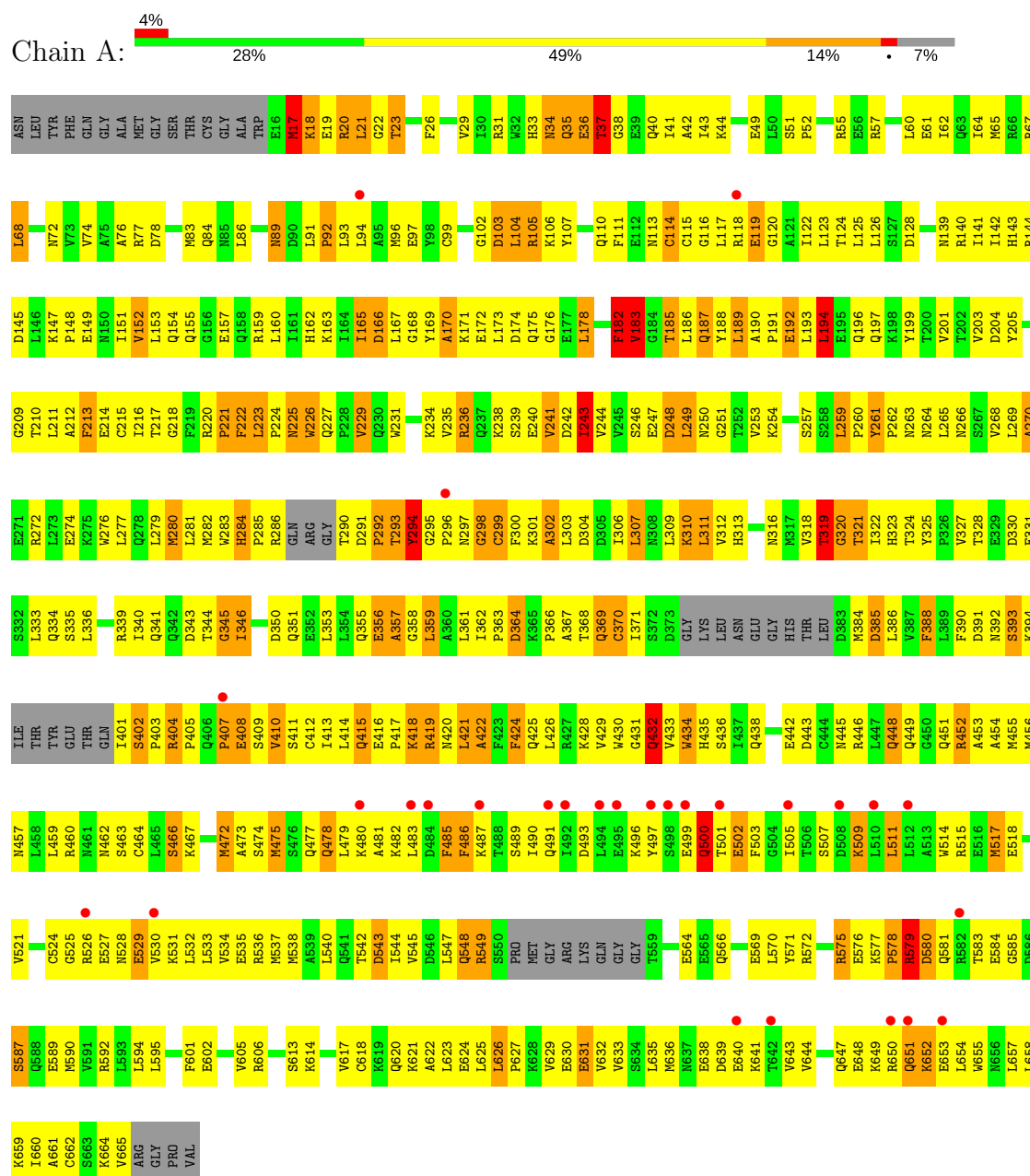
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	181	GLU	SER	ENGINEERED MUTATION	UNP O14920
F	1	ASN	-	EXPRESSION TAG	UNP O14920
F	2	LEU	-	EXPRESSION TAG	UNP O14920
F	3	TYR	-	EXPRESSION TAG	UNP O14920
F	4	PHE	-	EXPRESSION TAG	UNP O14920
F	5	GLN	-	EXPRESSION TAG	UNP O14920
F	6	GLY	-	EXPRESSION TAG	UNP O14920
F	7	ALA	-	EXPRESSION TAG	UNP O14920
F	8	MET	-	EXPRESSION TAG	UNP O14920
F	9	GLY	-	EXPRESSION TAG	UNP O14920
F	10	SER	-	EXPRESSION TAG	UNP O14920
F	177	GLU	SER	ENGINEERED MUTATION	UNP O14920
F	181	GLU	SER	ENGINEERED MUTATION	UNP O14920

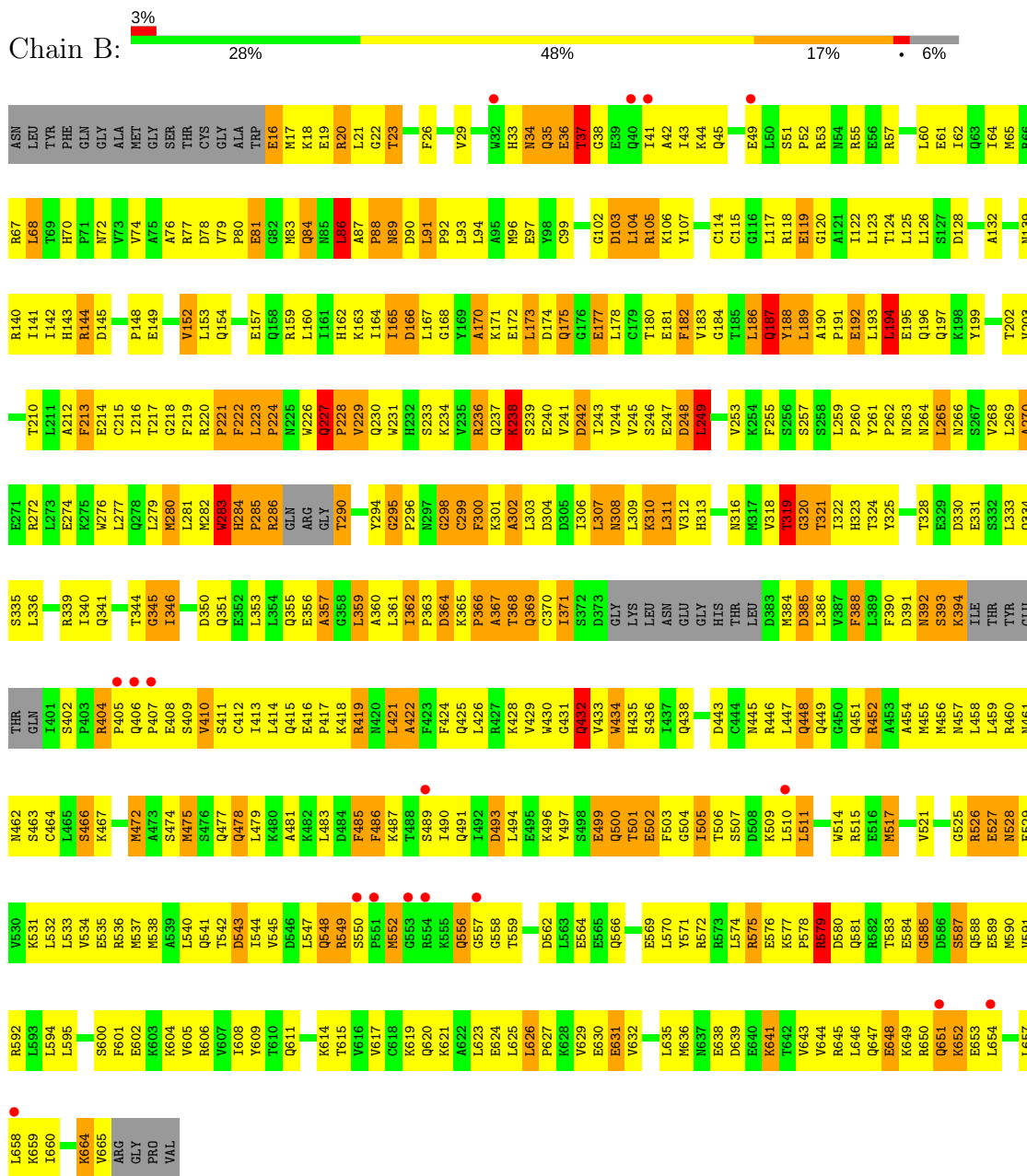
3 Residue-property plots

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.

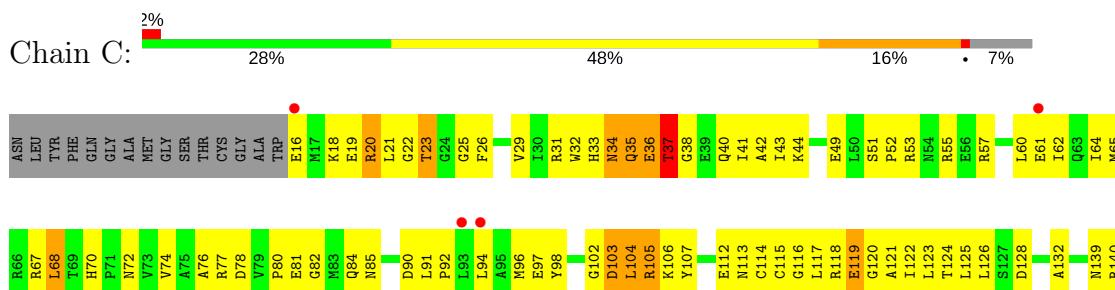
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

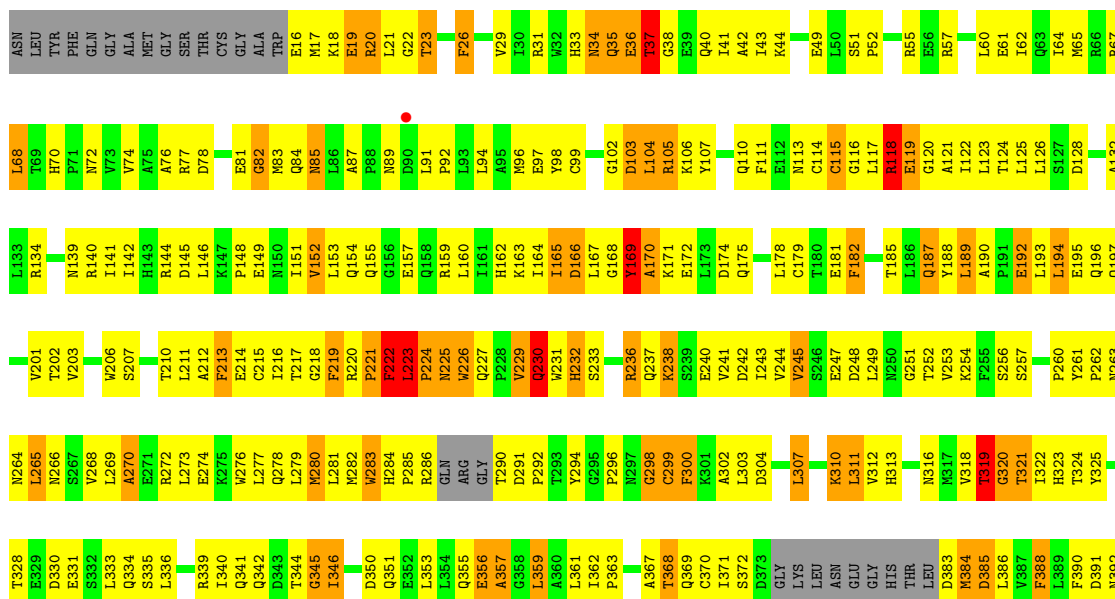


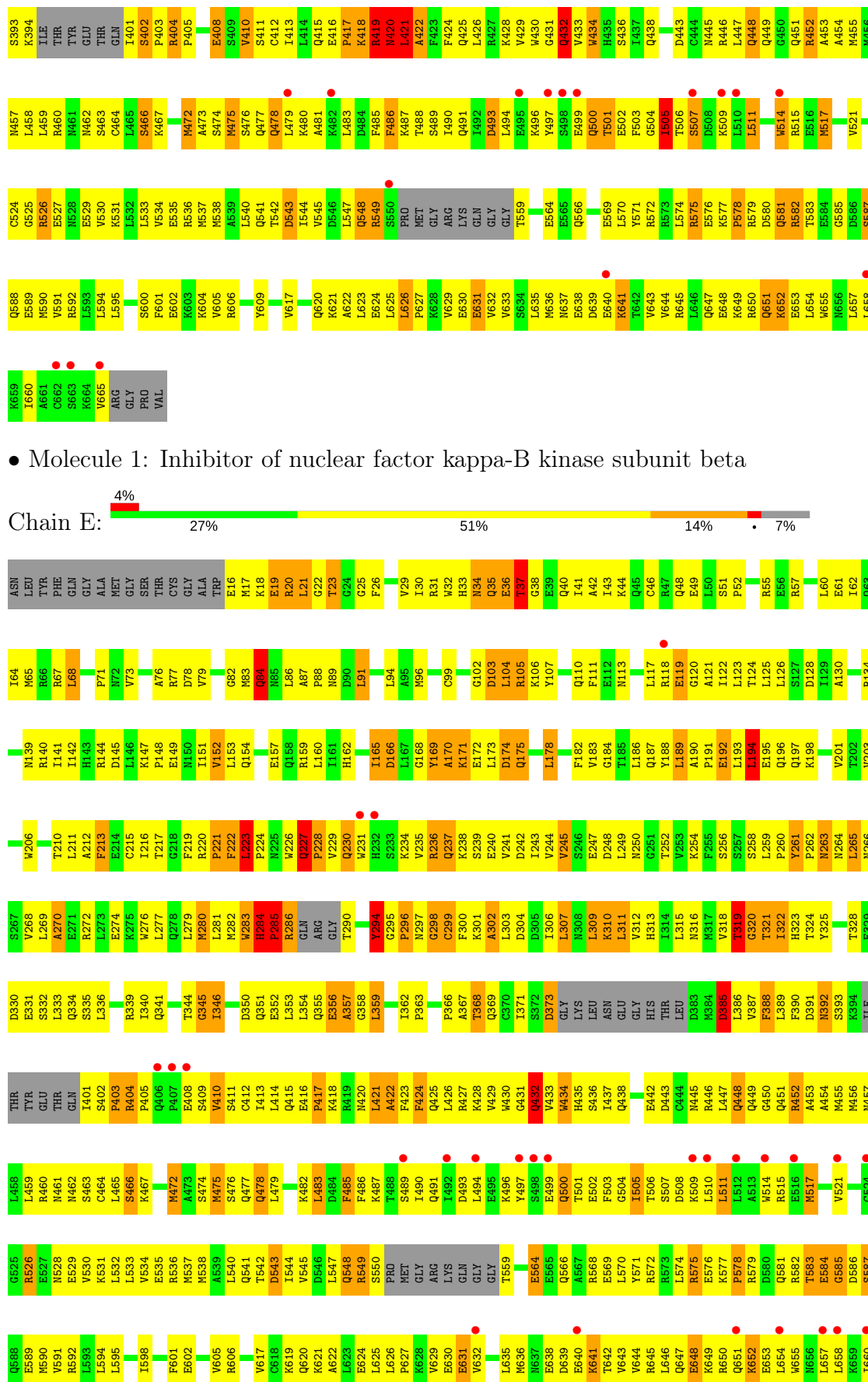
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

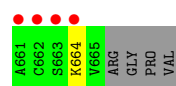


- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

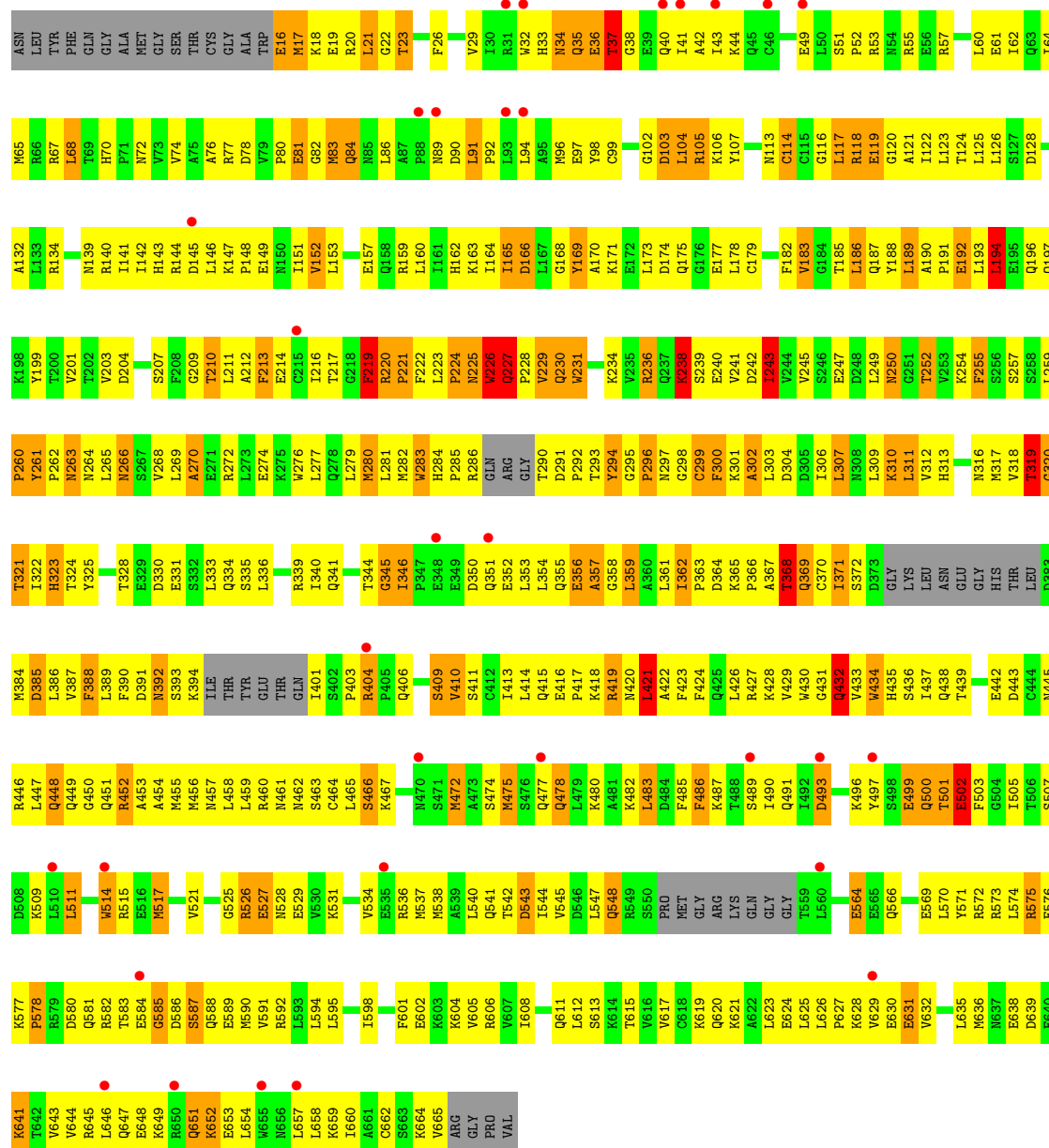








● Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.81Å 170.81Å 509.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.98 49.73 – 3.97	Depositor EDS
% Data completeness (in resolution range)	81.0 (29.84-3.98) 88.5 (49.73-3.97)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 4.00Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.267 , 0.299 0.285 , 0.316	Depositor DCC
R_{free} test set	2221 reflections (3.82%)	DCC
Wilson B-factor (Å ²)	113.9	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 155.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	30416	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	0/5142	0.61	3/6937 (0.0%)
1	B	0.47	0/5200	0.69	3/7014 (0.0%)
1	C	0.44	0/5142	0.58	0/6937
1	D	0.45	0/5142	0.69	3/6937 (0.0%)
1	E	0.44	0/5142	0.57	0/6937
1	F	0.42	0/5142	0.57	0/6937
All	All	0.45	0/30910	0.62	9/41699 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	118	ARG	NE-CZ-NH1	-21.84	109.38	120.30
1	D	118	ARG	NE-CZ-NH2	21.77	131.18	120.30
1	B	144	ARG	NE-CZ-NH1	-20.91	109.84	120.30
1	B	144	ARG	NE-CZ-NH2	19.92	130.26	120.30
1	D	118	ARG	CD-NE-CZ	9.85	137.39	123.60
1	B	144	ARG	CD-NE-CZ	8.65	135.72	123.60
1	A	500	GLN	CA-C-N	-7.28	101.18	117.20
1	A	422	ALA	N-CA-C	-6.32	93.93	111.00
1	A	500	GLN	CA-C-O	5.59	131.84	120.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5060	0	5109	581	0
1	B	5116	0	5169	569	0
1	C	5060	0	5109	522	0
1	D	5060	0	5109	557	0
1	E	5060	0	5107	554	0
1	F	5060	0	5107	584	0
All	All	30416	0	30710	3237	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 53.

All (3237) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:ARG:NH1	1:B:419:ARG:HB2	1.55	1.18
1:B:366:PRO:HB2	1:B:368:THR:HG23	1.29	1.14
1:C:496:LYS:HE2	1:C:654:LEU:HD21	1.20	1.14
1:F:626:LEU:H	1:F:627:PRO:HD2	1.13	1.13
1:D:479:LEU:HD11	1:D:641:LYS:HG2	1.28	1.11
1:C:479:LEU:HD11	1:C:641:LYS:HG2	1.30	1.08
1:A:417:PRO:HA	1:B:320:GLY:HA3	1.35	1.08
1:F:401:ILE:HG12	1:F:403:PRO:HD3	1.31	1.08
1:E:284:HIS:HB3	1:E:285:PRO:HD2	1.42	1.02
1:E:265:LEU:HG	1:E:266:ASN:H	1.23	1.02
1:B:479:LEU:HD11	1:B:641:LYS:HG2	1.41	1.02
1:C:418:LYS:HZ2	1:C:421:LEU:HD12	1.25	1.01
1:A:533:LEU:HD22	1:A:629:VAL:HG12	1.41	1.01
1:B:571:TYR:HB3	1:B:575:ARG:HH21	1.24	1.01
1:B:419:ARG:HH11	1:B:419:ARG:HB2	1.24	1.00
1:A:279:LEU:HA	1:A:286:ARG:HH12	1.24	1.00
1:F:279:LEU:HD22	1:F:292:PRO:HD3	1.43	1.00
1:F:387:VAL:HG11	1:F:450:GLY:HA2	1.43	0.99
1:A:419:ARG:H	1:A:419:ARG:NE	1.59	0.99
1:C:402:SER:H	1:C:403:PRO:HD2	1.27	0.99
1:C:417:PRO:HA	1:D:320:GLY:HA3	1.44	0.98
1:C:259:LEU:HD22	1:C:260:PRO:HD2	1.41	0.98
1:C:571:TYR:HB3	1:C:575:ARG:HH21	1.29	0.98
1:F:389:LEU:HD21	1:F:454:ALA:HB2	1.45	0.98
1:A:571:TYR:HB3	1:A:575:ARG:HH21	1.28	0.98
1:E:387:VAL:HG11	1:E:450:GLY:HA2	1.46	0.98
1:A:402:SER:H	1:A:403:PRO:HD3	1.30	0.97
1:A:417:PRO:HA	1:B:320:GLY:CA	1.94	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:ARG:HH22	1:D:345:GLY:HA3	1.30	0.97
1:E:571:TYR:HB3	1:E:575:ARG:HH21	1.27	0.97
1:F:266:ASN:HB3	1:F:269:LEU:HB2	1.47	0.96
1:F:389:LEU:HD21	1:F:454:ALA:CB	1.94	0.96
1:F:142:ILE:HG13	1:F:173:LEU:HD11	1.44	0.96
1:D:571:TYR:HB3	1:D:575:ARG:HH21	1.29	0.96
1:F:571:TYR:HB3	1:F:575:ARG:HH21	1.31	0.96
1:B:165:ILE:HG22	1:B:166:ASP:H	1.30	0.96
1:D:229:VAL:HG23	1:D:230:GLN:H	1.30	0.96
1:F:357:ALA:HA	1:F:452:ARG:HH12	1.32	0.95
1:D:582:ARG:H	1:D:582:ARG:HE	1.00	0.95
1:F:427:ARG:HE	1:F:575:ARG:HG3	1.28	0.95
1:A:266:ASN:HB3	1:A:269:LEU:HB2	1.48	0.95
1:A:223:LEU:HD22	1:A:235:VAL:HG23	1.47	0.94
1:D:165:ILE:HG22	1:D:166:ASP:H	1.32	0.94
1:D:213:PHE:CE1	1:D:221:PRO:HB2	2.02	0.94
1:A:579:ARG:H	1:A:579:ARG:HD3	1.29	0.94
1:D:402:SER:H	1:D:403:PRO:HD2	1.32	0.93
1:D:266:ASN:HB3	1:D:269:LEU:HB2	1.49	0.93
1:B:654:LEU:HD23	1:C:654:LEU:HD23	1.48	0.93
1:F:80:PRO:HB2	1:F:83:MET:HB2	1.51	0.93
1:A:265:LEU:HD23	1:A:266:ASN:H	1.34	0.93
1:F:229:VAL:HG22	1:F:230:GLN:H	1.34	0.93
1:B:87:ALA:HB2	1:B:93:LEU:HD11	1.49	0.93
1:C:55:ARG:NH1	1:C:91:LEU:HD11	1.83	0.93
1:D:404:ARG:NH2	1:D:404:ARG:H	1.67	0.93
1:C:266:ASN:HB3	1:C:269:LEU:HB2	1.51	0.92
1:B:266:ASN:HB3	1:B:269:LEU:HB2	1.50	0.92
1:A:118:ARG:HB2	1:A:264:ASN:HB3	1.47	0.92
1:B:226:TRP:O	1:B:227:GLN:HG3	1.70	0.92
1:E:266:ASN:HB3	1:E:269:LEU:HB2	1.49	0.92
1:A:417:PRO:CA	1:B:320:GLY:HA3	1.98	0.91
1:C:165:ILE:HG22	1:C:166:ASP:H	1.35	0.91
1:C:511:LEU:HG	1:C:515:ARG:HH12	1.35	0.91
1:B:496:LYS:HE2	1:B:654:LEU:HD21	1.51	0.91
1:A:421:LEU:HD13	1:A:585:GLY:HA3	1.51	0.90
1:E:505:ILE:HD12	1:E:506:THR:H	1.36	0.90
1:A:292:PRO:HG3	1:A:297:ASN:HD22	1.37	0.90
1:E:165:ILE:HG22	1:E:166:ASP:H	1.35	0.90
1:C:500:GLN:HE22	1:C:504:GLY:HA3	1.34	0.90
1:E:17:MET:HG2	1:E:33:HIS:H	1.37	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:LEU:HG	1:B:515:ARG:HH12	1.36	0.90
1:F:165:ILE:HG22	1:F:166:ASP:H	1.37	0.90
1:E:244:VAL:HB	1:E:256:SER:HB3	1.51	0.89
1:E:410:VAL:HG12	1:E:411:SER:H	1.37	0.89
1:D:505:ILE:HD12	1:D:506:THR:H	1.38	0.89
1:E:259:LEU:HD22	1:E:274:GLU:HG3	1.55	0.89
1:C:447:LEU:HD23	1:C:609:TYR:HE1	1.37	0.89
1:E:295:GLY:H	1:E:296:PRO:HD2	1.37	0.88
1:B:80:PRO:HB2	1:B:83:MET:HB2	1.56	0.88
1:C:486:PHE:CE1	1:C:647:GLN:HB3	2.07	0.88
1:F:410:VAL:HG12	1:F:411:SER:H	1.39	0.88
1:A:473:ALA:HB1	1:A:530:VAL:HG11	1.56	0.88
1:A:213:PHE:HA	1:A:277:LEU:HD21	1.57	0.87
1:A:511:LEU:HG	1:A:515:ARG:HH12	1.40	0.87
1:E:265:LEU:HD11	1:E:270:ALA:HA	1.56	0.87
1:D:481:ALA:HB1	1:E:482:LYS:HD2	1.56	0.87
1:A:165:ILE:HG22	1:A:166:ASP:H	1.38	0.87
1:F:352:GLU:OE2	1:F:619:LYS:HE2	1.72	0.87
1:C:221:PRO:O	1:C:222:PHE:HB2	1.70	0.87
1:D:170:ALA:HB3	1:D:178:LEU:HD23	1.56	0.87
1:E:144:ARG:HD2	1:E:171:LYS:HB2	1.57	0.87
1:F:279:LEU:HD12	1:F:286:ARG:HG2	1.54	0.87
1:A:434:TRP:HB3	1:A:571:TYR:CZ	2.09	0.86
1:E:511:LEU:HG	1:E:515:ARG:HH12	1.40	0.86
1:F:626:LEU:N	1:F:627:PRO:HD2	1.85	0.86
1:C:410:VAL:HG12	1:C:411:SER:H	1.39	0.86
1:D:192:GLU:HG2	1:D:283:TRP:HB3	1.57	0.86
1:C:458:LEU:HD11	1:C:544:ILE:HG21	1.56	0.86
1:B:500:GLN:HE22	1:B:504:GLY:HA3	1.39	0.86
1:D:533:LEU:HD22	1:D:629:VAL:HG12	1.57	0.86
1:A:118:ARG:HH22	1:A:438:GLN:HG2	1.41	0.86
1:F:49:GLU:HG2	1:F:91:LEU:HD11	1.58	0.86
1:D:511:LEU:HG	1:D:515:ARG:HH12	1.39	0.86
1:F:511:LEU:HG	1:F:515:ARG:HH12	1.40	0.86
1:A:500:GLN:C	1:A:500:GLN:HE21	1.79	0.85
1:B:410:VAL:HG12	1:B:411:SER:H	1.40	0.85
1:D:227:GLN:HB2	1:D:229:VAL:HG22	1.58	0.85
1:D:410:VAL:HG12	1:D:411:SER:H	1.41	0.85
1:F:220:ARG:H	1:F:223:LEU:HD12	1.40	0.85
1:F:458:LEU:HD21	1:F:619:LYS:HA	1.57	0.85
1:A:319:THR:HG23	1:A:320:GLY:H	1.40	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:GLU:HG3	1:D:241:VAL:HG23	1.58	0.85
1:E:193:LEU:HD22	1:E:203:VAL:HG21	1.58	0.85
1:B:171:LYS:HG2	1:B:177:GLU:HA	1.58	0.85
1:B:419:ARG:HB2	1:B:419:ARG:CZ	2.05	0.85
1:D:582:ARG:N	1:D:582:ARG:HE	1.73	0.85
1:F:318:VAL:HG21	1:F:346:ILE:HD11	1.59	0.85
1:B:319:THR:HG23	1:B:320:GLY:H	1.42	0.85
1:C:18:LYS:HB2	1:C:31:ARG:HB3	1.59	0.85
1:A:318:VAL:HG21	1:A:346:ILE:HD11	1.58	0.85
1:F:387:VAL:CG1	1:F:450:GLY:HA2	2.07	0.84
1:E:321:THR:HG21	1:E:447:LEU:HD11	1.60	0.84
1:A:358:GLY:CA	1:A:457:ASN:HB2	2.08	0.84
1:D:144:ARG:HD2	1:D:171:LYS:HB3	1.59	0.84
1:E:530:VAL:HG22	1:E:632:VAL:HG12	1.59	0.84
1:F:67:ARG:HH21	1:F:68:LEU:HD12	1.43	0.84
1:A:481:ALA:HB1	1:F:482:LYS:NZ	1.92	0.84
1:B:172:GLU:HG3	1:B:175:GLN:H	1.42	0.84
1:D:193:LEU:HD22	1:D:203:VAL:HG21	1.60	0.84
1:E:111:PHE:CD1	1:E:575:ARG:HD2	2.13	0.83
1:A:193:LEU:HD22	1:A:203:VAL:HG21	1.60	0.83
1:C:418:LYS:NZ	1:C:421:LEU:HD12	1.92	0.83
1:F:126:LEU:HB3	1:F:303:LEU:HD21	1.60	0.83
1:C:496:LYS:HE2	1:C:654:LEU:CD2	2.06	0.83
1:D:657:LEU:HD23	1:E:658:LEU:HD21	1.59	0.83
1:A:655:TRP:CD1	1:F:500:GLN:HG2	2.14	0.83
1:E:430:TRP:HE1	1:E:587:SER:HA	1.40	0.83
1:F:427:ARG:HH21	1:F:575:ARG:HG2	1.43	0.83
1:A:652:LYS:HA	1:F:496:LYS:HE2	1.59	0.83
1:E:279:LEU:HD11	1:E:290:THR:HB	1.61	0.83
1:A:67:ARG:HH21	1:A:68:LEU:HD12	1.44	0.82
1:A:659:LYS:HD3	1:F:500:GLN:HE22	1.41	0.82
1:B:353:LEU:HB3	1:B:386:LEU:HD11	1.59	0.82
1:A:419:ARG:CZ	1:A:419:ARG:H	1.93	0.82
1:D:318:VAL:HG21	1:D:346:ILE:HD11	1.60	0.82
1:F:32:TRP:HZ3	1:F:83:MET:HB3	1.44	0.82
1:A:410:VAL:HG12	1:A:411:SER:H	1.44	0.82
1:B:318:VAL:HG21	1:B:346:ILE:HD11	1.62	0.82
1:C:193:LEU:HD22	1:C:203:VAL:HG21	1.60	0.82
1:B:193:LEU:HD22	1:B:203:VAL:HG21	1.60	0.82
1:E:427:ARG:HE	1:E:575:ARG:HG3	1.43	0.82
1:A:657:LEU:O	1:F:658:LEU:HD11	1.79	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ALA:HB1	1:F:482:LYS:HZ2	1.45	0.82
1:E:265:LEU:HG	1:E:266:ASN:N	1.94	0.81
1:A:213:PHE:CE1	1:A:221:PRO:HB2	2.15	0.81
1:C:67:ARG:HH21	1:C:68:LEU:HD12	1.44	0.81
1:D:115:CYS:O	1:D:218:GLY:HA3	1.80	0.81
1:F:213:PHE:HA	1:F:277:LEU:HD21	1.61	0.81
1:F:249:LEU:HD21	1:F:418:LYS:HE2	1.61	0.81
1:C:421:LEU:HG	1:D:342:GLN:O	1.80	0.81
1:B:67:ARG:HH21	1:B:68:LEU:HD12	1.45	0.81
1:C:402:SER:N	1:C:403:PRO:HD2	1.94	0.81
1:E:126:LEU:HB3	1:E:303:LEU:HD21	1.63	0.81
1:E:309:LEU:HD22	1:E:310:LYS:N	1.95	0.81
1:F:282:MET:HG2	1:F:286:ARG:CZ	2.11	0.81
1:F:321:THR:HG21	1:F:447:LEU:HD11	1.62	0.80
1:D:319:THR:HG23	1:D:320:GLY:H	1.45	0.80
1:F:421:LEU:HB3	1:F:586:ASP:HA	1.61	0.80
1:A:61:GLU:HB2	1:A:178:LEU:HD21	1.60	0.80
1:E:431:GLY:HA2	1:E:571:TYR:CE2	2.15	0.80
1:F:319:THR:HG23	1:F:320:GLY:H	1.46	0.80
1:F:353:LEU:HB3	1:F:386:LEU:HD11	1.62	0.80
1:A:292:PRO:HG3	1:A:296:PRO:O	1.81	0.80
1:C:401:ILE:O	1:C:401:ILE:HD13	1.82	0.80
1:F:236:ARG:HH22	1:F:283:TRP:HE1	1.29	0.80
1:F:193:LEU:HD22	1:F:203:VAL:HG21	1.61	0.79
1:C:318:VAL:HG21	1:C:346:ILE:HD11	1.62	0.79
1:D:654:LEU:HD23	1:E:654:LEU:HD23	1.63	0.79
1:A:547:LEU:HD22	1:A:614:LYS:HE2	1.65	0.79
1:C:279:LEU:O	1:C:286:ARG:HD2	1.82	0.79
1:B:360:ALA:HB3	1:E:36:GLU:HG3	1.62	0.79
1:F:467:LYS:HD3	1:F:541:GLN:CG	2.13	0.79
1:C:418:LYS:O	1:C:419:ARG:HB3	1.81	0.79
1:D:536:ARG:NH1	1:D:625:LEU:HD13	1.96	0.79
1:E:319:THR:HG23	1:E:320:GLY:H	1.47	0.79
1:F:116:GLY:HA3	1:F:217:THR:O	1.82	0.79
1:A:627:PRO:HA	1:A:630:GLU:HB3	1.65	0.79
1:E:282:MET:HB3	1:E:286:ARG:HG3	1.63	0.79
1:A:320:GLY:HA3	1:B:417:PRO:HA	1.65	0.79
1:A:479:LEU:HB3	1:A:640:GLU:HG2	1.65	0.79
1:B:490:ILE:HD11	1:B:651:GLN:HG2	1.64	0.79
1:F:354:LEU:HD22	1:F:457:ASN:HB2	1.65	0.79
1:A:490:ILE:HG21	1:A:518:GLU:HB2	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:GLY:HA3	1:D:417:PRO:HA	1.64	0.78
1:A:480:LYS:HG2	1:A:527:GLU:HB2	1.64	0.78
1:A:657:LEU:HB3	1:F:658:LEU:HD21	1.63	0.78
1:B:481:ALA:CB	1:C:478:GLN:HG3	2.13	0.78
1:D:517:MET:HG2	1:D:650:ARG:CZ	2.14	0.78
1:D:279:LEU:O	1:D:286:ARG:HD2	1.82	0.78
1:F:430:TRP:HE1	1:F:587:SER:HA	1.48	0.78
1:E:427:ARG:HH21	1:E:575:ARG:HG2	1.46	0.78
1:F:426:LEU:HA	1:F:429:VAL:HB	1.66	0.78
1:C:649:LYS:HA	1:C:652:LYS:HB3	1.66	0.78
1:E:318:VAL:HG21	1:E:346:ILE:HD11	1.66	0.78
1:E:424:PHE:HD1	1:E:582:ARG:CZ	1.97	0.78
1:F:17:MET:O	1:F:18:LYS:HD2	1.83	0.78
1:F:486:PHE:HZ	1:F:651:GLN:OE1	1.67	0.78
1:A:479:LEU:HD12	1:A:640:GLU:CG	2.14	0.78
1:E:578:PRO:HB2	1:E:581:GLN:OE1	1.83	0.77
1:C:458:LEU:HD11	1:C:544:ILE:CG2	2.14	0.77
1:D:479:LEU:CD1	1:D:641:LYS:HG2	2.14	0.77
1:A:192:GLU:HG2	1:A:283:TRP:HB2	1.67	0.77
1:C:419:ARG:NH2	1:D:345:GLY:HA3	1.99	0.77
1:A:353:LEU:HB3	1:A:386:LEU:HD11	1.67	0.77
1:C:259:LEU:HB2	1:C:274:GLU:HG3	1.65	0.77
1:D:290:THR:HG23	1:D:296:PRO:HA	1.67	0.77
1:F:89:ASN:HB2	1:F:91:LEU:HG	1.66	0.77
1:D:67:ARG:HH21	1:D:68:LEU:HD12	1.47	0.77
1:D:478:GLN:HA	1:E:478:GLN:HG3	1.66	0.77
1:E:356:GLU:HA	1:E:453:ALA:HB2	1.65	0.77
1:D:261:TYR:N	1:D:262:PRO:HD2	2.00	0.77
1:C:21:LEU:HG	1:C:165:ILE:HD13	1.67	0.76
1:D:404:ARG:H	1:D:404:ARG:HH21	1.29	0.76
1:B:213:PHE:CE2	1:B:221:PRO:HG2	2.20	0.76
1:C:185:THR:O	1:C:186:LEU:HD23	1.85	0.76
1:D:467:LYS:HD3	1:D:541:GLN:NE2	2.00	0.76
1:E:531:LYS:HB3	1:E:531:LYS:HZ3	1.50	0.76
1:E:223:LEU:H	1:E:224:PRO:HD2	1.48	0.76
1:F:263:ASN:ND2	1:F:265:LEU:HD22	2.00	0.76
1:F:626:LEU:H	1:F:627:PRO:CD	1.94	0.76
1:E:353:LEU:HB3	1:E:386:LEU:HD11	1.68	0.76
1:F:104:LEU:HD23	1:F:148:PRO:HB3	1.67	0.76
1:B:286:ARG:HA	1:B:290:THR:HG21	1.67	0.76
1:B:260:PRO:C	1:B:262:PRO:HD2	2.05	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:GLU:HG3	1:B:592:ARG:HH12	1.50	0.76
1:E:420:ASN:O	1:E:421:LEU:HB2	1.84	0.76
1:F:263:ASN:HD21	1:F:265:LEU:HD22	1.50	0.76
1:F:627:PRO:HA	1:F:630:GLU:HB3	1.67	0.76
1:E:387:VAL:CG1	1:E:450:GLY:HA2	2.15	0.76
1:E:574:LEU:HD21	1:E:582:ARG:HH22	1.50	0.76
1:A:402:SER:N	1:A:403:PRO:HD3	2.01	0.76
1:B:649:LYS:HA	1:B:652:LYS:HB3	1.66	0.76
1:D:21:LEU:HG	1:D:165:ILE:HD13	1.68	0.76
1:A:21:LEU:HG	1:A:165:ILE:HD13	1.66	0.76
1:C:362:ILE:HD12	1:C:362:ILE:H	1.51	0.76
1:E:362:ILE:H	1:E:362:ILE:HD12	1.50	0.76
1:C:486:PHE:CZ	1:C:647:GLN:HB3	2.21	0.75
1:C:319:THR:HG23	1:C:320:GLY:H	1.50	0.75
1:A:140:ARG:HE	1:A:173:LEU:HD23	1.51	0.75
1:E:105:ARG:HD2	1:E:148:PRO:HB2	1.67	0.75
1:F:192:GLU:HG2	1:F:283:TRP:HB3	1.68	0.75
1:A:61:GLU:OE1	1:A:168:GLY:HA2	1.87	0.75
1:C:570:LEU:HD22	1:C:590:MET:HE2	1.67	0.75
1:E:282:MET:HG2	1:E:286:ARG:HE	1.49	0.75
1:E:67:ARG:HH21	1:E:68:LEU:HD12	1.50	0.75
1:F:362:ILE:H	1:F:362:ILE:HD12	1.51	0.75
1:D:214:GLU:HG3	1:D:220:ARG:H	1.51	0.75
1:E:309:LEU:HD22	1:E:310:LYS:H	1.50	0.75
1:D:496:LYS:HA	1:E:655:TRP:NE1	2.02	0.75
1:E:540:LEU:HA	1:E:543:ASP:HB2	1.69	0.75
1:F:430:TRP:CZ3	1:F:570:LEU:HB3	2.22	0.75
1:A:282:MET:HG3	1:A:283:TRP:CE3	2.21	0.74
1:C:506:THR:HG22	1:C:507:SER:H	1.52	0.74
1:A:657:LEU:C	1:F:658:LEU:HD11	2.08	0.74
1:C:540:LEU:HA	1:C:543:ASP:HB2	1.69	0.74
1:F:214:GLU:HG3	1:F:219:PHE:HA	1.69	0.74
1:B:457:ASN:HD21	1:B:619:LYS:NZ	1.84	0.74
1:D:223:LEU:HD12	1:D:226:TRP:HB2	1.69	0.74
1:B:447:LEU:HD23	1:B:609:TYR:HE1	1.51	0.74
1:D:223:LEU:HB3	1:D:231:TRP:CZ3	2.22	0.74
1:D:232:HIS:O	1:D:236:ARG:HB2	1.88	0.74
1:B:367:ALA:C	1:B:369:GLN:H	1.90	0.74
1:E:505:ILE:HD12	1:E:506:THR:N	2.02	0.74
1:A:434:TRP:HB3	1:A:571:TYR:OH	1.88	0.74
1:A:417:PRO:C	1:B:320:GLY:HA3	2.08	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ILE:H	1:B:362:ILE:HD12	1.53	0.74
1:A:362:ILE:HD12	1:A:362:ILE:H	1.53	0.74
1:D:117:LEU:HB2	1:D:215:CYS:O	1.88	0.74
1:E:366:PRO:HG2	1:E:368:THR:HG22	1.70	0.74
1:A:490:ILE:HG12	1:A:517:MET:CE	2.17	0.74
1:B:451:GLN:NE2	1:B:611:GLN:HB3	2.03	0.74
1:C:496:LYS:NZ	1:C:654:LEU:HD11	2.03	0.74
1:E:265:LEU:CG	1:E:266:ASN:H	2.00	0.74
1:A:579:ARG:HH11	1:A:579:ARG:N	1.85	0.73
1:E:21:LEU:HB3	1:E:165:ILE:HG21	1.69	0.73
1:E:627:PRO:HA	1:E:630:GLU:HB3	1.68	0.73
1:A:309:LEU:HD11	1:A:311:LEU:HD23	1.70	0.73
1:A:358:GLY:HA3	1:A:457:ASN:HB2	1.70	0.73
1:B:261:TYR:N	1:B:262:PRO:HD2	2.03	0.73
1:D:242:ASP:OD1	1:D:257:SER:HB3	1.88	0.73
1:D:283:TRP:CE3	1:D:285:PRO:HD2	2.23	0.73
1:D:410:VAL:HA	1:D:413:ILE:HG22	1.68	0.73
1:F:570:LEU:HD22	1:F:590:MET:HE2	1.70	0.73
1:C:589:GLU:HG3	1:C:592:ARG:HH12	1.53	0.73
1:A:533:LEU:HD13	1:A:629:VAL:HA	1.69	0.73
1:B:226:TRP:C	1:B:227:GLN:HG3	2.07	0.73
1:D:265:LEU:HG	1:D:266:ASN:H	1.53	0.73
1:E:61:GLU:HB2	1:E:178:LEU:HD11	1.70	0.73
1:E:284:HIS:HB3	1:E:285:PRO:CD	2.17	0.73
1:E:626:LEU:H	1:E:627:PRO:HD2	1.54	0.73
1:F:29:VAL:HG12	1:F:44:LYS:HB2	1.70	0.73
1:F:540:LEU:HA	1:F:543:ASP:HB2	1.70	0.73
1:D:649:LYS:HA	1:D:652:LYS:HB3	1.70	0.73
1:A:589:GLU:HG3	1:A:592:ARG:HH12	1.53	0.73
1:B:410:VAL:HA	1:B:413:ILE:HG22	1.71	0.73
1:B:486:PHE:CZ	1:B:647:GLN:HB3	2.23	0.73
1:C:410:VAL:HA	1:C:413:ILE:HG22	1.71	0.73
1:E:368:THR:HG23	1:E:369:GLN:H	1.54	0.73
1:C:426:LEU:HA	1:C:429:VAL:HB	1.71	0.73
1:D:55:ARG:HH11	1:D:91:LEU:HD21	1.52	0.73
1:F:430:TRP:HZ3	1:F:570:LEU:HB3	1.52	0.73
1:A:417:PRO:O	1:B:320:GLY:HA3	1.89	0.73
1:E:192:GLU:HG2	1:E:283:TRP:HB3	1.70	0.73
1:A:205:TYR:HD1	1:A:290:THR:HG23	1.53	0.72
1:A:117:LEU:HD12	1:A:215:CYS:O	1.90	0.72
1:A:410:VAL:HA	1:A:413:ILE:HG22	1.69	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:LEU:HB3	1:D:386:LEU:HD11	1.71	0.72
1:A:294:TYR:O	1:A:301:LYS:HD3	1.88	0.72
1:F:223:LEU:N	1:F:224:PRO:HD2	2.04	0.72
1:F:265:LEU:O	1:F:266:ASN:HB2	1.88	0.72
1:A:290:THR:N	1:A:298:GLY:H	1.87	0.72
1:B:126:LEU:HB3	1:B:303:LEU:HD21	1.70	0.72
1:C:140:ARG:HH21	1:C:173:LEU:HD22	1.54	0.72
1:A:570:LEU:HD22	1:A:590:MET:HE2	1.72	0.72
1:B:422:ALA:O	1:B:585:GLY:HA2	1.90	0.72
1:C:223:LEU:HG	1:C:245:VAL:HG12	1.70	0.72
1:F:649:LYS:HA	1:F:652:LYS:HB3	1.72	0.72
1:A:340:ILE:HD11	1:A:351:GLN:OE1	1.90	0.72
1:A:659:LYS:HD3	1:F:500:GLN:NE2	2.03	0.72
1:B:506:THR:HG22	1:B:507:SER:H	1.55	0.72
1:E:19:GLU:O	1:E:20:ARG:HD3	1.89	0.72
1:F:245:VAL:HG13	1:F:255:PHE:HB3	1.70	0.72
1:C:186:LEU:HG	1:C:228:PRO:HG2	1.71	0.72
1:C:249:LEU:HD23	1:C:418:LYS:NZ	2.05	0.72
1:C:500:GLN:NE2	1:C:504:GLY:HA3	2.05	0.72
1:D:223:LEU:HD13	1:D:224:PRO:HD2	1.71	0.72
1:E:410:VAL:HA	1:E:413:ILE:HG22	1.70	0.72
1:A:540:LEU:HA	1:A:543:ASP:HB2	1.70	0.72
1:A:661:ALA:HB1	1:F:662:CYS:SG	2.30	0.72
1:C:457:ASN:HD21	1:C:619:LYS:NZ	1.86	0.72
1:E:118:ARG:HB2	1:E:264:ASN:HB3	1.70	0.72
1:E:649:LYS:HA	1:E:652:LYS:HB3	1.71	0.72
1:A:477:GLN:OE1	1:F:478:GLN:NE2	2.23	0.72
1:A:231:TRP:NE1	1:A:235:VAL:HG21	2.04	0.71
1:B:19:GLU:O	1:B:20:ARG:HD3	1.90	0.71
1:B:528:ASN:H	1:B:528:ASN:HD22	1.36	0.71
1:D:290:THR:HG22	1:D:291:ASP:H	1.54	0.71
1:A:480:LYS:CG	1:A:527:GLU:HB2	2.20	0.71
1:D:118:ARG:HH12	1:D:438:GLN:HG2	1.54	0.71
1:A:626:LEU:H	1:A:627:PRO:HD2	1.53	0.71
1:B:142:ILE:HG22	1:B:144:ARG:HG2	1.73	0.71
1:B:394:LYS:HD3	1:B:402:SER:H	1.54	0.71
1:F:279:LEU:HD21	1:F:291:ASP:HA	1.71	0.71
1:A:486:PHE:HE2	1:A:518:GLU:HA	1.56	0.71
1:B:140:ARG:HB3	1:B:173:LEU:HD11	1.72	0.71
1:B:627:PRO:HA	1:B:630:GLU:HB3	1.70	0.71
1:C:340:ILE:HD11	1:C:351:GLN:OE1	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:354:LEU:CD1	1:E:454:ALA:HA	2.20	0.71
1:A:312:VAL:HG22	1:A:313:HIS:H	1.56	0.71
1:B:120:GLY:O	1:B:123:LEU:HD23	1.91	0.71
1:D:419:ARG:NH2	1:D:420:ASN:HB2	2.06	0.71
1:F:467:LYS:HD3	1:F:541:GLN:HG2	1.73	0.71
1:F:589:GLU:HG3	1:F:592:ARG:HH12	1.55	0.71
1:C:118:ARG:HH22	1:C:438:GLN:HG2	1.56	0.71
1:B:478:GLN:HG3	1:C:481:ALA:CB	2.20	0.71
1:D:426:LEU:HA	1:D:429:VAL:HB	1.72	0.71
1:E:500:GLN:CD	1:E:505:ILE:HG12	2.10	0.71
1:E:46:CYS:SG	1:E:91:LEU:HD11	2.31	0.71
1:A:533:LEU:CD2	1:A:629:VAL:HG12	2.17	0.71
1:B:243:ILE:HG22	1:B:281:LEU:HD23	1.72	0.71
1:B:408:GLU:HG3	1:B:409:SER:H	1.55	0.71
1:E:426:LEU:HA	1:E:429:VAL:HB	1.72	0.71
1:F:357:ALA:C	1:F:456:MET:HG2	2.10	0.71
1:F:430:TRP:C	1:F:571:TYR:HE2	1.94	0.71
1:A:19:GLU:O	1:A:20:ARG:HD3	1.91	0.70
1:B:242:ASP:HA	1:B:257:SER:OG	1.91	0.70
1:B:426:LEU:HA	1:B:429:VAL:HB	1.71	0.70
1:C:447:LEU:HD23	1:C:609:TYR:CE1	2.25	0.70
1:D:187:GLN:HE21	1:D:220:ARG:HH11	1.38	0.70
1:D:627:PRO:HA	1:D:630:GLU:HB3	1.73	0.70
1:F:384:MET:HG2	1:F:385:ASP:N	2.04	0.70
1:A:355:GLN:HE22	1:A:370:CYS:HA	1.54	0.70
1:D:540:LEU:HD21	1:D:622:ALA:HB2	1.71	0.70
1:F:410:VAL:HA	1:F:413:ILE:HG22	1.74	0.70
1:E:240:GLU:HG3	1:E:241:VAL:HG23	1.74	0.70
1:F:16:GLU:HB3	1:F:33:HIS:H	1.55	0.70
1:B:221:PRO:O	1:B:222:PHE:HB2	1.91	0.70
1:D:479:LEU:HD11	1:D:641:LYS:CG	2.17	0.70
1:D:55:ARG:HD2	1:D:91:LEU:HD21	1.74	0.70
1:E:213:PHE:HA	1:E:277:LEU:HD21	1.72	0.70
1:F:220:ARG:NE	1:F:221:PRO:HD2	2.05	0.70
1:D:372:SER:H	1:D:384:MET:HE2	1.53	0.70
1:D:505:ILE:CD1	1:D:506:THR:H	2.04	0.70
1:D:540:LEU:HA	1:D:543:ASP:HB2	1.73	0.70
