



Full wwPDB X-ray Structure Validation Report i

Jul 16, 2023 – 08:25 PM EDT

PDB ID : 3QA8
Title : Crystal Structure of inhibitor of kappa B kinase beta
Authors : Xu, G.; Lo, Y.C.; Li, Q.; Napolitano, G.; Wu, X.; Jiang, X.; Dreano, M.; Karin, M.; Wu, H.
Deposited on : 2011-01-10
Resolution : 3.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the i symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.34
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

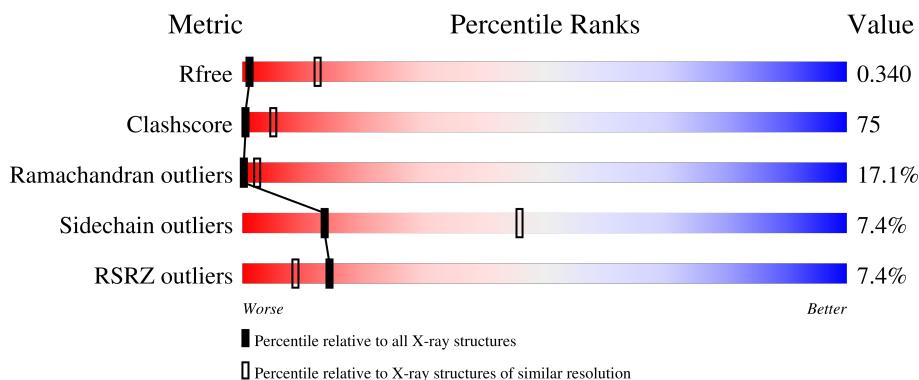
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



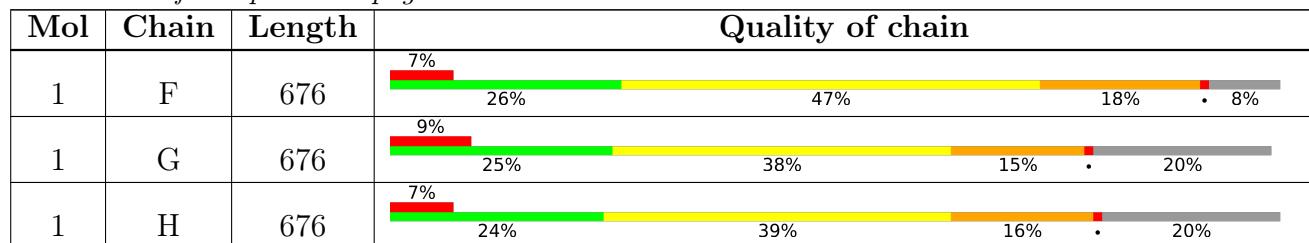
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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



Continued on next page...

Continued from previous page...



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 39026 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 MGC80376 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	622	Total	C	N	O	S	0	0	0
			5048	3189	899	929	31			
1	B	622	Total	C	N	O	S	0	0	0
			5048	3189	899	929	31			
1	C	622	Total	C	N	O	S	0	0	0
			5048	3189	899	929	31			
1	D	622	Total	C	N	O	S	0	0	0
			5048	3189	899	929	31			
1	E	622	Total	C	N	O	S	0	0	0
			5048	3189	899	929	31			
1	F	622	Total	C	N	O	S	0	0	0
			5048	3189	899	929	31			
1	G	541	Total	C	N	O	S	0	0	0
			4369	2764	779	800	26			
1	H	541	Total	C	N	O	S	0	0	0
			4369	2764	779	800	26			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q6INT1
A	1	GLY	-	expression tag	UNP Q6INT1
A	2	GLY	-	expression tag	UNP Q6INT1
A	3	ARG	-	expression tag	UNP Q6INT1
A	4	SER	-	expression tag	UNP Q6INT1
A	5	PRO	-	expression tag	UNP Q6INT1
A	6	SER	-	expression tag	UNP Q6INT1
A	7	LEU	-	expression tag	UNP Q6INT1
A	8	PRO	-	expression tag	UNP Q6INT1
A	9	THR	-	expression tag	UNP Q6INT1
A	10	GLN	-	expression tag	UNP Q6INT1
A	11	THR	-	expression tag	UNP Q6INT1
A	12	CYS	-	expression tag	UNP Q6INT1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	expression tag	UNP Q6INT1
A	14	PRO	-	expression tag	UNP Q6INT1
A	15	TRP	-	expression tag	UNP Q6INT1
A	16	GLU	-	expression tag	UNP Q6INT1
A	177	GLU	SER	engineered mutation	UNP Q6INT1
A	181	GLU	SER	engineered mutation	UNP Q6INT1
B	0	GLY	-	expression tag	UNP Q6INT1
B	1	GLY	-	expression tag	UNP Q6INT1
B	2	GLY	-	expression tag	UNP Q6INT1
B	3	ARG	-	expression tag	UNP Q6INT1
B	4	SER	-	expression tag	UNP Q6INT1
B	5	PRO	-	expression tag	UNP Q6INT1
B	6	SER	-	expression tag	UNP Q6INT1
B	7	LEU	-	expression tag	UNP Q6INT1
B	8	PRO	-	expression tag	UNP Q6INT1
B	9	THR	-	expression tag	UNP Q6INT1
B	10	GLN	-	expression tag	UNP Q6INT1
B	11	THR	-	expression tag	UNP Q6INT1
B	12	CYS	-	expression tag	UNP Q6INT1
B	13	GLY	-	expression tag	UNP Q6INT1
B	14	PRO	-	expression tag	UNP Q6INT1
B	15	TRP	-	expression tag	UNP Q6INT1
B	16	GLU	-	expression tag	UNP Q6INT1
B	177	GLU	SER	engineered mutation	UNP Q6INT1
B	181	GLU	SER	engineered mutation	UNP Q6INT1
C	0	GLY	-	expression tag	UNP Q6INT1
C	1	GLY	-	expression tag	UNP Q6INT1
C	2	GLY	-	expression tag	UNP Q6INT1
C	3	ARG	-	expression tag	UNP Q6INT1
C	4	SER	-	expression tag	UNP Q6INT1
C	5	PRO	-	expression tag	UNP Q6INT1
C	6	SER	-	expression tag	UNP Q6INT1
C	7	LEU	-	expression tag	UNP Q6INT1
C	8	PRO	-	expression tag	UNP Q6INT1
C	9	THR	-	expression tag	UNP Q6INT1
C	10	GLN	-	expression tag	UNP Q6INT1
C	11	THR	-	expression tag	UNP Q6INT1
C	12	CYS	-	expression tag	UNP Q6INT1
C	13	GLY	-	expression tag	UNP Q6INT1
C	14	PRO	-	expression tag	UNP Q6INT1
C	15	TRP	-	expression tag	UNP Q6INT1
C	16	GLU	-	expression tag	UNP Q6INT1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	177	GLU	SER	engineered mutation	UNP Q6INT1
C	181	GLU	SER	engineered mutation	UNP Q6INT1
D	0	GLY	-	expression tag	UNP Q6INT1
D	1	GLY	-	expression tag	UNP Q6INT1
D	2	GLY	-	expression tag	UNP Q6INT1
D	3	ARG	-	expression tag	UNP Q6INT1
D	4	SER	-	expression tag	UNP Q6INT1
D	5	PRO	-	expression tag	UNP Q6INT1
D	6	SER	-	expression tag	UNP Q6INT1
D	7	LEU	-	expression tag	UNP Q6INT1
D	8	PRO	-	expression tag	UNP Q6INT1
D	9	THR	-	expression tag	UNP Q6INT1
D	10	GLN	-	expression tag	UNP Q6INT1
D	11	THR	-	expression tag	UNP Q6INT1
D	12	CYS	-	expression tag	UNP Q6INT1
D	13	GLY	-	expression tag	UNP Q6INT1
D	14	PRO	-	expression tag	UNP Q6INT1
D	15	TRP	-	expression tag	UNP Q6INT1
D	16	GLU	-	expression tag	UNP Q6INT1
D	177	GLU	SER	engineered mutation	UNP Q6INT1
D	181	GLU	SER	engineered mutation	UNP Q6INT1
E	0	GLY	-	expression tag	UNP Q6INT1
E	1	GLY	-	expression tag	UNP Q6INT1
E	2	GLY	-	expression tag	UNP Q6INT1
E	3	ARG	-	expression tag	UNP Q6INT1
E	4	SER	-	expression tag	UNP Q6INT1
E	5	PRO	-	expression tag	UNP Q6INT1
E	6	SER	-	expression tag	UNP Q6INT1
E	7	LEU	-	expression tag	UNP Q6INT1
E	8	PRO	-	expression tag	UNP Q6INT1
E	9	THR	-	expression tag	UNP Q6INT1
E	10	GLN	-	expression tag	UNP Q6INT1
E	11	THR	-	expression tag	UNP Q6INT1
E	12	CYS	-	expression tag	UNP Q6INT1
E	13	GLY	-	expression tag	UNP Q6INT1
E	14	PRO	-	expression tag	UNP Q6INT1
E	15	TRP	-	expression tag	UNP Q6INT1
E	16	GLU	-	expression tag	UNP Q6INT1
E	177	GLU	SER	engineered mutation	UNP Q6INT1
E	181	GLU	SER	engineered mutation	UNP Q6INT1
F	0	GLY	-	expression tag	UNP Q6INT1
F	1	GLY	-	expression tag	UNP Q6INT1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	2	GLY	-	expression tag	UNP Q6INT1
F	3	ARG	-	expression tag	UNP Q6INT1
F	4	SER	-	expression tag	UNP Q6INT1
F	5	PRO	-	expression tag	UNP Q6INT1
F	6	SER	-	expression tag	UNP Q6INT1
F	7	LEU	-	expression tag	UNP Q6INT1
F	8	PRO	-	expression tag	UNP Q6INT1
F	9	THR	-	expression tag	UNP Q6INT1
F	10	GLN	-	expression tag	UNP Q6INT1
F	11	THR	-	expression tag	UNP Q6INT1
F	12	CYS	-	expression tag	UNP Q6INT1
F	13	GLY	-	expression tag	UNP Q6INT1
F	14	PRO	-	expression tag	UNP Q6INT1
F	15	TRP	-	expression tag	UNP Q6INT1
F	16	GLU	-	expression tag	UNP Q6INT1
F	177	GLU	SER	engineered mutation	UNP Q6INT1
F	181	GLU	SER	engineered mutation	UNP Q6INT1
G	0	GLY	-	expression tag	UNP Q6INT1
G	1	GLY	-	expression tag	UNP Q6INT1
G	2	GLY	-	expression tag	UNP Q6INT1
G	3	ARG	-	expression tag	UNP Q6INT1
G	4	SER	-	expression tag	UNP Q6INT1
G	5	PRO	-	expression tag	UNP Q6INT1
G	6	SER	-	expression tag	UNP Q6INT1
G	7	LEU	-	expression tag	UNP Q6INT1
G	8	PRO	-	expression tag	UNP Q6INT1
G	9	THR	-	expression tag	UNP Q6INT1
G	10	GLN	-	expression tag	UNP Q6INT1
G	11	THR	-	expression tag	UNP Q6INT1
G	12	CYS	-	expression tag	UNP Q6INT1
G	13	GLY	-	expression tag	UNP Q6INT1
G	14	PRO	-	expression tag	UNP Q6INT1
G	15	TRP	-	expression tag	UNP Q6INT1
G	16	GLU	-	expression tag	UNP Q6INT1
G	177	GLU	SER	engineered mutation	UNP Q6INT1
G	181	GLU	SER	engineered mutation	UNP Q6INT1
H	0	GLY	-	expression tag	UNP Q6INT1
H	1	GLY	-	expression tag	UNP Q6INT1
H	2	GLY	-	expression tag	UNP Q6INT1
H	3	ARG	-	expression tag	UNP Q6INT1
H	4	SER	-	expression tag	UNP Q6INT1
H	5	PRO	-	expression tag	UNP Q6INT1

Continued on next page...