1:E:105:ARG:CD	1:E:148:PRO:HB2	2.22	0.70
1:E:392:ASN:CG	1:E:393:SER:H	1.94	0.70
1:E:357:ALA:C	1:E:456:MET:HG2	2.11	0.70
1:C:407:PRO:HG2	1:C:408:GLU:H	1.56	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:GLU:HB2	1:D:178:LEU:HD11	1.73	0.70
1:E:333:LEU:HD23	1:E:363:PRO:HA	1.72	0.70
1:F:240:GLU:HG3	1:F:241:VAL:HG23	1.72	0.70
1:D:589:GLU:HG3	1:D:592:ARG:HH12	1.56	0.70
1:A:283:TRP:CD1	1:A:285:PRO:HD2	2.26	0.70
1:B:366:PRO:HB2	1:B:368:THR:CG2	2.14	0.70
1:F:17:MET:HG2	1:F:32:TRP:HE1	1.57	0.70
1:F:431:GLY:HA2	1:F:571:TYR:CE2	2.27	0.70
1:A:182:PHE:O	1:A:183:VAL:HG22	1.92	0.69
1:A:220:ARG:N	1:A:221:PRO:HD3	2.07	0.69
1:B:117:LEU:HB3	1:B:119:GLU:OE1	1.92	0.69
1:C:55:ARG:HH12	1:C:91:LEU:HD11	1.57	0.69
1:A:649:LYS:HA	1:A:652:LYS:HB3	1.73	0.69
1:E:589:GLU:HG3	1:E:592:ARG:HH12	1.56	0.69
1:F:279:LEU:O	1:F:286:ARG:HB3	1.91	0.69
1:B:558:GLY:HA2	1:B:562:ASP:HB2	1.74	0.69
1:D:227:GLN:H	1:D:227:GLN:CD	1.96	0.69
1:D:500:GLN:HB3	1:D:505:ILE:HG12	1.72	0.69
1:E:284:HIS:CB	1:E:285:PRO:HD2	2.20	0.69
1:F:70:HIS:HE1	1:F:132:ALA:HA	1.56	0.69
1:B:29:VAL:HG12	1:B:44:LYS:HB2	1.74	0.69
1:B:500:GLN:NE2	1:B:504:GLY:HA3	2.07	0.69
1:B:419:ARG:HH22	1:B:588:GLN:HG3	1.57	0.69
1:D:549:ARG:HB2	1:D:549:ARG:NH1	2.07	0.69
1:A:292:PRO:HG3	1:A:297:ASN:ND2	2.05	0.69
1:E:29:VAL:HG12	1:E:44:LYS:HB2	1.74	0.69
1:F:19:GLU:O	1:F:20:ARG:HD3	1.91	0.69
1:F:265:LEU:H	1:F:265:LEU:HD23	1.57	0.69
1:C:627:PRO:HA	1:C:630:GLU:HB3	1.75	0.69
1:D:118:ARG:HB2	1:D:264:ASN:OD1	1.91	0.69
1:D:626:LEU:O	1:D:629:VAL:HG22	1.92	0.69
1:F:17:MET:HG2	1:F:32:TRP:NE1	2.08	0.69
1:B:457:ASN:HD21	1:B:619:LYS:HZ1	1.40	0.69
1:A:285:PRO:O	1:A:290:THR:HB	1.93	0.69
1:B:540:LEU:HA	1:B:543:ASP:HB2	1.75	0.69
1:B:570:LEU:HD22	1:B:590:MET:HE2	1.74	0.69
1:C:290:THR:HG22	1:C:296:PRO:O	1.93	0.69
1:C:500:GLN:HB3	1:C:505:ILE:HG23	1.74	0.69
1:D:77:ARG:H	1:D:96:MET:HA	1.58	0.69
1:E:117:LEU:HB2	1:E:215:CYS:O	1.93	0.69
1:B:312:VAL:HG22	1:B:313:HIS:H	1.57	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:LYS:CE	1:B:654:LEU:HD21	2.22	0.69
1:C:434:TRP:HB3	1:C:571:TYR:CZ	2.26	0.69
1:D:17:MET:O	1:D:18:LYS:HD2	1.92	0.69
1:D:580:ASP:HA	1:D:582:ARG:CZ	2.22	0.69
1:B:279:LEU:HA	1:B:286:ARG:HH12	1.58	0.69
1:B:290:THR:HA	1:B:296:PRO:HA	1.75	0.69
1:C:526:ARG:HA	1:C:526:ARG:NE	2.07	0.69
1:D:187:GLN:HE21	1:D:220:ARG:NH1	1.90	0.69
1:F:430:TRP:CZ3	1:F:570:LEU:HD23	2.29	0.69
1:D:170:ALA:HB3	1:D:178:LEU:CD2	2.23	0.68
1:E:248:ASP:OD1	1:E:254:LYS:HE2	1.93	0.68
1:E:17:MET:HG2	1:E:33:HIS:N	2.08	0.68
1:A:394:LYS:CG	1:A:401:ILE:HG13	2.23	0.68
1:D:477:GLN:HG3	1:E:478:GLN:HB2	1.75	0.68
1:F:333:LEU:HD23	1:F:363:PRO:HA	1.74	0.68
1:A:333:LEU:HD23	1:A:363:PRO:HA	1.73	0.68
1:A:480:LYS:HG2	1:A:527:GLU:CD	2.14	0.68
1:D:403:PRO:HA	1:D:404:ARG:HH21	1.57	0.68
1:D:115:CYS:SG	1:D:116:GLY:N	2.65	0.68
1:E:226:TRP:CH2	1:E:228:PRO:HB2	2.28	0.68
1:C:353:LEU:HB3	1:C:386:LEU:HD11	1.75	0.68
1:D:333:LEU:HD23	1:D:363:PRO:HA	1.75	0.68
1:D:536:ARG:CZ	1:D:625:LEU:HD13	2.23	0.68
1:F:394:LYS:HE3	1:F:401:ILE:N	2.08	0.68
1:E:362:ILE:N	1:E:362:ILE:HD12	2.09	0.68
1:B:213:PHE:HA	1:B:277:LEU:HD21	1.76	0.68
1:D:486:PHE:CZ	1:D:647:GLN:HB3	2.28	0.68
1:A:259:LEU:HD13	1:A:259:LEU:O	1.94	0.68
1:A:361:LEU:HD23	1:A:369:GLN:HE21	1.59	0.68
1:B:467:LYS:HD3	1:B:541:GLN:NE2	2.08	0.68
1:C:19:GLU:O	1:C:20:ARG:HD3	1.93	0.68
1:F:362:ILE:N	1:F:362:ILE:HD12	2.09	0.68
1:A:356:GLU:HA	1:A:453:ALA:CB	2.24	0.68
1:D:16:GLU:N	1:D:33:HIS:H	1.91	0.68
1:E:366:PRO:HG2	1:E:368:THR:CG2	2.23	0.68
1:F:430:TRP:CH2	1:F:570:LEU:HD23	2.29	0.68
1:C:420:ASN:ND2	1:C:421:LEU:H	1.92	0.67
1:D:490:ILE:HG21	1:D:517:MET:HE2	1.76	0.67
1:D:221:PRO:O	1:D:222:PHE:HB2	1.93	0.67
1:D:362:ILE:H	1:D:362:ILE:HD12	1.59	0.67
1:D:480:LYS:HG2	1:D:527:GLU:CD	2.15	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ILE:HD12	1:A:362:ILE:N	2.09	0.67
1:A:29:VAL:HG12	1:A:44:LYS:HB2	1.76	0.67
1:B:325:TYR:CE2	1:B:340:ILE:HG22	2.29	0.67
1:C:249:LEU:HD23	1:C:418:LYS:HZ3	1.55	0.67
1:C:362:ILE:HD12	1:C:362:ILE:N	2.09	0.67
1:D:120:GLY:O	1:D:123:LEU:HD23	1.94	0.67
1:E:570:LEU:HD22	1:E:590:MET:HE2	1.75	0.67
1:F:602:GLU:O	1:F:606:ARG:HG2	1.95	0.67
1:A:49:GLU:OE2	1:A:89:ASN:HA	1.94	0.67
1:B:229:VAL:HG23	1:B:230:GLN:H	1.59	0.67
1:C:57:ARG:O	1:C:60:LEU:HB3	1.95	0.67
1:F:421:LEU:CB	1:F:586:ASP:HA	2.24	0.67
1:F:501:THR:O	1:F:502:GLU:HB2	1.93	0.67
1:A:279:LEU:HA	1:A:286:ARG:NH1	2.05	0.67
1:E:602:GLU:O	1:E:606:ARG:HG2	1.95	0.67
1:F:394:LYS:HD2	1:F:401:ILE:O	1.95	0.67
1:D:229:VAL:C	1:D:231:TRP:H	1.98	0.67
1:D:29:VAL:HG12	1:D:44:LYS:HB2	1.75	0.67
1:F:458:LEU:CD2	1:F:619:LYS:HA	2.23	0.67
1:B:171:LYS:HG3	1:B:199:TYR:OH	1.95	0.67
1:C:407:PRO:O	1:C:408:GLU:HB2	1.92	0.67
1:F:187:GLN:CD	1:F:223:LEU:HG	2.15	0.67
1:A:325:TYR:CE2	1:A:340:ILE:HG22	2.29	0.67
1:B:102:GLY:HA2	1:B:153:LEU:H	1.58	0.67
1:B:236:ARG:HD3	1:B:283:TRP:CZ3	2.30	0.67
1:E:102:GLY:HA2	1:E:153:LEU:H	1.60	0.67
1:B:479:LEU:CD1	1:B:641:LYS:HG2	2.21	0.67
1:C:419:ARG:N	1:C:419:ARG:HD3	2.08	0.67
1:D:416:GLU:C	1:D:418:LYS:H	1.98	0.67
1:F:236:ARG:NH2	1:F:283:TRP:HE1	1.93	0.67
1:A:118:ARG:CB	1:A:264:ASN:HB3	2.24	0.66
1:B:458:LEU:HD11	1:B:544:ILE:HG21	1.77	0.66
1:C:240:GLU:HG3	1:C:241:VAL:HG23	1.75	0.66
1:D:486:PHE:CE1	1:D:647:GLN:HB3	2.28	0.66
1:A:420:ASN:HD22	1:B:345:GLY:HA3	1.60	0.66
1:C:462:ASN:O	1:C:466:SER:HB3	1.95	0.66
1:F:480:LYS:HG2	1:F:527:GLU:HB3	1.77	0.66
1:E:295:GLY:N	1:E:296:PRO:HD2	2.08	0.66
1:F:422:ALA:O	1:F:585:GLY:HA3	1.95	0.66
1:C:213:PHE:HA	1:C:277:LEU:HD21	1.76	0.66
1:C:490:ILE:HG21	1:C:517:MET:HE2	1.75	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:THR:HG23	1:D:331:GLU:HG3	1.77	0.66
1:D:496:LYS:HD2	1:E:655:TRP:CD1	2.30	0.66
1:A:172:GLU:HG3	1:A:174:ASP:H	1.61	0.66
1:A:490:ILE:HG12	1:A:517:MET:HE1	1.77	0.66
1:A:420:ASN:ND2	1:B:345:GLY:HA3	2.10	0.66
1:D:310:LYS:HB2	1:D:310:LYS:HZ3	1.61	0.66
1:D:626:LEU:HB3	1:D:627:PRO:CD	2.26	0.66
1:F:227:GLN:HA	1:F:231:TRP:CE3	2.31	0.66
1:B:340:ILE:HD11	1:B:351:GLN:OE1	1.96	0.66
1:F:118:ARG:HB2	1:F:264:ASN:OD1	1.96	0.66
1:F:421:LEU:CG	1:F:586:ASP:HA	2.24	0.66
1:F:354:LEU:CD1	1:F:454:ALA:HA	2.26	0.66
1:A:117:LEU:HB3	1:A:119:GLU:OE1	1.95	0.66
1:B:415:GLN:O	1:B:419:ARG:HG3	1.95	0.66
1:D:404:ARG:N	1:D:404:ARG:HH21	1.93	0.66
1:D:496:LYS:HA	1:E:655:TRP:HE1	1.61	0.66
1:B:77:ARG:H	1:B:96:MET:HA	1.60	0.66
1:C:77:ARG:H	1:C:96:MET:HA	1.60	0.66
1:E:434:TRP:CZ3	1:E:568:ARG:HB2	2.31	0.66
1:F:312:VAL:HG22	1:F:313:HIS:H	1.61	0.66
1:B:282:MET:HG3	1:B:283:TRP:CD1	2.30	0.66
1:E:236:ARG:HH22	1:E:283:TRP:HE1	1.42	0.66
1:A:533:LEU:HD13	1:A:629:VAL:CB	2.26	0.66
1:A:246:SER:O	1:A:253:VAL:HA	1.96	0.65
1:A:528:ASN:O	1:A:532:LEU:HD23	1.96	0.65
1:B:362:ILE:N	1:B:362:ILE:HD12	2.11	0.65
1:D:182:PHE:HZ	1:D:194:LEU:HD23	1.61	0.65
1:B:220:ARG:N	1:B:221:PRO:HD3	2.11	0.65
1:C:517:MET:HG2	1:C:650:ARG:CZ	2.26	0.65
1:D:418:LYS:HE3	1:D:421:LEU:HD12	1.79	0.65
1:A:213:PHE:CE2	1:A:221:PRO:HG2	2.30	0.65
1:A:426:LEU:HA	1:A:429:VAL:HB	1.78	0.65
1:C:20:ARG:CB	1:C:23:THR:HB	2.27	0.65
1:C:479:LEU:CD1	1:C:641:LYS:HG2	2.17	0.65
1:E:57:ARG:O	1:E:60:LEU:HB3	1.96	0.65
1:F:357:ALA:CA	1:F:452:ARG:HH12	2.07	0.65
1:D:19:GLU:O	1:D:20:ARG:HD3	1.96	0.65
1:D:418:LYS:NZ	1:D:421:LEU:HD12	2.11	0.65
1:E:249:LEU:HD13	1:E:414:LEU:HG	1.78	0.65
1:F:427:ARG:HH21	1:F:575:ARG:CG	2.09	0.65
1:A:102:GLY:HA2	1:A:153:LEU:H	1.62	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:GLU:OE2	1:A:632:VAL:HG21	1.97	0.65
1:F:371:ILE:HA	1:F:384:MET:HE1	1.79	0.65
1:B:102:GLY:CA	1:B:153:LEU:H	2.09	0.65
1:B:245:VAL:O	1:B:245:VAL:HG12	1.96	0.65
1:B:451:GLN:HA	1:B:454:ALA:HB3	1.79	0.65
1:D:422:ALA:O	1:D:585:GLY:HA3	1.97	0.65
1:E:577:LYS:HG3	1:E:578:PRO:HD2	1.79	0.65
1:F:423:PHE:HD1	1:F:583:THR:HA	1.61	0.65
1:F:285:PRO:HG2	1:F:286:ARG:HE	1.62	0.65
1:F:428:LYS:HG3	1:F:429:VAL:N	2.10	0.65
1:A:243:ILE:HG22	1:A:281:LEU:HD23	1.78	0.65
1:A:77:ARG:H	1:A:96:MET:HA	1.61	0.65
1:B:602:GLU:O	1:B:606:ARG:HG2	1.97	0.65
1:F:212:ALA:O	1:F:216:ILE:HG13	1.97	0.65
1:F:310:LYS:HZ3	1:F:310:LYS:HB2	1.62	0.65
1:A:102:GLY:CA	1:A:153:LEU:H	2.10	0.65
1:B:36:GLU:OE2	1:E:359:LEU:HA	1.97	0.65
1:A:231:TRP:CE2	1:A:235:VAL:HG21	2.32	0.64
1:A:89:ASN:H	1:A:89:ASN:HD22	1.43	0.64
1:C:217:THR:HA	1:C:263:ASN:CG	2.17	0.64
1:C:365:LYS:HE2	1:C:365:LYS:HA	1.79	0.64
1:F:102:GLY:HA2	1:F:153:LEU:H	1.61	0.64
1:F:389:LEU:HD21	1:F:454:ALA:HB1	1.74	0.64
1:F:57:ARG:O	1:F:60:LEU:HB3	1.97	0.64
1:A:451:GLN:HA	1:A:454:ALA:HB3	1.79	0.64
1:B:626:LEU:HB3	1:B:627:PRO:CD	2.27	0.64
1:D:451:GLN:HA	1:D:454:ALA:HB3	1.78	0.64
1:F:394:LYS:HG2	1:F:401:ILE:N	2.12	0.64
1:E:77:ARG:H	1:E:96:MET:HA	1.61	0.64
1:A:20:ARG:CB	1:A:23:THR:HB	2.28	0.64
1:B:392:ASN:CG	1:B:393:SER:H	2.01	0.64
1:C:29:VAL:HG12	1:C:44:LYS:HB2	1.79	0.64
1:D:213:PHE:CE2	1:D:221:PRO:HG2	2.33	0.64
1:D:545:VAL:HA	1:D:548:GLN:HE22	1.62	0.64
1:D:481:ALA:CB	1:E:482:LYS:HD2	2.25	0.64
1:F:21:LEU:HG	1:F:165:ILE:HD13	1.80	0.64
1:F:626:LEU:N	1:F:627:PRO:CD	2.50	0.64
1:C:114:CYS:SG	1:C:115:CYS:N	2.71	0.64
1:E:577:LYS:HE3	1:E:584:GLU:OE1	1.96	0.64
1:B:20:ARG:CB	1:B:23:THR:HB	2.28	0.64
1:C:282:MET:HG3	1:C:283:TRP:CE3	2.33	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:426:LEU:O	1:F:430:TRP:HB2	1.98	0.64
1:F:80:PRO:CB	1:F:83:MET:HB2	2.27	0.64
1:B:104:LEU:HD23	1:B:148:PRO:HB3	1.78	0.64
1:C:517:MET:HG2	1:C:650:ARG:NE	2.12	0.64
1:D:602:GLU:O	1:D:606:ARG:HG2	1.97	0.64
1:F:577:LYS:HG3	1:F:578:PRO:HD2	1.80	0.64
1:A:394:LYS:HG2	1:A:401:ILE:HG13	1.80	0.64
1:A:417:PRO:HA	1:B:320:GLY:HA2	1.79	0.64
1:B:428:LYS:HG3	1:B:429:VAL:N	2.12	0.64
1:C:570:LEU:HD22	1:C:590:MET:CE	2.28	0.64
1:E:286:ARG:HB3	1:E:286:ARG:HH11	1.62	0.64
1:F:465:LEU:O	1:F:626:LEU:HD11	1.98	0.64
1:A:655:TRP:O	1:F:500:GLN:OE1	2.16	0.64
1:C:402:SER:H	1:C:403:PRO:CD	2.06	0.64
1:E:368:THR:O	1:E:371:ILE:HG22	1.98	0.64
1:E:426:LEU:O	1:E:430:TRP:HB2	1.98	0.64
1:E:60:LEU:HD13	1:E:175:GLN:HG2	1.80	0.64
1:E:328:THR:HG23	1:E:331:GLU:HG3	1.80	0.64
1:A:263:ASN:OD1	1:A:265:LEU:HD22	1.96	0.63
1:A:265:LEU:HD23	1:A:266:ASN:N	2.10	0.63
1:C:312:VAL:HG22	1:C:313:HIS:H	1.61	0.63
1:C:126:LEU:HB3	1:C:303:LEU:HD21	1.80	0.63
1:C:320:GLY:HA2	1:C:405:PRO:HG3	1.79	0.63
1:D:655:TRP:CD1	1:E:496:LYS:HD2	2.33	0.63
1:E:631:GLU:O	1:E:635:LEU:HG	1.98	0.63
1:C:402:SER:N	1:C:403:PRO:CD	2.62	0.63
1:C:496:LYS:HZ3	1:C:654:LEU:HD11	1.62	0.63
1:D:655:TRP:CE2	1:E:496:LYS:HD2	2.34	0.63
1:E:102:GLY:CA	1:E:153:LEU:H	2.12	0.63
1:E:120:GLY:O	1:E:123:LEU:HD23	1.98	0.63
1:E:21:LEU:HD23	1:E:165:ILE:HG23	1.81	0.63
1:E:310:LYS:HZ3	1:E:310:LYS:HB2	1.63	0.63
1:B:193:LEU:HD22	1:B:203:VAL:CG2	2.29	0.63
1:B:528:ASN:HD22	1:B:528:ASN:N	1.95	0.63
1:C:104:LEU:HD23	1:C:148:PRO:HB3	1.81	0.63
1:D:193:LEU:HD22	1:D:203:VAL:CG2	2.27	0.63
1:E:16:GLU:HG3	1:E:32:TRP:NE1	2.14	0.63
1:B:333:LEU:HD23	1:B:363:PRO:HA	1.79	0.63
1:D:223:LEU:CD1	1:D:226:TRP:HB2	2.29	0.63
1:E:340:ILE:HD11	1:E:351:GLN:OE1	1.99	0.63
1:A:117:LEU:HB2	1:A:215:CYS:O	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:LYS:HG3	1:D:429:VAL:N	2.13	0.63
1:A:651:GLN:HB2	1:F:493:ASP:OD2	1.99	0.63
1:A:57:ARG:O	1:A:60:LEU:HB3	1.98	0.63
1:C:602:GLU:O	1:C:606:ARG:HG2	1.99	0.63
1:A:193:LEU:HD22	1:A:203:VAL:CG2	2.29	0.63
1:C:451:GLN:HA	1:C:454:ALA:HB3	1.79	0.63
1:F:77:ARG:H	1:F:96:MET:HA	1.64	0.63
1:E:462:ASN:O	1:E:466:SER:HB3	1.99	0.63
1:C:511:LEU:CG	1:C:515:ARG:HH12	2.11	0.62
1:C:533:LEU:HD22	1:C:629:VAL:HG12	1.80	0.62
1:C:418:LYS:HA	1:D:344:THR:HG23	1.80	0.62
1:A:480:LYS:HG2	1:A:527:GLU:CG	2.30	0.62
1:C:114:CYS:SG	1:C:575:ARG:NH1	2.70	0.62
1:D:517:MET:HG2	1:D:650:ARG:NE	2.14	0.62
1:E:20:ARG:CB	1:E:23:THR:HB	2.28	0.62
1:F:570:LEU:HD22	1:F:590:MET:CE	2.29	0.62
1:B:213:PHE:CD2	1:B:221:PRO:HG2	2.33	0.62
1:B:310:LYS:HZ3	1:B:310:LYS:HB2	1.65	0.62
1:B:434:TRP:HB3	1:B:571:TYR:CZ	2.34	0.62
1:D:21:LEU:HB3	1:D:165:ILE:HG21	1.80	0.62
1:F:296:PRO:HG2	1:F:297:ASN:H	1.63	0.62
1:F:455:MET:O	1:F:459:LEU:HD13	1.99	0.62
1:F:544:ILE:O	1:F:547:LEU:HG	1.99	0.62
1:A:169:TYR:OH	1:A:183:VAL:HG21	1.99	0.62
1:A:286:ARG:HA	1:A:290:THR:OG1	1.99	0.62
1:C:120:GLY:O	1:C:123:LEU:HD23	1.99	0.62
1:C:545:VAL:HA	1:C:548:GLN:HE22	1.64	0.62
1:D:182:PHE:CZ	1:D:195:GLU:HG2	2.35	0.62
1:D:408:GLU:CG	1:D:413:ILE:HD13	2.29	0.62
1:F:210:THR:HG22	1:F:220:ARG:HB2	1.80	0.62
1:F:401:ILE:HG12	1:F:403:PRO:CD	2.20	0.62
1:C:90:ASP:O	1:C:91:LEU:HD22	2.00	0.62
1:F:340:ILE:HD11	1:F:351:GLN:OE1	1.99	0.62
1:A:434:TRP:HB3	1:A:571:TYR:CE1	2.34	0.62
1:B:355:GLN:O	1:B:359:LEU:HD11	1.99	0.62
1:F:185:THR:HG22	1:F:187:GLN:H	1.65	0.62
1:D:213:PHE:CD1	1:D:221:PRO:HB2	2.35	0.62
1:D:325:TYR:CE2	1:D:340:ILE:HG22	2.35	0.62
1:D:84:GLN:HE22	1:D:85:ASN:HB2	1.63	0.62
1:F:309:LEU:HD11	1:F:311:LEU:HD23	1.82	0.62
1:F:631:GLU:O	1:F:635:LEU:HG	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:TYR:CE2	1:C:340:ILE:HG22	2.34	0.62
1:C:417:PRO:CA	1:D:320:GLY:HA3	2.26	0.62
1:D:418:LYS:CE	1:D:421:LEU:HD12	2.30	0.62
1:F:542:THR:HA	1:F:545:VAL:HG22	1.81	0.62
1:A:361:LEU:HD22	1:A:369:GLN:HG3	1.82	0.62
1:A:480:LYS:HG2	1:A:527:GLU:CB	2.29	0.62
1:A:540:LEU:HD21	1:A:622:ALA:HB2	1.80	0.62
1:A:583:THR:HG23	1:A:584:GLU:H	1.64	0.62
1:B:328:THR:HG23	1:B:331:GLU:HG3	1.79	0.62
1:D:213:PHE:HA	1:D:277:LEU:HD21	1.81	0.62
1:D:244:VAL:HB	1:D:256:SER:HB2	1.81	0.62
1:E:237:GLN:HG2	1:E:238:LYS:HD2	1.81	0.62
1:F:486:PHE:CZ	1:F:651:GLN:OE1	2.52	0.62
1:A:212:ALA:O	1:A:216:ILE:HG13	2.00	0.62
1:B:227:GLN:NE2	1:B:229:VAL:HG13	2.15	0.62
1:B:545:VAL:HA	1:B:548:GLN:HE22	1.64	0.62
1:C:223:LEU:HD21	1:C:253:VAL:HG12	1.81	0.62
1:C:276:TRP:CE2	1:C:280:MET:HG3	2.35	0.62
1:C:123:LEU:HD12	1:C:307:LEU:HD13	1.81	0.62
1:C:366:PRO:O	1:C:368:THR:HG23	2.00	0.62
1:C:426:LEU:O	1:C:430:TRP:HB2	2.00	0.62
1:D:245:VAL:HA	1:D:254:LYS:O	2.00	0.62
1:F:354:LEU:HD13	1:F:453:ALA:O	2.00	0.62
1:A:363:PRO:HG2	1:A:364:ASP:OD1	2.00	0.61
1:A:505:ILE:HG12	1:A:511:LEU:HD13	1.82	0.61
1:E:186:LEU:HD12	1:E:189:LEU:HD23	1.82	0.61
1:E:526:ARG:HD2	1:E:636:MET:HG2	1.82	0.61
1:E:649:LYS:O	1:E:653:GLU:HG3	2.00	0.61
1:F:282:MET:HG2	1:F:286:ARG:NH2	2.14	0.61
1:A:486:PHE:HZ	1:A:517:MET:SD	2.23	0.61
1:A:533:LEU:HD13	1:A:629:VAL:HG12	1.82	0.61
1:B:17:MET:N	1:B:17:MET:SD	2.73	0.61
1:D:105:ARG:HD2	1:D:148:PRO:HB2	1.82	0.61
1:D:118:ARG:HH12	1:D:438:GLN:CG	2.14	0.61
1:E:21:LEU:HG	1:E:165:ILE:HD13	1.81	0.61
1:E:467:LYS:HD3	1:E:541:GLN:NE2	2.15	0.61
1:F:451:GLN:HA	1:F:454:ALA:HB3	1.81	0.61
1:A:602:GLU:O	1:A:606:ARG:HG2	2.00	0.61
1:C:570:LEU:N	1:C:570:LEU:HD12	2.16	0.61
1:D:126:LEU:HB3	1:D:303:LEU:HD21	1.81	0.61
1:E:312:VAL:HG22	1:E:313:HIS:H	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:357:ALA:HA	1:E:452:ARG:HH12	1.65	0.61
1:E:451:GLN:HA	1:E:454:ALA:HB3	1.82	0.61
1:E:49:GLU:HG3	1:E:89:ASN:HD22	1.65	0.61
1:F:325:TYR:CE2	1:F:340:ILE:HG22	2.35	0.61
1:F:34:ASN:OD1	1:F:83:MET:SD	2.58	0.61
1:A:244:VAL:HG21	1:A:260:PRO:HD3	1.82	0.61
1:B:81:GLU:CD	1:B:81:GLU:H	2.04	0.61
1:D:84:GLN:NE2	1:D:85:ASN:HB2	2.15	0.61
1:E:401:ILE:HG22	1:E:402:SER:H	1.65	0.61
1:A:658:LEU:HD21	1:F:497:TYR:HE1	1.66	0.61
1:B:61:GLU:OE1	1:B:168:GLY:HA2	2.01	0.61
1:B:421:LEU:HD12	1:B:421:LEU:H	1.64	0.61
1:C:21:LEU:HB3	1:C:165:ILE:HG21	1.81	0.61
1:D:107:TYR:CE2	1:D:153:LEU:HD22	2.35	0.61
1:E:542:THR:HA	1:E:545:VAL:HG22	1.83	0.61
1:E:427:ARG:HH21	1:E:575:ARG:CG	2.14	0.61
1:A:126:LEU:HB3	1:A:303:LEU:HD21	1.82	0.61
1:E:387:VAL:HG11	1:E:450:GLY:CA	2.25	0.61
1:F:57:ARG:HD2	1:F:177:GLU:O	2.01	0.61
1:B:57:ARG:O	1:B:60:LEU:HB3	2.00	0.61
1:F:61:GLU:OE1	1:F:168:GLY:HA2	2.01	0.61
1:F:626:LEU:O	1:F:629:VAL:HG22	2.00	0.61
1:F:82:GLY:C	1:F:84:GLN:H	2.04	0.61
1:B:165:ILE:HG22	1:B:166:ASP:N	2.11	0.61
1:B:84:GLN:O	1:B:86:LEU:HG	2.00	0.61
1:C:490:ILE:CG1	1:C:650:ARG:HB3	2.31	0.61
1:C:80:PRO:HB2	1:C:84:GLN:NE2	2.16	0.61
1:D:244:VAL:CG2	1:D:260:PRO:HD3	2.31	0.61
1:E:193:LEU:HD22	1:E:203:VAL:CG2	2.28	0.61
1:E:401:ILE:HB	1:E:403:PRO:HD3	1.82	0.61
1:F:120:GLY:O	1:F:123:LEU:HD23	2.00	0.61
1:F:328:THR:HG23	1:F:331:GLU:HG3	1.82	0.61
1:F:514:TRP:CH2	1:F:653:GLU:HB2	2.36	0.61
1:A:107:TYR:CE2	1:A:153:LEU:HD22	2.36	0.61
1:A:486:PHE:CE2	1:A:518:GLU:HA	2.36	0.61
1:A:545:VAL:HA	1:A:548:GLN:HE22	1.63	0.61
1:B:213:PHE:CE1	1:B:221:PRO:HB2	2.35	0.61
1:C:286:ARG:N	1:C:290:THR:HG23	2.15	0.61
1:C:542:THR:HA	1:C:545:VAL:HG22	1.83	0.61
1:F:32:TRP:CZ3	1:F:83:MET:HB3	2.33	0.61
1:B:187:GLN:HB3	1:B:220:ARG:CZ	2.31	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:GLU:HG2	1:D:413:ILE:HD13	1.82	0.61
1:D:57:ARG:O	1:D:60:LEU:HB3	2.01	0.61
1:E:22:GLY:N	1:E:165:ILE:HG21	2.15	0.61
1:F:21:LEU:HD23	1:F:165:ILE:HG23	1.82	0.61
1:C:526:ARG:HH11	1:C:529:GLU:HG2	1.66	0.60
1:E:325:TYR:CE2	1:E:340:ILE:HG22	2.36	0.60
1:F:276:TRP:CE2	1:F:280:MET:HG3	2.36	0.60
1:F:123:LEU:HD12	1:F:307:LEU:HD13	1.81	0.60
1:A:528:ASN:HA	1:A:531:LYS:HZ2	1.65	0.60
1:C:316:ASN:ND2	1:C:344:THR:HG21	2.16	0.60
1:A:402:SER:H	1:A:403:PRO:CD	2.10	0.60
1:A:533:LEU:HD13	1:A:629:VAL:CA	2.30	0.60
1:B:21:LEU:HG	1:B:165:ILE:HD13	1.82	0.60
1:B:283:TRP:HB2	1:B:284:HIS:ND1	2.16	0.60
1:B:477:GLN:HE21	1:C:477:GLN:NE2	1.99	0.60
1:C:118:ARG:HD3	1:C:435:HIS:NE2	2.16	0.60
1:F:117:LEU:O	1:F:118:ARG:HB3	2.01	0.60
1:F:279:LEU:CD2	1:F:292:PRO:HD3	2.26	0.60
1:A:419:ARG:N	1:A:419:ARG:NE	2.41	0.60
1:B:286:ARG:HA	1:B:290:THR:CG2	2.32	0.60
1:B:415:GLN:NE2	1:B:419:ARG:HG2	2.16	0.60
1:C:222:PHE:HA	1:C:245:VAL:HB	1.84	0.60
1:A:481:ALA:C	1:F:482:LYS:HZ1	2.05	0.60
1:F:526:ARG:HH22	1:F:635:LEU:HB3	1.67	0.60
1:A:192:GLU:HG2	1:A:283:TRP:CB	2.31	0.60
1:F:426:LEU:HD11	1:F:574:LEU:HD11	1.82	0.60
1:A:316:ASN:ND2	1:A:344:THR:HG21	2.16	0.60
1:B:415:GLN:HE21	1:B:419:ARG:CG	2.14	0.60
1:C:310:LYS:HB2	1:C:310:LYS:HZ3	1.66	0.60
1:C:417:PRO:HG3	1:D:405:PRO:HG3	1.82	0.60
1:C:626:LEU:O	1:C:629:VAL:HG22	2.01	0.60
1:D:340:ILE:HD11	1:D:351:GLN:OE1	2.00	0.60
1:D:402:SER:N	1:D:403:PRO:HD2	2.11	0.60
1:E:276:TRP:CE2	1:E:280:MET:HG3	2.37	0.60
1:E:430:TRP:C	1:E:571:TYR:HE2	2.04	0.60
1:A:120:GLY:O	1:A:123:LEU:HD23	2.00	0.60
1:A:292:PRO:C	1:A:294:TYR:H	2.04	0.60
1:E:416:GLU:C	1:E:418:LYS:H	2.04	0.60
1:A:658:LEU:HA	1:F:658:LEU:CD1	2.31	0.60
1:A:213:PHE:CE1	1:A:243:ILE:HB	2.37	0.60
1:B:626:LEU:O	1:B:629:VAL:HG22	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:VAL:HB	1:C:256:SER:HB3	1.84	0.60
1:C:333:LEU:HD23	1:C:363:PRO:HA	1.83	0.60
1:A:428:LYS:HG3	1:A:429:VAL:N	2.16	0.60
1:D:244:VAL:HG21	1:D:260:PRO:HD3	1.83	0.60
1:D:434:TRP:HB3	1:D:571:TYR:CZ	2.37	0.60
1:D:517:MET:HB3	1:D:650:ARG:NH2	2.17	0.60
1:E:16:GLU:HG3	1:E:32:TRP:HE1	1.65	0.60
1:A:503:PHE:HB2	1:F:659:LYS:CD	2.31	0.60
1:A:283:TRP:CD1	1:A:284:HIS:N	2.69	0.60
1:A:479:LEU:HD12	1:A:640:GLU:HG2	1.83	0.60
1:B:367:ALA:C	1:B:369:GLN:N	2.56	0.60
1:B:455:MET:O	1:B:459:LEU:HD13	2.02	0.60
1:C:366:PRO:C	1:C:368:THR:H	2.06	0.60
1:D:631:GLU:O	1:D:635:LEU:HG	2.02	0.60
1:E:16:GLU:N	1:E:30:ILE:HG21	2.17	0.60
1:D:665:VAL:HG13	1:E:664:LYS:O	2.02	0.60
1:F:193:LEU:HD22	1:F:203:VAL:CG2	2.29	0.60
1:A:170:ALA:O	1:A:178:LEU:HB2	2.02	0.59
1:D:224:PRO:HG2	1:D:225:ASN:H	1.67	0.59
1:D:236:ARG:HH22	1:D:283:TRP:HE1	1.47	0.59
1:D:496:LYS:HE2	1:D:654:LEU:HD21	1.84	0.59
1:E:545:VAL:HA	1:E:548:GLN:HE22	1.66	0.59
1:F:526:ARG:NH2	1:F:635:LEU:HB3	2.16	0.59
1:F:421:LEU:HG	1:F:586:ASP:HA	1.82	0.59
1:A:291:ASP:C	1:A:293:THR:H	2.04	0.59
1:A:533:LEU:HD22	1:A:629:VAL:CG1	2.25	0.59
1:B:35:GLN:HG2	1:E:465:LEU:HG	1.83	0.59
1:B:447:LEU:HD23	1:B:609:TYR:CE1	2.34	0.59
1:C:193:LEU:HD22	1:C:203:VAL:CG2	2.30	0.59
1:D:21:LEU:HG	1:D:165:ILE:CD1	2.32	0.59
1:F:102:GLY:CA	1:F:153:LEU:H	2.15	0.59
1:A:503:PHE:HB2	1:F:659:LYS:HD2	1.83	0.59
1:C:510:LEU:HB3	1:C:653:GLU:OE2	2.02	0.59
1:D:282:MET:HB2	1:D:286:ARG:CZ	2.31	0.59
1:E:229:VAL:HG22	1:E:230:GLN:OE1	2.03	0.59
1:A:655:TRP:HD1	1:F:500:GLN:HG2	1.62	0.59
1:A:361:LEU:CD2	1:A:369:GLN:HE21	2.15	0.59
1:C:486:PHE:CE2	1:C:521:VAL:HG21	2.37	0.59
1:D:426:LEU:O	1:D:430:TRP:HB2	2.03	0.59
1:F:284:HIS:CG	1:F:285:PRO:HD3	2.38	0.59
1:A:631:GLU:O	1:A:635:LEU:HG	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:HIS:H	1:B:285:PRO:HD2	1.68	0.59
1:B:365:LYS:C	1:B:367:ALA:H	2.06	0.59
1:E:428:LYS:HG3	1:E:429:VAL:N	2.16	0.59
1:E:626:LEU:O	1:E:629:VAL:HG22	2.03	0.59
1:C:404:ARG:O	1:C:404:ARG:HD3	2.01	0.59
1:F:20:ARG:CB	1:F:23:THR:HB	2.33	0.59