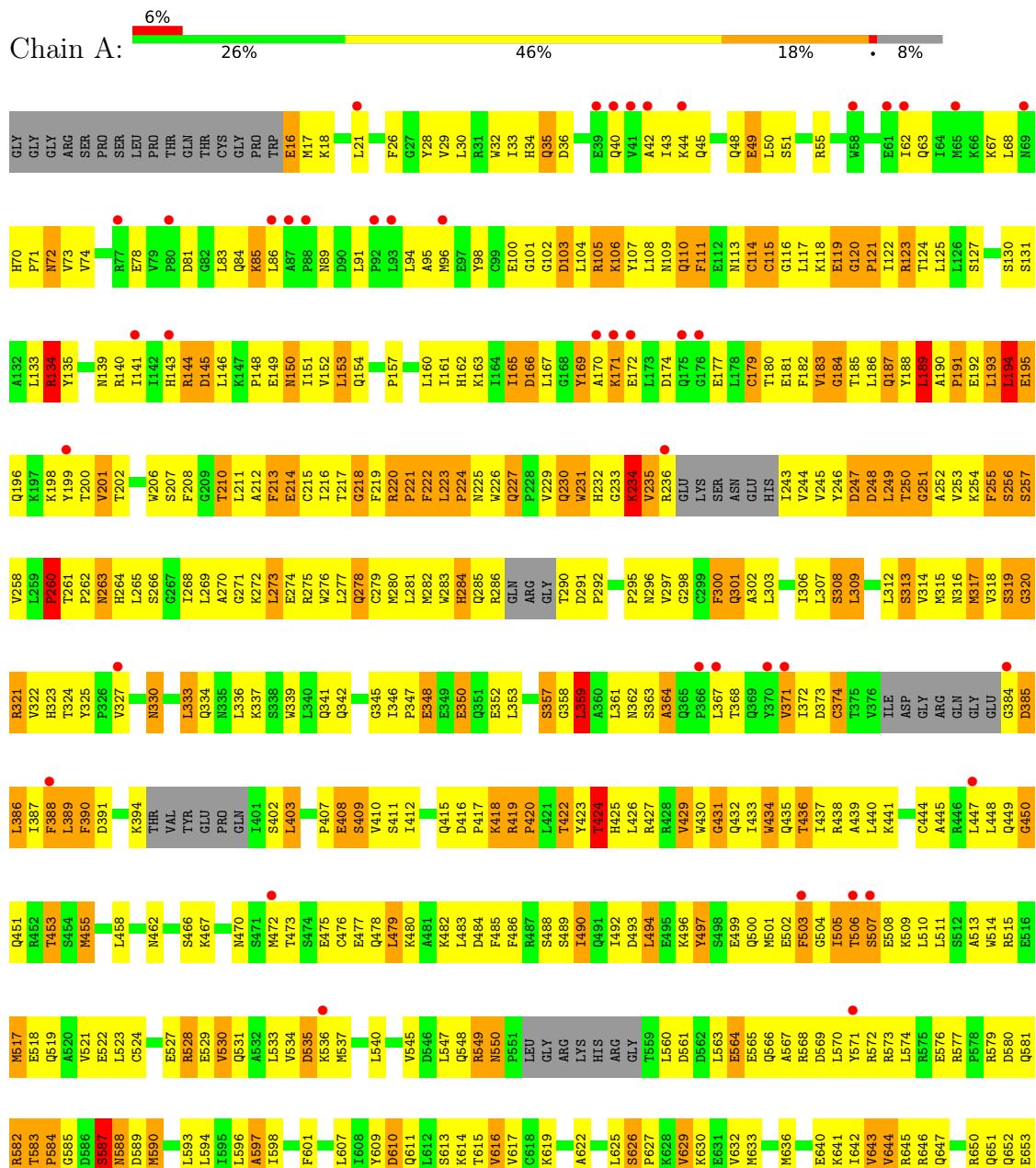
Continued from previous page...

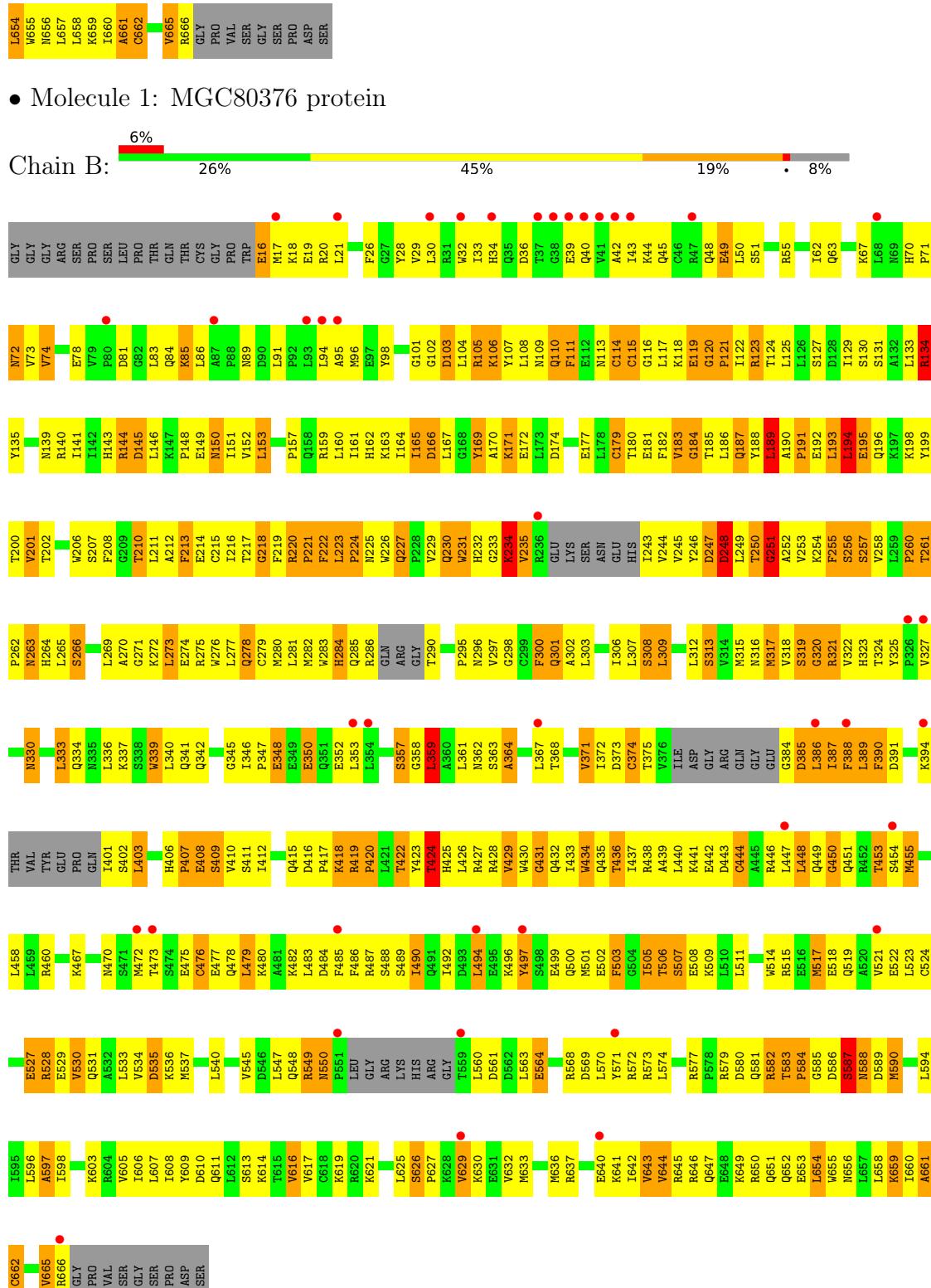
Chain	Residue	Modelled	Actual	Comment	Reference
H	6	SER	-	expression tag	UNP Q6INT1
H	7	LEU	-	expression tag	UNP Q6INT1
H	8	PRO	-	expression tag	UNP Q6INT1
H	9	THR	-	expression tag	UNP Q6INT1
H	10	GLN	-	expression tag	UNP Q6INT1
H	11	THR	-	expression tag	UNP Q6INT1
H	12	CYS	-	expression tag	UNP Q6INT1
H	13	GLY	-	expression tag	UNP Q6INT1
H	14	PRO	-	expression tag	UNP Q6INT1
H	15	TRP	-	expression tag	UNP Q6INT1
H	16	GLU	-	expression tag	UNP Q6INT1
H	177	GLU	SER	engineered mutation	UNP Q6INT1
H	181	GLU	SER	engineered mutation	UNP Q6INT1