1:F:427:ARG:HE	1:F:575:ARG:CG	2.10	0.59
1:A:367:ALA:O	1:A:369:GLN:N	2.35	0.59
1:A:579:ARG:HD3	1:A:579:ARG:N	2.10	0.59
1:D:171:LYS:HD2	1:D:172:GLU:H	1.68	0.59
1:D:362:ILE:N	1:D:362:ILE:HD12	2.17	0.59
1:D:416:GLU:O	1:D:418:LYS:N	2.36	0.59
1:D:500:GLN:HE22	1:D:504:GLY:HA3	1.66	0.59
1:D:581:GLN:H	1:D:582:ARG:NE	2.01	0.59
1:B:202:THR:HG21	1:B:284:HIS:HA	1.84	0.59
1:C:113:ASN:OD1	1:C:117:LEU:HD23	2.02	0.59
1:C:366:PRO:O	1:C:368:THR:N	2.33	0.59
1:D:488:THR:HG22	1:E:648:GLU:HB3	1.84	0.59
1:F:223:LEU:H	1:F:224:PRO:HD2	1.67	0.59
1:B:118:ARG:HD3	1:B:435:HIS:NE2	2.18	0.59
1:E:186:LEU:HD11	1:E:189:LEU:HB2	1.85	0.59
1:F:458:LEU:HD23	1:F:619:LYS:CB	2.33	0.59
1:A:105:ARG:HD2	1:A:148:PRO:HB2	1.85	0.59
1:A:462:ASN:O	1:A:466:SER:HB3	2.03	0.59
1:C:500:GLN:O	1:C:502:GLU:N	2.36	0.59
1:D:140:ARG:O	1:D:172:GLU:HG3	2.03	0.59
1:D:172:GLU:HG2	1:D:174:ASP:H	1.66	0.59
1:D:402:SER:H	1:D:403:PRO:CD	2.12	0.59
1:E:316:ASN:ND2	1:E:344:THR:HG21	2.18	0.59
1:A:282:MET:CE	1:A:286:ARG:HH21	2.16	0.58
1:A:402:SER:N	1:A:403:PRO:CD	2.65	0.58
1:C:239:SER:HA	1:C:242:ASP:OD1	2.03	0.58
1:D:649:LYS:O	1:D:653:GLU:HG3	2.03	0.58
1:E:352:GLU:OE2	1:E:619:LYS:HE2	2.03	0.58
1:F:21:LEU:HB3	1:F:165:ILE:HG21	1.85	0.58
1:F:213:PHE:CZ	1:F:243:ILE:HB	2.38	0.58
1:A:419:ARG:N	1:A:419:ARG:CZ	2.64	0.58
1:B:268:VAL:HG13	1:B:269:LEU:N	2.17	0.58
1:B:279:LEU:HA	1:B:286:ARG:NH1	2.18	0.58
1:B:577:LYS:HG2	1:B:581:GLN:HE21	1.67	0.58
1:C:531:LYS:HB3	1:C:531:LYS:HZ3	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:LEU:HD11	1:D:226:TRP:CE3	2.38	0.58
1:E:410:VAL:HG12	1:E:411:SER:N	2.14	0.58
1:A:21:LEU:HB3	1:A:165:ILE:HG21	1.85	0.58
1:B:458:LEU:HD11	1:B:544:ILE:CG2	2.34	0.58
1:B:542:THR:HA	1:B:545:VAL:HG22	1.85	0.58
1:C:223:LEU:HB3	1:C:226:TRP:CD1	2.38	0.58
1:C:421:LEU:O	1:C:585:GLY:HA3	2.03	0.58
1:D:41:ILE:HG22	1:D:42:ALA:H	1.68	0.58
1:E:118:ARG:HD3	1:E:435:HIS:NE2	2.18	0.58
1:E:455:MET:O	1:E:459:LEU:HD13	2.04	0.58
1:F:229:VAL:HG22	1:F:230:GLN:N	2.11	0.58
1:A:21:LEU:HD23	1:A:165:ILE:HG23	1.85	0.58
1:A:426:LEU:O	1:A:430:TRP:HB2	2.03	0.58
1:B:276:TRP:CE2	1:B:280:MET:HG3	2.39	0.58
1:B:321:THR:H	1:B:405:PRO:HG3	1.68	0.58
1:B:511:LEU:CG	1:B:515:ARG:HH12	2.12	0.58
1:D:20:ARG:CB	1:D:23:THR:HB	2.34	0.58
1:D:655:TRP:CD2	1:E:496:LYS:HD2	2.38	0.58
1:E:276:TRP:NE1	1:E:280:MET:HG3	2.19	0.58
1:A:328:THR:HG23	1:A:331:GLU:HG3	1.86	0.58
1:A:358:GLY:HA2	1:A:457:ASN:HB2	1.82	0.58
1:A:490:ILE:HG12	1:A:517:MET:HE2	1.85	0.58
1:B:426:LEU:O	1:B:430:TRP:HB2	2.02	0.58
1:D:102:GLY:CA	1:D:153:LEU:H	2.15	0.58
1:D:104:LEU:HD23	1:D:148:PRO:HB3	1.85	0.58
1:F:20:ARG:HB3	1:F:29:VAL:O	2.03	0.58
1:F:421:LEU:HB3	1:F:586:ASP:CA	2.33	0.58
1:C:18:LYS:CB	1:C:31:ARG:HD3	2.33	0.58
1:C:475:MET:O	1:C:478:GLN:HB3	2.04	0.58
1:D:276:TRP:CE2	1:D:280:MET:HG3	2.38	0.58
1:D:36:GLU:HG3	1:D:37:THR:H	1.68	0.58
1:E:356:GLU:O	1:E:452:ARG:NH1	2.35	0.58
1:C:37:THR:HG22	1:F:362:ILE:HG13	1.86	0.58
1:A:60:LEU:HD13	1:A:175:GLN:NE2	2.19	0.58
1:B:312:VAL:HG22	1:B:313:HIS:N	2.18	0.58
1:D:462:ASN:O	1:D:466:SER:HB3	2.03	0.58
1:F:279:LEU:CD2	1:F:291:ASP:HA	2.33	0.58
1:F:317:MET:SD	1:F:450:GLY:HA3	2.43	0.58
1:F:410:VAL:HG12	1:F:411:SER:N	2.15	0.58
1:A:455:MET:O	1:A:459:LEU:HD13	2.04	0.58
1:A:481:ALA:CB	1:F:482:LYS:NZ	2.64	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LYS:HG2	1:B:177:GLU:CA	2.32	0.58
1:B:316:ASN:ND2	1:B:344:THR:HG21	2.18	0.58
1:B:570:LEU:HD22	1:B:590:MET:CE	2.34	0.58
1:D:165:ILE:HG22	1:D:166:ASP:N	2.12	0.58
1:F:355:GLN:O	1:F:359:LEU:HD11	2.03	0.58
1:A:355:GLN:O	1:A:359:LEU:HD11	2.03	0.58
1:A:511:LEU:CG	1:A:515:ARG:HH12	2.16	0.58
1:C:102:GLY:HA2	1:C:153:LEU:H	1.68	0.58
1:D:282:MET:HG2	1:D:286:ARG:NH2	2.18	0.58
1:D:542:THR:HA	1:D:545:VAL:HG22	1.85	0.58
1:F:217:THR:HB	1:F:260:PRO:HG3	1.86	0.58
1:F:306:ILE:O	1:F:309:LEU:HD23	2.03	0.58
1:F:458:LEU:HD23	1:F:619:LYS:HB2	1.86	0.58
1:B:80:PRO:HB3	1:B:83:MET:SD	2.44	0.58
1:C:223:LEU:HD23	1:C:246:SER:HA	1.86	0.58
1:C:419:ARG:HH21	1:C:420:ASN:HB3	1.68	0.58
1:C:428:LYS:HG3	1:C:429:VAL:N	2.18	0.58
1:D:167:LEU:O	1:D:170:ALA:HB2	2.04	0.58
1:D:213:PHE:CE1	1:D:243:ILE:HB	2.39	0.58
1:E:430:TRP:CZ3	1:E:570:LEU:HB3	2.39	0.58
1:A:194:LEU:HB3	1:A:196:GLN:HE22	1.68	0.57
1:A:312:VAL:HG22	1:A:313:HIS:N	2.19	0.57
1:B:321:THR:N	1:B:405:PRO:HG3	2.19	0.57
1:C:214:GLU:OE1	1:C:220:ARG:HD3	2.04	0.57
1:A:21:LEU:HG	1:A:165:ILE:CD1	2.34	0.57
1:D:265:LEU:HG	1:D:266:ASN:N	2.19	0.57
1:E:420:ASN:O	1:E:421:LEU:CB	2.52	0.57
1:B:311:LEU:O	1:B:311:LEU:HD12	2.04	0.57
1:C:430:TRP:CZ3	1:C:574:LEU:HD12	2.40	0.57
1:C:636:MET:C	1:C:638:GLU:H	2.07	0.57
1:E:36:GLU:O	1:E:38:GLY:N	2.38	0.57
1:F:545:VAL:HA	1:F:548:GLN:HE22	1.69	0.57
1:F:65:MET:HB3	1:F:76:ALA:HB2	1.86	0.57
1:A:186:LEU:HD13	1:A:186:LEU:C	2.25	0.57
1:A:294:TYR:N	1:A:294:TYR:CD2	2.68	0.57
1:A:542:THR:HA	1:A:545:VAL:HG22	1.87	0.57
1:B:213:PHE:CE2	1:B:217:THR:HG21	2.40	0.57
1:B:501:THR:O	1:B:505:ILE:HG12	2.03	0.57
1:E:234:LYS:O	1:E:237:GLN:HB3	2.05	0.57
1:D:655:TRP:CG	1:E:496:LYS:HD2	2.39	0.57
1:F:316:ASN:ND2	1:F:344:THR:HG21	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LEU:HB3	1:B:196:GLN:HE22	1.69	0.57
1:C:270:ALA:O	1:C:274:GLU:HB2	2.05	0.57
1:D:316:ASN:ND2	1:D:344:THR:HG21	2.19	0.57
1:E:570:LEU:HD22	1:E:590:MET:CE	2.33	0.57
1:F:89:ASN:HD22	1:F:91:LEU:HB2	1.68	0.57
1:A:394:LYS:NZ	1:A:613:SER:HB2	2.19	0.57
1:C:169:TYR:HE1	1:C:183:VAL:HB	1.69	0.57
1:C:328:THR:HG23	1:C:331:GLU:HG3	1.85	0.57
1:E:220:ARG:HG2	1:E:220:ARG:NH1	2.19	0.57
1:A:265:LEU:HD21	1:A:270:ALA:HB2	1.87	0.57
1:A:649:LYS:O	1:A:653:GLU:HG3	2.05	0.57
1:B:448:GLN:OE1	1:B:608:ILE:HD12	2.04	0.57
1:C:21:LEU:HG	1:C:165:ILE:CD1	2.34	0.57
1:D:144:ARG:HD3	1:D:169:TYR:O	2.05	0.57
1:D:394:LYS:HG2	1:D:401:ILE:N	2.20	0.57
1:F:502:GLU:HA	1:F:502:GLU:OE1	2.03	0.57
1:C:21:LEU:HD23	1:C:165:ILE:HG23	1.86	0.57
1:D:408:GLU:HA	1:D:408:GLU:OE1	2.04	0.57
1:D:500:GLN:OE1	1:D:505:ILE:HG23	2.05	0.57
1:E:355:GLN:O	1:E:359:LEU:HD11	2.05	0.57
1:F:229:VAL:HG13	1:F:230:GLN:N	2.19	0.57
1:A:312:VAL:HG23	1:A:370:CYS:SG	2.45	0.57
1:A:531:LYS:HB3	1:A:531:LYS:HZ3	1.69	0.57
1:B:631:GLU:O	1:B:635:LEU:HG	2.05	0.57
1:C:36:GLU:HG3	1:C:37:THR:H	1.70	0.57
1:E:117:LEU:HB3	1:E:119:GLU:OE1	2.05	0.57
1:A:292:PRO:O	1:A:294:TYR:N	2.38	0.57
1:A:500:GLN:CD	1:A:502:GLU:HG3	2.25	0.57
1:B:408:GLU:HG3	1:B:409:SER:N	2.19	0.57
1:C:631:GLU:O	1:C:635:LEU:HG	2.04	0.57
1:D:17:MET:HG3	1:D:17:MET:O	2.05	0.57
1:D:247:GLU:HA	1:D:252:THR:O	2.05	0.57
1:F:276:TRP:NE1	1:F:280:MET:HG3	2.19	0.57
1:F:649:LYS:O	1:F:653:GLU:HG3	2.05	0.57
1:A:225:ASN:ND2	1:A:225:ASN:N	2.52	0.56
1:A:225:ASN:ND2	1:A:225:ASN:H	2.02	0.56
1:A:259:LEU:HD12	1:A:259:LEU:N	2.20	0.56
1:A:626:LEU:O	1:A:629:VAL:HG22	2.05	0.56
1:B:489:SER:C	1:B:490:ILE:HD12	2.26	0.56
1:B:571:TYR:HB3	1:B:575:ARG:NH2	2.08	0.56
1:B:62:ILE:HG13	1:B:94:LEU:HD13	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:GLU:C	1:C:418:LYS:H	2.07	0.56
1:C:490:ILE:HG12	1:C:650:ARG:HB3	1.87	0.56
1:D:636:MET:C	1:D:638:GLU:H	2.07	0.56
1:E:294:TYR:CG	1:E:296:PRO:HD2	2.39	0.56
1:B:20:ARG:HB3	1:B:29:VAL:O	2.04	0.56
1:B:36:GLU:HG3	1:B:37:THR:H	1.69	0.56
1:C:428:LYS:O	1:C:432:GLN:HG2	2.05	0.56
1:C:489:SER:C	1:C:490:ILE:HD12	2.26	0.56
1:D:21:LEU:HD23	1:D:165:ILE:HG23	1.88	0.56
1:E:245:VAL:HA	1:E:254:LYS:O	2.04	0.56
1:E:270:ALA:O	1:E:274:GLU:HB2	2.05	0.56
1:A:268:VAL:O	1:A:272:ARG:HB2	2.05	0.56
1:A:544:ILE:O	1:A:547:LEU:HG	2.05	0.56
1:B:419:ARG:CB	1:B:419:ARG:CZ	2.82	0.56
1:B:462:ASN:O	1:B:466:SER:HB3	2.05	0.56
1:C:649:LYS:O	1:C:653:GLU:HG3	2.05	0.56
1:D:41:ILE:HG22	1:D:42:ALA:N	2.19	0.56
1:D:455:MET:O	1:D:459:LEU:HD13	2.06	0.56
1:D:549:ARG:HB2	1:D:549:ARG:CZ	2.35	0.56
1:D:570:LEU:N	1:D:570:LEU:HD12	2.20	0.56
1:D:65:MET:HB3	1:D:76:ALA:HB2	1.87	0.56
1:D:99:CYS:HB3	1:D:154:GLN:HB2	1.86	0.56
1:E:229:VAL:HG13	1:E:230:GLN:CD	2.25	0.56
1:E:626:LEU:N	1:E:627:PRO:HD2	2.20	0.56
1:C:221:PRO:O	1:C:222:PHE:CB	2.48	0.56
1:C:41:ILE:HG22	1:C:42:ALA:H	1.70	0.56
1:C:592:ARG:NH1	1:C:592:ARG:HB3	2.21	0.56
1:D:511:LEU:CG	1:D:515:ARG:HH12	2.16	0.56
1:E:21:LEU:C	1:E:165:ILE:HD13	2.26	0.56
1:E:430:TRP:HE1	1:E:587:SER:CA	2.15	0.56
1:E:570:LEU:N	1:E:570:LEU:HD12	2.21	0.56
1:F:389:LEU:CD2	1:F:454:ALA:HB1	2.35	0.56
1:C:245:VAL:HA	1:C:254:LYS:O	2.05	0.56
1:C:392:ASN:CG	1:C:393:SER:H	2.08	0.56
1:C:404:ARG:HE	1:C:601:PHE:HE2	1.53	0.56
1:D:26:PHE:CE1	1:D:179:CYS:HB3	2.41	0.56
1:E:170:ALA:HB3	1:E:178:LEU:HG	1.88	0.56
1:E:220:ARG:HB2	1:E:221:PRO:HD2	1.87	0.56
1:E:223:LEU:HA	1:E:227:GLN:OE1	2.06	0.56
1:E:284:HIS:CB	1:E:285:PRO:CD	2.82	0.56
1:F:335:SER:O	1:F:339:ARG:HG3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:GLU:C	1:B:17:MET:SD	2.84	0.56
1:B:533:LEU:HD22	1:B:629:VAL:HG12	1.87	0.56
1:C:309:LEU:HD11	1:C:311:LEU:HD23	1.86	0.56
1:C:451:GLN:NE2	1:C:611:GLN:HB3	2.21	0.56
1:D:182:PHE:CZ	1:D:194:LEU:HD23	2.40	0.56
1:D:383:ASP:O	1:D:384:MET:HB2	2.06	0.56
1:D:55:ARG:HB3	1:D:91:LEU:HD21	1.88	0.56
1:F:290:THR:HG23	1:F:296:PRO:O	2.04	0.56
1:F:36:GLU:HG3	1:F:37:THR:H	1.70	0.56
1:A:430:TRP:HE1	1:A:587:SER:HB3	1.69	0.56
1:A:570:LEU:N	1:A:570:LEU:HD12	2.21	0.56
1:B:559:THR:HG22	1:B:600:SER:OG	2.05	0.56
1:B:88:PRO:HG2	1:B:89:ASN:H	1.71	0.56
1:C:213:PHE:CD1	1:C:221:PRO:HG2	2.41	0.56
1:D:506:THR:HG22	1:D:507:SER:H	1.68	0.56
1:E:653:GLU:O	1:E:657:LEU:HD13	2.05	0.56
1:F:220:ARG:NH2	1:F:221:PRO:HB2	2.21	0.56
1:F:265:LEU:HD11	1:F:270:ALA:HA	1.88	0.56
1:A:186:LEU:HD22	1:A:186:LEU:O	2.06	0.56
1:B:649:LYS:O	1:B:653:GLU:HG3	2.05	0.56
1:C:276:TRP:NE1	1:C:280:MET:HG3	2.20	0.56
1:C:410:VAL:O	1:C:411:SER:HB3	2.06	0.56
1:F:220:ARG:CZ	1:F:221:PRO:HB2	2.36	0.56
1:F:392:ASN:CG	1:F:393:SER:H	2.09	0.56
1:F:643:VAL:O	1:F:647:GLN:HG2	2.05	0.56
1:A:213:PHE:CA	1:A:277:LEU:HD21	2.33	0.56
1:B:187:GLN:HB3	1:B:220:ARG:NH1	2.20	0.56
1:B:118:ARG:HB2	1:B:264:ASN:OD1	2.05	0.56
1:B:636:MET:C	1:B:638:GLU:H	2.08	0.56
1:F:428:LYS:O	1:F:432:GLN:HG2	2.06	0.56
1:A:171:LYS:HD2	1:A:199:TYR:OH	2.06	0.56
1:B:41:ILE:HG22	1:B:42:ALA:H	1.71	0.56
1:C:486:PHE:HE1	1:C:647:GLN:HB3	1.67	0.56
1:D:570:LEU:HD22	1:D:590:MET:HE2	1.87	0.56
1:E:171:LYS:NZ	1:E:173:LEU:HD23	2.21	0.56
1:A:20:ARG:HB3	1:A:29:VAL:O	2.06	0.56
1:B:227:GLN:HE22	1:B:229:VAL:HG13	1.70	0.56
1:B:648:GLU:HB3	1:C:488:THR:CG2	2.36	0.56
1:C:265:LEU:HD11	1:C:270:ALA:HA	1.86	0.56
1:D:229:VAL:HG23	1:D:230:GLN:N	2.12	0.56
1:D:478:GLN:HB2	1:E:478:GLN:HA	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:489:SER:C	1:E:490:ILE:HD12	2.26	0.56
1:A:422:ALA:O	1:A:585:GLY:HA2	2.06	0.55
1:A:544:ILE:HG22	1:A:618:CYS:SG	2.46	0.55
1:B:186:LEU:N	1:B:187:GLN:HE21	2.04	0.55
1:B:55:ARG:HD2	1:B:91:LEU:HD11	1.87	0.55
1:C:118:ARG:HB2	1:C:264:ASN:HB3	1.87	0.55
1:C:122:ILE:HD13	1:C:216:ILE:HG12	1.87	0.55
1:C:350:ASP:HB2	1:C:391:ASP:H	1.70	0.55
1:C:65:MET:HB3	1:C:76:ALA:HB2	1.88	0.55
1:E:216:ILE:HG22	1:E:263:ASN:OD1	2.05	0.55
1:E:434:TRP:HB3	1:E:571:TYR:CE1	2.41	0.55
1:A:239:SER:HB2	1:A:242:ASP:HB2	1.88	0.55
1:A:286:ARG:C	1:A:290:THR:HG21	2.25	0.55
1:A:335:SER:O	1:A:339:ARG:HG3	2.06	0.55
1:B:272:ARG:HH11	1:B:272:ARG:HG3	1.72	0.55
1:B:285:PRO:O	1:B:286:ARG:HG3	2.06	0.55
1:B:394:LYS:C	1:B:394:LYS:HZ3	2.09	0.55
1:C:118:ARG:HA	1:C:264:ASN:O	2.05	0.55
1:C:286:ARG:HA	1:C:290:THR:N	2.21	0.55
1:C:418:LYS:C	1:C:419:ARG:HD3	2.26	0.55
1:D:335:SER:O	1:D:339:ARG:HG3	2.06	0.55
1:D:570:LEU:HD22	1:D:590:MET:CE	2.36	0.55
1:E:220:ARG:HH11	1:E:220:ARG:HG2	1.70	0.55
1:F:627:PRO:HA	1:F:630:GLU:CB	2.34	0.55
1:A:213:PHE:CZ	1:A:243:ILE:HB	2.42	0.55
1:A:276:TRP:CE2	1:A:280:MET:HG3	2.41	0.55
1:A:292:PRO:C	1:A:294:TYR:N	2.60	0.55
1:A:486:PHE:CZ	1:A:517:MET:SD	2.99	0.55
1:A:489:SER:C	1:A:490:ILE:HD12	2.27	0.55
1:B:122:ILE:HD13	1:B:216:ILE:HG12	1.88	0.55
1:B:249:LEU:HD12	1:B:414:LEU:HD21	1.87	0.55
1:B:426:LEU:HD11	1:B:574:LEU:HD11	1.88	0.55
1:C:290:THR:HB	1:C:296:PRO:HA	1.88	0.55
1:C:457:ASN:HD21	1:C:619:LYS:HZ1	1.53	0.55
1:D:404:ARG:N	1:D:404:ARG:HD3	2.21	0.55
1:E:483:LEU:HD13	1:E:640:GLU:OE1	2.05	0.55
1:E:111:PHE:HD1	1:E:575:ARG:HD2	1.68	0.55
1:F:68:LEU:HD13	1:F:139:ASN:CG	2.27	0.55
1:B:415:GLN:HE21	1:B:419:ARG:HG2	1.70	0.55
1:B:536:ARG:CZ	1:B:625:LEU:HD13	2.36	0.55
1:C:626:LEU:HB3	1:C:627:PRO:CD	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:644:VAL:O	1:C:647:GLN:HB2	2.07	0.55
1:D:236:ARG:O	1:D:237:GLN:C	2.45	0.55
1:D:261:TYR:N	1:D:262:PRO:CD	2.69	0.55
1:D:62:ILE:HG13	1:D:94:LEU:HD13	1.88	0.55
1:E:592:ARG:NH1	1:E:592:ARG:HB3	2.22	0.55
1:E:87:ALA:HB1	1:E:88:PRO:HD2	1.89	0.55
1:F:294:TYR:HE1	1:F:301:LYS:HZ2	1.55	0.55
1:C:455:MET:O	1:C:459:LEU:HD13	2.06	0.55
1:C:490:ILE:HG21	1:C:517:MET:CE	2.36	0.55
1:E:187:GLN:HG2	1:E:220:ARG:HH21	1.72	0.55
1:F:583:THR:O	1:F:585:GLY:N	2.40	0.55
1:B:487:LYS:HA	1:B:491:GLN:HB2	1.89	0.55
1:C:222:PHE:HB3	1:C:231:TRP:CZ2	2.41	0.55
1:E:213:PHE:CE2	1:E:217:THR:HG21	2.40	0.55
1:E:294:TYR:CE1	1:E:301:LYS:HB3	2.42	0.55
1:E:549:ARG:CZ	1:E:549:ARG:HA	2.37	0.55
1:C:105:ARG:HD3	1:C:149:GLU:CD	2.27	0.55
1:D:168:GLY:C	1:D:170:ALA:H	2.10	0.55
1:D:592:ARG:NH1	1:D:592:ARG:HB3	2.22	0.55
1:E:51:SER:HB2	1:E:52:PRO:HD2	1.89	0.55
1:E:627:PRO:HA	1:E:630:GLU:CB	2.36	0.55
1:F:431:GLY:N	1:F:571:TYR:HE2	2.05	0.55
1:B:118:ARG:HB2	1:B:264:ASN:ND2	2.21	0.55
1:C:222:PHE:HE2	1:C:281:LEU:HD21	1.70	0.55
1:D:19:GLU:H	1:D:19:GLU:CD	2.10	0.55
1:D:276:TRP:NE1	1:D:280:MET:HG3	2.22	0.55
1:D:316:ASN:HA	1:D:388:PHE:CE1	2.42	0.55
1:E:387:VAL:HG21	1:E:449:GLN:O	2.07	0.55
1:E:65:MET:HB3	1:E:76:ALA:HB2	1.89	0.55
1:A:320:GLY:HA2	1:A:405:PRO:HG3	1.89	0.55
1:A:626:LEU:HB3	1:A:627:PRO:CD	2.37	0.55
1:B:265:LEU:HD21	1:B:270:ALA:HB2	1.88	0.55
1:B:34:ASN:ND2	1:B:83:MET:SD	2.80	0.55
1:D:312:VAL:HG22	1:D:313:HIS:H	1.71	0.55
1:E:226:TRP:CE3	1:E:229:VAL:HG12	2.42	0.55
1:F:636:MET:C	1:F:638:GLU:H	2.09	0.55
1:A:114:CYS:SG	1:A:575:ARG:NH1	2.79	0.55
1:A:310:LYS:HZ3	1:A:310:LYS:HB2	1.70	0.55
1:B:213:PHE:CD1	1:B:221:PRO:HB2	2.41	0.55
1:C:434:TRP:HB3	1:C:571:TYR:OH	2.05	0.55
1:C:548:GLN:O	1:C:549:ARG:HG3	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:GLN:HA	1:E:89:ASN:HD21	1.72	0.55
1:E:60:LEU:O	1:E:64:ILE:HG12	2.07	0.55
1:F:117:LEU:HG	1:F:119:GLU:OE2	2.07	0.55
1:F:295:GLY:N	1:F:296:PRO:CD	2.70	0.55
1:F:462:ASN:O	1:F:466:SER:HB3	2.07	0.55
1:C:165:ILE:CG2	1:C:166:ASP:H	2.12	0.54
1:C:170:ALA:O	1:C:178:LEU:HB2	2.07	0.54
1:D:122:ILE:HD13	1:D:216:ILE:HG12	1.89	0.54
1:D:219:PHE:O	1:D:220:ARG:C	2.45	0.54
1:D:272:ARG:HG3	1:D:272:ARG:HH11	1.71	0.54
1:D:55:ARG:HH11	1:D:91:LEU:CD2	2.19	0.54
1:E:216:ILE:HD12	1:E:277:LEU:HD22	1.87	0.54
1:A:286:ARG:O	1:A:290:THR:OG1	2.25	0.54
1:A:592:ARG:NH1	1:A:592:ARG:HB3	2.21	0.54
1:B:213:PHE:CE1	1:B:243:ILE:HB	2.42	0.54
1:D:111:PHE:O	1:D:114:CYS:HB2	2.07	0.54
1:D:559:THR:HB	1:D:604:LYS:NZ	2.22	0.54
1:D:404:ARG:HD2	1:D:605:VAL:HG11	1.89	0.54
1:E:295:GLY:N	1:E:296:PRO:CD	2.70	0.54
1:F:259:LEU:HD11	1:F:270:ALA:HB1	1.89	0.54
1:B:172:GLU:HG2	1:B:175:GLN:OE1	2.07	0.54
1:B:366:PRO:O	1:B:368:THR:N	2.40	0.54
1:A:311:LEU:HD12	1:A:311:LEU:O	2.07	0.54
1:A:410:VAL:O	1:A:411:SER:HB3	2.08	0.54
1:B:282:MET:HB2	1:B:286:ARG:HH21	1.73	0.54
1:B:570:LEU:N	1:B:570:LEU:HD12	2.23	0.54
1:B:477:GLN:NE2	1:C:477:GLN:HE21	2.05	0.54
1:E:220:ARG:HB2	1:E:221:PRO:CD	2.38	0.54
1:F:213:PHE:CE2	1:F:217:THR:HG21	2.43	0.54
1:A:297:ASN:O	1:A:298:GLY:O	2.26	0.54
1:A:316:ASN:CG	1:A:344:THR:HG21	2.27	0.54
1:A:530:VAL:CG1	1:A:633:VAL:HG12	2.38	0.54
1:B:276:TRP:NE1	1:B:280:MET:HG3	2.23	0.54
1:B:41:ILE:HG22	1:B:42:ALA:N	2.22	0.54
1:E:494:LEU:HD21	1:E:515:ARG:HG2	1.90	0.54
1:F:142:ILE:CG1	1:F:173:LEU:HD11	2.28	0.54
1:A:659:LYS:CD	1:F:500:GLN:HE22	2.15	0.54
1:A:291:ASP:O	1:A:293:THR:N	2.41	0.54
1:B:118:ARG:HH22	1:B:438:GLN:HG2	1.73	0.54
1:B:234:LYS:O	1:B:237:GLN:HB3	2.08	0.54
1:B:118:ARG:HD2	1:B:264:ASN:HD21	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:LEU:HD12	1:B:286:ARG:HG2	1.90	0.54
1:B:581:GLN:H	1:B:581:GLN:CD	2.10	0.54
1:C:212:ALA:O	1:C:216:ILE:HG13	2.07	0.54
1:C:241:VAL:O	1:C:241:VAL:HG12	2.08	0.54
1:C:312:VAL:HG22	1:C:313:HIS:N	2.22	0.54
1:C:457:ASN:HA	1:C:460:ARG:HG3	1.89	0.54
1:D:123:LEU:HD12	1:D:307:LEU:HD13	1.90	0.54
1:E:17:MET:HB3	1:E:31:ARG:O	2.08	0.54
1:E:194:LEU:HB3	1:E:196:GLN:HE22	1.72	0.54
1:E:20:ARG:HB3	1:E:29:VAL:O	2.07	0.54
1:E:18:LYS:CB	1:E:31:ARG:HD3	2.38	0.54
1:E:511:LEU:CG	1:E:515:ARG:HH12	2.17	0.54
1:E:530:VAL:HG22	1:E:632:VAL:CG1	2.36	0.54
1:E:544:ILE:O	1:E:547:LEU:HG	2.08	0.54
1:F:118:ARG:HH22	1:F:438:GLN:HG2	1.73	0.54
1:F:511:LEU:CG	1:F:515:ARG:HH12	2.16	0.54
1:F:625:LEU:HD22	1:F:628:LYS:HD2	1.88	0.54
1:B:18:LYS:HB3	1:B:19:GLU:OE2	2.08	0.54
1:B:294:TYR:CG	1:B:301:LYS:HD3	2.43	0.54
1:C:220:ARG:N	1:C:221:PRO:CD	2.71	0.54
1:E:434:TRP:HB3	1:E:571:TYR:CZ	2.42	0.54
1:F:467:LYS:HA	1:F:541:GLN:NE2	2.23	0.54
1:A:239:SER:HA	1:A:242:ASP:OD2	2.06	0.54
1:A:279:LEU:C	1:A:281:LEU:H	2.10	0.54
1:B:114:CYS:O	1:B:115:CYS:HB3	2.08	0.54
1:B:335:SER:O	1:B:339:ARG:HG3	2.07	0.54
1:B:428:LYS:O	1:B:432:GLN:HG2	2.08	0.54
1:C:410:VAL:HG12	1:C:411:SER:N	2.17	0.54
1:C:394:LYS:HE2	1:C:612:LEU:CD1	2.38	0.54
1:D:213:PHE:CE2	1:D:217:THR:HG21	2.43	0.54
1:D:268:VAL:HG13	1:D:269:LEU:N	2.23	0.54
1:F:243:ILE:O	1:F:245:VAL:HG23	2.07	0.54
1:F:259:LEU:H	1:F:274:GLU:HG3	1.73	0.54
1:B:118:ARG:HB2	1:B:264:ASN:CG	2.29	0.54
1:C:41:ILE:HG22	1:C:42:ALA:N	2.22	0.54
1:D:194:LEU:HB3	1:D:196:GLN:HE22	1.72	0.54
1:D:282:MET:CB	1:D:286:ARG:CZ	2.85	0.54
1:C:81:GLU:CD	1:F:364:ASP:HB2	2.28	0.54
1:F:316:ASN:HA	1:F:388:PHE:CE1	2.43	0.54
1:A:36:GLU:HG3	1:A:37:THR:H	1.72	0.54
1:A:394:LYS:HZ3	1:A:613:SER:HB2	1.71	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:LEU:HB3	1:B:165:ILE:HG21	1.90	0.54
1:B:51:SER:HB2	1:B:52:PRO:HD2	1.89	0.54
1:B:548:GLN:O	1:B:549:ARG:HD2	2.08	0.54
1:B:434:TRP:HB3	1:B:571:TYR:OH	2.08	0.54
1:C:261:TYR:N	1:C:262:PRO:HD2	2.23	0.54
1:C:506:THR:O	1:C:508:ASP:N	2.41	0.54
1:D:514:TRP:HA	1:D:650:ARG:NH1	2.22	0.54
1:E:430:TRP:CZ3	1:E:570:LEU:HD23	2.43	0.54
1:A:118:ARG:NH2	1:A:438:GLN:HG2	2.16	0.53
1:A:570:LEU:HD22	1:A:590:MET:CE	2.36	0.53
1:D:105:ARG:HD3	1:D:149:GLU:CD	2.28	0.53
1:D:355:GLN:O	1:D:359:LEU:HD11	2.09	0.53
1:E:431:GLY:CA	1:E:571:TYR:CE2	2.88	0.53
1:F:501:THR:HG23	1:F:505:ILE:HG21	1.90	0.53
1:F:60:LEU:O	1:F:64:ILE:HG12	2.08	0.53
1:A:114:CYS:SG	1:A:115:CYS:N	2.81	0.53
1:A:43:ILE:HD12	1:A:43:ILE:N	2.24	0.53
1:A:65:MET:HB3	1:A:76:ALA:HB2	1.90	0.53
1:B:65:MET:HB3	1:B:76:ALA:HB2	1.89	0.53
1:C:173:LEU:HD23	1:C:173:LEU:O	2.07	0.53
1:C:20:ARG:HB3	1:C:29:VAL:O	2.08	0.53
1:C:231:TRP:C	1:C:233:SER:H	2.10	0.53
1:D:474:SER:O	1:D:477:GLN:HG2	2.09	0.53
1:E:160:LEU:HD12	1:E:160:LEU:N	2.23	0.53
1:E:504:GLY:O	1:E:505:ILE:HG23	2.09	0.53
1:F:105:ARG:HD3	1:F:149:GLU:CD	2.29	0.53
1:F:62:ILE:HG13	1:F:94:LEU:HD13	1.90	0.53
1:A:517:MET:HG2	1:A:650:ARG:CZ	2.38	0.53
1:B:286:ARG:HA	1:B:290:THR:OG1	2.08	0.53
1:D:487:LYS:HA	1:D:491:GLN:HB2	1.91	0.53
1:B:35:GLN:HG2	1:E:465:LEU:CG	2.38	0.53
1:F:238:LYS:HE3	1:F:238:LYS:HA	1.89	0.53
1:A:547:LEU:HD22	1:A:614:LYS:CE	2.38	0.53
1:B:626:LEU:HB3	1:B:627:PRO:HD3	1.91	0.53
1:E:113:ASN:OD1	1:E:117:LEU:HG	2.09	0.53
1:E:279:LEU:C	1:E:281:LEU:H	2.12	0.53
1:E:316:ASN:CG	1:E:344:THR:HG21	2.29	0.53
1:E:415:GLN:O	1:E:418:LYS:O	2.26	0.53
1:E:431:GLY:CA	1:E:571:TYR:HE2	2.20	0.53
1:E:517:MET:HG2	1:E:650:ARG:CZ	2.39	0.53
1:F:312:VAL:HG22	1:F:313:HIS:N	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:TRP:NE1	1:A:280:MET:HG3	2.24	0.53
1:C:487:LYS:HA	1:C:491:GLN:HB2	1.90	0.53
1:F:316:ASN:CG	1:F:344:THR:HG21	2.29	0.53
1:F:387:VAL:HG11	1:F:450:GLY:CA	2.28	0.53
1:A:578:PRO:O	1:A:580:ASP:N	2.41	0.53
1:C:37:THR:CG2	1:F:362:ILE:HG13	2.39	0.53
1:D:410:VAL:HG12	1:D:411:SER:N	2.19	0.53
1:D:500:GLN:CA	1:D:500:GLN:HE21	2.21	0.53
1:D:500:GLN:C	1:D:500:GLN:HE21	2.12	0.53
1:D:620:GLN:O	1:D:624:GLU:HG2	2.08	0.53
1:E:227:GLN:HA	1:E:231:TRP:HB2	1.91	0.53
1:E:620:GLN:O	1:E:624:GLU:HG2	2.07	0.53
1:F:261:TYR:H	1:F:262:PRO:HD2	1.74	0.53
1:A:430:TRP:HE1	1:A:587:SER:CB	2.21	0.53
1:B:294:TYR:OH	1:B:302:ALA:HB2	2.08	0.53
1:B:316:ASN:HA	1:B:388:PHE:CE1	2.44	0.53
1:B:419:ARG:NH2	1:B:588:GLN:HG3	2.24	0.53
1:B:67:ARG:NH2	1:B:68:LEU:HD12	2.21	0.53
1:C:213:PHE:CE2	1:C:221:PRO:HG3	2.44	0.53
1:C:547:LEU:HD22	1:C:614:LYS:HE2	1.91	0.53
1:E:636:MET:C	1:E:638:GLU:H	2.11	0.53
1:A:118:ARG:HD3	1:A:435:HIS:CE1	2.44	0.53
1:A:23:THR:HA	1:A:29:VAL:HG22	1.90	0.53
1:B:270:ALA:O	1:B:274:GLU:HB2	2.09	0.53
1:B:355:GLN:HB3	1:B:359:LEU:CD1	2.38	0.53
1:B:355:GLN:HB3	1:B:359:LEU:HD13	1.91	0.53
1:C:272:ARG:HH11	1:C:272:ARG:HG3	1.73	0.53
1:C:335:SER:O	1:C:339:ARG:HG3	2.09	0.53
1:D:544:ILE:O	1:D:547:LEU:HG	2.09	0.53
1:D:644:VAL:O	1:D:647:GLN:HB2	2.09	0.53
1:E:226:TRP:HE3	1:E:229:VAL:HG12	1.73	0.53
1:A:118:ARG:HB2	1:A:264:ASN:CB	2.31	0.53
1:A:533:LEU:CD1	1:A:629:VAL:HA	2.38	0.53
1:A:549:ARG:NE	1:A:549:ARG:HA	2.23	0.53
1:B:70:HIS:HE1	1:B:132:ALA:HA	1.73	0.53
1:B:433:VAL:O	1:B:436:SER:HB3	2.09	0.53
1:B:536:ARG:HG2	1:B:536:ARG:HH11	1.73	0.53
1:B:644:VAL:O	1:B:647:GLN:HB2	2.08	0.53
1:C:192:GLU:HG2	1:C:283:TRP:HB2	1.91	0.53
1:C:474:SER:O	1:C:477:GLN:HG2	2.09	0.53
1:C:49:GLU:OE2	1:C:90:ASP:HB2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:VAL:O	1:D:411:SER:HB3	2.08	0.53
1:D:457:ASN:HA	1:D:460:ARG:HG3	1.91	0.53
1:D:480:LYS:HG2	1:D:527:GLU:OE2	2.09	0.53
1:E:122:ILE:HD13	1:E:216:ILE:HG12	1.90	0.53
1:E:430:TRP:NE1	1:E:587:SER:HA	2.17	0.53
1:F:430:TRP:CE2	1:F:590:MET:HB2	2.44	0.53
1:A:105:ARG:HD3	1:A:149:GLU:CD	2.28	0.53
1:A:185:THR:O	1:A:186:LEU:HB3	2.08	0.53
1:A:221:PRO:HB3	1:A:244:VAL:HA	1.89	0.53
1:B:57:ARG:HH21	1:B:177:GLU:HG2	1.74	0.53
1:B:298:GLY:O	1:B:299:CYS:C	2.47	0.53
1:B:365:LYS:O	1:B:367:ALA:N	2.42	0.53
1:B:490:ILE:CD1	1:B:651:GLN:HG2	2.36	0.53
1:C:227:GLN:O	1:C:231:TRP:HB2	2.09	0.53
1:C:239:SER:HB2	1:C:242:ASP:HB2	1.91	0.53
1:C:577:LYS:HG3	1:C:578:PRO:HD2	1.91	0.53
1:D:102:GLY:HA2	1:D:153:LEU:H	1.72	0.53
1:E:36:GLU:HG3	1:E:37:THR:H	1.73	0.53
1:F:145:ASP:HB3	1:F:169:TYR:HB3	1.91	0.53
1:A:658:LEU:HD21	1:F:497:TYR:CE1	2.43	0.53
1:A:261:TYR:N	1:A:262:PRO:HD2	2.24	0.52
1:A:636:MET:C	1:A:638:GLU:H	2.10	0.52
1:C:643:VAL:O	1:C:647:GLN:HG2	2.09	0.52
1:B:496:LYS:HD2	1:C:655:TRP:HA	1.90	0.52
1:D:540:LEU:CD2	1:D:622:ALA:HB2	2.39	0.52
1:A:474:SER:O	1:A:477:GLN:HG2	2.10	0.52
1:A:620:GLN:O	1:A:624:GLU:HG2	2.08	0.52
1:B:316:ASN:CG	1:B:344:THR:HG21	2.29	0.52
1:B:653:GLU:O	1:B:657:LEU:HD13	2.09	0.52
1:C:213:PHE:CE2	1:C:217:THR:HG21	2.44	0.52
1:C:279:LEU:C	1:C:281:LEU:H	2.11	0.52
1:C:61:GLU:HB2	1:C:178:LEU:HD21	1.90	0.52
1:D:213:PHE:CG	1:D:221:PRO:HD2	2.44	0.52
1:D:536:ARG:HG2	1:D:536:ARG:HH11	1.75	0.52
1:D:654:LEU:HB3	1:E:654:LEU:HD23	1.90	0.52
1:F:214:GLU:HG3	1:F:219:PHE:CA	2.39	0.52
1:F:487:LYS:HA	1:F:491:GLN:HB2	1.91	0.52
1:A:223:LEU:HB3	1:A:231:TRP:CZ3	2.44	0.52
1:A:249:LEU:HD11	1:A:414:LEU:HG	1.92	0.52
1:B:286:ARG:HA	1:B:290:THR:CB	2.38	0.52
1:B:457:ASN:ND2	1:B:619:LYS:NZ	2.55	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:ILE:O	1:B:547:LEU:HG	2.09	0.52
1:B:91:LEU:HB3	1:B:92:PRO:CD	2.38	0.52
1:C:226:TRP:HD1	1:C:226:TRP:H	1.58	0.52
1:C:367:ALA:C	1:C:369:GLN:H	2.11	0.52
1:C:536:ARG:HG2	1:C:536:ARG:HH11	1.74	0.52
1:E:298:GLY:O	1:E:299:CYS:C	2.48	0.52
1:E:500:GLN:C	1:E:500:GLN:HE21	2.12	0.52
1:A:51:SER:HB2	1:A:52:PRO:HD2	1.91	0.52
1:A:661:ALA:CB	1:F:662:CYS:SG	2.97	0.52
1:B:493:ASP:HA	1:B:496:LYS:HG3	1.92	0.52
1:B:579:ARG:HG2	1:B:579:ARG:O	2.10	0.52
1:C:368:THR:C	1:C:370:CYS:H	2.12	0.52
1:C:62:ILE:HG13	1:C:94:LEU:HD13	1.91	0.52
1:D:152:VAL:HG13	1:D:165:ILE:HD11	1.91	0.52
1:E:371:ILE:C	1:E:373:ASP:H	2.11	0.52
1:E:431:GLY:HA2	1:E:571:TYR:CD2	2.43	0.52
1:F:270:ALA:O	1:F:274:GLU:HB2	2.09	0.52
1:F:282:MET:HB3	1:F:286:ARG:HB2	1.90	0.52
1:A:643:VAL:O	1:A:647:GLN:HG2	2.10	0.52
1:B:475:MET:O	1:B:478:GLN:HB3	2.09	0.52
1:C:316:ASN:CG	1:C:344:THR:HG21	2.30	0.52
1:C:18:LYS:HG3	1:C:31:ARG:HG2	1.91	0.52
1:C:407:PRO:O	1:C:408:GLU:CB	2.58	0.52
1:D:283:TRP:HE3	1:D:285:PRO:HD2	1.72	0.52
1:E:369:GLN:C	1:E:371:ILE:H	2.12	0.52
1:E:354:LEU:HD22	1:E:457:ASN:HB2	1.90	0.52
1:F:268:VAL:O	1:F:272:ARG:HB2	2.09	0.52
1:F:489:SER:C	1:F:490:ILE:HD12	2.29	0.52
1:F:528:ASN:O	1:F:531:LYS:HB3	2.10	0.52
1:A:533:LEU:HD13	1:A:629:VAL:CG1	2.40	0.52
1:A:62:ILE:HG13	1:A:94:LEU:HD13	1.90	0.52
1:B:659:LYS:HE2	1:C:499:GLU:OE1	2.09	0.52
1:C:72:ASN:HA	1:C:163:LYS:HA	1.91	0.52
1:D:582:ARG:H	1:D:582:ARG:NE	1.85	0.52
1:D:626:LEU:HD23	1:D:627:PRO:N	2.25	0.52
1:F:72:ASN:HA	1:F:163:LYS:HA	1.91	0.52
1:F:261:TYR:N	1:F:262:PRO:HD2	2.25	0.52
1:F:592:ARG:NH1	1:F:592:ARG:HB3	2.24	0.52
1:A:214:GLU:OE1	1:A:220:ARG:HD3	2.09	0.52
1:A:282:MET:HE3	1:A:286:ARG:HH21	1.73	0.52
1:A:407:PRO:O	1:A:408:GLU: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:665:VAL:HG23	1:F:665:VAL:HB	1.90	0.52
1:B:556:GLN:NE2	1:B:559:THR:OG1	2.42	0.52
1:B:547:LEU:HD22	1:B:614:LYS:HE2	1.91	0.52
1:B:86:LEU:HD12	1:B:87:ALA:H	1.75	0.52
1:C:74:VAL:HG23	1:C:164:ILE:O	2.09	0.52
1:D:643:VAL:O	1:D:647:GLN:HG2	2.09	0.52
1:F:142:ILE:HG12	1:F:201:VAL:HG13	1.92	0.52
1:F:362:ILE:HD12	1:F:369:GLN:HE22	1.75	0.52
1:A:626:LEU:N	1:A:627:PRO:HD2	2.24	0.52
1:B:500:GLN:CA	1:B:500:GLN:HE21	2.23	0.52
1:C:262:PRO:HB2	1:C:432:GLN:NE2	2.25	0.52
1:C:355:GLN:O	1:C:359:LEU:HD11	2.09	0.52
1:C:366:PRO:O	1:C:367:ALA:HB3	2.10	0.52
1:C:36:GLU:O	1:C:38:GLY:N	2.43	0.52
1:D:171:LYS:HD2	1:D:172:GLU:N	2.25	0.52
1:D:493:ASP:HA	1:D:496:LYS:HG3	1.91	0.52
1:E:105:ARG:HD3	1:E:149:GLU:CD	2.31	0.52
1:F:265:LEU:H	1:F:265:LEU:CD2	2.22	0.52
1:F:294:TYR:CZ	1:F:301:LYS:HD3	2.44	0.52
1:A:343:ASP:O	1:B:418:LYS:HB3	2.10	0.52
1:B:107:TYR:CE2	1:B:153:LEU:HD22	2.45	0.52
1:B:74:VAL:HG23	1:B:164:ILE:O	2.10	0.52
1:E:187:GLN:CG	1:E:220:ARG:HH21	2.23	0.52
1:E:23:THR:HA	1:E:29:VAL:HG22	1.91	0.52
1:B:362:ILE:HG23	1:E:37:THR:HG21	1.91	0.52
1:F:229:VAL:C	1:F:231:TRP:H	2.13	0.52
1:F:434:TRP:HZ3	1:F:564:GLU:OE1	1.93	0.52
1:A:104:LEU:HD23	1:A:148:PRO:HB3	1.92	0.52
1:A:286:ARG:HA	1:A:290:THR:CB	2.40	0.52
1:A:627:PRO:HA	1:A:630:GLU:CB	2.37	0.52
1:A:657:LEU:CB	1:F:658:LEU:HD21	2.37	0.52
1:B:213:PHE:CE1	1:B:221:PRO:CB	2.93	0.52
1:D:270:ALA:O	1:D:274:GLU:HB2	2.10	0.52
1:D:36:GLU:O	1:D:38:GLY:N	2.43	0.52
1:E:335:SER:O	1:E:339:ARG:HG3	2.10	0.52
1:E:355:GLN:HB3	1:E:359:LEU:CD1	2.40	0.52
1:E:424:PHE:CD1	1:E:582:ARG:CZ	2.86	0.52
1:F:624:GLU:O	1:F:627:PRO:HG2	2.10	0.52
1:A:241:VAL:HG12	1:A:241:VAL:O	2.10	0.51
1:A:270:ALA:O	1:A:274:GLU:HB2	2.10	0.51
1:B:160:LEU:HD12	1:B:160:LEU:N	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ASN:HD22	1:B:90:ASP:N	2.08	0.51
1:F:350:ASP:HB2	1:F:391:ASP:H	1.75	0.51
1:F:430:TRP:HE1	1:F:587:SER:CA	2.21	0.51
1:F:456:MET:HE3	1:F:459:LEU:HD22	1.92	0.51
1:A:428:LYS:O	1:A:432:GLN:HG2	2.10	0.51
1:A:487:LYS:HA	1:A:491:GLN:HB2	1.91	0.51
1:B:243:ILE:HG22	1:B:281:LEU:CD2	2.41	0.51
1:B:460:ARG:C	1:B:462:ASN:H	2.13	0.51
1:B:559:THR:HB	1:B:604:LYS:HZ1	1.75	0.51
1:B:627:PRO:HA	1:B:630:GLU:CB	2.39	0.51
1:C:279:LEU:HD11	1:C:290:THR:N	2.25	0.51
1:D:404:ARG:HB3	1:D:405:PRO:HD2	1.93	0.51
1:E:316:ASN:HA	1:E:388:PHE:CE1	2.45	0.51
1:E:355:GLN:HB3	1:E:359:LEU:HD13	1.92	0.51
1:B:173:LEU:HD12	1:B:174:ASP:H	1.75	0.51
1:B:214:GLU:O	1:B:218:GLY:HA2	2.10	0.51
1:B:216:ILE:HD12	1:B:277:LEU:HD22	1.93	0.51
1:B:500:GLN:C	1:B:500:GLN:HE21	2.14	0.51
1:C:102:GLY:CA	1:C:153:LEU:H	2.22	0.51
1:C:226:TRP:CD1	1:C:226:TRP:N	2.77	0.51
1:C:231:TRP:CD1	1:C:235:VAL:HG21	2.45	0.51
1:C:371:ILE:HG12	1:C:384:MET:O	2.10	0.51
1:D:489:SER:C	1:D:490:ILE:HD12	2.30	0.51
1:D:559:THR:HG22	1:D:600:SER:OG	2.11	0.51
1:E:272:ARG:HH11	1:E:272:ARG:HG3	1.75	0.51
1:E:500:GLN:HE21	1:E:500:GLN:CA	2.22	0.51
1:F:223:LEU:N	1:F:224:PRO:CD	2.74	0.51
1:F:295:GLY:N	1:F:296:PRO:HD2	2.26	0.51
1:F:321:THR:HG21	1:F:447:LEU:CD1	2.35	0.51
1:A:295:GLY:CA	1:A:301:LYS:HD3	2.41	0.51
1:A:295:GLY:HA3	1:A:301:LYS:HD3	1.93	0.51
1:B:658:LEU:HD23	1:C:496:LYS:NZ	2.25	0.51
1:C:152:VAL:HG13	1:C:165:ILE:HD11	1.91	0.51
1:C:371:ILE:HG22	1:C:372:SER:H	1.74	0.51
1:D:125:LEU:C	1:D:125:LEU:HD13	2.31	0.51
1:D:43:ILE:N	1:D:43:ILE:HD12	2.25	0.51
1:E:125:LEU:HD13	1:E:125:LEU:C	2.31	0.51
1:E:528:ASN:O	1:E:532:LEU:HD23	2.10	0.51
1:F:16:GLU:CB	1:F:33:HIS:H	2.20	0.51
1:A:284:HIS:HB3	1:A:285:PRO:CD	2.40	0.51
1:A:355:GLN:HB3	1:A:359:LEU:CD1	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ASN:HD22	1:B:308:ASN:N	2.09	0.51
1:B:89:ASN:OD1	1:B:91:LEU:HB2	2.10	0.51
1:C:514:TRP:HA	1:C:650:ARG:NH1	2.25	0.51
1:D:475:MET:O	1:D:478:GLN:HB3	2.11	0.51
1:E:41:ILE:HG22	1:E:42:ALA:H	1.76	0.51
1:E:476:SER:HB2	1:E:636:MET:CE	2.40	0.51
1:F:418:LYS:HB3	1:F:420:ASN:OD1	2.11	0.51
1:F:483:LEU:HD12	1:F:644:VAL:HG21	1.92	0.51
1:A:225:ASN:N	1:A:225:ASN:HD22	2.09	0.51
1:A:369:GLN:HA	1:A:369:GLN:OE1	2.10	0.51
1:A:41:ILE:HG22	1:A:42:ALA:N	2.25	0.51
1:B:213:PHE:CZ	1:B:221:PRO:HG2	2.45	0.51
1:C:500:GLN:HE21	1:C:500:GLN:CA	2.24	0.51
1:C:81:GLU:CG	1:F:364:ASP:HB2	2.40	0.51
1:E:219:PHE:CE2	1:E:260:PRO:HG3	2.46	0.51
1:E:428:LYS:O	1:E:432:GLN:HG2	2.10	0.51
1:F:536:ARG:HH11	1:F:536:ARG:HG2	1.76	0.51
1:F:620:GLN:O	1:F:624:GLU:HG2	2.11	0.51
1:B:418:LYS:O	1:B:419:ARG:HD3	2.10	0.51
1:B:68:LEU:HD13	1:B:139:ASN:CG	2.31	0.51
1:D:316:ASN:CG	1:D:344:THR:HG21	2.30	0.51
1:D:434:TRP:HB3	1:D:571:TYR:OH	2.09	0.51
1:E:434:TRP:CE3	1:E:568:ARG:HB2	2.45	0.51
1:E:426:LEU:HD11	1:E:574:LEU:HD11	1.91	0.51
1:F:279:LEU:C	1:F:281:LEU:H	2.13	0.51
1:F:460:ARG:C	1:F:462:ASN:H	2.14	0.51
1:A:213:PHE:CE2	1:A:217:THR:HG21	2.45	0.51
1:A:223:LEU:HG	1:A:226:TRP:CD1	2.46	0.51
1:A:384:MET:O	1:A:384:MET:HG3	2.11	0.51
1:A:493:ASP:HA	1:A:496:LYS:HG3	1.92	0.51
1:C:51:SER:HB2	1:C:52:PRO:HD2	1.92	0.51
1:C:570:LEU:H	1:C:570:LEU:HD12	1.73	0.51
1:D:144:ARG:HD2	1:D:171:LYS:CB	2.37	0.51
1:D:20:ARG:HB3	1:D:29:VAL:O	2.10	0.51
1:D:627:PRO:HA	1:D:630:GLU:CB	2.41	0.51
1:E:434:TRP:CZ3	1:E:568:ARG:NE	2.79	0.51
1:E:497:TYR:CE2	1:E:511:LEU:HD21	2.46	0.51
1:E:438:GLN:HA	1:E:564:GLU:HG3	1.93	0.51
1:F:23:THR:HA	1:F:29:VAL:HG22	1.93	0.51
1:F:500:GLN:CA	1:F:500:GLN:HE21	2.23	0.51
1:A:292:PRO:CG	1:A:296:PRO:O	2.57	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LEU:HD13	1:B:125:LEU:C	2.31	0.51
1:B:592:ARG:NH1	1:B:592:ARG:HB3	2.26	0.51
1:B:486:PHE:CE1	1:B:647:GLN:HB3	2.44	0.51
1:C:60:LEU:O	1:C:64:ILE:HG12	2.11	0.51
1:E:408:GLU:HG3	1:E:409:SER:N	2.25	0.51
1:A:268:VAL:HG13	1:A:269:LEU:N	2.26	0.51
1:A:41:ILE:HG22	1:A:42:ALA:H	1.76	0.51
1:A:534:VAL:O	1:A:538:MET:HB2	2.11	0.51
1:B:510:LEU:HB3	1:B:653:GLU:OE2	2.11	0.51
1:C:213:PHE:CZ	1:C:243:ILE:HB	2.46	0.51
1:C:431:GLY:C	1:C:433:VAL:H	2.14	0.51
1:C:517:MET:HB3	1:C:650:ARG:NH2	2.26	0.51
1:C:80:PRO:HB2	1:C:84:GLN:HE21	1.76	0.51
1:D:115:CYS:O	1:D:217:THR:O	2.28	0.51
1:E:165:ILE:HG22	1:E:166:ASP:N	2.15	0.51
1:E:268:VAL:HG13	1:E:269:LEU:N	2.26	0.51
1:E:282:MET:HG2	1:E:286:ARG:NE	2.23	0.51
1:E:493:ASP:HA	1:E:496:LYS:HG3	1.93	0.51
1:F:113:ASN:HB3	1:F:117:LEU:HD12	1.93	0.51
1:F:230:GLN:O	1:F:234:LYS:N	2.39	0.51
1:F:394:LYS:CG	1:F:401:ILE:HG22	2.41	0.51
1:F:426:LEU:HD22	1:F:586:ASP:O	2.11	0.51
1:A:583:THR:HG23	1:A:584:GLU:OE2	2.10	0.50
1:A:430:TRP:HE1	1:A:587:SER:HA	1.76	0.50
1:B:249:LEU:HD23	1:B:418:LYS:HZ1	1.76	0.50
1:B:410:VAL:HG12	1:B:411:SER:N	2.18	0.50
1:B:556:GLN:NE2	1:B:604:LYS:NZ	2.59	0.50
1:D:219:PHE:CD1	1:D:221:PRO:HG3	2.47	0.50
1:D:361:LEU:HD22	1:D:370:CYS:SG	2.51	0.50
1:D:578:PRO:C	1:D:580:ASP:H	2.14	0.50
1:E:117:LEU:HD23	1:E:119:GLU:OE1	2.11	0.50
1:E:245:VAL:HG12	1:E:245:VAL:O	2.10	0.50
1:F:227:GLN:O	1:F:231:TRP:HB3	2.11	0.50
1:F:420:ASN:C	1:F:421:LEU:HD22	2.32	0.50
1:B:152:VAL:HG13	1:B:165:ILE:HD11	1.92	0.50
1:D:418:LYS:HZ1	1:D:421:LEU:HD12	1.76	0.50
1:D:428:LYS:O	1:D:432:GLN:HG2	2.10	0.50
1:E:223:LEU:HD13	1:E:224:PRO:N	2.26	0.50
1:E:265:LEU:HD11	1:E:270:ALA:CA	2.34	0.50
1:E:41:ILE:HG22	1:E:42:ALA:N	2.26	0.50
1:E:77:ARG:HD2	1:E:78:ASP:H	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:355:GLN:HB3	1:F:359:LEU:HD13	1.93	0.50
1:A:336:LEU:HD23	1:A:340:ILE:HG23	1.93	0.50
1:A:410:VAL:HG12	1:A:411:SER:N	2.22	0.50
1:A:477:GLN:CD	1:F:478:GLN:NE2	2.65	0.50
1:B:20:ARG:HB2	1:B:23:THR:HB	1.92	0.50
1:B:366:PRO:C	1:B:368:THR:H	2.15	0.50
1:B:367:ALA:O	1:B:369:GLN:N	2.44	0.50
1:B:457:ASN:HA	1:B:460:ARG:HG3	1.93	0.50
1:B:536:ARG:NH1	1:B:625:LEU:HD13	2.27	0.50
1:C:365:LYS:HD3	1:C:366:PRO:HD2	1.93	0.50
1:C:443:ASP:HA	1:C:446:ARG:HG3	1.94	0.50
1:C:577:LYS:O	1:C:579:ARG:N	2.40	0.50
1:D:419:ARG:HE	1:D:419:ARG:N	2.09	0.50
1:D:654:LEU:HD23	1:E:654:LEU:HB3	1.93	0.50
1:D:49:GLU:HG2	1:D:91:LEU:HD13	1.91	0.50
1:E:371:ILE:HG23	1:E:371:ILE:O	2.11	0.50
1:F:475:MET:O	1:F:478:GLN:HB3	2.11	0.50
1:F:493:ASP:HA	1:F:496:LYS:HG3	1.94	0.50
1:B:474:SER:O	1:B:477:GLN:HG2	2.12	0.50
1:B:536:ARG:NH2	1:B:625:LEU:HD13	2.27	0.50
1:B:455:MET:HB2	1:B:615:THR:HG21	1.93	0.50
1:C:653:GLU:O	1:C:657:LEU:HD13	2.11	0.50
1:D:582:ARG:N	1:D:582:ARG:NE	2.52	0.50
1:E:643:VAL:O	1:E:647:GLN:HG2	2.11	0.50
1:F:336:LEU:HD23	1:F:340:ILE:HG23	1.92	0.50
1:F:41:ILE:HG22	1:F:42:ALA:H	1.76	0.50
1:A:350:ASP:HB2	1:A:391:ASP:H	1.76	0.50
1:A:36:GLU:O	1:A:38:GLY:N	2.44	0.50
1:B:99:CYS:HB3	1:B:154:GLN:HB2	1.93	0.50
1:B:350:ASP:HB2	1:B:391:ASP:H	1.77	0.50
1:C:493:ASP:HA	1:C:496:LYS:HG3	1.93	0.50
1:D:231:TRP:O	1:D:233:SER:N	2.44	0.50
1:F:294:TYR:HD2	1:F:296:PRO:HD2	1.75	0.50
1:F:423:PHE:CD1	1:F:583:THR:HA	2.46	0.50
1:A:189:LEU:HD22	1:A:189:LEU:N	2.27	0.50
1:A:220:ARG:N	1:A:221:PRO:CD	2.71	0.50
1:A:635:LEU:O	1:A:639:ASP:HB3	2.12	0.50
1:B:548:GLN:N	1:B:548:GLN:OE1	2.45	0.50
1:C:192:GLU:HG2	1:C:283:TRP:CB	2.42	0.50
1:C:311:LEU:O	1:C:311:LEU:HD12	2.11	0.50
1:C:641:LYS:HD2	1:C:645:ARG:NH1	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:MET:SD	1:D:385:ASP:N	2.85	0.50
1:D:60:LEU:O	1:D:64:ILE:HG12	2.12	0.50
1:E:433:VAL:O	1:E:436:SER:HB3	2.11	0.50
1:A:125:LEU:HA	1:A:162:HIS:CD2	2.46	0.50
1:A:122:ILE:HD13	1:A:216:ILE:HG12	1.94	0.50
1:A:236:ARG:NH1	1:A:236:ARG:HG3	2.26	0.50
1:A:536:ARG:HG2	1:A:536:ARG:HH11	1.76	0.50
1:B:189:LEU:HD22	1:B:189:LEU:N	2.27	0.50
1:B:284:HIS:N	1:B:285:PRO:HD2	2.26	0.50
1:B:578:PRO:C	1:B:580:ASP:H	2.15	0.50
1:D:117:LEU:HB3	1:D:119:GLU:OE1	2.11	0.50
1:D:139:ASN:O	1:D:141:ILE:HD12	2.11	0.50
1:D:167:LEU:O	1:D:170:ALA:CB	2.60	0.50
1:D:23:THR:HA	1:D:29:VAL:HG22	1.94	0.50
1:D:626:LEU:HD23	1:D:626:LEU:C	2.32	0.50
1:E:373:ASP:O	1:E:385:ASP:N	2.45	0.50
1:E:392:ASN:CG	1:E:393:SER:N	2.64	0.50
1:E:517:MET:HG2	1:E:650:ARG:NE	2.27	0.50
1:F:170:ALA:HB3	1:F:178:LEU:HD12	1.94	0.50
1:F:194:LEU:HB3	1:F:196:GLN:HE22	1.77	0.50
1:F:213:PHE:CA	1:F:277:LEU:HD21	2.38	0.50
1:F:355:GLN:HB3	1:F:359:LEU:CD1	2.41	0.50
1:B:103:ASP:O	1:B:105:ARG:N	2.45	0.50
1:B:282:MET:HB2	1:B:286:ARG:NH2	2.27	0.50
1:B:479:LEU:HD11	1:B:641:LYS:CG	2.28	0.50
1:C:234:LYS:NZ	1:C:237:GLN:HE22	2.10	0.50
1:C:417:PRO:HA	1:D:320:GLY:CA	2.28	0.50
1:C:544:ILE:O	1:C:547:LEU:HG	2.12	0.50
1:C:77:ARG:HD2	1:C:78:ASP:H	1.77	0.50
1:A:355:GLN:HB3	1:A:359:LEU:HD13	1.93	0.50
1:A:419:ARG:NH1	1:A:419:ARG:O	2.45	0.50
1:A:653:GLU:O	1:A:657:LEU:HD13	2.12	0.50
1:A:665:VAL:HG21	1:F:664:LYS:HB3	1.94	0.50
1:B:285:PRO:O	1:B:290:THR:HG21	2.12	0.50
1:B:365:LYS:C	1:B:367:ALA:N	2.66	0.50
1:B:643:VAL:O	1:B:647:GLN:HG2	2.12	0.50
1:C:320:GLY:CA	1:D:417:PRO:HA	2.37	0.50
1:C:620:GLN:O	1:C:624:GLU:HG2	2.11	0.50
1:C:631:GLU:HG3	1:C:632:VAL:N	2.27	0.50
1:D:350:ASP:HB2	1:D:391:ASP:H	1.77	0.50
1:D:525:GLY:HA2	1:D:640:GLU:OE2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:GLU:CD	1:E:19:GLU:H	2.16	0.50
1:F:249:LEU:HG	1:F:414:LEU:HG	1.93	0.50
1:F:41:ILE:HG22	1:F:42:ALA:N	2.26	0.50
1:F:577:LYS:CG	1:F:578:PRO:HD2	2.42	0.50
1:F:635:LEU:O	1:F:639:ASP:HB3	2.12	0.50
1:F:77:ARG:HD2	1:F:78:ASP:H	1.76	0.50
1:A:144:ARG:HD3	1:A:169:TYR:O	2.12	0.49
1:A:316:ASN:HA	1:A:388:PHE:CE1	2.47	0.49
1:A:644:VAL:O	1:A:647:GLN:HB2	2.11	0.49
1:B:117:LEU:HD12	1:B:215:CYS:O	2.12	0.49
1:B:268:VAL:O	1:B:272:ARG:HB2	2.11	0.49
1:B:410:VAL:O	1:B:411:SER:HB3	2.11	0.49
1:C:20:ARG:HB2	1:C:23:THR:HB	1.92	0.49
1:C:298:GLY:O	1:C:299:CYS:C	2.49	0.49
1:D:534:VAL:O	1:D:538:MET:HB2	2.12	0.49
1:D:533:LEU:HD13	1:D:629:VAL:HG12	1.94	0.49
1:D:77:ARG:N	1:D:96:MET:HA	2.26	0.49
1:E:311:LEU:O	1:E:311:LEU:HD12	2.12	0.49
1:E:434:TRP:HB3	1:E:571:TYR:OH	2.12	0.49
1:F:480:LYS:HG2	1:F:527:GLU:CB	2.42	0.49
1:A:282:MET:HG3	1:A:283:TRP:CZ3	2.47	0.49
1:B:272:ARG:NH1	1:B:272:ARG:HG3	2.27	0.49
1:B:658:LEU:HD23	1:C:496:LYS:HZ2	1.78	0.49
1:D:51:SER:HB2	1:D:52:PRO:HD2	1.94	0.49
1:D:621:LYS:O	1:D:625:LEU:HD12	2.12	0.49
1:E:239:SER:O	1:E:242:ASP:HB2	2.11	0.49
1:F:116:GLY:O	1:F:216:ILE:O	2.30	0.49
1:F:118:ARG:HD2	1:F:264:ASN:OD1	2.13	0.49
1:F:467:LYS:CD	1:F:541:GLN:HG2	2.41	0.49
1:A:20:ARG:HB2	1:A:23:THR:HB	1.93	0.49
1:A:243:ILE:HG22	1:A:281:LEU:CD2	2.42	0.49
1:A:367:ALA:C	1:A:369:GLN:N	2.66	0.49
1:B:594:LEU:C	1:B:594:LEU:HD13	2.33	0.49
1:C:103:ASP:O	1:C:105:ARG:N	2.45	0.49
1:C:23:THR:HA	1:C:29:VAL:HG22	1.93	0.49
1:D:103:ASP:O	1:D:106:LYS:N	2.44	0.49
1:D:128:ASP:HB3	1:D:162:HIS:HB2	1.93	0.49
1:D:16:GLU:HG3	1:D:33:HIS:O	2.12	0.49
1:E:306:ILE:O	1:E:309:LEU:HB3	2.11	0.49
1:E:358:GLY:HA2	1:E:453:ALA:O	2.12	0.49
1:E:463:SER:HA	1:E:467:LYS:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:487:LYS:HA	1:E:491:GLN:HB2	1.94	0.49
1:E:111:PHE:CE1	1:E:575:ARG:HD2	2.47	0.49
1:F:389:LEU:CD2	1:F:454:ALA:CB	2.79	0.49
1:A:655:TRP:HZ2	1:F:499:GLU:CD	2.14	0.49
1:B:36:GLU:O	1:B:38:GLY:N	2.45	0.49
1:B:462:ASN:C	1:B:464:CYS:H	2.16	0.49
1:B:528:ASN:O	1:B:532:LEU:HD23	2.12	0.49
1:B:620:GLN:O	1:B:624:GLU:HG2	2.12	0.49
1:B:496:LYS:NZ	1:C:658:LEU:HD23	2.28	0.49
1:C:67:ARG:NH2	1:C:68:LEU:HD12	2.22	0.49
1:D:476:SER:HB2	1:D:636:MET:CE	2.43	0.49
1:E:99:CYS:HB3	1:E:154:GLN:HB2	1.95	0.49
1:E:312:VAL:HG22	1:E:313:HIS:N	2.28	0.49
1:F:122:ILE:HD13	1:F:216:ILE:HG12	1.95	0.49
1:F:36:GLU:O	1:F:38:GLY:N	2.45	0.49
1:F:51:SER:HB2	1:F:52:PRO:HD2	1.93	0.49
1:F:621:LYS:O	1:F:625:LEU:HD12	2.12	0.49
1:A:657:LEU:HA	1:A:660:ILE:HG22	1.94	0.49
1:B:355:GLN:O	1:B:357:ALA:N	2.46	0.49
1:C:105:ARG:HD2	1:C:148:PRO:HB2	1.93	0.49
1:C:525:GLY:O	1:C:527:GLU:N	2.46	0.49
1:C:627:PRO:HA	1:C:630:GLU:CB	2.41	0.49
1:D:105:ARG:CD	1:D:148:PRO:HB2	2.42	0.49
1:D:371:ILE:HB	1:D:384:MET:HE2	1.94	0.49
1:D:394:LYS:HZ3	1:D:401:ILE:N	2.11	0.49
1:D:55:ARG:HD2	1:D:91:LEU:HD11	1.94	0.49
1:E:118:ARG:HH22	1:E:438:GLN:HG2	1.78	0.49
1:E:241:VAL:HG12	1:E:241:VAL:O	2.13	0.49
1:E:357:ALA:O	1:E:456:MET:HG2	2.10	0.49
1:E:548:GLN:OE1	1:E:548:GLN:N	2.46	0.49
1:E:434:TRP:HZ3	1:E:568:ARG:HE	1.59	0.49
1:F:18:LYS:HB3	1:F:19:GLU:OE2	2.12	0.49
1:F:294:TYR:HB2	1:F:296:PRO:HD2	1.93	0.49
1:F:457:ASN:HA	1:F:460:ARG:HG3	1.94	0.49
1:F:570:LEU:HD12	1:F:570:LEU:N	2.27	0.49
1:A:214:GLU:O	1:A:218:GLY:HA2	2.11	0.49
1:A:123:LEU:HD12	1:A:307:LEU:HD13	1.94	0.49
1:B:265:LEU:HD23	1:B:265:LEU:N	2.27	0.49
1:B:431:GLY:C	1:B:433:VAL:H	2.15	0.49
1:B:80:PRO:CB	1:B:83:MET:HB2	2.36	0.49
1:C:265:LEU:HG	1:C:266:ASN:N	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:SER:HA	1:C:467:LYS:HB3	1.93	0.49
1:D:229:VAL:CG2	1:D:230:GLN:H	2.09	0.49
1:D:223:LEU:O	1:D:231:TRP:CH2	2.66	0.49
1:D:559:THR:HB	1:D:604:LYS:HZ1	1.78	0.49
1:D:653:GLU:O	1:D:657:LEU:HD13	2.12	0.49
1:E:460:ARG:C	1:E:462:ASN:H	2.16	0.49
1:E:536:ARG:HH11	1:E:536:ARG:HG2	1.77	0.49
1:E:644:VAL:O	1:E:647:GLN:HB2	2.12	0.49
1:F:294:TYR:HB2	1:F:296:PRO:CD	2.42	0.49
1:F:341:GLN:HA	1:F:345:GLY:O	2.12	0.49
1:A:272:ARG:HG3	1:A:272:ARG:HH11	1.78	0.49
1:A:341:GLN:HA	1:A:345:GLY:O	2.12	0.49
1:A:412:CYS:O	1:A:415:GLN:HB3	2.13	0.49
1:A:626:LEU:HB3	1:A:627:PRO:HD3	1.95	0.49
1:B:477:GLN:HE21	1:C:477:GLN:HE21	1.59	0.49
1:C:490:ILE:HG13	1:C:650:ARG:HB3	1.95	0.49
1:D:419:ARG:HH11	1:D:588:GLN:NE2	2.10	0.49
1:D:458:LEU:HD11	1:D:544:ILE:HG21	1.94	0.49
1:E:474:SER:O	1:E:477:GLN:HG2	2.12	0.49
1:E:49:GLU:H	1:E:89:ASN:ND2	2.11	0.49
1:E:49:GLU:HG3	1:E:89:ASN:ND2	2.26	0.49
1:F:117:LEU:HD23	1:F:119:GLU:OE1	2.13	0.49
1:F:51:SER:O	1:F:55:ARG:HG3	2.12	0.49
1:F:577:LYS:HG3	1:F:578:PRO:CD	2.40	0.49
1:B:366:PRO:CB	1:B:368:THR:HG23	2.20	0.49
1:B:421:LEU:HD12	1:B:421:LEU:N	2.28	0.49
1:B:621:LYS:O	1:B:625:LEU:HD12	2.13	0.49
1:D:241:VAL:HG12	1:D:278:GLN:HG2	1.95	0.49
1:D:490:ILE:HG21	1:D:517:MET:CE	2.43	0.49
1:E:170:ALA:O	1:E:171:LYS:HB2	2.13	0.49
1:E:20:ARG:HB2	1:E:23:THR:HB	1.94	0.49
1:E:537:MET:SD	1:E:537:MET:C	2.91	0.49
1:D:496:LYS:HD2	1:E:655:TRP:CG	2.47	0.49
1:A:481:ALA:HB3	1:F:482:LYS:HD2	1.93	0.49