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

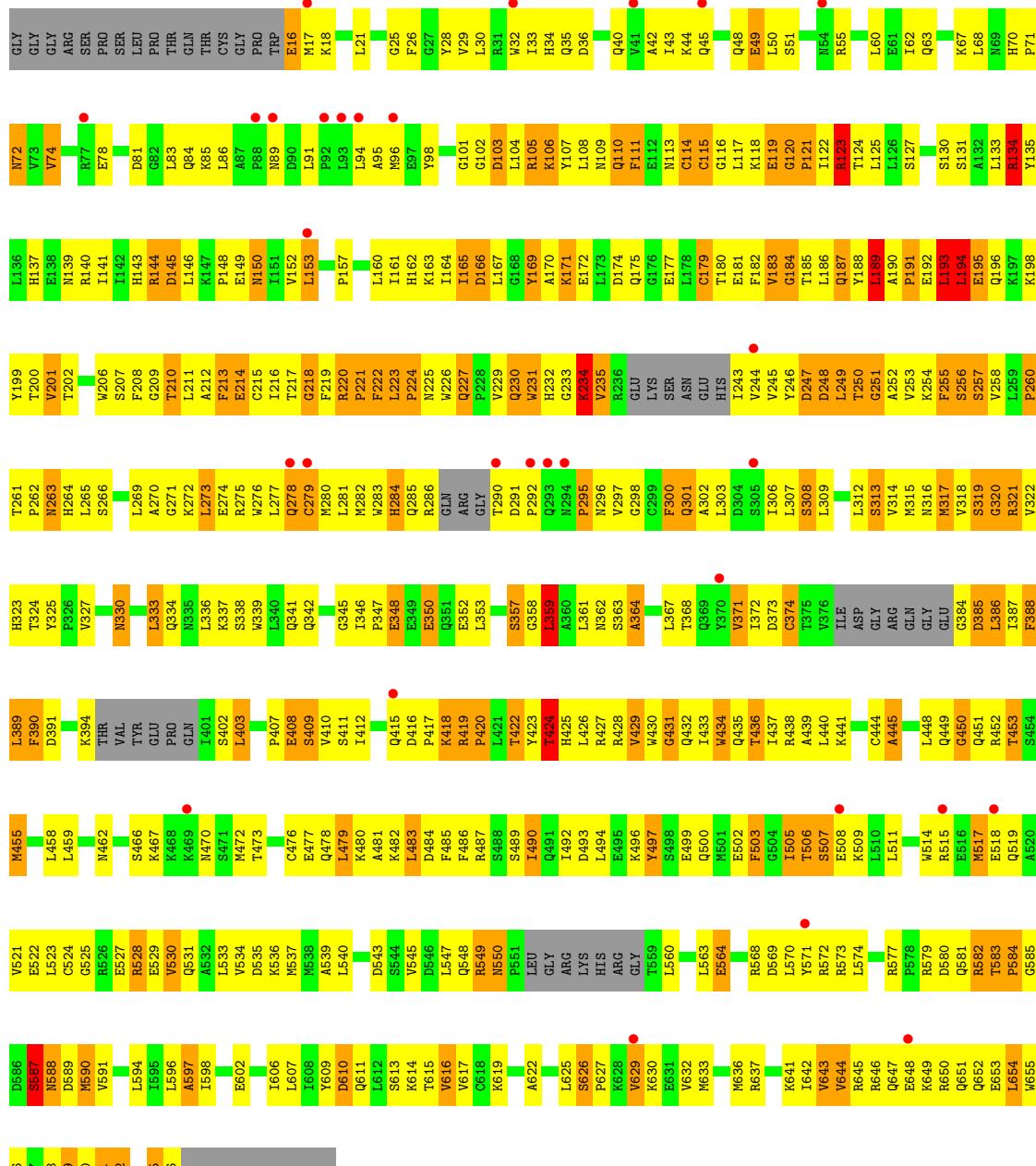
- Molecule 1: MG C80376 protein





- Molecule 1: MGCG80376 protein

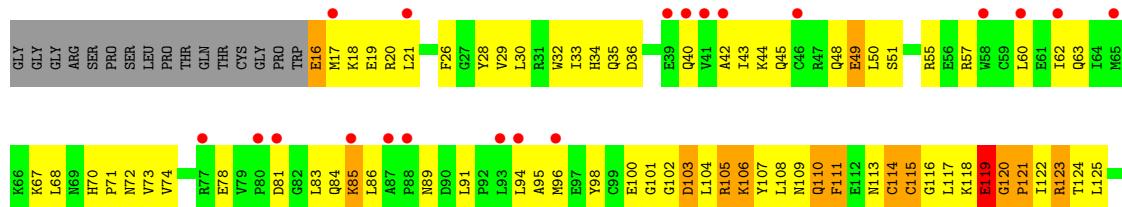


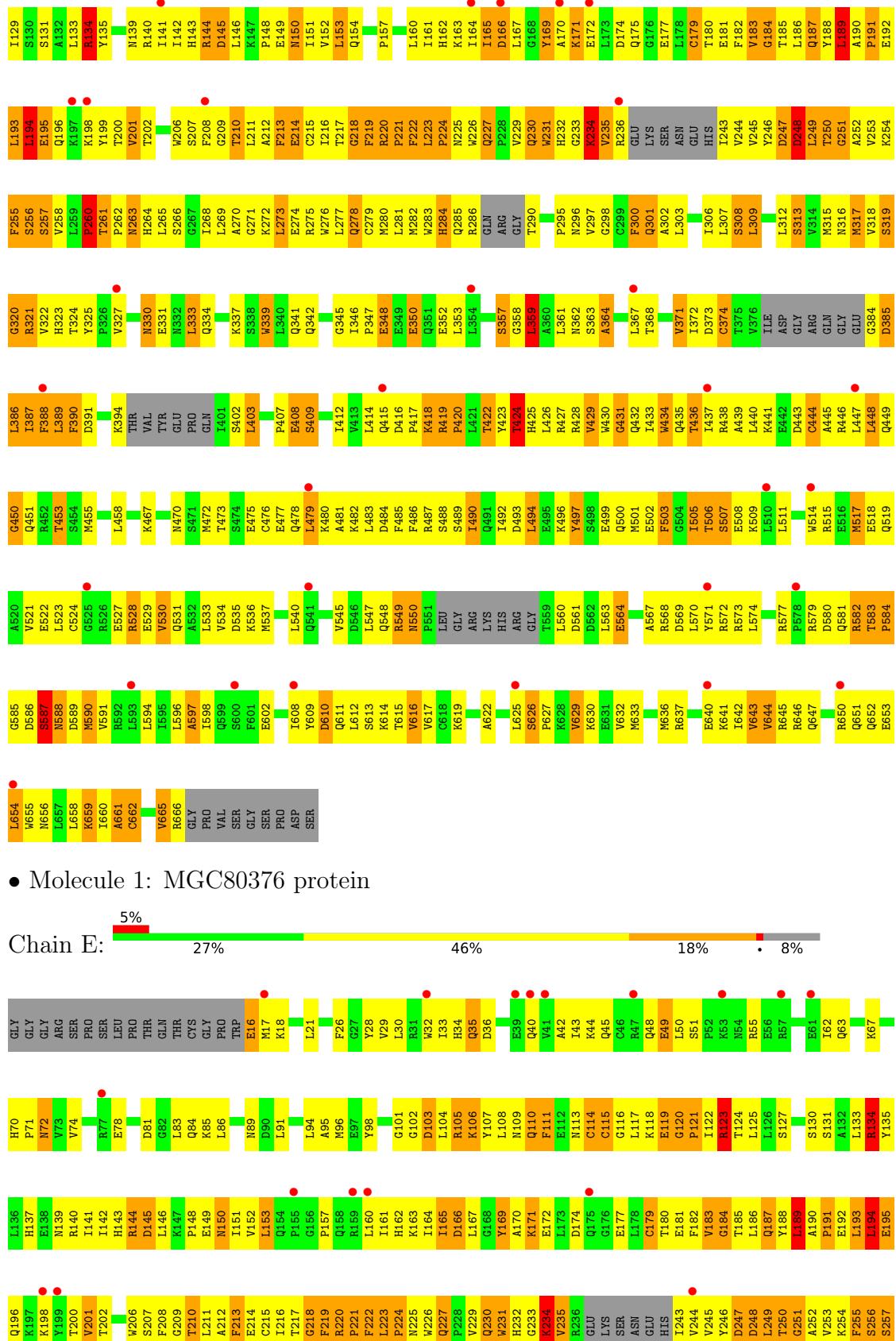


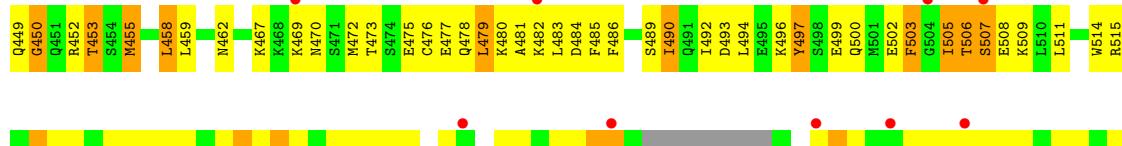
- Molecule 1: MGC80376 protein

Chain D:

Category	Percentage
Red	7%
Green	26%
Yellow	46%
Orange	18%
Black	8%

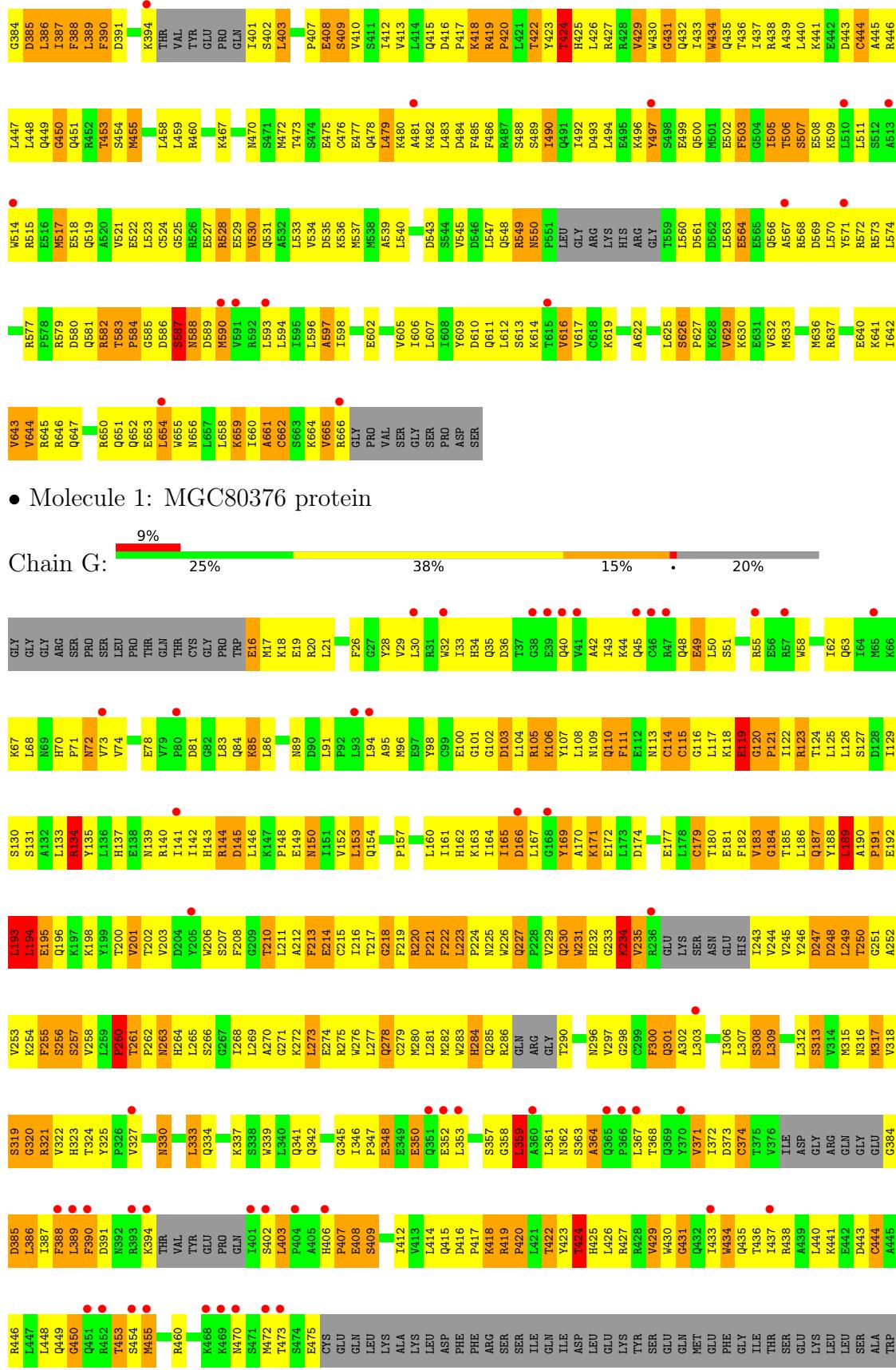






- Molecule 1: MGC80376 protein







4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	103.17Å 140.34Å 161.17Å 71.28° 79.56° 86.04°	Depositor
Resolution (Å)	15.00 – 3.60 48.67 – 3.50	Depositor EDS
% Data completeness (in resolution range)	78.7 (15.00-3.60) 76.9 (48.67-3.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle^1$	1.18 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R , R_{free}	0.308 , 0.344 0.302 , 0.340	Depositor DCC
R_{free} test set	4846 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	84.5	Xtriage
Anisotropy	0.749	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 118.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	39026	wwPDB-VP
Average B, all atoms (Å ²)	199.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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 i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.74	0/5136	0.97	9/6931 (0.1%)
1	B	0.76	0/5136	0.97	10/6931 (0.1%)
1	C	0.78	1/5136 (0.0%)	0.98	11/6931 (0.2%)
1	D	0.74	2/5136 (0.0%)	0.96	10/6931 (0.1%)
1	E	0.77	1/5136 (0.0%)	0.98	10/6931 (0.1%)
1	F	0.75	0/5136	0.96	10/6931 (0.1%)
1	G	0.74	1/4448 (0.0%)	0.96	7/6012 (0.1%)
1	H	0.75	0/4448	0.97	8/6012 (0.1%)
All	All	0.75	5/39712 (0.0%)	0.97	75/53610 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
1	B	0	11
1	C	0	10
1	D	0	11
1	E	0	10
1	F	0	11
1	G	0	11
1	H	0	11
All	All	0	86

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	279	CYS	CB-SG	-6.95	1.70	1.82
1	C	279	CYS	CB-SG	-5.47	1.73	1.81
1	G	119	GLU	CG-CD	5.22	1.59	1.51
1	D	119	GLU	CG-CD	5.14	1.59	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	331	GLU	CG-CD	5.14	1.59	1.51

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	123	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	E	153	LEU	CA-CB-CG	6.42	130.08	115.30
1	A	153	LEU	CA-CB-CG	6.28	129.73	115.30
1	C	153	LEU	CA-CB-CG	6.27	129.72	115.30
1	D	153	LEU	CA-CB-CG	6.27	129.71	115.30
1	B	153	LEU	CA-CB-CG	6.23	129.62	115.30
1	F	153	LEU	CA-CB-CG	6.15	129.44	115.30
1	G	153	LEU	CA-CB-CG	6.15	129.44	115.30
1	D	189	LEU	CA-CB-CG	-6.14	101.17	115.30
1	H	193	LEU	N-CA-C	-6.13	94.44	111.00
1	C	189	LEU	CA-CB-CG	-6.06	101.36	115.30
1	A	193	LEU	N-CA-C	-6.00	94.81	111.00
1	G	193	LEU	N-CA-C	-6.00	94.81	111.00
1	H	153	LEU	CA-CB-CG	5.99	129.07	115.30
1	D	193	LEU	N-CA-C	-5.97	94.88	111.00
1	E	193	LEU	N-CA-C	-5.94	94.96	111.00
1	C	256	SER	N-CA-C	5.94	127.03	111.00
1	C	193	LEU	N-CA-C	-5.94	94.97	111.00
1	B	193	LEU	N-CA-C	-5.93	94.98	111.00
1	A	189	LEU	CA-CB-CG	-5.88	101.77	115.30
1	F	193	LEU	N-CA-C	-5.86	95.17	111.00
1	E	256	SER	N-CA-C	5.86	126.82	111.00
1	G	194	LEU	CA-CB-CG	5.84	128.74	115.30
1	H	256	SER	N-CA-C	5.81	126.68	111.00
1	A	194	LEU	CA-CB-CG	5.78	128.60	115.30
1	D	256	SER	N-CA-C	5.75	126.54	111.00
1	C	249	LEU	CA-CB-CG	5.75	128.52	115.30
1	E	189	LEU	CA-CB-CG	-5.75	102.08	115.30
1	F	194	LEU	CA-CB-CG	5.70	128.40	115.30
1	H	194	LEU	CA-CB-CG	5.70	128.40	115.30
1	D	194	LEU	CA-CB-CG	5.69	128.39	115.30
1	C	194	LEU	CA-CB-CG	5.67	128.34	115.30
1	G	189	LEU	CA-CB-CG	-5.67	102.26	115.30
1	E	194	LEU	CA-CB-CG	5.66	128.32	115.30
1	B	189	LEU	CA-CB-CG	-5.64	102.32	115.30
1	C	123	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	256	SER	N-CA-C	5.64	126.23	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	LEU	CA-CB-CG	5.61	128.20	115.30
1	C	359	LEU	CA-CB-CG	5.61	128.20	115.30
1	G	256	SER	N-CA-C	5.60	126.12	111.00
1	B	359	LEU	CA-CB-CG	5.60	128.18	115.30
1	G	359	LEU	CA-CB-CG	5.58	128.14	115.30
1	A	256	SER	N-CA-C	5.57	126.05	111.00
1	F	256	SER	N-CA-C	5.56	126.02	111.00
1	H	359	LEU	CA-CB-CG	5.55	128.06	115.30
1	E	359	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	458	LEU	CA-CB-CG	5.52	127.99	115.30
1	F	458	LEU	CA-CB-CG	5.46	127.87	115.30
1	H	189	LEU	CA-CB-CG	-5.46	102.74	115.30
1	F	189	LEU	CA-CB-CG	-5.42	102.83	115.30
1	C	445	ALA	O-C-N	-5.42	114.04	122.70
1	C	458	LEU	CA-CB-CG	5.40	127.71	115.30
1	D	458	LEU	CA-CB-CG	5.39	127.69	115.30
1	E	458	LEU	CA-CB-CG	5.38	127.68	115.30
1	F	359	LEU	CA-CB-CG	5.36	127.64	115.30
1	D	248	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	458	LEU	CA-CB-CG	5.34	127.59	115.30
1	H	458	LEU	CA-CB-CG	5.28	127.45	115.30
1	E	224	PRO	N-CA-C	-5.28	98.39	112.10
1	F	249	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	248	ASP	CB-CG-OD1	5.26	123.03	118.30
1	F	105	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	E	249	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	359	LEU	CA-CB-CG	5.23	127.32	115.30
1	D	359	LEU	CA-CB-CG	5.21	127.29	115.30
1	B	224	PRO	N-CA-C	-5.21	98.55	112.10
1	A	249	LEU	CA-CB-CG	5.20	127.26	115.30
1	A	224	PRO	N-CA-C	-5.19	98.61	112.10
1	C	224	PRO	N-CA-C	-5.16	98.68	112.10
1	G	249	LEU	CA-CB-CG	5.16	127.16	115.30
1	D	249	LEU	CA-CB-CG	5.13	127.10	115.30
1	H	224	PRO	N-CA-C	-5.10	98.85	112.10
1	B	251	GLY	N-CA-C	-5.07	100.42	113.10
1	F	248	ASP	CB-CG-OD1	5.07	122.86	118.30
1	D	224	PRO	N-CA-C	-5.05	98.98	112.10