1:B:105:ARG:HD3	1:B:149:GLU:CD	2.33	0.49
1:B:220:ARG:N	1:B:221:PRO:CD	2.73	0.49
1:D:103:ASP:O	1:D:104:LEU:C	2.51	0.49
1:D:310:LYS:HZ2	1:D:310:LYS:H	1.59	0.49
1:F:356:GLU:OE2	1:F:384:MET:HG3	2.13	0.49
1:A:105:ARG:CD	1:A:148:PRO:HB2	2.43	0.49
1:A:170:ALA:HB3	1:A:178:LEU:HD12	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:ARG:O	1:A:580:ASP:HB3	2.11	0.49
1:B:22:GLY:N	1:B:165:ILE:HG21	2.28	0.49
1:B:279:LEU:C	1:B:281:LEU:H	2.15	0.49
1:C:43:ILE:HD12	1:C:43:ILE:N	2.28	0.49
1:C:77:ARG:N	1:C:96:MET:HA	2.27	0.49
1:D:268:VAL:O	1:D:272:ARG:HB2	2.12	0.49
1:E:350:ASP:HB2	1:E:391:ASP:H	1.78	0.49
1:F:242:ASP:OD2	1:F:257:SER:HB3	2.13	0.49
1:F:387:VAL:HG21	1:F:449:GLN:O	2.12	0.49
1:F:527:GLU:HG3	1:F:528:ASN:N	2.28	0.49
1:A:356:GLU:HA	1:A:453:ALA:HB1	1.95	0.48
1:B:186:LEU:O	1:B:188:TYR:N	2.46	0.48
1:B:212:ALA:O	1:B:216:ILE:HG13	2.12	0.48
1:B:310:LYS:H	1:B:310:LYS:HZ2	1.60	0.48
1:C:194:LEU:HB3	1:C:196:GLN:HE22	1.77	0.48
1:C:286:ARG:O	1:C:290:THR:N	2.46	0.48
1:C:418:LYS:O	1:C:419:ARG:CB	2.55	0.48
1:C:536:ARG:CZ	1:C:625:LEU:HD13	2.42	0.48
1:D:279:LEU:C	1:D:281:LEU:H	2.15	0.48
1:E:285:PRO:O	1:E:290:THR:OG1	2.31	0.48
1:F:294:TYR:CD2	1:F:296:PRO:HD2	2.48	0.48
1:F:298:GLY:O	1:F:299:CYS:C	2.51	0.48
1:F:350:ASP:CB	1:F:391:ASP:HB2	2.43	0.48
1:F:419:ARG:NH1	1:F:588:GLN:HA	2.28	0.48
1:F:467:LYS:HD3	1:F:541:GLN:CD	2.33	0.48
1:A:60:LEU:O	1:A:64:ILE:HG12	2.13	0.48
1:C:265:LEU:HG	1:C:266:ASN:H	1.77	0.48
1:D:213:PHE:CD2	1:D:221:PRO:HG2	2.48	0.48
1:E:103:ASP:O	1:E:106:LYS:N	2.42	0.48
1:E:422:ALA:O	1:E:585:GLY:HA3	2.12	0.48
1:F:43:ILE:N	1:F:43:ILE:HD12	2.27	0.48
1:F:501:THR:HG23	1:F:505:ILE:CG2	2.43	0.48
1:A:431:GLY:O	1:A:433:VAL:N	2.46	0.48
1:B:16:GLU:OE2	1:B:83:MET:HE3	2.12	0.48
1:B:89:ASN:C	1:B:91:LEU:H	2.16	0.48
1:C:572:ARG:O	1:C:576:GLU:HB2	2.13	0.48
1:C:594:LEU:C	1:C:594:LEU:HD13	2.34	0.48
1:D:418:LYS:C	1:D:419:ARG:HG3	2.34	0.48
1:D:262:PRO:HB2	1:D:432:GLN:NE2	2.28	0.48
1:E:107:TYR:CE2	1:E:153:LEU:HD22	2.47	0.48
1:E:418:LYS:HZ1	1:E:421:LEU:HD22	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:572:ARG:O	1:F:576:GLU:HB2	2.13	0.48
1:A:234:LYS:HE2	1:A:253:VAL:HG11	1.96	0.48
1:A:205:TYR:CD1	1:A:290:THR:HG23	2.42	0.48
1:A:72:ASN:HA	1:A:163:LYS:HA	1.96	0.48
1:B:248:ASP:O	1:B:249:LEU:C	2.51	0.48
1:B:319:THR:HG23	1:B:320:GLY:N	2.22	0.48
1:B:531:LYS:NZ	1:B:531:LYS:HB3	2.28	0.48
1:B:577:LYS:HG3	1:B:578:PRO:HD2	1.96	0.48
1:C:268:VAL:O	1:C:272:ARG:HB2	2.13	0.48
1:D:168:GLY:O	1:D:179:CYS:SG	2.71	0.48
1:D:279:LEU:HD11	1:D:290:THR:O	2.13	0.48
1:D:284:HIS:HB3	1:D:285:PRO:HD3	1.95	0.48
1:D:416:GLU:C	1:D:418:LYS:N	2.67	0.48
1:B:362:ILE:HG13	1:E:37:THR:HG22	1.96	0.48
1:F:227:GLN:HG3	1:F:231:TRP:CZ3	2.48	0.48
1:F:462:ASN:C	1:F:464:CYS:H	2.17	0.48
1:A:89:ASN:HD22	1:A:89:ASN:N	2.08	0.48
1:B:172:GLU:HG3	1:B:175:GLN:N	2.20	0.48
1:B:286:ARG:CA	1:B:290:THR:HG21	2.40	0.48
1:B:496:LYS:HG2	1:C:655:TRP:CD1	2.49	0.48
1:C:117:LEU:HB3	1:C:119:GLU:OE1	2.13	0.48
1:C:357:ALA:HB3	1:C:359:LEU:HD11	1.96	0.48
1:C:316:ASN:HA	1:C:388:PHE:CE1	2.48	0.48
1:C:394:LYS:O	1:C:394:LYS:HG2	2.13	0.48
1:C:486:PHE:CE1	1:C:647:GLN:CB	2.91	0.48
1:D:145:ASP:HA	1:D:189:LEU:HD11	1.94	0.48
1:D:168:GLY:O	1:D:170:ALA:N	2.47	0.48
1:E:294:TYR:CD2	1:E:294:TYR:N	2.79	0.48
1:E:79:VAL:HG23	1:E:84:GLN:HG2	1.96	0.48
1:F:285:PRO:O	1:F:290:THR:HB	2.14	0.48
1:F:429:VAL:O	1:F:433:VAL:HG23	2.14	0.48
1:A:431:GLY:C	1:A:433:VAL:H	2.16	0.48
1:A:463:SER:HA	1:A:467:LYS:HB3	1.95	0.48
1:A:594:LEU:HD13	1:A:594:LEU:O	2.14	0.48
1:B:23:THR:HA	1:B:29:VAL:HG22	1.94	0.48
1:B:55:ARG:NH1	1:B:91:LEU:HD11	2.28	0.48
1:E:128:ASP:HB3	1:E:162:HIS:HB2	1.96	0.48
1:F:18:LYS:HB3	1:F:19:GLU:CD	2.34	0.48
1:A:160:LEU:N	1:A:160:LEU:HD12	2.29	0.48
1:A:369:GLN:O	1:A:370:CYS:HB3	2.13	0.48
1:A:394:LYS:CD	1:A:401:ILE:HG13	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LEU:HD23	1:B:340:ILE:HG23	1.96	0.48
1:B:366:PRO:C	1:B:368:THR:N	2.66	0.48
1:B:478:GLN:HG3	1:C:481:ALA:HB2	1.95	0.48
1:B:77:ARG:HD2	1:B:78:ASP:H	1.79	0.48
1:C:240:GLU:OE1	1:C:241:VAL:N	2.47	0.48
1:C:462:ASN:C	1:C:464:CYS:H	2.16	0.48
1:C:55:ARG:HH11	1:C:91:LEU:HD11	1.76	0.48
1:D:570:LEU:HD12	1:D:570:LEU:H	1.77	0.48
1:D:641:LYS:HD2	1:D:645:ARG:NH1	2.29	0.48
1:D:74:VAL:HG23	1:D:164:ILE:O	2.14	0.48
1:E:118:ARG:HA	1:E:264:ASN:O	2.14	0.48
1:E:152:VAL:HG13	1:E:165:ILE:HD11	1.94	0.48
1:F:22:GLY:N	1:F:165:ILE:HG21	2.29	0.48
1:A:125:LEU:C	1:A:125:LEU:HD13	2.33	0.48
1:A:306:ILE:O	1:A:309:LEU:HD23	2.13	0.48
1:C:139:ASN:O	1:C:141:ILE:HD12	2.14	0.48
1:C:22:GLY:N	1:C:165:ILE:HG21	2.29	0.48
1:D:311:LEU:O	1:D:311:LEU:HD12	2.14	0.48
1:D:571:TYR:HB3	1:D:575:ARG:NH2	2.13	0.48
1:D:657:LEU:HA	1:D:660:ILE:HG22	1.95	0.48
1:E:105:ARG:NH2	1:E:188:TYR:OH	2.46	0.48
1:E:125:LEU:HA	1:E:162:HIS:CD2	2.49	0.48
1:E:410:VAL:O	1:E:411:SER:HB3	2.13	0.48
1:D:496:LYS:HD2	1:E:655:TRP:HA	1.96	0.48
1:E:657:LEU:HA	1:E:660:ILE:HG22	1.95	0.48
1:F:16:GLU:N	1:F:16:GLU:OE2	2.47	0.48
1:F:80:PRO:HB2	1:F:83:MET:CB	2.34	0.48
1:A:103:ASP:O	1:A:105:ARG:N	2.47	0.48
1:A:217:THR:HB	1:A:260:PRO:HG3	1.96	0.48
1:A:415:GLN:NE2	1:A:419:ARG:HB3	2.29	0.48
1:A:577:LYS:HG2	1:A:581:GLN:HB2	1.96	0.48
1:B:213:PHE:HE2	1:B:217:THR:HG21	1.78	0.48
1:B:394:LYS:HZ1	1:B:402:SER:HB3	1.78	0.48
1:B:517:MET:HG2	1:B:650:ARG:CZ	2.43	0.48
1:C:145:ASP:HA	1:C:189:LEU:HD11	1.96	0.48
1:C:410:VAL:HA	1:C:413:ILE:CG2	2.43	0.48
1:D:431:GLY:C	1:D:433:VAL:H	2.16	0.48
1:E:191:PRO:O	1:E:194:LEU:HB2	2.14	0.48
1:E:430:TRP:HZ3	1:E:570:LEU:HB3	1.76	0.48
1:F:169:TYR:CD1	1:F:179:CYS:SG	3.05	0.48
1:F:354:LEU:CD2	1:F:457:ASN:HB2	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ASP:HB3	1:A:162:HIS:HB2	1.96	0.48
1:A:247:GLU:O	1:A:247:GLU:HG2	2.13	0.48
1:B:249:LEU:CD1	1:B:414:LEU:HD21	2.43	0.48
1:B:434:TRP:HB3	1:B:571:TYR:CE1	2.49	0.48
1:C:268:VAL:HG13	1:C:269:LEU:N	2.29	0.48
1:D:223:LEU:HD13	1:D:224:PRO:CD	2.43	0.48
1:D:635:LEU:O	1:D:639:ASP:HB3	2.14	0.48
1:E:111:PHE:CE1	1:E:575:ARG:HB3	2.49	0.48
1:E:21:LEU:HG	1:E:165:ILE:CD1	2.43	0.48
1:E:212:ALA:O	1:E:216:ILE:HG13	2.13	0.48
1:E:284:HIS:O	1:E:285:PRO:C	2.52	0.48
1:F:587:SER:O	1:F:591:VAL:HG23	2.14	0.48
1:F:74:VAL:HG23	1:F:164:ILE:O	2.14	0.48
1:F:89:ASN:C	1:F:91:LEU:H	2.16	0.48
1:A:145:ASP:HA	1:A:189:LEU:HD11	1.96	0.47
1:A:460:ARG:HH11	1:A:460:ARG:HG2	1.78	0.47
1:A:579:ARG:H	1:A:579:ARG:CD	2.13	0.47
1:A:601:PHE:O	1:A:605:VAL:HG23	2.14	0.47
1:B:460:ARG:HG2	1:B:460:ARG:HH11	1.79	0.47
1:C:531:LYS:NZ	1:C:531:LYS:HB3	2.29	0.47
1:C:594:LEU:O	1:C:594:LEU:HD13	2.14	0.47
1:D:241:VAL:HG12	1:D:278:GLN:CG	2.44	0.47
1:E:497:TYR:HA	1:E:500:GLN:HB2	1.96	0.47
1:F:144:ARG:HD2	1:F:171:LYS:HB2	1.96	0.47
1:F:534:VAL:O	1:F:538:MET:HB2	2.13	0.47
1:A:220:ARG:O	1:A:221:PRO:O	2.31	0.47
1:B:72:ASN:HA	1:B:163:LYS:HA	1.96	0.47
1:C:128:ASP:HB3	1:C:162:HIS:HB2	1.96	0.47
1:C:236:ARG:HH22	1:C:283:TRP:HE3	1.61	0.47
1:C:367:ALA:C	1:C:369:GLN:N	2.68	0.47
1:C:433:VAL:O	1:C:436:SER:HB3	2.15	0.47
1:D:282:MET:HB2	1:D:286:ARG:NH1	2.29	0.47
1:D:566:GLN:O	1:D:569:GLU:HB2	2.15	0.47
1:E:21:LEU:HB3	1:E:165:ILE:CG2	2.39	0.47
1:E:313:HIS:ND1	1:E:324:THR:HG22	2.29	0.47
1:F:134:ARG:HG2	1:F:300:PHE:CD1	2.49	0.47
1:F:644:VAL:O	1:F:647:GLN:HB2	2.14	0.47
1:F:653:GLU:O	1:F:657:LEU:HD13	2.13	0.47
1:B:173:LEU:HD12	1:B:174:ASP:N	2.28	0.47
1:C:160:LEU:N	1:C:160:LEU:HD12	2.29	0.47
1:D:117:LEU:HD12	1:D:215:CYS:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:LEU:N	1:D:160:LEU:HD12	2.29	0.47
1:D:462:ASN:C	1:D:464:CYS:H	2.18	0.47
1:D:472:MET:O	1:D:475:MET:HG3	2.14	0.47
1:E:259:LEU:HD22	1:E:274:GLU:CG	2.36	0.47
1:F:165:ILE:HG22	1:F:166:ASP:N	2.17	0.47
1:F:227:GLN:CB	1:F:228:PRO:HD3	2.44	0.47
1:F:472:MET:O	1:F:475:MET:HG3	2.14	0.47
1:A:165:ILE:HG22	1:A:166:ASP:N	2.17	0.47
1:A:185:THR:C	1:A:187:GLN:H	2.18	0.47
1:A:353:LEU:N	1:A:353:LEU:HD12	2.29	0.47
1:A:655:TRP:HD1	1:F:500:GLN:CG	2.27	0.47
1:B:190:ALA:HB3	1:B:203:VAL:HG23	1.95	0.47
1:B:213:PHE:CZ	1:B:243:ILE:HB	2.49	0.47
1:B:410:VAL:HA	1:B:413:ILE:CG2	2.41	0.47
1:C:366:PRO:C	1:C:368:THR:N	2.67	0.47
1:C:394:LYS:HB2	1:C:401:ILE:CB	2.43	0.47
1:C:408:GLU:O	1:C:409:SER:OG	2.25	0.47
1:D:346:ILE:HD13	1:D:388:PHE:HZ	1.79	0.47
1:D:587:SER:O	1:D:591:VAL:HG23	2.15	0.47
1:E:621:LYS:O	1:E:625:LEU:HD12	2.14	0.47
1:E:517:MET:HB3	1:E:650:ARG:NH2	2.29	0.47
1:F:357:ALA:O	1:F:456:MET:HG2	2.13	0.47
1:C:360:ALA:O	1:F:37:THR:HG22	2.13	0.47
1:F:431:GLY:CA	1:F:571:TYR:CE2	2.96	0.47
1:F:430:TRP:NE1	1:F:587:SER:HA	2.24	0.47
1:A:570:LEU:HD12	1:A:570:LEU:H	1.78	0.47
1:B:392:ASN:ND2	1:B:393:SER:H	2.11	0.47
1:B:499:GLU:OE1	1:C:659:LYS:HE2	2.14	0.47
1:C:118:ARG:HH22	1:C:438:GLN:CG	2.26	0.47
1:C:371:ILE:HG12	1:C:384:MET:HE3	1.96	0.47
1:C:460:ARG:C	1:C:462:ASN:H	2.17	0.47
1:F:142:ILE:HG23	1:F:204:ASP:OD2	2.15	0.47
1:F:152:VAL:HG13	1:F:165:ILE:HD11	1.95	0.47
1:F:285:PRO:O	1:F:286:ARG:HG3	2.15	0.47
1:F:467:LYS:NZ	1:F:541:GLN:HG2	2.29	0.47
1:F:517:MET:O	1:F:521:VAL:HG23	2.15	0.47
1:F:601:PHE:O	1:F:605:VAL:HG23	2.14	0.47
1:F:617:VAL:O	1:F:621:LYS:HB2	2.13	0.47
1:B:463:SER:HA	1:B:467:LYS:HB3	1.96	0.47
1:B:635:LEU:O	1:B:639:ASP:HB3	2.13	0.47
1:C:70:HIS:HE1	1:C:132:ALA:HA	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:TYR:O	1:C:301:LYS:HD3	2.15	0.47
1:C:355:GLN:HB3	1:C:359:LEU:HD13	1.97	0.47
1:E:151:ILE:HD12	1:E:211:LEU:HD11	1.96	0.47
1:E:631:GLU:HG3	1:E:632:VAL:N	2.30	0.47
1:E:649:LYS:HA	1:E:652:LYS:HE3	1.95	0.47
1:F:245:VAL:HA	1:F:255:PHE:HA	1.96	0.47
1:F:261:TYR:HB3	1:F:409:SER:CB	2.45	0.47
1:F:77:ARG:N	1:F:96:MET:HA	2.30	0.47
1:A:490:ILE:HG21	1:A:518:GLU:CB	2.40	0.47
1:B:246:SER:OG	1:B:247:GLU:N	2.46	0.47
1:B:357:ALA:HB3	1:B:359:LEU:HD11	1.96	0.47
1:B:445:ASN:HA	1:B:448:GLN:HB2	1.97	0.47
1:B:490:ILE:HD11	1:B:651:GLN:CG	2.40	0.47
1:C:346:ILE:HD13	1:C:388:PHE:HZ	1.78	0.47
1:C:416:GLU:HB2	1:D:405:PRO:HB3	1.97	0.47
1:C:472:MET:O	1:C:475:MET:HG3	2.15	0.47
1:D:70:HIS:HE1	1:D:132:ALA:HA	1.79	0.47
1:D:272:ARG:HG3	1:D:272:ARG:NH1	2.29	0.47
1:E:357:ALA:HB3	1:E:359:LEU:HD11	1.97	0.47
1:E:43:ILE:N	1:E:43:ILE:HD12	2.30	0.47
1:E:457:ASN:HA	1:E:460:ARG:HG3	1.97	0.47
1:E:571:TYR:HB3	1:E:575:ARG:NH2	2.11	0.47
1:A:443:ASP:HA	1:A:446:ARG:HG3	1.96	0.47
1:A:485:PHE:CD1	1:A:485:PHE:C	2.88	0.47
1:A:91:LEU:HA	1:A:92:PRO:HD3	1.73	0.47
1:A:77:ARG:N	1:A:96:MET:HA	2.29	0.47
1:B:408:GLU:CG	1:B:409:SER:H	2.26	0.47
1:B:572:ARG:O	1:B:576:GLU:HB2	2.15	0.47
1:C:103:ASP:O	1:C:104:LEU:C	2.53	0.47
1:C:635:LEU:O	1:C:639:ASP:HB3	2.14	0.47
1:D:350:ASP:CB	1:D:391:ASP:HB2	2.45	0.47
1:D:77:ARG:HD2	1:D:78:ASP:H	1.80	0.47
1:E:145:ASP:HA	1:E:189:LEU:HD11	1.97	0.47
1:E:190:ALA:HB3	1:E:203:VAL:HG23	1.96	0.47
1:E:241:VAL:HA	1:E:286:ARG:HH22	1.80	0.47
1:E:353:LEU:HD12	1:E:353:LEU:N	2.30	0.47
1:E:385:ASP:CG	1:E:386:LEU:N	2.67	0.47
1:E:566:GLN:O	1:E:569:GLU:HB2	2.14	0.47
1:F:294:TYR:HE1	1:F:301:LYS:NZ	2.12	0.47
1:F:566:GLN:O	1:F:569:GLU:HB2	2.15	0.47
1:F:49:GLU:OE1	1:F:91:LEU:HD21	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ASN:CG	1:B:393:SER:N	2.67	0.47
1:B:558:GLY:CA	1:B:562:ASP:HB2	2.43	0.47
1:C:190:ALA:HB3	1:C:203:VAL:HG23	1.96	0.47
1:C:272:ARG:NH1	1:C:272:ARG:HG3	2.29	0.47
1:D:355:GLN:HB3	1:D:359:LEU:CD1	2.44	0.47
1:D:418:LYS:NZ	1:D:421:LEU:CD1	2.77	0.47
1:E:77:ARG:N	1:E:96:MET:HA	2.29	0.47
1:F:189:LEU:N	1:F:189:LEU:HD22	2.30	0.47
1:A:460:ARG:C	1:A:462:ASN:H	2.18	0.47
1:C:577:LYS:CD	1:C:581:GLN:HE22	2.28	0.47
1:D:217:THR:HA	1:D:263:ASN:CG	2.36	0.47
1:D:283:TRP:CZ3	1:D:285:PRO:HD2	2.50	0.47
1:D:517:MET:O	1:D:521:VAL:HG23	2.15	0.47
1:E:169:TYR:OH	1:E:183:VAL:HB	2.13	0.47
1:E:17:MET:O	1:E:18:LYS:HG2	2.15	0.47
1:E:416:GLU:C	1:E:418:LYS:N	2.69	0.47
1:E:475:MET:O	1:E:478:GLN:HB3	2.15	0.47
1:D:655:TRP:NE1	1:E:496:LYS:HD2	2.30	0.47
1:E:430:TRP:O	1:E:571:TYR:HE2	1.97	0.47
1:E:635:LEU:O	1:E:639:ASP:HB3	2.14	0.47
1:F:128:ASP:HB3	1:F:162:HIS:HB2	1.96	0.47
1:F:169:TYR:HA	1:F:179:CYS:HB3	1.95	0.47
1:F:460:ARG:HH11	1:F:460:ARG:HG2	1.80	0.47
1:A:531:LYS:HB3	1:A:531:LYS:NZ	2.29	0.47
1:A:594:LEU:HD13	1:A:594:LEU:C	2.35	0.47
1:B:221:PRO:O	1:B:222:PHE:CB	2.61	0.47
1:B:229:VAL:C	1:B:231:TRP:H	2.18	0.47
1:B:369:GLN:O	1:B:369:GLN:HG3	2.15	0.47
1:C:153:LEU:HD12	1:C:153:LEU:N	2.30	0.47
1:C:168:GLY:O	1:C:178:LEU:HD22	2.14	0.47
1:C:341:GLN:HA	1:C:345:GLY:O	2.15	0.47
1:C:355:GLN:HB3	1:C:359:LEU:CD1	2.45	0.47
1:C:431:GLY:O	1:C:433:VAL:N	2.48	0.47
1:C:548:GLN:OE1	1:C:548:GLN:N	2.47	0.47
1:C:657:LEU:HA	1:C:660:ILE:HG22	1.96	0.47
1:D:192:GLU:H	1:D:192:GLU:HG3	1.42	0.47
1:D:408:GLU:HG3	1:D:413:ILE:HD13	1.95	0.47
1:D:460:ARG:C	1:D:462:ASN:H	2.17	0.47
1:D:84:GLN:CD	1:D:85:ASN:N	2.68	0.47
1:E:165:ILE:CG2	1:E:166:ASP:H	2.12	0.47
1:E:229:VAL:HG13	1:E:230:GLN:N	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:216:ILE:HD12	1:F:277:LEU:HD22	1.95	0.47
1:F:631:GLU:HG3	1:F:632:VAL:N	2.30	0.47
1:B:170:ALA:N	1:B:178:LEU:HD12	2.30	0.46
1:B:259:LEU:H	1:B:274:GLU:HG3	1.80	0.46
1:B:284:HIS:C	1:B:286:ARG:H	2.18	0.46
1:B:306:ILE:O	1:B:309:LEU:HB2	2.15	0.46
1:B:341:GLN:HA	1:B:345:GLY:O	2.15	0.46
1:B:566:GLN:O	1:B:569:GLU:HB2	2.14	0.46
1:B:60:LEU:O	1:B:64:ILE:HG12	2.15	0.46
1:B:89:ASN:N	1:B:89:ASN:HD22	2.11	0.46
1:D:421:LEU:O	1:D:422:ALA:O	2.32	0.46
1:D:477:GLN:OE1	1:E:475:MET:HA	2.15	0.46
1:A:490:ILE:HG22	1:A:518:GLU:CD	2.35	0.46
1:A:566:GLN:O	1:A:569:GLU:HB2	2.15	0.46
1:A:623:LEU:O	1:A:623:LEU:HD23	2.15	0.46
1:A:626:LEU:HD23	1:A:626:LEU:C	2.36	0.46
1:B:114:CYS:SG	1:B:431:GLY:HA3	2.55	0.46
1:B:517:MET:HG2	1:B:650:ARG:NE	2.31	0.46
1:B:55:ARG:HH11	1:B:91:LEU:HD11	1.80	0.46
1:C:631:GLU:HG3	1:C:632:VAL:H	1.80	0.46
1:D:473:ALA:HB2	1:D:633:VAL:HG11	1.97	0.46
1:D:72:ASN:HA	1:D:163:LYS:HA	1.97	0.46
1:E:410:VAL:HA	1:E:413:ILE:CG2	2.42	0.46
1:E:583:THR:O	1:E:584:GLU:O	2.33	0.46
1:F:431:GLY:C	1:F:433:VAL:H	2.17	0.46
1:A:319:THR:HG23	1:A:320:GLY:N	2.20	0.46
1:B:123:LEU:HD12	1:B:307:LEU:HD13	1.96	0.46
1:B:312:VAL:HG12	1:B:325:TYR:O	2.15	0.46
1:B:43:ILE:HD12	1:B:43:ILE:N	2.31	0.46
1:C:217:THR:HA	1:C:263:ASN:ND2	2.29	0.46
1:C:310:LYS:HZ2	1:C:310:LYS:H	1.63	0.46
1:D:105:ARG:HH22	1:D:220:ARG:HH21	1.62	0.46
1:D:17:MET:C	1:D:18:LYS:HD2	2.35	0.46
1:D:476:SER:HB2	1:D:636:MET:HE3	1.97	0.46
1:E:186:LEU:CD1	1:E:189:LEU:HB2	2.45	0.46
1:F:419:ARG:NE	1:F:591:VAL:HG21	2.30	0.46
1:A:151:ILE:HD12	1:A:211:LEU:HD11	1.98	0.46
1:A:481:ALA:HB1	1:F:482:LYS:HZ1	1.75	0.46
1:B:141:ILE:HG22	1:B:142:ILE:N	2.30	0.46
1:B:353:LEU:HD12	1:B:353:LEU:N	2.29	0.46
1:C:103:ASP:O	1:C:106:LYS:N	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:385:ASP:CG	1:D:386:LEU:N	2.69	0.46
1:E:221:PRO:HG3	1:E:243:ILE:O	2.15	0.46
1:E:261:TYR:N	1:E:262:PRO:HD2	2.29	0.46
1:E:295:GLY:H	1:E:296:PRO:CD	2.17	0.46
1:F:139:ASN:O	1:F:141:ILE:HD12	2.15	0.46
1:F:265:LEU:N	1:F:265:LEU:HD23	2.27	0.46
1:F:433:VAL:O	1:F:436:SER:HB3	2.15	0.46
1:A:633:VAL:HA	1:A:636:MET:HE2	1.97	0.46
1:B:21:LEU:C	1:B:165:ILE:HD13	2.36	0.46
1:B:501:THR:HA	1:B:505:ILE:CG2	2.45	0.46
1:B:649:LYS:HA	1:B:652:LYS:HE3	1.96	0.46
1:C:313:HIS:ND1	1:C:324:THR:HG22	2.30	0.46
1:D:577:LYS:HG3	1:D:578:PRO:HD2	1.95	0.46
1:D:72:ASN:C	1:D:163:LYS:HA	2.36	0.46
1:E:265:LEU:HD21	1:E:270:ALA:HB2	1.98	0.46
1:E:534:VAL:O	1:E:538:MET:HB2	2.16	0.46
1:E:641:LYS:HD2	1:E:645:ARG:NH1	2.31	0.46
1:F:474:SER:O	1:F:477:GLN:HG2	2.16	0.46
1:F:68:LEU:HD13	1:F:139:ASN:OD1	2.15	0.46
1:A:530:VAL:HG13	1:A:633:VAL:HG12	1.98	0.46
1:A:67:ARG:NH2	1:A:68:LEU:HD12	2.22	0.46
1:A:77:ARG:HD2	1:A:78:ASP:H	1.81	0.46
1:C:452:ARG:C	1:C:452:ARG:HD3	2.35	0.46
1:D:229:VAL:O	1:D:231:TRP:N	2.47	0.46
1:E:142:ILE:HG12	1:E:201:VAL:HG13	1.97	0.46
1:E:18:LYS:HB2	1:E:31:ARG:HB3	1.97	0.46
1:B:360:ALA:O	1:E:37:THR:HA	2.16	0.46
1:F:21:LEU:HG	1:F:165:ILE:CD1	2.44	0.46
1:F:462:ASN:ND2	1:F:544:ILE:CD1	2.79	0.46
1:F:537:MET:C	1:F:537:MET:SD	2.94	0.46
1:A:103:ASP:O	1:A:104:LEU:C	2.53	0.46
1:A:142:ILE:HG12	1:A:201:VAL:HG13	1.97	0.46
1:B:243:ILE:HG13	1:B:244:VAL:H	1.80	0.46
1:B:284:HIS:O	1:B:286:ARG:N	2.45	0.46
1:B:285:PRO:C	1:B:290:THR:HG21	2.36	0.46
1:B:594:LEU:O	1:B:594:LEU:HD13	2.16	0.46
1:D:243:ILE:HG13	1:D:244:VAL:N	2.31	0.46
1:D:284:HIS:HB3	1:D:285:PRO:CD	2.45	0.46
1:D:394:LYS:HZ1	1:D:402:SER:HB2	1.81	0.46
1:D:445:ASN:HA	1:D:448:GLN:HB2	1.97	0.46
1:D:636:MET:C	1:D:638:GLU:N	2.69	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:355:GLN:O	1:E:357:ALA:N	2.48	0.46
1:E:431:GLY:N	1:E:571:TYR:HE2	2.13	0.46
1:A:152:VAL:HG13	1:A:165:ILE:HD11	1.97	0.46
1:A:17:MET:C	1:A:18:LYS:HD2	2.36	0.46
1:A:248:ASP:O	1:A:249:LEU:C	2.54	0.46
1:A:662:CYS:C	1:A:664:LYS:H	2.19	0.46
1:B:547:LEU:HB2	1:B:548:GLN:OE1	2.16	0.46
1:C:189:LEU:HD22	1:C:189:LEU:N	2.31	0.46
1:C:534:VAL:O	1:C:538:MET:HB2	2.15	0.46
1:C:649:LYS:HA	1:C:652:LYS:HE3	1.98	0.46
1:E:105:ARG:HD3	1:E:149:GLU:OE2	2.15	0.46
1:E:475:MET:SD	1:E:479:LEU:HD23	2.56	0.46
1:E:572:ARG:HD2	1:E:572:ARG:O	2.16	0.46
1:E:533:LEU:HD11	1:E:632:VAL:HG21	1.98	0.46
1:F:103:ASP:O	1:F:106:LYS:N	2.42	0.46
1:F:80:PRO:HB3	1:F:83:MET:SD	2.56	0.46
1:A:298:GLY:O	1:A:299:CYS:C	2.54	0.46
1:A:355:GLN:NE2	1:A:370:CYS:HA	2.27	0.46
1:A:655:TRP:HZ2	1:F:499:GLU:OE1	1.98	0.46
1:A:99:CYS:HB3	1:A:154:GLN:HB2	1.97	0.46
1:B:294:TYR:OH	1:B:298:GLY:HA2	2.16	0.46
1:C:116:GLY:HA3	1:C:217:THR:O	2.16	0.46
1:C:125:LEU:HD13	1:C:125:LEU:C	2.35	0.46
1:C:186:LEU:CG	1:C:228:PRO:HG2	2.44	0.46
1:D:213:PHE:CZ	1:D:221:PRO:HB2	2.50	0.46
1:D:221:PRO:O	1:D:222:PHE:CB	2.64	0.46
1:E:219:PHE:O	1:E:220:ARG:HB3	2.16	0.46
1:F:107:TYR:CE2	1:F:153:LEU:HD22	2.51	0.46
1:F:370:CYS:C	1:F:371:ILE:HD12	2.36	0.46
1:A:291:ASP:C	1:A:293:THR:N	2.70	0.46
1:A:500:GLN:OE1	1:A:502:GLU:HG3	2.15	0.46
1:B:227:GLN:HE21	1:B:227:GLN:HB2	1.58	0.46
1:B:227:GLN:O	1:B:229:VAL:HG22	2.16	0.46
1:D:151:ILE:HD12	1:D:211:LEU:HD11	1.97	0.46
1:D:310:LYS:NZ	1:D:310:LYS:HB2	2.31	0.46
1:D:16:GLU:CA	1:D:33:HIS:H	2.28	0.46
1:D:356:GLU:HA	1:D:453:ALA:HB2	1.97	0.46
1:D:496:LYS:CG	1:E:655:TRP:CD1	2.99	0.46
1:D:658:LEU:HD11	1:E:657:LEU:HB3	1.97	0.46
1:D:82:GLY:O	1:D:84:GLN:N	2.49	0.46
1:E:123:LEU:HD12	1:E:307:LEU:HD13	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:415:GLN:O	1:E:415:GLN:HG2	2.16	0.46
1:D:657:LEU:HB3	1:E:658:LEU:HD11	1.98	0.46
1:F:406:GLN:NE2	1:F:439:THR:HG22	2.31	0.46
1:A:327:VAL:HG21	1:A:367:ALA:HB1	1.98	0.45
1:C:415:GLN:HG2	1:C:415:GLN:O	2.16	0.45
1:C:537:MET:SD	1:C:537:MET:C	2.95	0.45
1:C:636:MET:C	1:C:638:GLU:N	2.70	0.45
1:D:113:ASN:OD1	1:D:117:LEU:HA	2.16	0.45
1:D:260:PRO:C	1:D:262:PRO:HD2	2.37	0.45
1:D:531:LYS:HB3	1:D:531:LYS:NZ	2.31	0.45
1:E:517:MET:O	1:E:521:VAL:HG23	2.16	0.45
1:F:191:PRO:O	1:F:194:LEU:HB2	2.16	0.45
1:F:531:LYS:HB3	1:F:531:LYS:NZ	2.30	0.45
1:A:173:LEU:O	1:A:173:LEU:HG	2.16	0.45
1:A:462:ASN:C	1:A:464:CYS:H	2.19	0.45
1:A:533:LEU:CD1	1:A:629:VAL:HG12	2.46	0.45
1:A:111:PHE:CE1	1:A:575:ARG:HD2	2.51	0.45
1:B:128:ASP:HB3	1:B:162:HIS:HB2	1.97	0.45
1:B:236:ARG:HD3	1:B:283:TRP:CH2	2.51	0.45
1:B:246:SER:O	1:B:253:VAL:HA	2.16	0.45
1:B:363:PRO:HG2	1:B:364:ASP:H	1.81	0.45
1:B:452:ARG:HD3	1:B:452:ARG:C	2.36	0.45
1:B:517:MET:O	1:B:521:VAL:HG23	2.16	0.45
1:B:641:LYS:HD2	1:B:645:ARG:NH1	2.30	0.45
1:C:234:LYS:HD2	1:C:237:GLN:OE1	2.17	0.45
1:C:434:TRP:HB3	1:C:571:TYR:CE1	2.50	0.45
1:C:74:VAL:HG13	1:C:97:GLU:CG	2.46	0.45
1:D:103:ASP:O	1:D:105:ARG:N	2.48	0.45
1:D:500:GLN:CB	1:D:505:ILE:HG12	2.44	0.45
1:E:153:LEU:HD12	1:E:153:LEU:N	2.32	0.45
1:E:243:ILE:HG22	1:E:281:LEU:HD23	1.98	0.45
1:E:356:GLU:HB2	1:E:449:GLN:HE21	1.81	0.45
1:A:547:LEU:HB2	1:A:548:GLN:OE1	2.16	0.45
1:B:140:ARG:HB3	1:B:173:LEU:CD1	2.43	0.45
1:C:174:ASP:O	1:C:175:GLN:HB2	2.16	0.45
1:C:231:TRP:CD1	1:C:231:TRP:C	2.89	0.45
1:C:51:SER:O	1:C:55:ARG:HG3	2.16	0.45
1:D:105:ARG:HG2	1:D:105:ARG:HH11	1.81	0.45
1:D:169:TYR:CD2	1:D:181:GLU:HG2	2.51	0.45
1:D:22:GLY:N	1:D:165:ILE:HG21	2.31	0.45
1:D:434:TRP:HB3	1:D:571:TYR:CE1	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:572:ARG:O	1:D:576:GLU:HB2	2.17	0.45
1:D:601:PHE:O	1:D:605:VAL:HG23	2.16	0.45
1:E:226:TRP:CD2	1:E:228:PRO:HD2	2.51	0.45
1:E:192:GLU:CG	1:E:283:TRP:HB3	2.44	0.45
1:E:294:TYR:HE1	1:E:301:LYS:HB3	1.81	0.45
1:E:356:GLU:HB2	1:E:449:GLN:NE2	2.32	0.45
1:F:160:LEU:HD12	1:F:160:LEU:N	2.31	0.45
1:F:284:HIS:CE1	1:F:285:PRO:HD3	2.52	0.45
1:F:445:ASN:HA	1:F:448:GLN:HB2	1.98	0.45