There are no chirality outliers.

All (86) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	GLU	Peptide
1	A	120	GLY	Peptide
1	A	169	TYR	Peptide
1	A	221	PRO	Peptide
1	A	223	LEU	Peptide
1	A	247	ASP	Peptide
1	A	255	PHE	Peptide
1	A	257	SER	Peptide
1	A	260	PRO	Peptide
1	A	389	LEU	Peptide
1	A	587	SER	Peptide
1	B	119	GLU	Peptide
1	B	120	GLY	Peptide
1	B	169	TYR	Peptide
1	B	221	PRO	Peptide
1	B	223	LEU	Peptide
1	B	247	ASP	Peptide
1	B	255	PHE	Peptide
1	B	257	SER	Peptide
1	B	389	LEU	Peptide
1	B	527	GLU	Mainchain
1	B	587	SER	Peptide
1	C	119	GLU	Peptide
1	C	120	GLY	Peptide
1	C	169	TYR	Peptide
1	C	221	PRO	Peptide
1	C	223	LEU	Peptide
1	C	247	ASP	Peptide
1	C	255	PHE	Peptide
1	C	257	SER	Peptide
1	C	389	LEU	Peptide
1	C	587	SER	Peptide
1	D	119	GLU	Peptide
1	D	120	GLY	Peptide
1	D	169	TYR	Peptide
1	D	221	PRO	Peptide
1	D	223	LEU	Peptide
1	D	247	ASP	Peptide
1	D	255	PHE	Peptide
1	D	257	SER	Peptide
1	D	260	PRO	Peptide
1	D	389	LEU	Peptide
1	D	587	SER	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	E	119	GLU	Peptide
1	E	120	GLY	Peptide
1	E	169	TYR	Peptide
1	E	221	PRO	Peptide
1	E	223	LEU	Peptide
1	E	247	ASP	Peptide
1	E	255	PHE	Peptide
1	E	257	SER	Peptide
1	E	389	LEU	Peptide
1	E	587	SER	Peptide
1	F	119	GLU	Peptide
1	F	120	GLY	Peptide
1	F	169	TYR	Peptide
1	F	221	PRO	Peptide
1	F	223	LEU	Peptide
1	F	247	ASP	Peptide
1	F	255	PHE	Peptide
1	F	257	SER	Peptide
1	F	260	PRO	Peptide
1	F	389	LEU	Peptide
1	F	587	SER	Peptide
1	G	119	GLU	Peptide
1	G	120	GLY	Peptide
1	G	169	TYR	Peptide
1	G	221	PRO	Peptide
1	G	223	LEU	Peptide
1	G	247	ASP	Peptide
1	G	255	PHE	Peptide
1	G	257	SER	Peptide
1	G	260	PRO	Peptide
1	G	389	LEU	Peptide
1	G	587	SER	Peptide
1	H	119	GLU	Peptide
1	H	120	GLY	Peptide
1	H	169	TYR	Peptide
1	H	221	PRO	Peptide
1	H	223	LEU	Peptide
1	H	247	ASP	Peptide
1	H	255	PHE	Peptide
1	H	257	SER	Peptide
1	H	260	PRO	Peptide
1	H	389	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	H	587	SER	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5048	0	5120	770	3
1	B	5048	0	5120	807	2
1	C	5048	0	5120	837	4
1	D	5048	0	5120	861	0
1	E	5048	0	5120	820	2
1	F	5048	0	5120	801	0
1	G	4369	0	4430	607	0
1	H	4369	0	4430	616	1
All	All	39026	0	39580	5868	6

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 75.

All (5868) 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:E:547:LEU:CD1	1:E:615:THR:HG22	1.18	1.61
1:E:547:LEU:HD13	1:E:615:THR:CG2	1.16	1.54
1:C:496:LYS:CB	1:D:655:TRP:HE1	1.25	1.48
1:A:524:CYS:SG	1:A:643:VAL:HG11	1.55	1.46
1:C:496:LYS:HB2	1:D:655:TRP:NE1	1.23	1.43
1:C:573:ARG:HH12	1:D:573:ARG:NH2	1.26	1.33
1:C:573:ARG:NH1	1:D:573:ARG:HH22	1.25	1.33
1:D:434:TRP:CZ3	1:D:568:ARG:HA	1.63	1.32
1:E:655:TRP:NE1	1:F:496:LYS:HB2	1.48	1.29
1:B:434:TRP:CZ3	1:B:568:ARG:HA	1.67	1.29
1:A:230:GLN:O	1:A:232:HIS:N	1.66	1.28
1:H:434:TRP:CE3	1:H:568:ARG:HA	1.66	1.28
1:D:230:GLN:O	1:D:232:HIS:N	1.67	1.27
1:C:654:LEU:CD2	1:D:654:LEU:HD21	1.63	1.26