1:A:114:CYS:C	1:A:116:GLY:N	2.69	0.45
1:A:117:LEU:CD1	1:A:215:CYS:O	2.62	0.45
1:A:22:GLY:N	1:A:165:ILE:HG21	2.32	0.45
1:A:416:GLU:N	1:A:417:PRO:CD	2.80	0.45
1:A:475:MET:O	1:A:478:GLN:HB3	2.16	0.45
1:A:477:GLN:CD	1:F:478:GLN:HE21	2.20	0.45
1:B:241:VAL:HG12	1:B:241:VAL:O	2.16	0.45
1:B:290:THR:HG23	1:B:296:PRO:O	2.17	0.45
1:B:587:SER:O	1:B:591:VAL:HG23	2.17	0.45
1:C:213:PHE:CZ	1:C:221:PRO:HG3	2.51	0.45
1:D:654:LEU:HD23	1:E:654:LEU:CD2	2.41	0.45
1:E:142:ILE:HG22	1:E:144:ARG:HG3	1.98	0.45
1:E:578:PRO:O	1:E:579:ARG:HB2	2.17	0.45
1:E:62:ILE:HG13	1:E:94:LEU:HD13	1.98	0.45
1:F:20:ARG:HB2	1:F:23:THR:HB	1.97	0.45
1:F:350:ASP:N	1:F:350:ASP:OD2	2.48	0.45
1:F:365:LYS:CD	1:F:366:PRO:HD2	2.47	0.45
1:F:410:VAL:HA	1:F:413:ILE:CG2	2.44	0.45
1:C:36:GLU:CD	1:F:460:ARG:HE	2.19	0.45
1:F:463:SER:HA	1:F:467:LYS:HB3	1.98	0.45
1:F:548:GLN:OE1	1:F:548:GLN:N	2.49	0.45
1:F:573:ARG:O	1:F:577:LYS:HB2	2.17	0.45
1:A:350:ASP:OD2	1:A:350:ASP:N	2.49	0.45
1:A:393:SER:O	1:A:394:LYS:HB2	2.17	0.45
1:A:537:MET:SD	1:A:537:MET:C	2.95	0.45
1:B:143:HIS:O	1:B:145:ASP:N	2.49	0.45
1:B:191:PRO:O	1:B:194:LEU:HB2	2.16	0.45
1:B:485:PHE:CD1	1:C:485:PHE:CD1	3.04	0.45
1:C:336:LEU:HD23	1:C:340:ILE:HG23	1.99	0.45
1:C:467:LYS:HD3	1:C:541:GLN:NE2	2.32	0.45
1:C:526:ARG:HD3	1:C:529:GLU:CG	2.46	0.45
1:C:621:LYS:O	1:C:625:LEU:HD12	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:ARG:HB2	1:D:23:THR:HB	1.99	0.45
1:E:638:GLU:O	1:E:643:VAL:HG23	2.16	0.45
1:F:190:ALA:HB3	1:F:203:VAL:HG23	1.97	0.45
1:F:213:PHE:CD1	1:F:221:PRO:HD3	2.51	0.45
1:F:284:HIS:ND1	1:F:285:PRO:HD3	2.31	0.45
1:F:419:ARG:HB3	1:F:419:ARG:NH1	2.32	0.45
1:F:657:LEU:HA	1:F:660:ILE:HG22	1.98	0.45
1:A:279:LEU:O	1:A:281:LEU:N	2.45	0.45
1:A:460:ARG:O	1:A:464:CYS:HB2	2.17	0.45
1:A:480:LYS:CD	1:A:527:GLU:HB2	2.46	0.45
1:A:548:GLN:N	1:A:548:GLN:OE1	2.50	0.45
1:A:621:LYS:O	1:A:625:LEU:HD12	2.17	0.45
1:B:310:LYS:HB2	1:B:310:LYS:NZ	2.32	0.45
1:B:646:LEU:O	1:B:646:LEU:HD12	2.16	0.45
1:E:140:ARG:NH2	1:E:174:ASP:OD2	2.50	0.45
1:E:418:LYS:HZ2	1:E:421:LEU:HD13	1.81	0.45
1:F:102:GLY:HA3	1:F:152:VAL:HG12	1.97	0.45
1:F:34:ASN:O	1:F:35:GLN:C	2.54	0.45
1:F:467:LYS:HD3	1:F:541:GLN:NE2	2.32	0.45
1:F:631:GLU:HG3	1:F:632:VAL:H	1.81	0.45
1:A:216:ILE:HD12	1:A:277:LEU:HD22	1.99	0.45
1:B:368:THR:C	1:B:370:CYS:N	2.70	0.45
1:B:490:ILE:N	1:B:490:ILE:HD12	2.32	0.45
1:B:494:LEU:O	1:B:494:LEU:HD13	2.16	0.45
1:B:570:LEU:H	1:B:570:LEU:HD12	1.82	0.45
1:C:242:ASP:OD1	1:C:255:PHE:HB3	2.17	0.45
1:C:309:LEU:HD12	1:C:309:LEU:C	2.37	0.45
1:C:353:LEU:N	1:C:353:LEU:HD12	2.32	0.45
1:D:102:GLY:HA3	1:D:153:LEU:H	1.81	0.45
1:D:60:LEU:HD21	1:D:175:GLN:HB2	1.97	0.45
1:D:283:TRP:HB2	1:D:284:HIS:H	1.44	0.45
1:D:368:THR:O	1:D:371:ILE:HG12	2.17	0.45
1:D:429:VAL:O	1:D:433:VAL:HG23	2.17	0.45
1:E:540:LEU:HD21	1:E:622:ALA:HB2	1.99	0.45
1:E:631:GLU:HG3	1:E:632:VAL:H	1.81	0.45
1:F:449:GLN:HE22	1:F:452:ARG:HD2	1.81	0.45
1:F:419:ARG:NH2	1:F:587:SER:OG	2.50	0.45
1:A:303:LEU:HD11	1:A:307:LEU:HD23	1.98	0.45
1:A:369:GLN:O	1:A:370:CYS:CB	2.65	0.45
1:A:460:ARG:HG2	1:A:460:ARG:NH1	2.31	0.45
1:A:473:ALA:HB1	1:A:530:VAL:CG1	2.37	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LEU:CG	1:A:629:VAL:HG12	2.46	0.45
1:B:350:ASP:CB	1:B:391:ASP:HB2	2.46	0.45
1:C:229:VAL:O	1:C:230:GLN:HB3	2.16	0.45
1:D:223:LEU:HD21	1:D:226:TRP:CE3	2.52	0.45
1:D:18:LYS:CB	1:D:31:ARG:HD3	2.47	0.45
1:D:431:GLY:O	1:D:433:VAL:N	2.50	0.45
1:D:451:GLN:HA	1:D:454:ALA:CB	2.47	0.45
1:E:328:THR:H	1:E:331:GLU:HG3	1.82	0.45
1:E:350:ASP:CB	1:E:391:ASP:HB2	2.46	0.45
1:F:186:LEU:C	1:F:188:TYR:N	2.70	0.45
1:F:226:TRP:HB3	1:F:227:GLN:H	1.42	0.45
1:F:310:LYS:NZ	1:F:310:LYS:HB2	2.31	0.45
1:F:311:LEU:O	1:F:311:LEU:HD12	2.16	0.45
1:F:394:LYS:HG2	1:F:401:ILE:HG22	1.98	0.45
1:F:570:LEU:H	1:F:570:LEU:HD12	1.82	0.45
1:A:62:ILE:HA	1:A:94:LEU:HD13	1.98	0.45
1:A:530:VAL:HG22	1:A:632:VAL:HG12	1.99	0.45
1:B:283:TRP:HB2	1:B:284:HIS:H	1.42	0.45
1:B:556:GLN:HE21	1:B:556:GLN:HB3	1.63	0.45
1:B:665:VAL:HG13	1:C:665:VAL:O	2.16	0.45
1:C:105:ARG:CD	1:C:148:PRO:HB2	2.47	0.45
1:C:463:SER:HA	1:C:467:LYS:CB	2.47	0.45
1:D:319:THR:O	1:D:321:THR:N	2.50	0.45
1:D:336:LEU:HD23	1:D:340:ILE:HG23	1.98	0.45
1:D:341:GLN:HA	1:D:345:GLY:O	2.17	0.45
1:D:368:THR:OG1	1:D:369:GLN:N	2.49	0.45
1:E:103:ASP:O	1:E:104:LEU:C	2.54	0.45
1:E:113:ASN:HD21	1:E:117:LEU:HG	1.81	0.45
1:E:490:ILE:N	1:E:490:ILE:HD12	2.32	0.45
1:E:89:ASN:HB3	1:E:91:LEU:HD22	1.99	0.45
1:F:70:HIS:CE1	1:F:132:ALA:HA	2.43	0.45
1:F:213:PHE:HE2	1:F:217:THR:HG21	1.81	0.45
1:F:249:LEU:HB3	1:F:250:ASN:H	1.50	0.45
1:A:655:TRP:HB2	1:F:496:LYS:NZ	2.31	0.45
1:F:74:VAL:HG13	1:F:97:GLU:CG	2.47	0.45
1:A:475:MET:SD	1:A:479:LEU:HD23	2.57	0.45
1:B:240:GLU:OE1	1:B:241:VAL:HG23	2.17	0.45
1:B:416:GLU:N	1:B:417:PRO:CD	2.80	0.45
1:B:501:THR:HA	1:B:505:ILE:HG21	1.99	0.45
1:B:534:VAL:O	1:B:538:MET:HB2	2.17	0.45
1:C:282:MET:HB3	1:C:286:ARG:HG3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:VAL:HG12	1:D:325:TYR:O	2.16	0.45
1:D:316:ASN:HA	1:D:388:PHE:CD1	2.51	0.45
1:D:460:ARG:HG2	1:D:460:ARG:HH11	1.82	0.45
1:D:533:LEU:CD2	1:D:629:VAL:HG12	2.38	0.45
1:E:189:LEU:N	1:E:189:LEU:HD22	2.32	0.45
1:E:213:PHE:CZ	1:E:243:ILE:HB	2.52	0.45
1:E:262:PRO:O	1:E:263:ASN:HB2	2.17	0.45
1:E:272:ARG:NH1	1:E:272:ARG:HG3	2.32	0.45
1:E:547:LEU:HB2	1:E:548:GLN:OE1	2.17	0.45
1:E:594:LEU:HD13	1:E:594:LEU:O	2.17	0.45
1:F:231:TRP:CD1	1:F:231:TRP:C	2.90	0.45
1:F:316:ASN:HA	1:F:388:PHE:CD1	2.51	0.45
1:F:443:ASP:HA	1:F:446:ARG:HG3	1.98	0.45
1:F:456:MET:CE	1:F:459:LEU:HD22	2.47	0.45
1:F:641:LYS:HD2	1:F:645:ARG:NH1	2.32	0.45
1:F:89:ASN:HD22	1:F:91:LEU:CB	2.29	0.45
1:A:235:VAL:HG12	1:A:236:ARG:N	2.32	0.44
1:B:460:ARG:HG2	1:B:460:ARG:NH1	2.32	0.44
1:B:636:MET:C	1:B:638:GLU:N	2.71	0.44
1:C:34:ASN:O	1:C:35:GLN:C	2.56	0.44
1:C:587:SER:O	1:C:591:VAL:HG23	2.17	0.44
1:C:90:ASP:C	1:C:91:LEU:HD22	2.38	0.44
1:D:155:GLN:HA	1:D:155:GLN:OE1	2.16	0.44
1:D:537:MET:SD	1:D:537:MET:C	2.96	0.44
1:E:606:ARG:HG3	1:E:606:ARG:HH21	1.81	0.44
1:D:658:LEU:HD21	1:E:657:LEU:HD23	1.99	0.44
1:F:114:CYS:O	1:F:116:GLY:N	2.51	0.44
1:F:313:HIS:ND1	1:F:324:THR:HG22	2.32	0.44
1:A:103:ASP:O	1:A:106:LYS:N	2.45	0.44
1:A:191:PRO:O	1:A:194:LEU:HB2	2.16	0.44
1:A:356:GLU:HA	1:A:453:ALA:HB2	1.99	0.44
1:A:475:MET:SD	1:A:636:MET:HE1	2.58	0.44
1:A:490:ILE:N	1:A:490:ILE:HD12	2.32	0.44
1:A:60:LEU:HD22	1:A:175:GLN:HG2	1.99	0.44
1:B:219:PHE:O	1:B:220:ARG:HB3	2.17	0.44
1:B:239:SER:HB3	1:B:255:PHE:CD1	2.51	0.44
1:B:448:GLN:HE21	1:B:552:MET:CE	2.29	0.44
1:B:497:TYR:HA	1:B:500:GLN:HB2	1.98	0.44
1:C:490:ILE:HG12	1:C:650:ARG:CB	2.48	0.44
1:D:290:THR:HA	1:D:296:PRO:HA	1.99	0.44
1:E:279:LEU:O	1:E:281:LEU:N	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:570:LEU:H	1:E:570:LEU:HD12	1.80	0.44
1:F:173:LEU:HD12	1:F:173:LEU:N	2.32	0.44
1:F:185:THR:HG22	1:F:186:LEU:N	2.32	0.44
1:F:416:GLU:N	1:F:417:PRO:CD	2.80	0.44
1:A:229:VAL:C	1:A:231:TRP:H	2.21	0.44
1:A:292:PRO:CG	1:A:297:ASN:HD22	2.19	0.44
1:B:360:ALA:HB3	1:E:36:GLU:CG	2.39	0.44
1:B:578:PRO:O	1:B:580:ASP:N	2.41	0.44
1:B:657:LEU:HA	1:B:660:ILE:HG22	1.99	0.44
1:B:86:LEU:CD1	1:B:87:ALA:H	2.30	0.44
1:C:490:ILE:CG2	1:C:517:MET:HE2	2.47	0.44
1:D:212:ALA:O	1:D:216:ILE:HG13	2.18	0.44
1:D:313:HIS:ND1	1:D:324:THR:HG22	2.32	0.44
1:D:355:GLN:HB3	1:D:359:LEU:HD13	1.99	0.44
1:D:606:ARG:HH21	1:D:606:ARG:HG3	1.82	0.44
1:F:139:ASN:C	1:F:141:ILE:HD12	2.38	0.44
1:F:357:ALA:HB3	1:F:359:LEU:HD11	1.98	0.44
1:F:361:LEU:HD22	1:F:369:GLN:NE2	2.32	0.44
1:F:571:TYR:HB3	1:F:575:ARG:NH2	2.15	0.44
1:F:652:LYS:C	1:F:654:LEU:H	2.20	0.44
1:A:320:GLY:HA2	1:A:405:PRO:CG	2.47	0.44
1:A:486:PHE:CE2	1:A:521:VAL:HB	2.52	0.44
1:A:531:LYS:O	1:A:535:GLU:HG3	2.17	0.44
1:A:659:LYS:HB2	1:F:500:GLN:HE22	1.83	0.44
1:B:180:THR:O	1:B:180:THR:HG22	2.17	0.44
1:B:192:GLU:O	1:B:196:GLN:HB2	2.18	0.44
1:C:68:LEU:HD13	1:C:139:ASN:CG	2.38	0.44
1:C:328:THR:H	1:C:331:GLU:HG3	1.81	0.44
1:C:416:GLU:N	1:C:417:PRO:CD	2.80	0.44
1:C:487:LYS:HE2	1:C:487:LYS:HB3	1.83	0.44
1:C:490:ILE:HD12	1:C:490:ILE:N	2.32	0.44
1:D:292:PRO:C	1:D:294:TYR:H	2.20	0.44
1:D:490:ILE:HG12	1:D:650:ARG:HB3	1.99	0.44
1:F:229:VAL:C	1:F:231:TRP:N	2.71	0.44
1:F:209:GLY:O	1:F:277:LEU:HD11	2.17	0.44
1:F:303:LEU:HD11	1:F:307:LEU:HD23	1.99	0.44
1:A:192:GLU:HG3	1:A:192:GLU:H	1.48	0.44
1:A:247:GLU:HG3	1:A:251:GLY:HA2	1.99	0.44
1:A:415:GLN:O	1:A:415:GLN:HG2	2.17	0.44
1:B:103:ASP:O	1:B:104:LEU:C	2.56	0.44
1:B:105:ARG:HG2	1:B:105:ARG:HH11	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:LEU:HG	1:B:165:ILE:CD1	2.46	0.44
1:B:238:LYS:HB3	1:B:239:SER:H	1.56	0.44
1:B:268:VAL:CG1	1:B:269:LEU:N	2.80	0.44
1:B:316:ASN:HA	1:B:388:PHE:CD1	2.52	0.44
1:B:534:VAL:HG13	1:B:535:GLU:N	2.32	0.44
1:B:68:LEU:HD13	1:B:139:ASN:OD1	2.17	0.44
1:C:237:GLN:O	1:C:238:LYS:C	2.56	0.44
1:C:579:ARG:HG3	1:C:579:ARG:HH11	1.83	0.44
1:C:601:PHE:O	1:C:605:VAL:HG23	2.16	0.44
1:D:312:VAL:HG22	1:D:313:HIS:N	2.32	0.44
1:D:319:THR:HG23	1:D:320:GLY:N	2.24	0.44
1:D:416:GLU:N	1:D:417:PRO:CD	2.80	0.44
1:D:533:LEU:HD13	1:D:629:VAL:CB	2.47	0.44
1:F:285:PRO:C	1:F:286:ARG:HG3	2.38	0.44
1:F:32:TRP:HZ3	1:F:83:MET:CB	2.22	0.44
1:F:649:LYS:HA	1:F:652:LYS:HE3	2.00	0.44
1:A:457:ASN:HA	1:A:460:ARG:HG3	1.98	0.44
1:B:145:ASP:HA	1:B:189:LEU:HD11	2.00	0.44
1:B:19:GLU:C	1:B:20:ARG:HD3	2.38	0.44
1:B:361:LEU:HD22	1:B:367:ALA:HB1	1.99	0.44
1:B:631:GLU:HG3	1:B:632:VAL:N	2.33	0.44
1:C:192:GLU:HG3	1:C:192:GLU:H	1.49	0.44
1:C:319:THR:O	1:C:321:THR:N	2.51	0.44
1:C:350:ASP:CB	1:C:391:ASP:HB2	2.48	0.44
1:C:490:ILE:HD11	1:C:651:GLN:HG2	1.98	0.44
1:D:87:ALA:C	1:D:89:ASN:H	2.21	0.44
1:D:65:MET:HG3	1:D:94:LEU:HD21	1.99	0.44
1:E:105:ARG:HG2	1:E:105:ARG:HH11	1.82	0.44
1:E:430:TRP:CH2	1:E:570:LEU:HD23	2.52	0.44
1:E:594:LEU:HD13	1:E:594:LEU:C	2.38	0.44
1:F:328:THR:H	1:F:331:GLU:HG3	1.82	0.44
1:A:143:HIS:O	1:A:145:ASP:N	2.50	0.44
1:A:190:ALA:HB3	1:A:203:VAL:HG23	1.99	0.44
1:B:181:GLU:C	1:B:183:VAL:H	2.21	0.44
1:B:429:VAL:O	1:B:433:VAL:HG23	2.18	0.44
1:D:490:ILE:HD11	1:D:651:GLN:HG2	1.99	0.44
1:E:268:VAL:O	1:E:272:ARG:HB2	2.18	0.44
1:E:312:VAL:HG12	1:E:325:TYR:O	2.17	0.44
1:E:341:GLN:HA	1:E:345:GLY:O	2.18	0.44
1:E:531:LYS:O	1:E:535:GLU:HG3	2.17	0.44
1:F:105:ARG:HH11	1:F:105:ARG:HG2	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:ILE:HD12	1:F:211:LEU:HD11	1.99	0.44
1:A:72:ASN:C	1:A:163:LYS:HA	2.37	0.44
1:A:36:GLU:CG	1:A:37:THR:H	2.29	0.44
1:A:419:ARG:HB2	1:A:419:ARG:HH11	1.82	0.44
1:A:482:LYS:O	1:A:485:PHE:HD2	2.01	0.44
1:B:102:GLY:HA3	1:B:153:LEU:H	1.83	0.44
1:B:265:LEU:HD21	1:B:270:ALA:CB	2.48	0.44
1:B:77:ARG:N	1:B:96:MET:HA	2.29	0.44
1:C:25:GLY:HA2	1:C:169:TYR:CZ	2.52	0.44
1:C:16:GLU:N	1:C:32:TRP:HE1	2.15	0.44
1:C:60:LEU:CD1	1:C:175:GLN:HG2	2.47	0.44
1:C:261:TYR:OH	1:C:407:PRO:HG3	2.17	0.44
1:D:60:LEU:HD11	1:D:175:GLN:HG3	2.00	0.44
1:D:189:LEU:N	1:D:189:LEU:HD22	2.32	0.44
1:D:97:GLU:OE2	1:D:163:LYS:HE2	2.18	0.44
1:E:18:LYS:HB2	1:E:31:ARG:HD3	1.99	0.44
1:E:223:LEU:HD13	1:E:223:LEU:C	2.38	0.44
1:F:421:LEU:N	1:F:421:LEU:HD13	2.33	0.44
1:F:81:GLU:OE1	1:F:81:GLU:HA	2.18	0.44
1:A:313:HIS:ND1	1:A:324:THR:HG22	2.33	0.44
1:A:319:THR:O	1:A:321:THR:N	2.51	0.44
1:A:544:ILE:HG13	1:A:545:VAL:N	2.33	0.44
1:B:404:ARG:HH22	1:B:406:GLN:HB3	1.83	0.44
1:C:213:PHE:HE2	1:C:217:THR:HG21	1.83	0.44
1:D:36:GLU:CG	1:D:37:THR:H	2.28	0.44
1:D:404:ARG:N	1:D:404:ARG:CD	2.80	0.44
1:E:336:LEU:HD23	1:E:340:ILE:HG23	1.98	0.44
1:E:445:ASN:HA	1:E:448:GLN:HB2	1.99	0.44
1:F:16:GLU:HB2	1:F:17:MET:H	1.56	0.44
1:F:220:ARG:HE	1:F:221:PRO:HD2	1.81	0.44
1:A:283:TRP:CG	1:A:284:HIS:N	2.86	0.43
1:A:507:SER:C	1:A:509:LYS:N	2.71	0.43
1:A:572:ARG:O	1:A:576:GLU:HB2	2.18	0.43
1:A:631:GLU:HG3	1:A:632:VAL:N	2.33	0.43
1:B:153:LEU:HD12	1:B:153:LEU:N	2.33	0.43
1:B:294:TYR:CE2	1:B:301:LYS:HB3	2.53	0.43
1:C:291:ASP:C	1:C:293:THR:H	2.22	0.43
1:C:419:ARG:CD	1:C:419:ARG:N	2.78	0.43
1:C:422:ALA:O	1:C:426:LEU:HD23	2.18	0.43
1:D:18:LYS:HB3	1:D:19:GLU:H	1.57	0.43
1:D:243:ILE:HG13	1:D:244:VAL:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:VAL:O	1:D:245:VAL:HG12	2.17	0.43
1:D:449:GLN:HE22	1:D:452:ARG:HD2	1.82	0.43
1:E:139:ASN:O	1:E:141:ILE:HD12	2.18	0.43
1:E:34:ASN:O	1:E:35:GLN:C	2.57	0.43
1:F:125:LEU:HA	1:F:162:HIS:CD2	2.53	0.43
1:F:353:LEU:HD12	1:F:353:LEU:N	2.33	0.43
1:F:569:GLU:HA	1:F:569:GLU:OE1	2.18	0.43
1:F:636:MET:C	1:F:638:GLU:N	2.71	0.43
1:F:82:GLY:C	1:F:84:GLN:N	2.71	0.43
1:F:89:ASN:C	1:F:91:LEU:N	2.70	0.43
1:A:172:GLU:CG	1:A:175:GLN:H	2.31	0.43
1:A:227:GLN:OE1	1:A:227:GLN:HA	2.18	0.43
1:A:286:ARG:HA	1:A:290:THR:HB	2.00	0.43
1:B:34:ASN:O	1:B:35:GLN:C	2.56	0.43
1:B:606:ARG:HG3	1:B:606:ARG:HH21	1.83	0.43
1:B:45:GLN:OE1	1:B:88:PRO:HD3	2.18	0.43
1:C:350:ASP:N	1:C:350:ASP:OD2	2.50	0.43
1:C:359:LEU:HD12	1:C:359:LEU:N	2.32	0.43
1:D:223:LEU:CG	1:D:226:TRP:HE3	2.31	0.43
1:D:292:PRO:O	1:D:294:TYR:N	2.46	0.43
1:D:430:TRP:HE1	1:D:587:SER:HB3	1.82	0.43
1:D:463:SER:HA	1:D:467:LYS:HB3	2.00	0.43
1:D:631:GLU:HG3	1:D:632:VAL:H	1.83	0.43
1:D:649:LYS:HA	1:D:652:LYS:HE3	1.98	0.43
1:E:404:ARG:HD3	1:E:404:ARG:N	2.33	0.43
1:E:443:ASP:HA	1:E:446:ARG:HG3	1.99	0.43
1:E:456:MET:HE3	1:E:459:LEU:HD22	2.01	0.43
1:F:103:ASP:O	1:F:105:ARG:N	2.51	0.43
1:F:186:LEU:O	1:F:188:TYR:N	2.51	0.43
1:F:350:ASP:HB2	1:F:391:ASP:HB2	1.99	0.43
1:F:346:ILE:HD13	1:F:388:PHE:HZ	1.83	0.43
1:F:404:ARG:HG2	1:F:605:VAL:HG21	2.00	0.43
1:F:40:GLN:O	1:F:98:TYR:HB3	2.18	0.43
1:F:472:MET:C	1:F:474:SER:H	2.21	0.43
1:A:404:ARG:N	1:A:404:ARG:HD3	2.34	0.43
1:A:524:CYS:HB2	1:A:639:ASP:OD1	2.18	0.43
1:B:624:GLU:HG3	1:B:625:LEU:HG	2.00	0.43
1:C:283:TRP:HD1	1:C:284:HIS:H	1.55	0.43
1:C:460:ARG:HG2	1:C:460:ARG:HH11	1.84	0.43
1:C:617:VAL:O	1:C:621:LYS:HB2	2.18	0.43
1:D:231:TRP:O	1:D:232:HIS:C	2.55	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:THR:H	1:D:331:GLU:HG3	1.81	0.43
1:D:356:GLU:HA	1:D:453:ALA:CB	2.48	0.43
1:D:361:LEU:HD22	1:D:370:CYS:HB3	2.00	0.43
1:D:631:GLU:HG3	1:D:632:VAL:N	2.32	0.43
1:E:139:ASN:C	1:E:141:ILE:HD12	2.38	0.43
1:E:213:PHE:HE2	1:E:217:THR:HG21	1.78	0.43
1:E:236:ARG:O	1:E:238:LYS:N	2.51	0.43
1:F:145:ASP:HA	1:F:189:LEU:HD11	2.01	0.43
1:F:268:VAL:HG13	1:F:269:LEU:N	2.33	0.43
1:A:117:LEU:HD12	1:A:215:CYS:HA	2.01	0.43
1:A:283:TRP:HD1	1:A:284:HIS:H	1.59	0.43
1:A:286:ARG:CA	1:A:290:THR:OG1	2.66	0.43
1:A:649:LYS:HA	1:A:652:LYS:HE3	2.01	0.43
1:B:350:ASP:OD2	1:B:350:ASP:N	2.51	0.43
1:B:385:ASP:CG	1:B:386:LEU:N	2.69	0.43
1:C:105:ARG:HG2	1:C:105:ARG:HH11	1.83	0.43
1:C:279:LEU:O	1:C:281:LEU:N	2.46	0.43
1:C:447:LEU:CD2	1:C:609:TYR:HE1	2.21	0.43
1:D:298:GLY:O	1:D:299:CYS:C	2.56	0.43
1:D:402:SER:N	1:D:403:PRO:CD	2.79	0.43
1:D:452:ARG:HD3	1:D:452:ARG:C	2.39	0.43
1:E:213:PHE:CD1	1:E:221:PRO:HD3	2.53	0.43
1:E:368:THR:HG23	1:E:369:GLN:N	2.29	0.43
1:E:431:GLY:C	1:E:433:VAL:H	2.22	0.43
1:A:655:TRP:NE1	1:F:500:GLN:HG2	2.34	0.43
1:A:155:GLN:HA	1:A:155:GLN:OE1	2.18	0.43
1:A:186:LEU:O	1:A:187:GLN:C	2.57	0.43
1:A:394:LYS:HD2	1:A:613:SER:OG	2.19	0.43
1:A:606:ARG:HG3	1:A:606:ARG:HH21	1.82	0.43
1:A:655:TRP:HZ2	1:F:499:GLU:OE2	2.01	0.43
1:A:84:GLN:NE2	1:A:93:LEU:HD12	2.33	0.43
1:B:192:GLU:HG2	1:B:283:TRP:HB3	2.00	0.43
1:B:49:GLU:HG2	1:B:89:ASN:HB2	2.00	0.43
1:B:79:VAL:HB	1:B:84:GLN:NE2	2.33	0.43
1:C:422:ALA:HB1	1:C:426:LEU:HB3	1.99	0.43
1:C:475:MET:SD	1:C:479:LEU:HD23	2.59	0.43
1:E:103:ASP:O	1:E:105:ARG:N	2.51	0.43
1:E:168:GLY:O	1:E:178:LEU:HB3	2.19	0.43
1:E:389:LEU:HD21	1:E:454:ALA:CB	2.49	0.43
1:E:354:LEU:HD13	1:E:454:ALA:HA	2.00	0.43
1:E:68:LEU:HD13	1:E:139:ASN:OD1	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:238:LYS:HB3	1:F:239:SER:H	1.59	0.43
1:F:282:MET:CB	1:F:286:ARG:HB2	2.48	0.43
1:A:236:ARG:HH11	1:A:236:ARG:HG3	1.82	0.43
1:A:500:GLN:NE2	1:A:501:THR:N	2.67	0.43
1:B:36:GLU:CG	1:B:37:THR:H	2.28	0.43
1:B:472:MET:O	1:B:475:MET:HG3	2.18	0.43
1:C:244:VAL:CG2	1:C:260:PRO:HD3	2.49	0.43
1:C:291:ASP:C	1:C:293:THR:N	2.71	0.43
1:C:524:CYS:HB2	1:C:639:ASP:OD2	2.19	0.43
1:D:422:ALA:O	1:D:585:GLY:CA	2.66	0.43
1:E:459:LEU:HD12	1:E:459:LEU:N	2.34	0.43
1:E:475:MET:HB2	1:E:478:GLN:NE2	2.34	0.43
1:F:221:PRO:HB3	1:F:243:ILE:O	2.19	0.43
1:F:67:ARG:NH2	1:F:68:LEU:HD12	2.22	0.43
1:A:113:ASN:ND2	1:A:117:LEU:HD23	2.33	0.43
1:A:433:VAL:O	1:A:436:SER:HB3	2.19	0.43
1:A:636:MET:C	1:A:638:GLU:N	2.71	0.43
1:A:86:LEU:O	1:A:86:LEU:HD23	2.19	0.43
1:B:276:TRP:CD1	1:B:302:ALA:HB1	2.54	0.43
1:C:460:ARG:O	1:C:464:CYS:HB2	2.18	0.43
1:C:572:ARG:HD2	1:C:572:ARG:O	2.19	0.43
1:D:152:VAL:CG1	1:D:165:ILE:HD11	2.48	0.43
1:D:460:ARG:O	1:D:464:CYS:HB2	2.19	0.43
1:D:623:LEU:HD23	1:D:623:LEU:O	2.18	0.43
1:E:104:LEU:O	1:E:107:TYR:HB2	2.18	0.43
1:E:265:LEU:CG	1:E:266:ASN:N	2.65	0.43
1:E:357:ALA:O	1:E:456:MET:CG	2.66	0.43
1:E:359:LEU:HD12	1:E:359:LEU:N	2.33	0.43
1:E:601:PHE:O	1:E:605:VAL:HG23	2.19	0.43
1:E:652:LYS:C	1:E:654:LEU:H	2.21	0.43
1:F:225:ASN:O	1:F:226:TRP:C	2.57	0.43
1:F:187:GLN:HA	1:F:227:GLN:CD	2.39	0.43
1:F:452:ARG:HD3	1:F:452:ARG:C	2.39	0.43
1:A:102:GLY:HA3	1:A:153:LEU:H	1.81	0.43
1:A:350:ASP:CB	1:A:391:ASP:HB2	2.48	0.43
1:A:449:GLN:HE22	1:A:452:ARG:HD2	1.83	0.43
1:A:500:GLN:HG2	1:A:502:GLU:HG3	2.01	0.43
1:B:193:LEU:O	1:B:195:GLU:N	2.51	0.43
1:B:261:TYR:N	1:B:262:PRO:CD	2.79	0.43
1:B:34:ASN:CG	1:B:83:MET:SD	2.97	0.43
1:B:460:ARG:O	1:B:464:CYS:HB2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:LEU:C	1:B:494:LEU:HD13	2.39	0.43
1:B:541:GLN:OE1	1:B:541:GLN:HA	2.18	0.43
1:B:486:PHE:HZ	1:B:647:GLN:HB3	1.77	0.43
1:B:72:ASN:C	1:B:163:LYS:HA	2.39	0.43
1:C:36:GLU:CG	1:C:37:THR:H	2.29	0.43
1:C:392:ASN:CG	1:C:393:SER:N	2.72	0.43
1:C:445:ASN:HA	1:C:448:GLN:HB2	1.99	0.43
1:C:479:LEU:HD11	1:C:641:LYS:CG	2.22	0.43
1:B:665:VAL:HB	1:C:503:PHE:CE2	2.54	0.43
1:C:664:LYS:O	1:C:665:VAL:C	2.57	0.43
1:C:74:VAL:HG13	1:C:97:GLU:HG2	2.01	0.43
1:D:336:LEU:HD12	1:D:367:ALA:HB1	2.00	0.43
1:D:531:LYS:O	1:D:535:GLU:HG3	2.18	0.43
1:D:62:ILE:HA	1:D:94:LEU:HD13	2.00	0.43
1:E:119:GLU:HG2	1:E:121:ALA:H	1.83	0.43
1:E:51:SER:O	1:E:55:ARG:HG3	2.19	0.43
1:F:355:GLN:O	1:F:357:ALA:N	2.52	0.43
1:F:358:GLY:CA	1:F:456:MET:HB3	2.49	0.43
1:A:367:ALA:C	1:A:369:GLN:H	2.22	0.43
1:A:410:VAL:HA	1:A:413:ILE:CG2	2.45	0.43
1:A:502:GLU:HB2	1:A:503:PHE:H	1.68	0.43
1:A:652:LYS:C	1:A:654:LEU:H	2.21	0.43
1:B:231:TRP:C	1:B:233:SER:H	2.22	0.43
1:B:244:VAL:CG2	1:B:260:PRO:HD3	2.49	0.43
1:C:102:GLY:HA3	1:C:152:VAL:HG12	2.01	0.43
1:C:165:ILE:HG22	1:C:166:ASP:N	2.16	0.43
1:C:18:LYS:HG3	1:C:31:ARG:CG	2.49	0.43
1:D:467:LYS:HD3	1:D:541:GLN:HE22	1.79	0.43
1:E:294:TYR:HD2	1:E:294:TYR:N	2.16	0.43
1:E:408:GLU:HG3	1:E:409:SER:H	1.84	0.43
1:E:416:GLU:N	1:E:417:PRO:CD	2.82	0.43
1:F:213:PHE:CE1	1:F:221:PRO:HG3	2.54	0.43
1:F:418:LYS:O	1:F:419:ARG:HB2	2.17	0.43
1:F:394:LYS:HA	1:F:613:SER:OG	2.19	0.43
1:F:80:PRO:O	1:F:81:GLU:C	2.55	0.43
1:A:221:PRO:O	1:A:222:PHE:HB2	2.18	0.43
1:B:328:THR:H	1:B:331:GLU:HG3	1.84	0.43
1:C:214:GLU:O	1:C:218:GLY:HA2	2.18	0.43
1:C:420:ASN:CG	1:C:421:LEU:N	2.72	0.43
1:D:125:LEU:HA	1:D:162:HIS:CD2	2.54	0.43
1:D:192:GLU:O	1:D:196:GLN:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:TRP:CD1	1:D:232:HIS:N	2.86	0.43
1:D:223:LEU:O	1:D:231:TRP:CZ3	2.72	0.43
1:D:372:SER:H	1:D:384:MET:CE	2.27	0.43
1:D:419:ARG:CZ	1:D:420:ASN:HB2	2.49	0.43
1:D:421:LEU:HB3	1:D:422:ALA:H	1.70	0.43
1:E:141:ILE:HG22	1:E:142:ILE:N	2.33	0.43
1:E:446:ARG:HG2	1:E:446:ARG:NH1	2.33	0.43
1:F:104:LEU:HB3	1:F:148:PRO:O	2.18	0.43
1:F:434:TRP:CZ3	1:F:564:GLU:OE1	2.71	0.43
1:A:231:TRP:CD1	1:A:235:VAL:HG21	2.54	0.42
1:A:272:ARG:HG3	1:A:272:ARG:NH1	2.34	0.42
1:A:34:ASN:O	1:A:35:GLN:C	2.56	0.42
1:C:490:ILE:CG1	1:C:650:ARG:CB	2.96	0.42
1:C:60:LEU:HD13	1:C:175:GLN:HG2	2.00	0.42
1:D:21:LEU:C	1:D:165:ILE:HD13	2.39	0.42
1:D:412:CYS:O	1:D:415:GLN:HB3	2.19	0.42
1:D:490:ILE:HD12	1:D:490:ILE:N	2.34	0.42
1:D:594:LEU:HD13	1:D:594:LEU:C	2.39	0.42
1:F:276:TRP:CD1	1:F:302:ALA:HB1	2.54	0.42
1:F:319:THR:O	1:F:321:THR:N	2.52	0.42
1:A:185:THR:OG1	1:A:187:GLN:HG2	2.19	0.42
1:A:117:LEU:HD12	1:A:215:CYS:CA	2.48	0.42
1:A:213:PHE:HE2	1:A:217:THR:HG21	1.83	0.42
1:A:355:GLN:O	1:A:357:ALA:N	2.53	0.42
1:A:479:LEU:HD12	1:A:640:GLU:HG3	1.96	0.42
1:A:65:MET:HG3	1:A:94:LEU:HD21	2.01	0.42
1:B:220:ARG:H	1:B:221:PRO:HD3	1.80	0.42
1:B:344:THR:O	1:B:345:GLY:C	2.57	0.42
1:B:451:GLN:HA	1:B:454:ALA:CB	2.48	0.42
1:B:525:GLY:C	1:B:527:GLU:H	2.22	0.42
1:B:79:VAL:HB	1:B:84:GLN:CG	2.49	0.42
1:C:420:ASN:HD22	1:C:421:LEU:H	1.65	0.42
1:C:500:GLN:HE22	1:C:504:GLY:CA	2.18	0.42
1:D:213:PHE:HE2	1:D:217:THR:HG21	1.83	0.42
1:D:480:LYS:HE2	1:D:527:GLU:OE1	2.19	0.42
1:D:547:LEU:O	1:D:549:ARG:NH2	2.52	0.42
1:D:548:GLN:O	1:D:549:ARG:NH2	2.51	0.42
1:E:309:LEU:HD13	1:E:309:LEU:C	2.39	0.42
1:E:408:GLU:CG	1:E:409:SER:N	2.82	0.42
1:E:40:GLN:HE21	1:E:40:GLN:HA	1.83	0.42
1:E:626:LEU:N	1:E:627:PRO:CD	2.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:TYR:HB3	1:F:409:SER:HB3	2.01	0.42
1:F:62:ILE:HA	1:F:94:LEU:HD13	2.00	0.42
1:A:167:LEU:O	1:A:169:TYR:N	2.52	0.42
1:B:125:LEU:HA	1:B:162:HIS:CD2	2.54	0.42
1:B:475:MET:SD	1:B:479:LEU:HD23	2.59	0.42
1:B:572:ARG:HD2	1:B:572:ARG:O	2.19	0.42
1:B:86:LEU:HG	1:B:86:LEU:H	1.67	0.42
1:C:219:PHE:O	1:C:220:ARG:C	2.57	0.42
1:C:231:TRP:NE1	1:C:235:VAL:HG21	2.34	0.42
1:C:547:LEU:HB2	1:C:548:GLN:OE1	2.20	0.42
1:C:577:LYS:HB3	1:C:582:ARG:HH22	1.84	0.42
1:C:652:LYS:C	1:C:654:LEU:H	2.22	0.42
1:D:139:ASN:C	1:D:141:ILE:HD12	2.40	0.42
1:D:249:LEU:HD22	1:D:418:LYS:HZ1	1.84	0.42
1:D:432:GLN:H	1:D:432:GLN:HG2	1.68	0.42
1:D:449:GLN:NE2	1:D:452:ARG:HD2	2.34	0.42
1:E:460:ARG:HH11	1:E:460:ARG:HG2	1.83	0.42
1:F:140:ARG:HH11	1:F:140:ARG:HG3	1.84	0.42
1:F:192:GLU:HG3	1:F:192:GLU:H	1.48	0.42
1:F:217:THR:HG22	1:F:260:PRO:HD2	2.01	0.42
1:A:253:VAL:CG2	1:A:254:LYS:N	2.82	0.42
1:A:279:LEU:HD11	1:A:291:ASP:CB	2.48	0.42
1:B:370:CYS:O	1:B:371:ILE:HB	2.20	0.42
1:C:21:LEU:C	1:C:165:ILE:HD13	2.38	0.42
1:C:62:ILE:HA	1:C:94:LEU:HD13	2.01	0.42
1:D:134:ARG:HG2	1:D:300:PHE:CD1	2.55	0.42
1:D:219:PHE:O	1:D:221:PRO:N	2.52	0.42
1:D:652:LYS:C	1:D:654:LEU:H	2.22	0.42
1:E:389:LEU:HD21	1:E:454:ALA:HB2	2.01	0.42
1:E:460:ARG:O	1:E:464:CYS:HB2	2.18	0.42
1:F:239:SER:HB2	1:F:242:ASP:HB2	2.02	0.42
1:F:118:ARG:HD3	1:F:435:HIS:NE2	2.35	0.42
1:F:74:VAL:HG13	1:F:97:GLU:HG2	2.01	0.42
1:A:296:PRO:O	1:A:297:ASN:ND2	2.53	0.42
1:A:442:GLU:O	1:A:446:ARG:HG3	2.19	0.42
1:A:658:LEU:HA	1:F:658:LEU:HD13	2.00	0.42
1:B:223:LEU:HD22	1:B:226:TRP:CG	2.55	0.42
1:B:290:THR:N	1:B:298:GLY:N	2.68	0.42
1:B:299:CYS:O	1:B:300:PHE:C	2.57	0.42
1:B:462:ASN:C	1:B:464:CYS:N	2.72	0.42
1:B:533:LEU:HD13	1:B:629:VAL:HG12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:652:LYS:C	1:B:654:LEU:H	2.22	0.42
1:C:146:LEU:HB3	1:C:207:SER:HB3	2.01	0.42
1:C:385:ASP:CG	1:C:386:LEU:N	2.72	0.42
1:C:394:LYS:HE2	1:C:612:LEU:HD12	2.00	0.42
1:C:497:TYR:CE1	1:C:505:ILE:HG22	2.54	0.42
1:C:577:LYS:HD2	1:C:581:GLN:HE22	1.84	0.42
1:D:110:GLN:HB2	1:D:113:ASN:HB2	2.01	0.42
1:E:183:VAL:O	1:E:183:VAL:HG12	2.20	0.42
1:E:249:LEU:HD13	1:E:414:LEU:CG	2.46	0.42
1:E:319:THR:O	1:E:321:THR:N	2.52	0.42
1:E:392:ASN:ND2	1:E:393:SER:H	2.18	0.42
1:E:587:SER:O	1:E:591:VAL:HG23	2.20	0.42
1:E:617:VAL:O	1:E:621:LYS:HB2	2.19	0.42
1:F:460:ARG:NH1	1:F:460:ARG:HG2	2.35	0.42
1:A:385:ASP:CG	1:A:386:LEU:N	2.73	0.42
1:A:456:MET:HE3	1:A:459:LEU:HD22	2.01	0.42
1:A:507:SER:C	1:A:509:LYS:H	2.21	0.42
1:B:228:PRO:HA	1:B:231:TRP:CB	2.49	0.42
1:B:528:ASN:H	1:B:528:ASN:ND2	2.11	0.42
1:B:537:MET:C	1:B:537:MET:SD	2.98	0.42
1:C:142:ILE:HG12	1:C:201:VAL:HG13	2.01	0.42
1:C:566:GLN:O	1:C:569:GLU:HB2	2.19	0.42
1:D:192:GLU:CG	1:D:283:TRP:HB3	2.39	0.42
1:D:426:LEU:HD11	1:D:574:LEU:HD11	2.02	0.42
1:D:447:LEU:HD23	1:D:609:TYR:HE1	1.85	0.42
1:D:617:VAL:O	1:D:621:LYS:HB2	2.18	0.42
1:E:123:LEU:HD22	1:E:123:LEU:N	2.34	0.42
1:E:17:MET:CB	1:E:32:TRP:HA	2.50	0.42
1:E:236:ARG:NH2	1:E:283:TRP:HE1	2.14	0.42
1:E:296:PRO:HG2	1:E:297:ASN:H	1.84	0.42
1:E:424:PHE:HD1	1:E:582:ARG:NE	2.17	0.42
1:F:272:ARG:HG3	1:F:272:ARG:HH11	1.84	0.42
1:F:279:LEU:HD21	1:F:291:ASP:CA	2.46	0.42
1:F:358:GLY:HA3	1:F:456:MET:CG	2.50	0.42
1:A:118:ARG:C	1:A:264:ASN:O	2.58	0.42
1:A:142:ILE:HG23	1:A:204:ASP:OD2	2.19	0.42
1:A:296:PRO:HG2	1:A:297:ASN:H	1.84	0.42
1:A:479:LEU:HD12	1:A:640:GLU:CB	2.50	0.42
1:B:103:ASP:O	1:B:106:LYS:N	2.47	0.42
1:B:118:ARG:HD3	1:B:435:HIS:CE1	2.54	0.42
1:B:18:LYS:HB3	1:B:19:GLU:CD	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:LYS:HZ3	1:B:531:LYS:HB3	1.85	0.42
1:B:559:THR:HG21	1:B:604:LYS:NZ	2.35	0.42
1:C:119:GLU:HG2	1:C:121:ALA:H	1.85	0.42
1:C:497:TYR:HA	1:C:500:GLN:HB2	2.01	0.42
1:C:480:LYS:HE2	1:C:527:GLU:OE2	2.20	0.42
1:D:146:LEU:HB3	1:D:207:SER:HB3	2.02	0.42
1:D:505:ILE:HD12	1:D:506:THR:N	2.19	0.42
1:D:525:GLY:O	1:D:527:GLU:N	2.47	0.42
1:D:547:LEU:O	1:D:549:ARG:NH1	2.53	0.42
1:E:110:GLN:HB2	1:E:113:ASN:HB3	2.01	0.42
1:E:36:GLU:CG	1:E:37:THR:H	2.31	0.42
1:F:125:LEU:HD13	1:F:125:LEU:C	2.39	0.42
1:F:146:LEU:HB3	1:F:207:SER:HB3	2.02	0.42
1:F:264:ASN:ND2	1:F:264:ASN:O	2.52	0.42
1:F:36:GLU:CG	1:F:37:THR:H	2.30	0.42
1:A:430:TRP:HE1	1:A:587:SER:CA	2.32	0.42
1:B:286:ARG:HH11	1:B:286:ARG:HG2	1.84	0.42
1:B:526:ARG:HH11	1:B:526:ARG:N	2.16	0.42
1:B:51:SER:O	1:B:55:ARG:HG3	2.18	0.42
1:C:125:LEU:HA	1:C:162:HIS:CD2	2.54	0.42
1:C:355:GLN:O	1:C:357:ALA:N	2.53	0.42
1:C:577:LYS:HA	1:C:578:PRO:HD3	1.79	0.42
1:D:104:LEU:O	1:D:107:TYR:HB2	2.20	0.42
1:D:117:LEU:HD23	1:D:119:GLU:OE2	2.20	0.42
1:D:190:ALA:HB3	1:D:203:VAL:HG23	2.02	0.42
1:D:236:ARG:NH2	1:D:283:TRP:CD1	2.86	0.42
1:D:526:ARG:HD3	1:D:635:LEU:HB2	2.01	0.42
1:D:578:PRO:C	1:D:580:ASP:N	2.73	0.42
1:E:25:GLY:HA3	1:E:166:ASP:OD1	2.20	0.42
1:E:265:LEU:HD23	1:E:265:LEU:N	2.35	0.42
1:E:463:SER:HA	1:E:467:LYS:CB	2.49	0.42
1:E:423:PHE:O	1:E:583:THR:O	2.37	0.42
1:E:83:MET:O	1:E:83:MET:SD	2.78	0.42
1:F:17:MET:C	1:F:18:LYS:HD2	2.39	0.42
1:F:219:PHE:N	1:F:219:PHE:CD2	2.86	0.42
1:F:220:ARG:HG3	1:F:221:PRO:N	2.34	0.42
1:F:242:ASP:O	1:F:243:ILE:HG23	2.20	0.42
1:F:458:LEU:CD2	1:F:619:LYS:CA	2.96	0.42
1:F:74:VAL:HG22	1:F:99:CYS:SG	2.59	0.42
1:A:432:GLN:H	1:A:432:GLN:HG2	1.62	0.42
1:B:181:GLU:C	1:B:183:VAL:N	2.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:TRP:CG	1:C:284:HIS:N	2.87	0.42
1:C:429:VAL:O	1:C:433:VAL:HG23	2.20	0.42
1:C:531:LYS:O	1:C:535:GLU:HG3	2.20	0.42
1:D:202:THR:HG21	1:D:284:HIS:O	2.19	0.42
1:E:19:GLU:N	1:E:19:GLU:CD	2.73	0.42
1:E:249:LEU:HB3	1:E:250:ASN:H	1.70	0.42
1:F:103:ASP:O	1:F:104:LEU:C	2.59	0.42
1:F:107:TYR:CD2	1:F:153:LEU:HD13	2.55	0.42
1:F:219:PHE:HB2	1:F:223:LEU:HD13	2.00	0.42
1:F:294:TYR:CE1	1:F:301:LYS:NZ	2.88	0.42
1:F:33:HIS:O	1:F:35:GLN:N	2.53	0.42
1:F:572:ARG:HD2	1:F:572:ARG:O	2.19	0.42
1:A:403:PRO:C	1:A:404:ARG:HG3	2.41	0.42
1:B:184:GLY:O	1:B:186:LEU:HD22	2.20	0.42
1:B:575:ARG:HE	1:B:575:ARG:HB2	1.78	0.42
1:B:601:PHE:O	1:B:605:VAL:HG23	2.20	0.42
1:B:641:LYS:O	1:B:645:ARG:HB2	2.20	0.42
1:B:664:LYS:C	1:B:664:LYS:HD3	2.40	0.42
1:C:456:MET:HE3	1:C:459:LEU:HD22	2.01	0.42
1:C:500:GLN:HE21	1:C:500:GLN:C	2.23	0.42
1:C:517:MET:O	1:C:521:VAL:HG23	2.20	0.42
1:D:227:GLN:CD	1:D:227:GLN:N	2.70	0.42
1:D:353:LEU:HD12	1:D:353:LEU:N	2.35	0.42
1:D:494:LEU:O	1:D:494:LEU:HD13	2.20	0.42
1:E:140:ARG:NH1	1:E:174:ASP:OD2	2.52	0.42
1:E:316:ASN:HA	1:E:388:PHE:CD1	2.55	0.42
1:F:171:LYS:HD3	1:F:199:TYR:OH	2.20	0.42
1:A:141:ILE:HG22	1:A:142:ILE:N	2.35	0.41
1:A:40:GLN:HE21	1:A:40:GLN:HA	1.85	0.41
1:A:472:MET:O	1:A:475:MET:HG3	2.19	0.41
1:B:16:GLU:OE2	1:B:35:GLN:OE1	2.38	0.41
1:B:33:HIS:O	1:B:35:GLN:N	2.53	0.41
1:B:443:ASP:HA	1:B:446:ARG:HG3	2.02	0.41
1:B:89:ASN:CG	1:B:91:LEU:HB2	2.41	0.41
1:C:104:LEU:O	1:C:107:TYR:HB2	2.20	0.41
1:C:416:GLU:O	1:C:418:LYS:N	2.53	0.41
1:B:659:LYS:HE2	1:C:499:GLU:CD	2.40	0.41
1:D:142:ILE:HG12	1:D:201:VAL:HG13	2.01	0.41
1:D:219:PHE:HD1	1:D:221:PRO:HG3	1.84	0.41
1:D:460:ARG:HG2	1:D:460:ARG:NH1	2.35	0.41
1:E:187:GLN:HG3	1:E:220:ARG:HE	1.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:321:THR:O	1:E:322:ILE:O	2.38	0.41
1:E:449:GLN:HE22	1:E:452:ARG:HD2	1.85	0.41
1:D:488:THR:CG2	1:E:648:GLU:HB3	2.49	0.41
1:F:245:VAL:HG22	1:F:255:PHE:HB3	2.02	0.41
1:F:359:LEU:N	1:F:359:LEU:HD12	2.35	0.41
1:F:459:LEU:HD12	1:F:459:LEU:N	2.35	0.41
1:F:606:ARG:HH21	1:F:606:ARG:HG3	1.84	0.41
1:F:611:GLN:O	1:F:615:THR:HG23	2.20	0.41
1:A:240:GLU:HG3	1:A:241:VAL:HG23	2.00	0.41
1:A:209:GLY:O	1:A:277:LEU:HD11	2.20	0.41
1:A:316:ASN:HA	1:A:388:PHE:CD1	2.55	0.41
1:A:517:MET:O	1:A:521:VAL:HG23	2.20	0.41
1:A:530:VAL:HG11	1:A:633:VAL:HG12	2.02	0.41
1:B:222:PHE:O	1:B:223:LEU:HB2	2.20	0.41
1:B:223:LEU:HA	1:B:224:PRO:HD2	1.85	0.41
1:C:451:GLN:HA	1:C:454:ALA:CB	2.46	0.41
1:D:316:ASN:HA	1:D:388:PHE:HE1	1.85	0.41
1:D:497:TYR:HA	1:D:500:GLN:HB2	2.02	0.41
1:D:501:THR:HA	1:D:505:ILE:HD11	2.02	0.41
1:D:60:LEU:HD22	1:D:175:GLN:HB3	2.02	0.41
1:D:622:ALA:O	1:D:626:LEU:HB2	2.18	0.41
1:D:526:ARG:HD3	1:D:635:LEU:CB	2.49	0.41
1:E:113:ASN:OD1	1:E:117:LEU:HA	2.20	0.41
1:E:139:ASN:O	1:E:140:ARG:HB2	2.20	0.41
1:E:223:LEU:HD22	1:E:223:LEU:O	2.19	0.41
1:E:266:ASN:HD21	1:E:313:HIS:HE1	1.68	0.41
1:E:433:VAL:O	1:E:437:ILE:HG13	2.20	0.41
1:E:426:LEU:CD1	1:E:574:LEU:HD11	2.48	0.41
1:E:646:LEU:HD12	1:E:646:LEU:O	2.19	0.41
1:F:19:GLU:CD	1:F:19:GLU:N	2.73	0.41
1:F:431:GLY:CA	1:F:571:TYR:HE2	2.33	0.41
1:F:427:ARG:NE	1:F:575:ARG:HG3	2.12	0.41
1:F:594:LEU:HD13	1:F:598:ILE:HD11	2.02	0.41
1:A:115:CYS:HB2	1:A:435:HIS:CD2	2.54	0.41
1:A:286:ARG:C	1:A:290:THR:OG1	2.58	0.41
1:A:328:THR:H	1:A:331:GLU:HG3	1.85	0.41
1:A:481:ALA:CB	1:F:482:LYS:HZ1	2.32	0.41
1:A:617:VAL:O	1:A:621:LYS:HB2	2.19	0.41
1:A:644:VAL:HG12	1:A:644:VAL:O	2.21	0.41
1:C:422:ALA:O	1:C:585:GLY:HA2	2.20	0.41
1:C:424:PHE:O	1:C:426:LEU:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:ASP:CB	1:D:162:HIS:HB2	2.51	0.41
1:D:541:GLN:HA	1:D:541:GLN:OE1	2.20	0.41
1:E:144:ARG:HD3	1:E:169:TYR:O	2.20	0.41
1:E:186:LEU:HG	1:E:187:GLN:N	2.35	0.41
1:E:192:GLU:HG3	1:E:192:GLU:H	1.48	0.41
1:E:462:ASN:C	1:E:464:CYS:H	2.22	0.41
1:F:419:ARG:HH12	1:F:588:GLN:HA	1.85	0.41
1:F:462:ASN:C	1:F:464:CYS:N	2.73	0.41
1:F:460:ARG:O	1:F:464:CYS:HB2	2.20	0.41
1:A:105:ARG:HG2	1:A:105:ARG:HH11	1.84	0.41
1:A:213:PHE:CD1	1:A:221:PRO:HB2	2.52	0.41
1:A:463:SER:HA	1:A:467:LYS:CB	2.49	0.41
1:B:165:ILE:O	1:B:166:ASP:C	2.59	0.41
1:B:313:HIS:ND1	1:B:324:THR:HG22	2.36	0.41
1:B:463:SER:HA	1:B:467:LYS:CB	2.50	0.41
1:C:139:ASN:C	1:C:141:ILE:HD12	2.41	0.41
1:C:19:GLU:N	1:C:19:GLU:CD	2.73	0.41
1:C:19:GLU:C	1:C:20:ARG:HD3	2.40	0.41
1:C:263:ASN:O	1:C:265:LEU:CD2	2.69	0.41
1:C:265:LEU:O	1:C:266:ASN:HB2	2.20	0.41
1:C:299:CYS:O	1:C:300:PHE:C	2.58	0.41
1:C:315:LEU:O	1:C:317:MET:N	2.53	0.41
1:D:168:GLY:C	1:D:170:ALA:N	2.73	0.41
1:D:496:LYS:HG2	1:E:655:TRP:CD1	2.55	0.41
1:E:227:GLN:HB2	1:E:227:GLN:HE21	1.62	0.41
1:E:247:GLU:HA	1:E:252:THR:O	2.20	0.41
1:F:291:ASP:HA	1:F:292:PRO:HD3	1.87	0.41
1:F:290:THR:N	1:F:298:GLY:N	2.68	0.41
1:F:449:GLN:NE2	1:F:452:ARG:HD2	2.36	0.41
1:F:356:GLU:C	1:F:452:ARG:NH1	2.74	0.41
1:A:445:ASN:HA	1:A:448:GLN:HB2	2.01	0.41
1:B:21:LEU:HD23	1:B:165:ILE:HG23	2.03	0.41
1:B:230:GLN:O	1:B:233:SER:HB3	2.20	0.41
1:B:260:PRO:C	1:B:262:PRO:CD	2.85	0.41
1:B:62:ILE:HA	1:B:94:LEU:HD13	2.02	0.41
1:C:418:LYS:NZ	1:C:421:LEU:CD1	2.75	0.41
1:D:268:VAL:CG1	1:D:269:LEU:N	2.84	0.41
1:D:284:HIS:CD2	1:D:285:PRO:HD3	2.56	0.41
1:E:147:LYS:HE2	1:E:184:GLY:HA3	2.01	0.41
1:E:226:TRP:CZ3	1:E:228:PRO:HB2	2.54	0.41
1:E:227:GLN:CA	1:E:231:TRP:HB2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:TRP:CD1	1:E:302:ALA:HB1	2.56	0.41
1:E:33:HIS:O	1:E:35:GLN:N	2.53	0.41
1:E:594:LEU:HD13	1:E:598:ILE:HD11	2.01	0.41
1:D:496:LYS:CD	1:E:655:TRP:CD1	3.01	0.41
1:F:145:ASP:OD1	1:F:147:LYS:HG2	2.20	0.41
1:F:261:TYR:O	1:F:263:ASN:N	2.54	0.41
1:F:366:PRO:HG2	1:F:368:THR:HG23	2.03	0.41
1:A:140:ARG:HG3	1:A:140:ARG:HH11	1.86	0.41
1:A:213:PHE:CZ	1:A:221:PRO:HB2	2.55	0.41
1:A:359:LEU:N	1:A:359:LEU:HD12	2.36	0.41
1:A:497:TYR:HA	1:A:500:GLN:HB2	2.02	0.41
1:B:140:ARG:HG3	1:B:140:ARG:HH11	1.85	0.41
1:B:181:GLU:O	1:B:183:VAL:N	2.53	0.41
1:B:350:ASP:HB3	1:B:391:ASP:HB2	2.02	0.41
1:B:531:LYS:O	1:B:535:GLU:HG3	2.21	0.41
1:B:65:MET:HG3	1:B:94:LEU:HD21	2.03	0.41
1:C:61:GLU:OE1	1:C:168:GLY:HA2	2.20	0.41
1:D:350:ASP:HB2	1:D:391:ASP:HB2	2.02	0.41
1:D:433:VAL:O	1:D:436:SER:HB3	2.20	0.41
1:D:526:ARG:O	1:D:530:VAL:HG23	2.21	0.41
1:D:430:TRP:HE1	1:D:587:SER:CB	2.34	0.41
1:D:524:CYS:HB2	1:D:639:ASP:OD1	2.20	0.41
1:E:18:LYS:HB3	1:E:19:GLU:H	1.54	0.41
1:E:231:TRP:HA	1:E:235:VAL:HG23	2.03	0.41
1:E:282:MET:CE	1:E:286:ARG:HH21	2.33	0.41
1:E:55:ARG:HB3	1:E:55:ARG:NH1	2.35	0.41
1:F:306:ILE:HA	1:F:309:LEU:HD23	2.03	0.41
1:F:442:GLU:O	1:F:446:ARG:HG3	2.20	0.41
1:F:426:LEU:CD1	1:F:574:LEU:HD11	2.49	0.41
1:A:145:ASP:OD1	1:A:147:LYS:HG2	2.21	0.41
1:A:223:LEU:HG	1:A:226:TRP:HD1	1.86	0.41
1:A:263:ASN:OD1	1:A:265:LEU:CD2	2.65	0.41
1:A:340:ILE:HG13	1:A:341:GLN:N	2.36	0.41
1:A:424:PHE:C	1:A:426:LEU:N	2.73	0.41
1:A:500:GLN:HE21	1:A:501:THR:N	2.15	0.41
1:A:89:ASN:C	1:A:91:LEU:H	2.23	0.41
1:A:420:ASN:HB3	1:B:345:GLY:N	2.36	0.41
1:C:332:SER:HB2	1:C:334:GLN:HG2	2.02	0.41
1:C:626:LEU:HB3	1:C:627:PRO:HD3	2.01	0.41
1:D:119:GLU:HG2	1:D:121:ALA:H	1.86	0.41
1:D:415:GLN:HG2	1:D:415:GLN:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:MET:HE3	1:D:637:ASN:HD21	1.85	0.41
1:D:624:GLU:HG3	1:D:625:LEU:HG	2.02	0.41
1:E:190:ALA:HB2	1:E:206:TRP:HB3	2.03	0.41
1:E:193:LEU:O	1:E:195:GLU:N	2.52	0.41
1:E:19:GLU:C	1:E:20:ARG:HD3	2.39	0.41
1:E:231:TRP:HA	1:E:235:VAL:CG2	2.51	0.41
1:E:332:SER:HA	1:E:366:PRO:HB3	2.01	0.41
1:E:426:LEU:HD22	1:E:586:ASP:O	2.20	0.41
1:E:482:LYS:O	1:E:485:PHE:HD2	2.03	0.41
1:E:572:ARG:O	1:E:576:GLU:HB2	2.21	0.41
1:F:294:TYR:CD1	1:F:294:TYR:N	2.88	0.41
1:F:367:ALA:O	1:F:369:GLN:N	2.53	0.41
1:A:276:TRP:CD1	1:A:302:ALA:HB1	2.56	0.41
1:A:357:ALA:HB3	1:A:359:LEU:HD11	2.01	0.41
1:B:249:LEU:HD23	1:B:418:LYS:NZ	2.34	0.41
1:B:412:CYS:SG	1:B:413:ILE:N	2.94	0.41
1:B:623:LEU:HD23	1:B:623:LEU:O	2.21	0.41
1:B:649:LYS:C	1:B:651:GLN:H	2.22	0.41
1:B:79:VAL:HB	1:B:84:GLN:HG3	2.02	0.41
1:C:447:LEU:HD12	1:C:447:LEU:H	1.86	0.41
1:C:569:GLU:HA	1:C:569:GLU:OE1	2.21	0.41
1:D:51:SER:O	1:D:55:ARG:HG3	2.20	0.41
1:D:641:LYS:O	1:D:645:ARG:HB2	2.21	0.41
1:E:130:ALA:C	1:E:134:ARG:HD3	2.41	0.41
1:E:350:ASP:OD2	1:E:350:ASP:N	2.50	0.41
1:E:403:PRO:O	1:E:404:ARG:HB3	2.20	0.41
1:E:65:MET:HG3	1:E:94:LEU:HD21	2.03	0.41
1:F:452:ARG:O	1:F:456:MET:HB2	2.21	0.41
1:F:583:THR:HB	1:F:584:GLU:H	1.63	0.41
1:F:623:LEU:O	1:F:623:LEU:HD23	2.21	0.41
1:F:647:GLN:OE1	1:F:647:GLN:HA	2.20	0.41
1:A:171:LYS:HG2	1:A:171:LYS:O	2.19	0.41
1:A:18:LYS:HB2	1:A:31:ARG:HB3	2.02	0.41
1:B:190:ALA:HA	1:B:191:PRO:HD3	1.96	0.41
1:B:431:GLY:O	1:B:433:VAL:N	2.52	0.41
1:B:626:LEU:HD23	1:B:626:LEU:C	2.41	0.41
1:C:112:GLU:OE2	1:C:112:GLU:N	2.54	0.41
1:C:191:PRO:O	1:C:194:LEU:HB2	2.21	0.41
1:C:231:TRP:C	1:C:233:SER:N	2.74	0.41
1:C:310:LYS:HB2	1:C:310:LYS:NZ	2.33	0.41
1:C:344:THR:HG23	1:D:418:LYS:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:462:ASN:C	1:C:464:CYS:N	2.73	0.41
1:C:506:THR:HG22	1:C:507:SER:N	2.29	0.41
1:C:68:LEU:HD13	1:C:139:ASN:OD1	2.21	0.41
1:D:19:GLU:N	1:D:19:GLU:CD	2.73	0.41
1:D:190:ALA:HB2	1:D:206:TRP:HB3	2.03	0.41
1:D:34:ASN:O	1:D:35:GLN:C	2.59	0.41
1:D:410:VAL:HA	1:D:413:ILE:CG2	2.44	0.41
1:D:443:ASP:HA	1:D:446:ARG:HG3	2.03	0.41
1:D:463:SER:HA	1:D:467:LYS:CB	2.51	0.41
1:E:104:LEU:HD23	1:E:148:PRO:HB3	2.02	0.41
1:E:303:LEU:HD11	1:E:307:LEU:HD23	2.03	0.41
1:E:544:ILE:HG13	1:E:545:VAL:N	2.36	0.41
1:E:64:ILE:O	1:E:67:ARG:HG3	2.20	0.41
1:E:79:VAL:HG21	1:E:84:GLN:CD	2.41	0.41
1:F:224:PRO:HG2	1:F:225:ASN:H	1.86	0.41
1:F:392:ASN:ND2	1:F:393:SER:H	2.19	0.41
1:F:430:TRP:O	1:F:433:VAL:HB	2.21	0.41
1:A:310:LYS:H	1:A:310:LYS:HZ2	1.68	0.41
1:A:51:SER:O	1:A:55:ARG:HG3	2.21	0.41
1:A:421:LEU:HD22	1:A:585:GLY:O	2.20	0.41
1:B:65:MET:CE	1:B:167:LEU:HB2	2.51	0.41
1:B:449:GLN:HE22	1:B:452:ARG:HD2	1.86	0.41
1:B:517:MET:HB3	1:B:650:ARG:NH2	2.36	0.41
1:B:55:ARG:NH1	1:B:91:LEU:HD21	2.36	0.41
1:B:74:VAL:HG13	1:B:97:GLU:CG	2.51	0.41
1:C:72:ASN:CA	1:C:163:LYS:HA	2.51	0.41
1:C:320:GLY:HA3	1:D:417:PRO:CA	2.41	0.41
1:C:528:ASN:O	1:C:532:LEU:HD23	2.20	0.41
1:C:80:PRO:O	1:C:84:GLN:HG2	2.21	0.41
1:E:22:GLY:H	1:E:165:ILE:HG21	1.86	0.41
1:E:452:ARG:C	1:E:452:ARG:HD3	2.41	0.41
1:E:430:TRP:O	1:E:571:TYR:CE2	2.74	0.41
1:E:624:GLU:HG3	1:E:625:LEU:HG	2.02	0.41
1:F:119:GLU:HG2	1:F:121:ALA:H	1.86	0.41
1:F:394:LYS:HG3	1:F:401:ILE:HG22	2.02	0.41
1:F:547:LEU:HB2	1:F:548:GLN:OE1	2.21	0.41
1:A:107:TYR:CD2	1:A:153:LEU:HD22	2.56	0.41
1:A:167:LEU:C	1:A:169:TYR:H	2.23	0.41
1:A:19:GLU:C	1:A:20:ARG:HD3	2.42	0.41
1:A:451:GLN:HA	1:A:454:ALA:CB	2.48	0.41
1:A:55:ARG:HB3	1:A:55:ARG:NH1	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PHE:CD1	1:A:575:ARG:HD2	2.56	0.41
1:A:631:GLU:HG3	1:A:632:VAL:H	1.86	0.41
1:A:649:LYS:C	1:A:651:GLN:H	2.24	0.41
1:A:64:ILE:O	1:A:67:ARG:HG3	2.21	0.41
1:B:104:LEU:O	1:B:107:TYR:HB2	2.21	0.41
1:B:239:SER:HB2	1:B:242:ASP:CB	2.51	0.41
1:B:303:LEU:HD11	1:B:307:LEU:HD23	2.03	0.41
1:B:346:ILE:HD13	1:B:388:PHE:HZ	1.86	0.41
1:B:359:LEU:HD12	1:B:359:LEU:N	2.36	0.41
1:B:319:THR:O	1:B:405:PRO:HD3	2.21	0.41
1:B:249:LEU:HG	1:B:414:LEU:HG	2.03	0.41
1:B:617:VAL:O	1:B:621:LYS:HB2	2.21	0.41
1:B:631:GLU:HG3	1:B:632:VAL:H	1.85	0.41
1:B:64:ILE:O	1:B:67:ARG:HG3	2.21	0.41
1:C:316:ASN:HA	1:C:388:PHE:CD1	2.56	0.41
1:C:33:HIS:O	1:C:35:GLN:N	2.54	0.41
1:C:55:ARG:NH1	1:C:55:ARG:HB3	2.36	0.41
1:C:496:LYS:CE	1:C:654:LEU:HD11	2.50	0.41
1:D:165:ILE:O	1:D:166:ASP:C	2.59	0.41
1:D:475:MET:SD	1:D:479:LEU:HD23	2.61	0.41
1:D:500:GLN:HB3	1:D:505:ILE:CG1	2.46	0.41
1:D:21:LEU:HD13	1:D:98:TYR:CD1	2.55	0.41
1:E:171:LYS:HZ1	1:E:173:LEU:HD23	1.85	0.41
1:E:367:ALA:O	1:E:368:THR:C	2.59	0.41
1:E:346:ILE:HD13	1:E:388:PHE:HZ	1.86	0.41
1:E:421:LEU:O	1:E:422:ALA:O	2.38	0.41
1:E:549:ARG:HB2	1:E:550:SER:H	1.62	0.41
1:F:239:SER:HA	1:F:242:ASP:OD1	2.21	0.41
1:F:426:LEU:HD11	1:F:574:LEU:CD1	2.50	0.41
1:F:490:ILE:HD12	1:F:490:ILE:N	2.36	0.41
1:F:500:GLN:HE21	1:F:500:GLN:C	2.24	0.41
1:F:451:GLN:HG3	1:F:612:LEU:HD23	2.03	0.41
1:A:294:TYR:O	1:A:301:LYS:CD	2.64	0.40
1:A:452:ARG:HD3	1:A:452:ARG:C	2.41	0.40
1:A:74:VAL:HG13	1:A:97:GLU:CG	2.51	0.40
1:B:105:ARG:HD2	1:B:148:PRO:HB2	2.03	0.40
1:B:294:TYR:CD2	1:B:295:GLY:N	2.90	0.40
1:B:408:GLU:CG	1:B:409:SER:N	2.84	0.40
1:B:432:GLN:HG2	1:B:432:GLN:H	1.65	0.40
1:C:165:ILE:O	1:C:166:ASP:C	2.59	0.40
1:C:247:GLU:HG2	1:C:247:GLU:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:583:THR:O	1:C:584:GLU:C	2.59	0.40
1:D:350:ASP:N	1:D:350:ASP:OD2	2.51	0.40
1:D:594:LEU:O	1:D:594:LEU:HD13	2.21	0.40
1:D:85:ASN:C	1:D:87:ALA:H	2.24	0.40
1:E:190:ALA:HA	1:E:206:TRP:CD1	2.56	0.40
1:E:362:ILE:N	1:E:362:ILE:CD1	2.76	0.40
1:E:472:MET:O	1:E:475:MET:HG3	2.20	0.40
1:F:419:ARG:HE	1:F:591:VAL:HG21	1.86	0.40
1:F:463:SER:HA	1:F:467:LYS:CB	2.51	0.40
1:F:433:VAL:CG1	1:F:594:LEU:HB2	2.51	0.40
1:F:594:LEU:C	1:F:594:LEU:HD13	2.42	0.40
1:A:110:GLN:HB2	1:A:113:ASN:HB2	2.03	0.40
1:A:259:LEU:N	1:A:259:LEU:CD1	2.83	0.40
1:A:419:ARG:NH1	1:A:419:ARG:C	2.75	0.40
1:A:479:LEU:HD12	1:A:640:GLU:HB3	2.03	0.40
1:A:84:GLN:OE1	1:A:84:GLN:O	2.39	0.40
1:A:74:VAL:HG13	1:A:97:GLU:HG2	2.03	0.40
1:B:368:THR:C	1:B:370:CYS:H	2.24	0.40
1:B:430:TRP:O	1:B:433:VAL:HB	2.22	0.40
1:B:487:LYS:HE2	1:B:487:LYS:HB3	1.86	0.40
1:C:392:ASN:C	1:C:393:SER:OG	2.60	0.40
1:C:457:ASN:ND2	1:C:619:LYS:NZ	2.63	0.40
1:C:649:LYS:C	1:C:651:GLN:H	2.24	0.40
1:C:65:MET:CE	1:C:167:LEU:HB2	2.50	0.40
1:D:241:VAL:O	1:D:241:VAL:HG12	2.20	0.40
1:D:462:ASN:C	1:D:464:CYS:N	2.75	0.40
1:E:315:LEU:HD12	1:E:321:THR:HA	2.02	0.40
1:E:416:GLU:O	1:E:418:LYS:N	2.54	0.40
1:E:577:LYS:HA	1:E:578:PRO:HD3	1.91	0.40
1:E:636:MET:C	1:E:638:GLU:N	2.73	0.40
1:F:403:PRO:C	1:F:404:ARG:HG3	2.42	0.40
1:F:433:VAL:O	1:F:437:ILE:HG13	2.21	0.40
1:F:89:ASN:O	1:F:91:LEU:N	2.55	0.40
1:A:231:TRP:CD1	1:A:231:TRP:C	2.93	0.40
1:A:331:GLU:HB2	1:A:367:ALA:HB2	2.03	0.40
1:A:320:GLY:HA2	1:A:405:PRO:CD	2.51	0.40
1:A:526:ARG:HH11	1:A:526:ARG:HG3	1.85	0.40
1:B:496:LYS:HZ2	1:C:658:LEU:HD23	1.86	0.40
1:B:647:GLN:HA	1:B:647:GLN:OE1	2.20	0.40
1:C:151:ILE:HD12	1:C:211:LEU:HD11	2.04	0.40
1:C:276:TRP:CD1	1:C:302:ALA:HB1	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:ARG:HH21	1:C:606:ARG:HG3	1.85	0.40
1:C:626:LEU:HD23	1:C:626:LEU:C	2.42	0.40