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:230:GLN:O	1:G:232:HIS:N	1.68	1.26
1:B:230:GLN:O	1:B:232:HIS:N	1.67	1.26
1:G:475:GLU:HG2	1:G:636:MET:CE	1.67	1.25
1:C:230:GLN:O	1:C:232:HIS:N	1.68	1.25
1:D:187:GLN:HB3	1:D:223:LEU:CD2	1.66	1.24
1:E:496:LYS:HB2	1:F:655:TRP:NE1	1.52	1.24
1:F:230:GLN:O	1:F:232:HIS:N	1.69	1.23
1:E:230:GLN:O	1:E:232:HIS:N	1.70	1.23
1:B:434:TRP:CE3	1:B:568:ARG:HA	1.73	1.22
1:D:434:TRP:CE3	1:D:568:ARG:HA	1.74	1.22
1:E:547:LEU:CD1	1:E:615:THR:CG2	1.86	1.22
1:A:654:LEU:HD21	1:B:654:LEU:CD2	1.68	1.21
1:A:655:TRP:CE3	1:B:654:LEU:HD11	1.74	1.21
1:H:230:GLN:O	1:H:232:HIS:N	1.69	1.21
1:E:246:TYR:HD1	1:E:258:VAL:HB	1.05	1.20
1:E:654:LEU:HD11	1:F:655:TRP:CE3	1.77	1.20
1:A:486:PHE:HZ	1:A:517:MET:HE2	1.03	1.20
1:A:517:MET:SD	1:A:650:ARG:HG3	1.82	1.19
1:G:434:TRP:CE3	1:G:568:ARG:HA	1.78	1.19
1:A:434:TRP:CE3	1:A:568:ARG:HA	1.76	1.19
1:C:654:LEU:HD21	1:D:654:LEU:CD2	1.73	1.18
1:B:187:GLN:HB3	1:B:223:LEU:HD21	1.24	1.18
1:H:246:TYR:CD1	1:H:258:VAL:HB	1.79	1.18
1:B:246:TYR:CD1	1:B:258:VAL:HB	1.79	1.17
1:F:570:LEU:HB3	1:F:590:MET:HE3	1.25	1.17
1:H:185:THR:HG23	1:H:187:GLN:HG3	1.18	1.17
1:E:496:LYS:CB	1:F:655:TRP:HE1	1.56	1.17
1:A:187:GLN:HB3	1:A:223:LEU:HD21	1.25	1.17
1:A:496:LYS:HB2	1:B:655:TRP:NE1	1.60	1.17
1:C:536:LYS:HB3	1:C:625:LEU:HD13	1.21	1.17
1:C:655:TRP:NE1	1:D:496:LYS:HB2	1.56	1.17
1:D:246:TYR:CD1	1:D:258:VAL:HB	1.79	1.17
1:G:475:GLU:HG2	1:G:636:MET:HE1	1.21	1.17
1:A:246:TYR:CD1	1:A:258:VAL:HB	1.79	1.17
1:B:219:PHE:O	1:B:220:ARG:HG2	1.44	1.17
1:F:219:PHE:O	1:F:220:ARG:HG2	1.45	1.17
1:A:655:TRP:HE1	1:B:496:LYS:HB2	1.10	1.16
1:A:185:THR:HG23	1:A:187:GLN:HG3	1.20	1.16
1:C:246:TYR:CD1	1:C:258:VAL:HB	1.80	1.16
1:E:655:TRP:HE1	1:F:496:LYS:CB	1.57	1.16
1:G:246:TYR:CD1	1:G:258:VAL:HB	1.80	1.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:246:TYR:CD1	1:F:258:VAL:HB	1.80	1.16
1:G:111:PHE:HZ	1:G:572:ARG:HG3	1.00	1.16
1:G:246:TYR:HD1	1:G:258:VAL:HB	1.03	1.16
1:C:246:TYR:HD1	1:C:258:VAL:HB	1.03	1.15
1:E:246:TYR:CD1	1:E:258:VAL:HB	1.80	1.15
1:F:185:THR:HG23	1:F:187:GLN:HG3	1.15	1.15
1:E:118:LYS:HG2	1:E:264:HIS:O	1.46	1.15
1:E:540:LEU:CD1	1:E:622:ALA:HB2	1.77	1.15
1:C:118:LYS:HG2	1:C:264:HIS:O	1.47	1.14
1:C:422:THR:HB	1:C:585:GLY:CA	1.77	1.14
1:C:219:PHE:O	1:C:220:ARG:HG2	1.42	1.14
1:E:187:GLN:HB3	1:E:223:LEU:HD21	1.15	1.14
1:H:563:LEU:HD21	1:H:596:LEU:HB2	1.21	1.14
1:B:479:LEU:HB3	1:B:640:GLU:OE2	1.48	1.14
1:D:219:PHE:O	1:D:220:ARG:HG2	1.47	1.14
1:B:547:LEU:CD1	1:B:614:LYS:HB3	1.75	1.14
1:E:219:PHE:O	1:E:220:ARG:HG2	1.45	1.14
1:C:547:LEU:CD1	1:C:615:THR:HG22	1.78	1.14
1:G:111:PHE:CZ	1:G:572:ARG:HG3	1.81	1.14
1:F:189:LEU:HG	1:F:190:ALA:H	1.10	1.13
1:H:187:GLN:HB3	1:H:223:LEU:HD21	1.26	1.13
1:A:547:LEU:CD1	1:A:615:THR:HG22	1.78	1.13
1:B:527:GLU:O	1:B:529:GLU:N	1.82	1.13
1:C:179:CYS:CB	1:C:181:GLU:HG2	1.77	1.13
1:C:187:GLN:HB3	1:C:223:LEU:HD21	1.25	1.13
1:B:434:TRP:HB3	1:B:571:TYR:CD1	1.84	1.13
1:C:646:ARG:HG3	1:C:647:GLN:NE2	1.64	1.12
1:D:185:THR:HG23	1:D:187:GLN:HG3	1.13	1.12
1:D:246:TYR:HD1	1:D:258:VAL:HB	1.03	1.12
1:E:187:GLN:HB3	1:E:223:LEU:CD2	1.78	1.12
1:H:179:CYS:CB	1:H:181:GLU:HG2	1.78	1.12
1:A:476:CYS:SG	1:A:477:GLU:OE2	2.06	1.12
1:D:476:CYS:SG	1:D:477:GLU:OE2	2.06	1.12
1:B:185:THR:HG23	1:B:187:GLN:HG3	1.16	1.12
1:B:189:LEU:HG	1:B:190:ALA:H	1.09	1.12
1:G:185:THR:HG23	1:G:187:GLN:HG3	1.16	1.12
1:A:179:CYS:CB	1:A:181:GLU:HG2	1.78	1.11
1:D:179:CYS:CB	1:D:181:GLU:HG2	1.79	1.11
1:A:263:ASN:HD21	1:A:265:LEU:HB2	1.16	1.11
1:A:434:TRP:CZ3	1:A:568:ARG:HA	1.86	1.11
1:B:646:ARG:HG3	1:B:647:GLN:HE22	0.95	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:473:THR:HG21	1:E:533:LEU:CD2	1.81	1.11
1:H:110:GLN:O	1:H:111:PHE:HB2	1.49	1.11
1:A:547:LEU:HD13	1:A:615:THR:CG2	1.81	1.11
1:F:179:CYS:CB	1:F:181:GLU:HG2	1.79	1.11
1:H:387:ILE:HD11	1:H:449:GLN:HG3	1.13	1.11
1:A:646:ARG:HG3	1:A:647:GLN:HE22	0.94	1.10
1:F:263:ASN:HD21	1:F:265:LEU:HB2	1.14	1.10
1:H:246:TYR:HD1	1:H:258:VAL:HB	1.03	1.10
1:H:189:LEU:HG	1:H:190:ALA:H	1.14	1.10
1:C:476:CYS:SG	1:C:477:GLU:OE2	2.09	1.10
1:H:134:ARG:HA	1:H:300:PHE:HZ	1.12	1.10
1:B:179:CYS:CB	1:B:181:GLU:HG2	1.81	1.10
1:D:262:PRO:HB3	1:D:409:SER:OG	1.52	1.10
1:F:434:TRP:CE3	1:F:568:ARG:HA	1.86	1.10
1:G:179:CYS:CB	1:G:181:GLU:HG2	1.80	1.10
1:A:646:ARG:HG3	1:A:647:GLN:NE2	1.65	1.10
1:B:246:TYR:HD1	1:B:258:VAL:HB	1.02	1.10
1:F:187:GLN:HB3	1:F:223:LEU:HD21	1.17	1.10
1:F:246:TYR:HD1	1:F:258:VAL:HB	1.04	1.10
1:F:646:ARG:HG3	1:F:647:GLN:HE22	0.95	1.10
1:G:219:PHE:O	1:G:220:ARG:HG2	1.52	1.10
1:C:189:LEU:HG	1:C:190:ALA:H	1.08	1.09
1:C:219:PHE:O	1:C:220:ARG:CG	2.00	1.09
1:C:646:ARG:HG3	1:C:647:GLN:HE22	0.93	1.09
1:E:185:THR:HG23	1:E:187:GLN:HG3	1.15	1.09
1:A:219:PHE:O	1:A:220:ARG:HG2	1.50	1.09
1:C:185:THR:HG23	1:C:187:GLN:HG3	1.15	1.09
1:C:654:LEU:CD2	1:D:654:LEU:CD2	2.28	1.09
1:H:434:TRP:HB3	1:H:571:TYR:CD1	1.87	1.09
1:A:111:PHE:HZ	1:A:572:ARG:HG3	1.15	1.09
1:A:246:TYR:HD1	1:A:258:VAL:HB	1.03	1.09
1:A:496:LYS:CB	1:B:655:TRP:HE1	1.64	1.09
1:B:547:LEU:HD13	1:B:614:LYS:CB	1.82	1.09
1:E:536:LYS:HB3	1:E:625:LEU:HD13	1.21	1.09
1:F:646:ARG:HG3	1:F:647:GLN:NE2	1.66	1.09
1:C:110:GLN:O	1:C:111:PHE:HB2	1.48	1.09
1:G:189:LEU:HG	1:G:190:ALA:H	1.13	1.09
1:D:219:PHE:O	1:D:220:ARG:CG	2.01	1.09
1:E:179:CYS:CB	1:E:181:GLU:HG2	1.80	1.09
1:F:219:PHE:O	1:F:220:ARG:CG	2.01	1.09
1:B:263:ASN:HD21	1:B:265:LEU:HB2	1.18	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:282:MET:HB2	1:E:286:ARG:HG3	1.36	1.08
1:D:434:TRP:HB3	1:D:571:TYR:CD1	1.88	1.08
1:H:219:PHE:O	1:H:220:ARG:HG2	1.51	1.08
1:A:666:ARG:HH12	1:B:502:GLU:HG3	1.15	1.08
1:B:219:PHE:O	1:B:220:ARG:CG	2.01	1.08
1:D:646:ARG:HG3	1:D:647:GLN:NE2	1.66	1.08
1:G:110:GLN:O	1:G:111:PHE:HB2	1.52	1.08
1:B:646:ARG:HG3	1:B:647:GLN:NE2	1.66	1.07
1:E:547:LEU:HD13	1:E:615:THR:HG21	1.31	1.07
1:F:473:THR:HG21	1:F:533:LEU:HD22	1.09	1.07
1:A:665:VAL:HG13	1:B:665:VAL:HG13	1.35	1.07
1:E:646:ARG:HG3	1:E:647:GLN:NE2	1.65	1.07
1:D:110:GLN:O	1:D:111:PHE:HB2	1.53	1.07
1:G:434:TRP:CZ3	1:G:568:ARG:HA	1.89	1.07
1:C:492:ILE:HG23	1:D:651:GLN:HE22	0.97	1.07
1:E:189:LEU:HG	1:E:190:ALA:H	1.08	1.07
1:F:110:GLN:O	1:F:111:PHE:HB2	1.50	1.07
1:A:189:LEU:HG	1:A:190:ALA:H	1.09	1.07
1:A:434:TRP:HB3	1:A:571:TYR:CD1	1.88	1.07
1:A:521:VAL:HA	1:A:524:CYS:SG	1.95	1.07
1:B:110:GLN:O	1:B:111:PHE:HB2	1.52	1.07
1:B:494:LEU:HD12	1:B:514:TRP:HE3	1.16	1.07
1:H:187:GLN:HB3	1:H:223:LEU:CD2	1.85	1.07
1:E:387:ILE:HD11	1:E:449:GLN:HG3	1.33	1.06
1:B:187:GLN:HB3	1:B:223:LEU:CD2	1.85	1.06
1:C:263:ASN:HD21	1:C:265:LEU:HB2	1.17	1.06
1:C:655:TRP:HE1	1:D:496:LYS:HB2	0.93	1.06
1:F:118:LYS:HG2	1:F:264:HIS:O	1.54	1.06
1:D:473:THR:HG21	1:D:533:LEU:HD22	1.22	1.06
1:E:547:LEU:HD12	1:E:615:THR:HG22	1.29	1.06
1:E:646:ARG:HG3	1:E:647:GLN:HE22	0.94	1.06
1:H:434:TRP:CZ3	1:H:568:ARG:HA	1.88	1.06
1:A:282:MET:HB2	1:A:286:ARG:HG3	1.37	1.06
1:G:187:GLN:HB3	1:G:223:LEU:HD21	1.34	1.06
1:A:187:GLN:HB3	1:A:223:LEU:CD2	1.85	1.06
1:A:524:CYS:SG	1:A:643:VAL:CG1	2.43	1.06
1:B:476:CYS:SG	1:B:477:GLU:OE2	2.13	1.06
1:C:547:LEU:HD13	1:C:615:THR:CG2	1.84	1.06
1:F:419:ARG:H	1:F:420:PRO:HD3	1.20	1.06
1:F:497:TYR:CE2	1:F:511:LEU:HD22	1.91	1.06
1:G:187:GLN:HB3	1:G:223:LEU:CD2	1.86	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:LEU:HG	1:D:190:ALA:H	1.09	1.05
1:F:187:GLN:HB3	1:F:223:LEU:CD2	1.84	1.05
1:A:479:LEU:HD12	1:A:640:GLU:HB3	1.38	1.05
1:C:492:ILE:HG23	1:D:651:GLN:NE2	1.70	1.05
1:E:422:THR:HB	1:E:585:GLY:CA	1.86	1.05
1:G:419:ARG:H	1:G:420:PRO:HD3	1.20	1.05
1:H:473:THR:HG21	1:H:533:LEU:HD22	1.38	1.05
1:A:486:PHE:HZ	1:A:517:MET:CE	1.70	1.05
1:C:434:TRP:CE3	1:C:568:ARG:HA	1.91	1.05
1:D:646:ARG:HG3	1:D:647:GLN:HE22	0.95	1.05
1:H:219:PHE:O	1:H:220:ARG:CG	2.05	1.05
1:H:419:ARG:H	1:H:420:PRO:HD3	1.20	1.05
1:A:570:LEU:HB3	1:A:590:MET:HE3	1.39	1.05
1:C:187:GLN:HB3	1:C:223:LEU:CD2	1.87	1.05
1:C:419:ARG:H	1:C:420:PRO:HD3	1.20	1.05
1:E:110:GLN:O	1:E:111:PHE:HB2	1.51	1.05
1:A:219:PHE:O	1:A:220:ARG:CG	2.04	1.04
1:E:219:PHE:O	1:E:220:ARG:CG	2.03	1.04
1:G:263:ASN:HD21	1:G:265:LEU:HB2	1.16	1.04
1:H:263:ASN:HD21	1:H:265:LEU:HB2	1.16	1.04
1:B:419:ARG:H	1:B:420:PRO:HD3	1.20	1.04
1:E:134:ARG:HA	1:E:300:PHE:HZ	1.18	1.04
1:F:134:ARG:HA	1:F:300:PHE:HZ	1.18	1.04
1:H:134:ARG:HA	1:H:300:PHE:CZ	1.92	1.04
1:A:533:LEU:HD23	1:A:629:VAL:CG1	1.86	1.04
1:C:434:TRP:HB3	1:C:571:TYR:CD1	1.92	1.04
1:G:282:MET:HB2	1:G:286:ARG:HG3	1.37	1.04
1:B:517:MET:HG3	1:B:646:ARG:HH11	1.22	1.04
1:D:263:ASN:HD21	1:D:265:LEU:HB2	1.17	1.04
1:E:263:ASN:HD21	1:E:265:LEU:HB2	1.20	1.04
1:F:476:CYS:SG	1:F:477:GLU:OE2	2.15	1.04
1:H:26:PHE:CZ	1:H:179:CYS:HB3	1.91	1.04
1:B:179:CYS:HB2	1:B:181:GLU:HG2	1.05	1.04
1:C:533:LEU:HD23	1:C:629:VAL:HG11	1.39	1.04
1:E:547:LEU:HD13	1:E:615:THR:HG23	1.35	1.04
1:E:655:TRP:CE3	1:F:654:LEU:HD11	1.93	1.04
1:H:434:TRP:HZ3	1:H:568:ARG:HG3	1.23	1.04
1:C:533:LEU:HD23	1:C:629:VAL:CG1	1.86	1.03
1:B:282:MET:HB2	1:B:286:ARG:HG3	1.40	1.03
1:D:185:THR:CG2	1:D:187:GLN:HG3	1.89	1.03
1:E:502:GLU:HG3	1:F:666:ARG:NH1	1.73	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:179:CYS:HB2	1:G:181:GLU:HG2	1.04	1.03
1:C:651:GLN:HE22	1:D:492:ILE:HG23	1.18	1.03
1:A:110:GLN:O	1:A:111:PHE:HB2	1.51	1.03
1:A:179:CYS:HB2	1:A:181:GLU:HG2	1.04	1.03
1:C:249:LEU:HD23	1:C:252:ALA:HA	1.40	1.03
1:D:179:CYS:HB2	1:D:181:GLU:HG2	1.04	1.03
1:E:419:ARG:H	1:E:420:PRO:HD3	1.21	1.03
1:F:229:VAL:HG13	1:G:229:VAL:HG13	1.40	1.03
1:F:387:ILE:HD12	1:F:450:GLY:HA2	1.41	1.03
1:A:486:PHE:CZ	1:A:517:MET:HE2	1.95	1.02
1:A:655:TRP:CE3	1:B:654:LEU:CD1	2.41	1.02
1:E:179:CYS:HB2	1:E:181:GLU:HG2	1.04	1.02
1:F:282:MET:HB2	1:F:286:ARG:HG3	1.37	1.02
1:G:249:LEU:HD23	1:G:252:ALA:HA	1.40	1.02
1:C:111:PHE:HZ	1:C:572:ARG:HG3	1.24	1.02
1:E:249:LEU:HD23	1:E:252:ALA:HA	1.40	1.02
1:A:249:LEU:HD23	1:A:252:ALA:HA	1.41	1.02
1:B:547:LEU:HD13	1:B:614:LYS:HB3	1.06	1.02
1:H:282:MET:HB2	1:H:286:ARG:HG3	1.40	1.02
1:A:654:LEU:CD2	1:B:654:LEU:HD21	1.87	1.02
1:C:492:ILE:CG2	1:D:651:GLN:HE22	1.72	1.02
1:D:249:LEU:HD23	1:D:252:ALA:HA	1.37	1.02
1:D:282:MET:HB2	1:D:286:ARG:HG3	1.37	1.02
1:D:419:ARG:H	1:D:420:PRO:HD3	1.21	1.02
1:E:134:ARG:HA	1:E:300:PHE:CZ	1.95	1.02
1:H:26:PHE:CE2	1:H:181:GLU:CD	2.33	1.02
1:F:249:LEU:HD23	1:F:252:ALA:HA	1.38	1.02
1:A:419:ARG:H	1:A:420:PRO:HD3	1.20	1.01
1:A:422:THR:HB	1:A:585:GLY:CA	1.89	1.01
1:C:651:GLN:NE2	1:D:492:ILE:HG23	1.73	1.01
1:D:187:GLN:HB3	1:D:223:LEU:HD21	1.05	1.01
1:A:654:LEU:CD2	1:B:654:LEU:CD2	2.38	1.01
1:C:492:ILE:HD13	1:D:651:GLN:HE21	1.24	1.01
1:E:185:THR:CG2	1:E:187:GLN:HG3	1.89	1.01
1:H:118:LYS:HG2	1:H:264:HIS:O	1.58	1.01
1:A:229:VAL:HG13	1:D:229:VAL:HG13	1.39	1.01
1:B:118:LYS:HG2	1:B:264:HIS:O	1.60	1.01
1:D:118:LYS:HG2	1:D:264:HIS:O	1.60	1.01
1:E:476:CYS:SG	1:E:477:GLU:OE2	2.19	1.01
1:B:249:LEU:HD23	1:B:252:ALA:HA	1.42	1.01
1:C:262:PRO:HB3	1:C:409:SER:OG	1.61	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:646:ARG:CG	1:C:647:GLN:HE22	1.73	1.01
1:G:219:PHE:O	1:G:220:ARG:CG	2.07	1.01
1:B:476:CYS:HB2	1:B:636:MET:SD	2.01	1.01
1:C:179:CYS:HB2	1:C:181:GLU:HG2	1.03	1.01
1:C:185:THR:CG2	1:C:187:GLN:HG3	1.89	1.01
1:C:521:VAL:HA	1:C:524:CYS:SG	2.01	1.01
1:E:530:VAL:HA	1:E:533:LEU:HD12	1.43	1.01
1:F:179:CYS:HB2	1:F:181:GLU:HG2	1.03	1.01
1:F:226:TRP:CD1	1:F:227:GLN:N	2.28	1.01
1:F:434:TRP:CZ3	1:F:568:ARG:HA	1.94	1.01
1:E:646:ARG:CG	1:E:647:GLN:HE22	1.74	1.00
1:H:179:CYS:HB2	1:H:181:GLU:HG2	1.03	1.00
1:B:185:THR:CG2	1:B:187:GLN:HG3	1.91	1.00
1:C:530:VAL:HA	1:C:533:LEU:HD12	1.43	1.00
1:H:226:TRP:CD1	1:H:227:GLN:N	2.28	1.00
1:C:226:TRP:CD1	1:C:227:GLN:N	2.29	1.00
1:F:646:ARG:CG	1:F:647:GLN:HE22	1.75	1.00
1:F:521:VAL:HA	1:F:524:CYS:SG	2.01	1.00
1:D:530:VAL:HA	1:D:533:LEU:HD12	1.43	1.00
1:F:262:PRO:HB3	1:F:409:SER:OG	1.61	1.00
1:A:118:LYS:HG2	1:A:264:HIS:O	1.61	1.00
1:F:524:CYS:SG	1:F:643:VAL:HG11	2.01	1.00
1:F:536:LYS:HB3	1:F:625:LEU:HD13	1.43	1.00
1:H:249:LEU:HD23	1:H:252:ALA:HA	1.40	1.00
1:C:655:TRP:HE1	1:D:496:LYS:CB	1.75	0.99
1:D:226:TRP:CD1	1:D:227:GLN:N	2.30	0.99
1:A:479:LEU:HB3	1:A:640:GLU:OE2	1.61	0.99
1:C:134:ARG:HA	1:C:300:PHE:HZ	1.21	0.99
1:C:282:MET:HB2	1:C:286:ARG:HG3	1.38	0.99
1:D:536:LYS:O	1:D:625:LEU:HD13	1.60	0.99
1:E:533:LEU:HD23	1:E:629:VAL:HG11	1.44	0.99
1:B:262:PRO:HB3	1:B:409:SER:OG	1.59	0.99
1:D:422:THR:HB	1:D:585:GLY:CA	1.91	0.99
1:G:434:TRP:HB3	1:G:571:TYR:CD1	1.96	0.99
1:F:185:THR:CG2	1:F:187:GLN:HG3	1.90	0.99
1:G:185:THR:CG2	1:G:187:GLN:HG3	1.90	0.99
1:G:530:VAL:HA	1:G:533:LEU:HD12	1.44	0.99
1:A:536:LYS:HB3	1:A:625:LEU:HD13	1.02	0.99
1:E:497:TYR:CE2	1:E:511:LEU:HD22	1.98	0.99
1:A:111:PHE:CZ	1:A:572:ARG:HG3	1.97	0.99
1:B:521:VAL:HA	1:B:524:CYS:SG	2.03	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:ARG:CG	1:B:647:GLN:HE22	1.75	0.99
1:C:434:TRP:CZ3	1:C:568:ARG:HA	1.97	0.99
1:B:226:TRP:CD1	1:B:227:GLN:N	2.31	0.99
1:C:479:LEU:HD11	1:C:641:LYS:HG3	1.44	0.99
1:H:111:PHE:HZ	1:H:572:ARG:HG3	1.27	0.99
1:G:359:LEU:HA	1:G:460:ARG:HH12	1.28	0.99
1:B:224:PRO:HG3	1:B:428:ARG:HH22	1.28	0.99
1:E:547:LEU:HD11	1:E:615:THR:HG22	1.41	0.99
1:C:654:LEU:HD11	1:D:655:TRP:CE3	1.97	0.98
1:F:530:VAL:HA	1:F:533:LEU:HD12	1.42	0.98
1:A:646:ARG:CG	1:A:647:GLN:HE22	1.75	0.98
1:B:387:ILE:HD12	1:B:450:GLY:HA2	1.45	0.98
1:B:134:ARG:HA	1:B:300:PHE:HZ	1.27	0.98
1:B:494:LEU:HD21	1:B:518:GLU:OE2	1.64	0.98
1:G:473:THR:HG21	1:G:533:LEU:HD22	1.42	0.98
1:C:473:THR:HG21	1:C:533:LEU:CD2	1.93	0.98
1:F:570:LEU:HD23	1:F:590:MET:HG2	1.42	0.98
1:G:387:ILE:HG21	1:G:450:GLY:HA2	1.45	0.98
1:E:226:TRP:CD1	1:E:227:GLN:N	2.30	0.98
1:B:530:VAL:HA	1:B:533:LEU:HD12	1.44	0.98
1:D:26:PHE:CZ	1:D:179:CYS:HB3	1.99	0.98
1:H:185:THR:CG2	1:H:187:GLN:HG3	1.93	0.98
1:A:185:THR:CG2	1:A:187:GLN:HG3	1.94	0.97
1:F:434:TRP:HB3	1:F:571:TYR:CD1	1.99	0.97
1:A:533:LEU:HD23	1:A:629:VAL:HG11	1.46	0.97
1:H:434:TRP:HE3	1:H:568:ARG:HA	1.20	0.97
1:D:646:ARG:CG	1:D:647:GLN:HE22	1.76	0.97
1:H:530:VAL:HA	1:H:533:LEU:HD12	1.43	0.97
1:D:521:VAL:HA	1:D:524:CYS:SG	2.04	0.97
1:E:654:LEU:CD1	1:F:655:TRP:CE3	2.47	0.97
1:A:473:THR:HG21	1:A:533:LEU:HD22	1.46	0.97
1:F:473:THR:HG21	1:F:533:LEU:CD2	1.94	0.97
1:A:530:VAL:HA	1:A:533:LEU:HD12	1.45	0.97
1:H:387:ILE:HG21	1:H:450:GLY:HA2	1.41	0.97
1:H:434:TRP:HD1	1:H:435:GLN:N	1.62	0.97
1:C:492:ILE:CG2	1:D:651:GLN:NE2	2.26	0.97
1:E:654:LEU:CD2	1:F:654:LEU:HD21	1.94	0.97
1:G:226:TRP:CD1	1:G:227:GLN:N	2.33	0.97
1:A:536:LYS:CB	1:A:625:LEU:HD13	1.95	0.96
1:F:443:ASP:O	1:F:446:ARG:HB2	1.64	0.96
1:A:547:LEU:HD13	1:A:615:THR:HG22	1.36	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:ASN:HD21	1:B:611:GLN:CD	1.67	0.96
1:C:134:ARG:HA	1:C:300:PHE:CZ	2.00	0.96