1:D:240:GLU:HG3	1:D:241:VAL:CG2	2.38	0.40
1:D:299:CYS:O	1:D:300:PHE:C	2.59	0.40
1:D:497:TYR:CE1	1:D:505:ILE:HD13	2.56	0.40
1:D:637:ASN:HA	1:D:641:LYS:HB2	2.04	0.40
1:D:40:GLN:O	1:D:98:TYR:HB3	2.21	0.40
1:E:241:VAL:H	1:E:286:ARG:NH2	2.19	0.40
1:E:321:THR:HG21	1:E:447:LEU:CD1	2.42	0.40
1:E:652:LYS:HD2	1:E:652:LYS:C	2.42	0.40
1:E:71:PRO:C	1:E:73:VAL:H	2.24	0.40
1:F:143:HIS:O	1:F:145:ASP:N	2.51	0.40
1:F:252:THR:O	1:F:254:LYS:HG3	2.21	0.40
1:F:350:ASP:HB3	1:F:391:ASP:HB2	2.03	0.40
1:F:646:LEU:O	1:F:646:LEU:HD12	2.20	0.40
1:A:213:PHE:CG	1:A:221:PRO:HD2	2.56	0.40
1:A:259:LEU:HB2	1:A:260:PRO:HD2	2.01	0.40
1:A:261:TYR:N	1:A:262:PRO:CD	2.84	0.40
1:A:284:HIS:CB	1:A:285:PRO:CD	2.98	0.40
1:A:418:LYS:HB3	1:B:344:THR:OG1	2.21	0.40
1:B:412:CYS:O	1:B:415:GLN:HB3	2.22	0.40
1:C:580:ASP:OD1	1:C:581:GLN:HG3	2.22	0.40
1:C:604:LYS:O	1:C:608:ILE:HG12	2.20	0.40
1:C:65:MET:HG3	1:C:94:LEU:HD21	2.03	0.40
1:C:40:GLN:O	1:C:98:TYR:HB3	2.22	0.40
1:D:350:ASP:HB3	1:D:391:ASP:HB2	2.04	0.40
1:D:547:LEU:HB2	1:D:548:GLN:OE1	2.22	0.40
1:E:442:GLU:O	1:E:446:ARG:HG3	2.22	0.40
1:E:460:ARG:NH1	1:E:460:ARG:HG2	2.37	0.40
1:F:104:LEU:HD23	1:F:148:PRO:CB	2.43	0.40
1:F:422:ALA:O	1:F:585:GLY:CA	2.68	0.40
1:A:139:ASN:O	1:A:140:ARG:HB2	2.21	0.40
1:A:33:HIS:O	1:A:35:GLN:N	2.55	0.40
1:B:237:GLN:O	1:B:238:LYS:C	2.60	0.40
1:B:452:ARG:O	1:B:456:MET:HB2	2.21	0.40
1:C:250:ASN:ND2	1:C:250:ASN:N	2.70	0.40
1:C:296:PRO:HG2	1:C:297:ASN:HD22	1.86	0.40
1:B:481:ALA:HB1	1:C:478:GLN:HG3	1.99	0.40
1:B:481:ALA:HB3	1:C:478:GLN:HG3	1.99	0.40
1:C:662:CYS:O	1:C:665:VAL:HG13	2.21	0.40
1:C:72:ASN:C	1:C:163:LYS:HA	2.40	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:ALA:HB3	1:D:359:LEU:HD11	2.03	0.40
1:D:447:LEU:HD12	1:D:447:LEU:H	1.87	0.40
1:D:548:GLN:OE1	1:D:548:GLN:N	2.55	0.40
1:D:626:LEU:HB3	1:D:627:PRO:HD3	2.01	0.40
1:E:412:CYS:O	1:E:415:GLN:HB3	2.21	0.40
1:E:510:LEU:HB3	1:E:653:GLU:OE2	2.21	0.40
1:E:642:THR:O	1:E:646:LEU:HD23	2.22	0.40
1:F:227:GLN:H	1:F:228:PRO:CD	2.35	0.40
1:F:415:GLN:O	1:F:415:GLN:HG2	2.22	0.40
1:F:604:LYS:O	1:F:608:ILE:HG12	2.22	0.40
1:F:89:ASN:HD22	1:F:91:LEU:CG	2.35	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	614/669 (92%)	427 (70%)	112 (18%)	75 (12%)	0	7
1	B	624/669 (93%)	411 (66%)	133 (21%)	80 (13%)	0	7
1	C	614/669 (92%)	423 (69%)	117 (19%)	74 (12%)	0	7
1	D	614/669 (92%)	421 (69%)	119 (19%)	74 (12%)	0	7
1	E	614/669 (92%)	417 (68%)	121 (20%)	76 (12%)	0	7
1	F	614/669 (92%)	421 (69%)	120 (20%)	73 (12%)	0	7
All	All	3694/4014 (92%)	2520 (68%)	722 (20%)	452 (12%)	0	7

All (452) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	35	GLN
1	A	92	PRO
1	A	166	ASP
1	A	182	PHE
1	A	183	VAL
1	A	221	PRO
1	A	250	ASN
1	A	299	CYS
1	A	300	PHE
1	A	302	ALA
1	A	319	THR
1	A	322	ILE
1	A	323	HIS
1	A	356	GLU
1	A	370	CYS
1	A	392	ASN
1	A	408	GLU
1	A	580	ASP
1	A	587	SER
1	A	641	LYS
1	B	35	GLN
1	B	68	LEU
1	B	84	GLN
1	B	86	LEU
1	B	104	LEU
1	B	166	ASP
1	B	186	LEU
1	B	187	GLN
1	B	188	TYR
1	B	222	PHE
1	B	224	PRO
1	B	283	TRP
1	B	299	CYS
1	B	300	PHE
1	B	302	ALA
1	B	319	THR
1	B	322	ILE
1	B	323	HIS
1	B	356	GLU
1	B	392	ASN
1	B	501	THR
1	B	505	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	550	SER
1	B	587	SER
1	B	641	LYS
1	C	35	GLN
1	C	37	THR
1	C	68	LEU
1	C	85	ASN
1	C	166	ASP
1	C	177	GLU
1	C	222	PHE
1	C	299	CYS
1	C	300	PHE
1	C	302	ALA
1	C	319	THR
1	C	322	ILE
1	C	323	HIS
1	C	356	GLU
1	C	371	ILE
1	C	402	SER
1	C	419	ARG
1	C	501	THR
1	C	505	ILE
1	C	578	PRO
1	C	583	THR
1	C	587	SER
1	C	641	LYS
1	D	34	ASN
1	D	35	GLN
1	D	37	THR
1	D	68	LEU
1	D	81	GLU
1	D	83	MET
1	D	166	ASP
1	D	170	ALA
1	D	224	PRO
1	D	299	CYS
1	D	300	PHE
1	D	302	ALA
1	D	319	THR
1	D	322	ILE
1	D	323	HIS
1	D	356	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	392	ASN
1	D	419	ARG
1	D	421	LEU
1	D	422	ALA
1	D	501	THR
1	D	581	GLN
1	D	587	SER
1	D	641	LYS
1	E	35	GLN
1	E	37	THR
1	E	68	LEU
1	E	86	LEU
1	E	166	ASP
1	E	263	ASN
1	E	285	PRO
1	E	294	TYR
1	E	299	CYS
1	E	300	PHE
1	E	302	ALA
1	E	319	THR
1	E	322	ILE
1	E	323	HIS
1	E	356	GLU
1	E	368	THR
1	E	421	LEU
1	E	422	ALA
1	E	501	THR
1	E	583	THR
1	E	584	GLU
1	E	587	SER
1	E	641	LYS
1	F	34	ASN
1	F	35	GLN
1	F	37	THR
1	F	68	LEU
1	F	114	CYS
1	F	118	ARG
1	F	166	ASP
1	F	221	PRO
1	F	225	ASN
1	F	227	GLN
1	F	229	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	243	ILE
1	F	296	PRO
1	F	299	CYS
1	F	300	PHE
1	F	302	ALA
1	F	319	THR
1	F	322	ILE
1	F	323	HIS
1	F	356	GLU
1	F	372	SER
1	F	501	THR
1	F	502	GLU
1	F	585	GLY
1	F	587	SER
1	F	641	LYS
1	A	34	ASN
1	A	37	THR
1	A	68	LEU
1	A	83	MET
1	A	104	LEU
1	A	157	GLU
1	A	188	TYR
1	A	197	GLN
1	A	224	PRO
1	A	243	ILE
1	A	298	GLY
1	A	320	GLY
1	A	330	ASP
1	A	368	THR
1	A	369	GLN
1	A	410	VAL
1	A	509	LYS
1	A	579	ARG
1	B	34	ASN
1	B	37	THR
1	B	88	PRO
1	B	157	GLU
1	B	197	GLN
1	B	221	PRO
1	B	228	PRO
1	B	295	GLY
1	B	320	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	330	ASP
1	B	345	GLY
1	B	364	ASP
1	B	367	ALA
1	B	410	VAL
1	B	509	LYS
1	B	584	GLU
1	C	34	ASN
1	C	104	LEU
1	C	157	GLU
1	C	168	GLY
1	C	175	GLN
1	C	197	GLN
1	C	221	PRO
1	C	320	GLY
1	C	330	ASP
1	C	345	GLY
1	C	392	ASN
1	C	407	PRO
1	C	408	GLU
1	C	410	VAL
1	C	422	ALA
1	C	507	SER
1	C	509	LYS
1	D	19	GLU
1	D	82	GLY
1	D	104	LEU
1	D	157	GLU
1	D	169	TYR
1	D	188	TYR
1	D	197	GLN
1	D	222	PHE
1	D	238	LYS
1	D	320	GLY
1	D	330	ASP
1	D	393	SER
1	D	410	VAL
1	D	503	PHE
1	D	505	ILE
1	D	509	LYS
1	E	34	ASN
1	E	82	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	104	LEU
1	E	157	GLU
1	E	174	ASP
1	E	197	GLN
1	E	237	GLN
1	E	284	HIS
1	E	298	GLY
1	E	320	GLY
1	E	330	ASP
1	E	410	VAL
1	E	505	ILE
1	E	509	LYS
1	E	578	PRO
1	F	86	LEU
1	F	104	LEU
1	F	157	GLU
1	F	197	GLN
1	F	226	TRP
1	F	238	LYS
1	F	250	ASN
1	F	263	ASN
1	F	266	ASN
1	F	320	GLY
1	F	330	ASP
1	F	392	ASN
1	F	409	SER
1	F	410	VAL
1	F	509	LYS
1	F	578	PRO
1	A	36	GLU
1	A	187	GLN
1	A	189	LEU
1	A	249	LEU
1	A	280	MET
1	A	293	THR
1	A	321	THR
1	A	357	ALA
1	A	366	PRO
1	A	393	SER
1	A	402	SER
1	A	407	PRO
1	A	432	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	466	SER
1	B	36	GLU
1	B	81	GLU
1	B	189	LEU
1	B	280	MET
1	B	321	THR
1	B	357	ALA
1	B	407	PRO
1	B	422	ALA
1	B	425	GLN
1	B	432	GLN
1	C	36	GLU
1	C	178	LEU
1	C	189	LEU
1	C	226	TRP
1	C	232	HIS
1	C	280	MET
1	C	321	THR
1	C	357	ALA
1	C	393	SER
1	C	432	GLN
1	C	466	SER
1	C	526	ARG
1	D	36	GLU
1	D	92	PRO
1	D	189	LEU
1	D	229	VAL
1	D	230	GLN
1	D	232	HIS
1	D	265	LEU
1	D	280	MET
1	D	357	ALA
1	D	417	PRO
1	D	418	LYS
1	D	425	GLN
1	D	432	GLN
1	D	466	SER
1	D	583	THR
1	D	626	LEU
1	E	36	GLU
1	E	84	GLN
1	E	159	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	171	LYS
1	E	189	LEU
1	E	222	PHE
1	E	223	LEU
1	E	227	GLN
1	E	280	MET
1	E	321	THR
1	E	357	ALA
1	E	392	ASN
1	E	425	GLN
1	E	502	GLU
1	E	508	ASP
1	F	17	MET
1	F	36	GLU
1	F	175	GLN
1	F	189	LEU
1	F	224	PRO
1	F	260	PRO
1	F	280	MET
1	F	357	ALA
1	F	368	THR
1	F	369	GLN
1	F	371	ILE
1	F	421	LEU
1	F	432	GLN
1	F	466	SER
1	A	159	ARG
1	A	170	ALA
1	A	223	LEU
1	A	270	ALA
1	A	284	HIS
1	A	292	PRO
1	A	425	GLN
1	B	159	ARG
1	B	170	ALA
1	B	175	GLN
1	B	177	GLU
1	B	182	PHE
1	B	194	LEU
1	B	223	LEU
1	B	238	LYS
1	B	249	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	270	ALA
1	B	298	GLY
1	B	368	THR
1	B	461	ASN
1	B	466	SER
1	B	579	ARG
1	C	159	ARG
1	C	186	LEU
1	C	249	LEU
1	C	263	ASN
1	C	270	ALA
1	C	369	GLN
1	C	425	GLN
1	D	159	ARG
1	D	223	LEU
1	D	251	GLY
1	D	270	ALA
1	D	298	GLY
1	D	321	THR
1	D	345	GLY
1	D	402	SER
1	D	578	PRO
1	D	579	ARG
1	E	19	GLU
1	E	221	PRO
1	E	296	PRO
1	E	345	GLY
1	E	385	ASP
1	E	432	GLN
1	E	461	ASN
1	E	466	SER
1	E	507	SER
1	F	83	MET
1	F	159	ARG
1	F	174	ASP
1	F	219	PHE
1	F	230	GLN
1	F	270	ALA
1	A	21	LEU
1	A	114	CYS
1	A	194	LEU
1	A	294	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	346	ILE
1	A	409	SER
1	A	626	LEU
1	B	227	GLN
1	B	285	PRO
1	B	346	ILE
1	B	626	LEU
1	C	194	LEU
1	C	265	LEU
1	C	298	GLY
1	C	346	ILE
1	C	420	ASN
1	C	584	GLU
1	C	626	LEU
1	D	185	THR
1	D	384	MET
1	D	507	SER
1	E	21	LEU
1	E	170	ALA
1	E	194	LEU
1	E	265	LEU
1	E	270	ALA
1	E	346	ILE
1	F	117	LEU
1	F	194	LEU
1	F	346	ILE
1	F	461	ASN
1	A	18	LYS
1	A	176	GLY
1	A	238	LYS
1	A	345	GLY
1	B	91	LEU
1	B	265	LEU
1	B	366	PRO
1	B	393	SER
1	B	502	GLU
1	C	238	LYS
1	C	417	PRO
1	D	221	PRO
1	D	346	ILE
1	D	420	ASN
1	E	198	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	403	PRO
1	F	21	LEU
1	F	321	THR
1	F	525	GLY
1	C	92	PRO
1	C	241	VAL
1	C	585	GLY
1	E	245	VAL
1	A	165	ILE
1	B	229	VAL
1	B	371	ILE
1	E	165	ILE
1	F	345	GLY
1	B	585	GLY
1	C	82	GLY
1	D	165	ILE
1	E	228	PRO
1	E	405	PRO
1	F	92	PRO
1	F	165	ILE
1	A	525	GLY
1	B	165	ILE
1	C	165	ILE
1	D	245	VAL
1	E	417	PRO
1	E	585	GLY
1	F	183	VAL
1	A	241	VAL
1	A	578	PRO
1	B	557	GLY
1	C	245	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	567/601 (94%)	491 (87%)	76 (13%)	4	28
1	B	572/601 (95%)	485 (85%)	87 (15%)	3	22
1	C	567/601 (94%)	490 (86%)	77 (14%)	4	27
1	D	567/601 (94%)	488 (86%)	79 (14%)	4	27
1	E	567/601 (94%)	492 (87%)	75 (13%)	5	28
1	F	567/601 (94%)	478 (84%)	89 (16%)	3	22
All	All	3407/3606 (94%)	2924 (86%)	483 (14%)	4	26

All (483) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	MET
1	A	20	ARG
1	A	23	THR
1	A	26	PHE
1	A	37	THR
1	A	89	ASN
1	A	103	ASP
1	A	105	ARG
1	A	119	GLU
1	A	124	THR
1	A	152	VAL
1	A	178	LEU
1	A	182	PHE
1	A	183	VAL
1	A	185	THR
1	A	192	GLU
1	A	194	LEU
1	A	210	THR
1	A	213	PHE
1	A	222	PHE
1	A	225	ASN
1	A	226	TRP
1	A	229	VAL
1	A	236	ARG
1	A	243	ILE
1	A	248	ASP
1	A	257	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	259	LEU
1	A	261	TYR
1	A	294	TYR
1	A	304	ASP
1	A	307	LEU
1	A	310	LYS
1	A	311	LEU
1	A	319	THR
1	A	334	GLN
1	A	359	LEU
1	A	364	ASP
1	A	371	ILE
1	A	385	ASP
1	A	388	PHE
1	A	390	PHE
1	A	404	ARG
1	A	415	GLN
1	A	418	LYS
1	A	419	ARG
1	A	421	LEU
1	A	424	PHE
1	A	432	GLN
1	A	434	TRP
1	A	448	GLN
1	A	452	ARG
1	A	472	MET
1	A	475	MET
1	A	478	GLN
1	A	483	LEU
1	A	485	PHE
1	A	486	PHE
1	A	499	GLU
1	A	500	GLN
1	A	502	GLU
1	A	511	LEU
1	A	514	TRP
1	A	517	MET
1	A	529	GLU
1	A	543	ASP
1	A	548	GLN
1	A	549	ARG
1	A	564	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	575	ARG
1	A	579	ARG
1	A	595	LEU
1	A	631	GLU
1	A	648	GLU
1	A	651	GLN
1	A	652	LYS
1	B	16	GLU
1	B	20	ARG
1	B	23	THR
1	B	26	PHE
1	B	37	THR
1	B	53	ARG
1	B	86	LEU
1	B	89	ASN
1	B	103	ASP
1	B	105	ARG
1	B	119	GLU
1	B	124	THR
1	B	152	VAL
1	B	173	LEU
1	B	182	PHE
1	B	187	GLN
1	B	192	GLU
1	B	194	LEU
1	B	210	THR
1	B	213	PHE
1	B	227	GLN
1	B	236	ARG
1	B	238	LYS
1	B	242	ASP
1	B	248	ASP
1	B	249	LEU
1	B	263	ASN
1	B	283	TRP
1	B	284	HIS
1	B	286	ARG
1	B	290	THR
1	B	304	ASP
1	B	307	LEU
1	B	308	ASN
1	B	310	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	311	LEU
1	B	319	THR
1	B	334	GLN
1	B	359	LEU
1	B	362	ILE
1	B	369	GLN
1	B	384	MET
1	B	385	ASP
1	B	388	PHE
1	B	390	PHE
1	B	394	LYS
1	B	404	ARG
1	B	419	ARG
1	B	421	LEU
1	B	424	PHE
1	B	432	GLN
1	B	434	TRP
1	B	448	GLN
1	B	452	ARG
1	B	472	MET
1	B	475	MET
1	B	478	GLN
1	B	483	LEU
1	B	485	PHE
1	B	486	PHE
1	B	493	ASP
1	B	499	GLU
1	B	500	GLN
1	B	502	GLU
1	B	503	PHE
1	B	511	LEU
1	B	514	TRP
1	B	517	MET
1	B	526	ARG
1	B	527	GLU
1	B	528	ASN
1	B	529	GLU
1	B	543	ASP
1	B	548	GLN
1	B	549	ARG
1	B	552	MET
1	B	556	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	564	GLU
1	B	575	ARG
1	B	579	ARG
1	B	583	THR
1	B	595	LEU
1	B	631	GLU
1	B	648	GLU
1	B	651	GLN
1	B	652	LYS
1	B	664	LYS
1	C	20	ARG
1	C	23	THR
1	C	26	PHE
1	C	37	THR
1	C	53	ARG
1	C	103	ASP
1	C	105	ARG
1	C	119	GLU
1	C	124	THR
1	C	152	VAL
1	C	169	TYR
1	C	174	ASP
1	C	178	LEU
1	C	181	GLU
1	C	186	LEU
1	C	192	GLU
1	C	194	LEU
1	C	210	THR
1	C	213	PHE
1	C	225	ASN
1	C	231	TRP
1	C	236	ARG
1	C	243	ILE
1	C	247	GLU
1	C	250	ASN
1	C	253	VAL
1	C	257	SER
1	C	304	ASP
1	C	307	LEU
1	C	309	LEU
1	C	310	LYS
1	C	311	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	319	THR
1	C	334	GLN
1	C	359	LEU
1	C	362	ILE
1	C	368	THR
1	C	385	ASP
1	C	388	PHE
1	C	390	PHE
1	C	394	LYS
1	C	401	ILE
1	C	404	ARG
1	C	419	ARG
1	C	424	PHE
1	C	432	GLN
1	C	434	TRP
1	C	448	GLN
1	C	452	ARG
1	C	472	MET
1	C	475	MET
1	C	478	GLN
1	C	483	LEU
1	C	485	PHE
1	C	486	PHE
1	C	493	ASP
1	C	499	GLU
1	C	500	GLN
1	C	502	GLU
1	C	503	PHE
1	C	511	LEU
1	C	514	TRP
1	C	517	MET
1	C	528	ASN
1	C	529	GLU
1	C	543	ASP
1	C	548	GLN
1	C	549	ARG
1	C	559	THR
1	C	564	GLU
1	C	575	ARG
1	C	581	GLN
1	C	595	LEU
1	C	631	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	648	GLU
1	C	651	GLN
1	C	652	LYS
1	D	20	ARG
1	D	23	THR
1	D	26	PHE
1	D	37	THR
1	D	85	ASN
1	D	103	ASP
1	D	105	ARG
1	D	115	CYS
1	D	118	ARG
1	D	119	GLU
1	D	124	THR
1	D	152	VAL
1	D	169	TYR
1	D	182	PHE
1	D	187	GLN
1	D	192	GLU
1	D	194	LEU
1	D	210	THR
1	D	213	PHE
1	D	219	PHE
1	D	222	PHE
1	D	223	LEU
1	D	225	ASN
1	D	226	TRP
1	D	230	GLN
1	D	236	ARG
1	D	238	LYS
1	D	248	ASP
1	D	253	VAL
1	D	273	LEU
1	D	283	TRP
1	D	304	ASP
1	D	307	LEU
1	D	310	LYS
1	D	311	LEU
1	D	319	THR
1	D	334	GLN
1	D	359	LEU
1	D	368	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	385	ASP
1	D	388	PHE
1	D	390	PHE
1	D	404	ARG
1	D	408	GLU
1	D	419	ARG
1	D	420	ASN
1	D	421	LEU
1	D	424	PHE
1	D	432	GLN
1	D	434	TRP
1	D	448	GLN
1	D	452	ARG
1	D	472	MET
1	D	475	MET
1	D	478	GLN
1	D	483	LEU
1	D	485	PHE
1	D	486	PHE
1	D	493	ASP
1	D	499	GLU
1	D	500	GLN
1	D	502	GLU
1	D	505	ILE
1	D	511	LEU
1	D	514	TRP
1	D	517	MET
1	D	526	ARG
1	D	529	GLU
1	D	543	ASP
1	D	548	GLN
1	D	549	ARG
1	D	564	GLU
1	D	575	ARG
1	D	582	ARG
1	D	595	LEU
1	D	631	GLU
1	D	648	GLU
1	D	651	GLN
1	D	652	LYS
1	E	20	ARG
1	E	23	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	26	PHE
1	E	37	THR
1	E	84	GLN
1	E	91	LEU
1	E	103	ASP
1	E	105	ARG
1	E	119	GLU
1	E	124	THR
1	E	152	VAL
1	E	169	TYR
1	E	172	GLU
1	E	175	GLN
1	E	178	LEU
1	E	182	PHE
1	E	192	GLU
1	E	194	LEU
1	E	210	THR
1	E	213	PHE
1	E	222	PHE
1	E	223	LEU
1	E	227	GLN
1	E	230	GLN
1	E	236	ARG
1	E	258	SER
1	E	261	TYR
1	E	283	TRP
1	E	284	HIS
1	E	285	PRO
1	E	286	ARG
1	E	294	TYR
1	E	304	ASP
1	E	307	LEU
1	E	309	LEU
1	E	310	LYS
1	E	311	LEU
1	E	319	THR
1	E	334	GLN
1	E	359	LEU
1	E	373	ASP
1	E	385	ASP
1	E	388	PHE
1	E	390	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	404	ARG
1	E	424	PHE
1	E	432	GLN
1	E	434	TRP
1	E	448	GLN
1	E	452	ARG
1	E	472	MET
1	E	475	MET
1	E	478	GLN
1	E	483	LEU
1	E	485	PHE
1	E	486	PHE
1	E	499	GLU
1	E	500	GLN
1	E	503	PHE
1	E	511	LEU
1	E	514	TRP
1	E	517	MET
1	E	526	ARG
1	E	529	GLU
1	E	543	ASP
1	E	548	GLN
1	E	549	ARG
1	E	559	THR
1	E	564	GLU
1	E	575	ARG
1	E	595	LEU
1	E	631	GLU
1	E	648	GLU
1	E	651	GLN
1	E	652	LYS
1	F	16	GLU
1	F	23	THR
1	F	26	PHE
1	F	37	THR
1	F	53	ARG
1	F	81	GLU
1	F	84	GLN
1	F	90	ASP
1	F	91	LEU
1	F	103	ASP
1	F	105	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	119	GLU
1	F	124	THR
1	F	152	VAL
1	F	169	TYR
1	F	182	PHE
1	F	183	VAL
1	F	186	LEU
1	F	192	GLU
1	F	194	LEU
1	F	210	THR
1	F	213	PHE
1	F	219	PHE
1	F	220	ARG
1	F	222	PHE
1	F	226	TRP
1	F	227	GLN
1	F	231	TRP
1	F	236	ARG
1	F	238	LYS
1	F	243	ILE
1	F	247	GLU
1	F	252	THR
1	F	255	PHE
1	F	261	TYR
1	F	283	TRP
1	F	293	THR
1	F	294	TYR
1	F	304	ASP
1	F	307	LEU
1	F	310	LYS
1	F	311	LEU
1	F	319	THR
1	F	323	HIS
1	F	334	GLN
1	F	359	LEU
1	F	362	ILE
1	F	368	THR
1	F	385	ASP
1	F	388	PHE
1	F	390	PHE
1	F	404	ARG
1	F	419	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	421	LEU
1	F	424	PHE
1	F	432	GLN
1	F	434	TRP
1	F	448	GLN
1	F	452	ARG
1	F	472	MET
1	F	475	MET
1	F	478	GLN
1	F	483	LEU
1	F	485	PHE
1	F	486	PHE
1	F	493	ASP
1	F	499	GLU
1	F	500	GLN
1	F	502	GLU
1	F	503	PHE
1	F	507	SER
1	F	511	LEU
1	F	514	TRP
1	F	517	MET
1	F	526	ARG
1	F	527	GLU
1	F	529	GLU
1	F	543	ASP
1	F	548	GLN
1	F	564	GLU
1	F	575	ARG
1	F	580	ASP
1	F	581	GLN
1	F	582	ARG
1	F	595	LEU
1	F	631	GLU
1	F	648	GLU
1	F	651	GLN
1	F	652	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	89	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	113	ASN
1	A	175	GLN
1	A	196	GLN
1	A	225	ASN
1	A	278	GLN
1	A	284	HIS
1	A	297	ASN
1	A	334	GLN
1	A	355	GLN
1	A	369	GLN
1	A	415	GLN
1	A	420	ASN
1	A	432	GLN
1	A	449	GLN
1	A	478	GLN
1	A	500	GLN
1	A	581	GLN
1	A	651	GLN
1	B	40	GLN
1	B	70	HIS
1	B	72	ASN
1	B	89	ASN
1	B	113	ASN
1	B	187	GLN
1	B	196	GLN
1	B	227	GLN
1	B	264	ASN
1	B	308	ASN
1	B	334	GLN
1	B	406	GLN
1	B	415	GLN
1	B	432	GLN
1	B	448	GLN
1	B	449	GLN
1	B	457	ASN
1	B	477	GLN
1	B	478	GLN
1	B	500	GLN
1	B	528	ASN
1	B	556	GLN
1	B	581	GLN
1	B	651	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	40	GLN
1	C	70	HIS
1	C	72	ASN
1	C	84	GLN
1	C	85	ASN
1	C	230	GLN
1	C	237	GLN
1	C	250	ASN
1	C	278	GLN
1	C	297	ASN
1	C	334	GLN
1	C	355	GLN
1	C	420	ASN
1	C	432	GLN
1	C	449	GLN
1	C	457	ASN
1	C	478	GLN
1	C	500	GLN
1	D	40	GLN
1	D	70	HIS
1	D	72	ASN
1	D	84	GLN
1	D	85	ASN
1	D	89	ASN
1	D	137	HIS
1	D	187	GLN
1	D	196	GLN
1	D	225	ASN
1	D	278	GLN
1	D	284	HIS
1	D	334	GLN
1	D	432	GLN
1	D	449	GLN
1	D	457	ASN
1	D	478	GLN
1	D	500	GLN
1	D	588	GLN
1	D	651	GLN
1	E	40	GLN
1	E	89	ASN
1	E	137	HIS
1	E	196	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	278	GLN
1	E	334	GLN
1	E	432	GLN
1	E	449	GLN
1	E	478	GLN
1	E	500	GLN
1	E	528	ASN
1	E	651	GLN
1	F	40	GLN
1	F	70	HIS
1	F	72	ASN
1	F	89	ASN
1	F	187	GLN
1	F	263	ASN
1	F	278	GLN
1	F	297	ASN
1	F	334	GLN
1	F	369	GLN
1	F	415	GLN
1	F	432	GLN
1	F	449	GLN
1	F	457	ASN
1	F	478	GLN
1	F	500	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	624/669 (93%)	0.32	28 (4%)	34	27	56, 129, 201, 287	0
1	B	632/669 (94%)	0.16	17 (2%)	55	44	56, 130, 204, 256	0
1	C	624/669 (93%)	0.11	14 (2%)	62	53	64, 133, 201, 267	0
1	D	624/669 (93%)	0.14	17 (2%)	55	44	62, 132, 201, 286	0
1	E	624/669 (93%)	0.27	30 (4%)	31	24	63, 134, 205, 264	0
1	F	624/669 (93%)	0.25	31 (4%)	30	23	64, 144, 206, 256	0
All	All	3752/4014 (93%)	0.21	137 (3%)	42	33	56, 133, 204, 287	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	510	LEU	9.2
1	A	505	ILE	7.1
1	A	497	TYR	6.2
1	D	665	VAL	6.0
1	A	495	GLU	5.9
1	D	507	SER	5.7
1	A	494	LEU	5.2
1	A	498	SER	5.1
1	A	491	GLN	5.1
1	B	510	LEU	4.7
1	D	550	SER	4.5
1	A	530	VAL	4.4
1	A	650	ARG	4.3
1	B	557	GLY	4.3
1	F	88	PRO	4.1
1	F	650	ARG	4.1
1	F	510	LEU	3.7
1	C	16	GLU	3.7
1	A	487	LYS	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	498	SER	3.7
1	C	510	LEU	3.7
1	F	49	GLU	3.7
1	E	662	CYS	3.6
1	C	655	TRP	3.6
1	E	510	LEU	3.5
1	D	509	LYS	3.3
1	B	553	GLY	3.3
1	C	550	SER	3.3
1	F	489	SER	3.3
1	D	658	LEU	3.2
1	F	89	ASN	3.2
1	B	658	LEU	3.2
1	F	477	GLN	3.2
1	E	516	GLU	3.2
1	F	93	LEU	3.2
1	D	514	TRP	3.1
1	E	232	HIS	3.0
1	D	497	TYR	3.0
1	C	232	HIS	3.0
1	E	514	TRP	3.0
1	F	404	ARG	3.0
1	C	488	THR	3.0
1	B	489	SER	3.0
1	B	554	ARG	3.0
1	C	521	VAL	3.0
1	E	651	GLN	3.0
1	A	492	ILE	3.0
1	E	231	TRP	2.9
1	E	654	LEU	2.9
1	B	551	PRO	2.9
1	F	497	TYR	2.9
1	A	640	GLU	2.9
1	D	479	LEU	2.9
1	D	640	GLU	2.8
1	E	660	ILE	2.8
1	D	662	CYS	2.8
1	F	41	ILE	2.8
1	F	535	GLU	2.8
1	F	31	ARG	2.8
1	E	509	LYS	2.8
1	F	470	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	494	LEU	2.7
1	D	482	LYS	2.7
1	A	407	PRO	2.7
1	F	94	LEU	2.7
1	F	493	ASP	2.7
1	F	215	CYS	2.7
1	D	498	SER	2.7
1	A	510	LEU	2.6
1	F	32	TRP	2.6
1	B	651	GLN	2.6
1	F	46	CYS	2.6
1	F	40	GLN	2.6
1	F	584	GLU	2.6
1	C	93	LEU	2.5
1	E	664	LYS	2.5
1	E	499	GLU	2.5
1	C	658	LEU	2.5
1	A	653	GLU	2.5
1	E	658	LEU	2.5
1	F	348	GLU	2.4
1	B	406	GLN	2.4
1	E	492	ILE	2.4
1	D	663	SER	2.4
1	B	49	GLU	2.4
1	A	296	PRO	2.4
1	F	560	LEU	2.4
1	A	483	LEU	2.4
1	E	661	ALA	2.4
1	B	407	PRO	2.4
1	E	497	TYR	2.4
1	A	499	GLU	2.3
1	F	351	GLN	2.3
1	F	514	TRP	2.3
1	E	118	ARG	2.3
1	E	408	GLU	2.3
1	A	94	LEU	2.3
1	E	640	GLU	2.3
1	B	32	TRP	2.3
1	C	94	LEU	2.3
1	F	43	ILE	2.3
1	E	632	VAL	2.3
1	E	406	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	550	SER	2.3
1	E	521	VAL	2.3
1	A	118	ARG	2.2
1	D	90	ASP	2.2
1	C	455	MET	2.2
1	E	407	PRO	2.2
1	E	489	SER	2.2
1	F	655	TRP	2.2
1	A	512	LEU	2.2
1	E	512	LEU	2.2
1	D	499	GLU	2.2
1	E	663	SER	2.2
1	B	405	PRO	2.2
1	D	495	GLU	2.2
1	A	642	THR	2.2
1	A	508	ASP	2.2
1	F	646	LEU	2.2
1	A	480	LYS	2.1
1	A	526	ARG	2.1
1	F	629	VAL	2.1
1	A	501	THR	2.1
1	E	524	CYS	2.1
1	B	41	ILE	2.1
1	A	651	GLN	2.1
1	F	145	ASP	2.1
1	C	61	GLU	2.1
1	A	582	ARG	2.1
1	C	506	THR	2.1
1	B	40	GLN	2.1
1	A	484	ASP	2.0
1	B	654	LEU	2.0
1	F	657	LEU	2.0
1	C	493	ASP	2.0
1	E	657	LEU	2.0

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

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.