1:G:475:GLU:CG	1:G:636:MET:HE1	1.95	0.96
1:A:226:TRP:CD1	1:A:227:GLN:N	2.33	0.96
1:C:26:PHE:CZ	1:C:179:CYS:HB3	2.00	0.96
1:B:473:THR:HG21	1:B:533:LEU:HD22	1.45	0.96
1:B:521:VAL:HG13	1:B:643:VAL:CG1	1.95	0.96
1:F:134:ARG:HA	1:F:300:PHE:CZ	2.00	0.96
1:B:434:TRP:HZ3	1:B:568:ARG:HA	1.30	0.96
1:A:134:ARG:HA	1:A:300:PHE:HZ	1.31	0.96
1:A:666:ARG:NH1	1:B:502:GLU:HG3	1.80	0.96
1:A:570:LEU:HB3	1:A:590:MET:CE	1.96	0.96
1:E:434:TRP:HD1	1:E:435:GLN:N	1.64	0.95
1:E:473:THR:HG21	1:E:533:LEU:HD22	1.47	0.95
1:A:563:LEU:HD21	1:A:596:LEU:HB2	1.48	0.95
1:D:441:LYS:HB2	1:D:560:LEU:CD2	1.96	0.95
1:D:434:TRP:CZ3	1:D:568:ARG:CA	2.49	0.95
1:E:262:PRO:HB3	1:E:409:SER:OG	1.66	0.95
1:E:521:VAL:HA	1:E:524:CYS:SG	2.06	0.95
1:E:222:PHE:CE2	1:E:225:ASN:HB2	2.02	0.95
1:H:111:PHE:CZ	1:H:572:ARG:HG3	2.00	0.95
1:D:494:LEU:HD12	1:D:514:TRP:HE3	1.31	0.95
1:F:111:PHE:HZ	1:F:572:ARG:HG3	1.31	0.95
1:A:262:PRO:HB3	1:A:409:SER:OG	1.66	0.95
1:B:222:PHE:CE2	1:B:225:ASN:HB2	2.02	0.94
1:A:655:TRP:HE3	1:B:654:LEU:HD11	1.31	0.94
1:B:494:LEU:HD12	1:B:514:TRP:CE3	2.02	0.94
1:H:193:LEU:HD22	1:H:231:TRP:CD1	2.02	0.94
1:A:17:MET:HB3	1:A:32:TRP:HB3	1.50	0.94
1:A:641:LYS:HB3	1:A:645:ARG:HH21	1.33	0.94
1:E:658:LEU:HD12	1:F:658:LEU:HD12	1.49	0.94
1:C:654:LEU:HD21	1:D:654:LEU:HD21	1.38	0.94
1:D:434:TRP:HD1	1:D:435:GLN:N	1.66	0.94
1:F:570:LEU:HB3	1:F:590:MET:CE	1.98	0.94
1:A:222:PHE:CE2	1:A:225:ASN:HB2	2.02	0.94
1:D:222:PHE:CE2	1:D:225:ASN:HB2	2.02	0.94
1:G:434:TRP:HD1	1:G:435:GLN:N	1.66	0.94
1:B:229:VAL:HG13	1:C:229:VAL:HG13	1.50	0.93
1:D:479:LEU:HD11	1:D:641:LYS:HG3	1.49	0.93
1:E:189:LEU:HG	1:E:190:ALA:N	1.82	0.93
1:G:222:PHE:CE2	1:G:225:ASN:HB2	2.03	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:222:PHE:CE2	1:H:225:ASN:HB2	2.03	0.93
1:B:134:ARG:HA	1:B:300:PHE:CZ	2.04	0.93
1:E:654:LEU:HD21	1:F:654:LEU:CD2	1.98	0.93
1:F:517:MET:HG3	1:F:646:ARG:HH11	1.32	0.93
1:F:641:LYS:HB3	1:F:645:ARG:HH21	1.34	0.93
1:H:327:VAL:HG11	1:H:367:LEU:HB2	1.50	0.93
1:C:473:THR:HG21	1:C:533:LEU:HD22	1.48	0.93
1:C:394:LYS:HG3	1:C:613:SER:HB2	1.49	0.92
1:H:434:TRP:HB3	1:H:571:TYR:HD1	1.33	0.92
1:A:658:LEU:HD12	1:B:658:LEU:HD12	1.51	0.92
1:B:434:TRP:CZ3	1:B:568:ARG:CA	2.52	0.92
1:C:497:TYR:CE2	1:C:511:LEU:HD22	2.04	0.92
1:B:434:TRP:HD1	1:B:435:GLN:N	1.67	0.92
1:D:430:TRP:HB3	1:D:571:TYR:HD2	1.30	0.92
1:D:570:LEU:HB3	1:D:590:MET:HE3	1.48	0.92
1:E:229:VAL:HG13	1:H:229:VAL:HG13	1.49	0.92
1:B:641:LYS:HB3	1:B:645:ARG:HH21	1.33	0.92
1:E:563:LEU:HD21	1:E:596:LEU:HB2	1.51	0.92
1:F:327:VAL:HG11	1:F:367:LEU:HB2	1.50	0.92
1:E:434:TRP:HB3	1:E:571:TYR:CD1	2.05	0.92
1:D:434:TRP:HZ3	1:D:568:ARG:HA	1.26	0.91
1:B:17:MET:HB3	1:B:32:TRP:HB3	1.52	0.91
1:B:387:ILE:HG21	1:B:450:GLY:HA2	1.52	0.91
1:D:641:LYS:HB3	1:D:645:ARG:HH21	1.33	0.91
1:E:540:LEU:HD11	1:E:622:ALA:HB2	1.50	0.91
1:A:540:LEU:CD1	1:A:622:ALA:HB2	2.00	0.91
1:G:327:VAL:HG11	1:G:367:LEU:HB2	1.49	0.91
1:D:17:MET:HB3	1:D:32:TRP:HB3	1.50	0.91
1:A:153:LEU:HA	1:A:162:HIS:HB3	1.53	0.91
1:A:486:PHE:CZ	1:A:517:MET:CE	2.52	0.91
1:C:222:PHE:CE2	1:C:225:ASN:HB2	2.05	0.91
1:F:17:MET:HB3	1:F:32:TRP:HB3	1.53	0.91
1:E:153:LEU:HD23	1:E:162:HIS:ND1	1.85	0.91
1:A:179:CYS:HB2	1:A:181:GLU:CG	1.99	0.91
1:B:327:VAL:HG11	1:B:367:LEU:HB2	1.52	0.91
1:E:17:MET:HB3	1:E:32:TRP:HB3	1.51	0.91
1:F:387:ILE:CD1	1:F:450:GLY:HA2	1.99	0.91
1:H:26:PHE:HE2	1:H:181:GLU:OE1	1.54	0.91
1:D:387:ILE:HD11	1:D:449:GLN:HG3	1.52	0.91
1:A:327:VAL:HG11	1:A:367:LEU:HB2	1.50	0.90
1:B:550:ASN:ND2	1:B:611:GLN:CD	2.25	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:CYS:HB2	1:C:181:GLU:CG	1.98	0.90
1:E:387:ILE:HD11	1:E:449:GLN:CG	2.00	0.90
1:G:17:MET:HB3	1:G:32:TRP:HB3	1.51	0.90
1:E:519:GLN:HA	1:E:522:GLU:HB2	1.52	0.90
1:B:153:LEU:HA	1:B:162:HIS:HB3	1.53	0.90
1:B:550:ASN:ND2	1:B:611:GLN:OE1	2.05	0.90
1:C:153:LEU:HD23	1:C:162:HIS:ND1	1.86	0.90
1:C:327:VAL:HG11	1:C:367:LEU:HB2	1.53	0.90
1:F:144:ARG:HD3	1:F:169:TYR:O	1.71	0.90
1:H:26:PHE:HE2	1:H:181:GLU:CD	1.69	0.90
1:D:134:ARG:HA	1:D:300:PHE:HZ	1.37	0.90
1:H:153:LEU:HA	1:H:162:HIS:HB3	1.53	0.90
1:F:519:GLN:HA	1:F:522:GLU:HB2	1.53	0.90
1:G:339:TRP:HA	1:G:342:GLN:HB2	1.52	0.90
1:F:387:ILE:HG21	1:F:450:GLY:HA2	1.51	0.90
1:A:150:ASN:HD22	1:A:167:LEU:HD12	1.37	0.90
1:C:153:LEU:HA	1:C:162:HIS:HB3	1.54	0.90
1:D:219:PHE:C	1:D:220:ARG:HG3	1.91	0.90
1:F:222:PHE:CE2	1:F:225:ASN:HB2	2.06	0.90
1:C:17:MET:HB3	1:C:32:TRP:HB3	1.51	0.90
1:D:327:VAL:HG11	1:D:367:LEU:HB2	1.51	0.90
1:E:654:LEU:CD2	1:F:654:LEU:CD2	2.50	0.90
1:G:125:LEU:HA	1:G:162:HIS:NE2	1.87	0.90
1:A:527:GLU:O	1:A:529:GLU:N	2.05	0.90
1:C:563:LEU:HD21	1:C:596:LEU:HB2	1.54	0.90
1:D:153:LEU:HA	1:D:162:HIS:HB3	1.54	0.90
1:A:434:TRP:HB3	1:A:571:TYR:HD1	1.37	0.89
1:B:26:PHE:CZ	1:B:179:CYS:HB3	2.06	0.89
1:C:419:ARG:HA	1:C:587:SER:OG	1.72	0.89
1:E:641:LYS:HB3	1:E:645:ARG:HH21	1.33	0.89
1:E:651:GLN:HE22	1:F:492:ILE:HG23	1.33	0.89
1:H:17:MET:HB3	1:H:32:TRP:HB3	1.52	0.89
1:C:272:LYS:HG2	1:C:273:LEU:N	1.87	0.89
1:E:339:TRP:HA	1:E:342:GLN:HB2	1.54	0.89
1:F:153:LEU:HA	1:F:162:HIS:HB3	1.52	0.89
1:F:339:TRP:HA	1:F:342:GLN:HB2	1.52	0.89
1:F:434:TRP:HD1	1:F:435:GLN:N	1.70	0.89
1:F:153:LEU:HD23	1:F:162:HIS:ND1	1.86	0.89
1:A:536:LYS:HB3	1:A:625:LEU:CD1	1.97	0.89
1:C:339:TRP:HA	1:C:342:GLN:HB2	1.55	0.89
1:D:153:LEU:HD23	1:D:162:HIS:ND1	1.88	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:434:TRP:CZ3	1:H:568:ARG:HG3	2.07	0.89
1:E:144:ARG:HD3	1:E:169:TYR:O	1.73	0.89
1:E:153:LEU:HA	1:E:162:HIS:HB3	1.52	0.89
1:E:272:LYS:HG2	1:E:273:LEU:N	1.87	0.89
1:B:111:PHE:HZ	1:B:572:ARG:HG3	1.34	0.89
1:C:434:TRP:HD1	1:C:435:GLN:N	1.70	0.89
1:E:118:LYS:CG	1:E:264:HIS:O	2.18	0.89
1:E:179:CYS:HB2	1:E:181:GLU:CG	2.00	0.89
1:H:125:LEU:HA	1:H:162:HIS:NE2	1.87	0.89
1:H:339:TRP:HA	1:H:342:GLN:HB2	1.53	0.89
1:A:189:LEU:HG	1:A:190:ALA:N	1.82	0.89
1:A:434:TRP:HE3	1:A:568:ARG:HA	1.36	0.89
1:B:153:LEU:HD23	1:B:162:HIS:ND1	1.87	0.89
1:D:179:CYS:HB2	1:D:181:GLU:CG	1.99	0.89
1:G:153:LEU:HA	1:G:162:HIS:HB3	1.54	0.89
1:G:153:LEU:HD23	1:G:162:HIS:ND1	1.86	0.89
1:C:219:PHE:C	1:C:220:ARG:HG3	1.94	0.89
1:C:459:LEU:HD11	1:C:548:GLN:OE1	1.73	0.89
1:G:475:GLU:HG2	1:G:636:MET:HE3	1.52	0.89
1:A:576:GLU:OE2	1:B:573:ARG:NH2	2.06	0.88
1:B:519:GLN:HA	1:B:522:GLU:HB2	1.53	0.88
1:C:519:GLN:HA	1:C:522:GLU:HB2	1.53	0.88
1:H:153:LEU:HD23	1:H:162:HIS:ND1	1.87	0.88
1:A:502:GLU:HG3	1:B:666:ARG:NH1	1.89	0.88
1:A:579:ARG:NH2	1:D:580:ASP:HB3	1.88	0.88
1:B:144:ARG:HD3	1:B:169:TYR:O	1.73	0.88
1:C:651:GLN:NE2	1:D:492:ILE:CG2	2.35	0.88
1:D:144:ARG:HD3	1:D:169:TYR:O	1.74	0.88
1:D:339:TRP:HA	1:D:342:GLN:HB2	1.55	0.88
1:F:125:LEU:HA	1:F:162:HIS:NE2	1.87	0.88
1:E:319:SER:OG	1:E:403:LEU:HB2	1.73	0.88
1:C:480:LYS:CE	1:C:527:GLU:HB2	2.03	0.88
1:G:144:ARG:HD3	1:G:169:TYR:O	1.73	0.88
1:A:144:ARG:HD3	1:A:169:TYR:O	1.73	0.88
1:C:658:LEU:HD12	1:D:658:LEU:HD12	1.56	0.88
1:B:125:LEU:HA	1:B:162:HIS:NE2	1.87	0.88
1:B:219:PHE:C	1:B:220:ARG:HG3	1.91	0.88
1:B:339:TRP:HA	1:B:342:GLN:HB2	1.54	0.88
1:C:641:LYS:HB3	1:C:645:ARG:HH21	1.36	0.88
1:F:533:LEU:CD2	1:F:629:VAL:HG13	2.04	0.88
1:D:519:GLN:HA	1:D:522:GLU:HB2	1.53	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:144:ARG:HD3	1:H:169:TYR:O	1.74	0.88
1:A:219:PHE:C	1:A:220:ARG:HG3	1.94	0.88
1:C:111:PHE:CZ	1:C:572:ARG:HG3	2.09	0.88
1:C:118:LYS:CG	1:C:264:HIS:O	2.21	0.88
1:E:125:LEU:HA	1:E:162:HIS:NE2	1.88	0.88
1:G:189:LEU:HG	1:G:190:ALA:N	1.86	0.88
1:A:434:TRP:HD1	1:A:435:GLN:N	1.69	0.87
1:C:235:VAL:HG11	1:C:243:ILE:N	1.88	0.87
1:D:125:LEU:HA	1:D:162:HIS:NE2	1.88	0.87
1:F:235:VAL:HG11	1:F:243:ILE:N	1.88	0.87
1:C:144:ARG:HD3	1:C:169:TYR:O	1.72	0.87
1:C:648:GLU:HB3	1:D:492:ILE:HD12	1.55	0.87
1:D:235:VAL:HG11	1:D:243:ILE:N	1.88	0.87
1:E:26:PHE:CZ	1:E:179:CYS:HB3	2.09	0.87
1:E:327:VAL:HG11	1:E:367:LEU:HB2	1.54	0.87
1:F:219:PHE:C	1:F:220:ARG:HG3	1.91	0.87
1:A:519:GLN:HA	1:A:522:GLU:HB2	1.54	0.87
1:C:368:THR:HA	1:C:371:VAL:HG23	1.57	0.87
1:H:179:CYS:HB2	1:H:181:GLU:CG	1.99	0.87
1:A:339:TRP:HA	1:A:342:GLN:HB2	1.54	0.87
1:D:189:LEU:HG	1:D:190:ALA:N	1.83	0.87
1:F:179:CYS:HB2	1:F:181:GLU:CG	1.99	0.87
1:F:189:LEU:HG	1:F:190:ALA:N	1.85	0.87
1:E:434:TRP:CE3	1:E:568:ARG:HA	2.09	0.87
1:E:394:LYS:HG3	1:E:613:SER:HB2	1.56	0.87
1:A:153:LEU:HD23	1:A:162:HIS:ND1	1.88	0.87
1:B:246:TYR:HD1	1:B:258:VAL:CB	1.88	0.87
1:B:494:LEU:CD2	1:B:518:GLU:OE2	2.23	0.87
1:G:150:ASN:HD22	1:G:167:LEU:HD12	1.39	0.87
1:H:536:LYS:O	1:H:625:LEU:HD13	1.75	0.87
1:H:570:LEU:HB3	1:H:590:MET:CE	2.04	0.87
1:C:655:TRP:CE3	1:D:654:LEU:HD11	2.10	0.87
1:E:536:LYS:CB	1:E:625:LEU:HD13	2.04	0.87
1:B:517:MET:HG3	1:B:646:ARG:NH1	1.89	0.86
1:H:235:VAL:HG11	1:H:243:ILE:N	1.89	0.86
1:B:500:GLN:HB3	1:B:505:ILE:HG12	1.57	0.86
1:C:644:VAL:HA	1:C:647:GLN:HE21	1.40	0.86
1:D:563:LEU:HD23	1:D:597:ALA:HB2	1.58	0.86
1:E:368:THR:HA	1:E:371:VAL:HG23	1.57	0.86
1:H:134:ARG:HB2	1:H:300:PHE:CE1	2.10	0.86
1:H:134:ARG:HB2	1:H:300:PHE:HE1	1.37	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:571:TYR:CZ	1:H:590:MET:SD	2.69	0.86
1:A:134:ARG:HA	1:A:300:PHE:CZ	2.09	0.86
1:D:644:VAL:HA	1:D:647:GLN:HE21	1.39	0.86
1:E:462:ASN:HD21	1:E:540:LEU:HB2	1.40	0.86
1:F:368:THR:HA	1:F:371:VAL:HG23	1.55	0.86
1:B:189:LEU:HG	1:B:190:ALA:N	1.83	0.86
1:G:434:TRP:HZ3	1:G:568:ARG:HG3	1.40	0.86
1:H:134:ARG:CA	1:H:300:PHE:HZ	1.87	0.86
1:H:150:ASN:HD22	1:H:167:LEU:HD12	1.41	0.86
1:A:368:THR:HA	1:A:371:VAL:HG23	1.57	0.86
1:B:235:VAL:HG11	1:B:243:ILE:N	1.90	0.86
1:D:497:TYR:CE2	1:D:511:LEU:HD22	2.10	0.86
1:E:473:THR:HG21	1:E:533:LEU:HD21	1.57	0.86
1:E:662:CYS:SG	1:F:661:ALA:HB1	2.16	0.86
1:F:272:LYS:HG2	1:F:273:LEU:N	1.88	0.86
1:F:644:VAL:HA	1:F:647:GLN:HE21	1.41	0.86
1:B:644:VAL:HA	1:B:647:GLN:HE21	1.40	0.86
1:C:219:PHE:C	1:C:220:ARG:CG	2.43	0.86
1:E:219:PHE:C	1:E:220:ARG:HG3	1.94	0.86
1:G:368:THR:HA	1:G:371:VAL:HG23	1.57	0.86
1:G:434:TRP:HE3	1:G:568:ARG:HA	1.37	0.86
1:E:644:VAL:HA	1:E:647:GLN:HE21	1.41	0.86
1:C:497:TYR:CD2	1:C:497:TYR:O	2.28	0.85
1:E:497:TYR:CD2	1:E:497:TYR:O	2.29	0.85
1:A:235:VAL:HG11	1:A:243:ILE:N	1.90	0.85
1:B:368:THR:HA	1:B:371:VAL:HG23	1.57	0.85
1:C:422:THR:HB	1:C:585:GLY:HA2	1.57	0.85
1:F:150:ASN:HD22	1:F:167:LEU:HD12	1.41	0.85
1:E:235:VAL:HG11	1:E:243:ILE:N	1.90	0.85
1:E:658:LEU:CD1	1:F:658:LEU:HA	2.06	0.85
1:G:570:LEU:HB3	1:G:590:MET:HE3	1.58	0.85
1:H:563:LEU:HD21	1:H:596:LEU:CB	2.07	0.85
1:A:497:TYR:O	1:A:497:TYR:CD2	2.30	0.85
1:B:394:LYS:HG2	1:B:401:ILE:N	1.91	0.85
1:C:125:LEU:HA	1:C:162:HIS:NE2	1.91	0.85
1:D:246:TYR:HD1	1:D:258:VAL:CB	1.89	0.85
1:E:111:PHE:HZ	1:E:572:ARG:HG3	1.41	0.85
1:D:187:GLN:CB	1:D:223:LEU:HD21	2.01	0.85
1:B:434:TRP:HZ3	1:B:568:ARG:CA	1.88	0.85
1:B:434:TRP:HB3	1:B:571:TYR:HD1	1.40	0.85
1:B:497:TYR:CD2	1:B:497:TYR:O	2.30	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:GLN:CB	1:B:505:ILE:HG12	2.06	0.85
1:C:148:PRO:HD3	1:C:188:TYR:CE2	2.10	0.85
1:H:387:ILE:HD11	1:H:449:GLN:CG	2.03	0.85
1:H:563:LEU:CD2	1:H:596:LEU:HB2	2.07	0.85
1:A:125:LEU:HA	1:A:162:HIS:NE2	1.90	0.85
1:D:368:THR:HA	1:D:371:VAL:HG23	1.57	0.85
1:B:230:GLN:C	1:B:232:HIS:H	1.80	0.85
1:C:480:LYS:HE3	1:C:527:GLU:HB2	1.57	0.85
1:A:510:LEU:HD13	1:A:653:GLU:O	1.77	0.85
1:A:644:VAL:HA	1:A:647:GLN:HE21	1.41	0.85
1:D:150:ASN:HD22	1:D:167:LEU:HD12	1.42	0.85
1:D:434:TRP:HZ3	1:D:568:ARG:CA	1.85	0.85
1:A:502:GLU:HG3	1:B:666:ARG:HH11	1.42	0.84
1:B:387:ILE:CD1	1:B:450:GLY:HA2	2.05	0.84
1:C:189:LEU:HG	1:C:190:ALA:N	1.81	0.84
1:D:272:LYS:HG2	1:D:273:LEU:N	1.91	0.84
1:D:497:TYR:CD2	1:D:497:TYR:O	2.30	0.84
1:H:153:LEU:HD23	1:H:162:HIS:CG	2.12	0.84
1:H:368:THR:HA	1:H:371:VAL:HG23	1.56	0.84
1:C:533:LEU:CD2	1:C:629:VAL:CG1	2.54	0.84
1:E:153:LEU:HD23	1:E:162:HIS:CG	2.12	0.84
1:B:111:PHE:CZ	1:B:572:ARG:HG3	2.12	0.84
1:C:150:ASN:HD22	1:C:167:LEU:HD12	1.40	0.84
1:F:357:SER:HA	1:F:453:THR:HB	1.58	0.84
1:F:503:PHE:O	1:F:505:ILE:HG13	1.77	0.84
1:H:219:PHE:C	1:H:220:ARG:HG3	1.95	0.84
1:C:153:LEU:HD23	1:C:162:HIS:CG	2.12	0.84
1:E:655:TRP:CE3	1:F:654:LEU:CD1	2.59	0.84
1:G:430:TRP:CE3	1:G:574:LEU:HD22	2.12	0.84
1:B:153:LEU:HD23	1:B:162:HIS:CG	2.13	0.84
1:E:170:ALA:O	1:E:172:GLU:N	2.11	0.84
1:F:230:GLN:C	1:F:232:HIS:H	1.81	0.84
1:H:434:TRP:CD1	1:H:435:GLN:N	2.45	0.84
1:E:219:PHE:C	1:E:220:ARG:CG	2.45	0.84
1:H:402:SER:HA	1:H:609:TYR:CG	2.11	0.84
1:D:119:GLU:CB	1:D:121:PRO:HD2	2.08	0.84
1:E:134:ARG:HB2	1:E:300:PHE:HE1	1.43	0.84
1:E:492:ILE:HD13	1:F:651:GLN:HE21	1.42	0.84
1:G:235:VAL:HG11	1:G:243:ILE:N	1.91	0.84
1:H:246:TYR:HD1	1:H:258:VAL:CB	1.89	0.84
1:F:480:LYS:NZ	1:F:527:GLU:HB2	1.92	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LEU:HD23	1:A:629:VAL:HG13	1.59	0.84
1:D:536:LYS:HB3	1:D:625:LEU:HD13	1.60	0.84
1:A:654:LEU:HD21	1:B:654:LEU:HD21	1.46	0.83
1:A:654:LEU:HD21	1:B:654:LEU:HD22	1.59	0.83
1:G:219:PHE:C	1:G:220:ARG:HG3	1.97	0.83
1:A:153:LEU:HD23	1:A:162:HIS:CG	2.13	0.83
1:E:230:GLN:C	1:E:232:HIS:H	1.81	0.83
1:E:249:LEU:HG	1:E:253:VAL:O	1.78	0.83
1:F:153:LEU:HD23	1:F:162:HIS:CG	2.13	0.83
1:B:394:LYS:HE2	1:B:401:ILE:HA	1.59	0.83
1:G:153:LEU:HD23	1:G:162:HIS:CG	2.13	0.83
1:G:246:TYR:HD1	1:G:258:VAL:CB	1.89	0.83
1:B:150:ASN:HD22	1:B:167:LEU:HD12	1.41	0.83
1:C:230:GLN:C	1:C:232:HIS:H	1.81	0.83
1:A:148:PRO:HD3	1:A:188:TYR:CE2	2.14	0.83
1:E:148:PRO:HD3	1:E:188:TYR:CE2	2.13	0.83
1:F:118:LYS:CG	1:F:264:HIS:O	2.26	0.83
1:C:153:LEU:CD2	1:C:162:HIS:ND1	2.42	0.83
1:D:547:LEU:HD13	1:D:615:THR:HG22	1.60	0.83
1:E:150:ASN:HD22	1:E:167:LEU:HD12	1.41	0.83
1:F:220:ARG:HH12	1:F:223:LEU:HD22	1.43	0.83
1:G:272:LYS:HG2	1:G:273:LEU:N	1.93	0.83
1:B:217:THR:OG1	1:B:218:GLY:N	2.04	0.83
1:C:462:ASN:HD21	1:C:540:LEU:HB2	1.43	0.83
1:C:502:GLU:HG3	1:D:666:ARG:NH1	1.92	0.83
1:A:433:ILE:HB	1:A:571:TYR:CZ	2.14	0.83
1:A:496:LYS:HB2	1:B:655:TRP:HE1	0.75	0.83
1:C:26:PHE:HE2	1:C:181:GLU:OE1	1.62	0.83
1:F:148:PRO:HD3	1:F:188:TYR:CE2	2.12	0.83
1:H:189:LEU:HG	1:H:190:ALA:N	1.89	0.83
1:H:272:LYS:HG2	1:H:273:LEU:N	1.92	0.83
1:A:42:ALA:O	1:A:95:ALA:HA	1.79	0.83
1:D:153:LEU:HD23	1:D:162:HIS:CG	2.13	0.83
1:H:422:THR:HB	1:H:585:GLY:CA	2.08	0.83
1:C:540:LEU:CD1	1:C:622:ALA:HB2	2.09	0.83
1:C:655:TRP:CE3	1:D:654:LEU:CD1	2.61	0.83
1:D:441:LYS:HB2	1:D:560:LEU:HD22	1.60	0.83
1:E:26:PHE:HE2	1:E:181:GLU:OE1	1.61	0.83
1:E:153:LEU:CD2	1:E:162:HIS:ND1	2.41	0.83
1:F:263:ASN:ND2	1:F:265:LEU:HB2	1.93	0.83
1:F:422:THR:HB	1:F:585:GLY:CA	2.09	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:444:CYS:C	1:F:446:ARG:H	1.80	0.83
1:H:230:GLN:C	1:H:232:HIS:H	1.81	0.83
1:C:263:ASN:ND2	1:C:265:LEU:HB2	1.94	0.82
1:D:473:THR:HG21	1:D:533:LEU:CD2	2.07	0.82
1:G:230:GLN:C	1:G:232:HIS:H	1.81	0.82
1:G:263:ASN:ND2	1:G:265:LEU:HB2	1.95	0.82
1:G:475:GLU:OE2	1:G:637:ARG:HG3	1.79	0.82
1:A:236:ARG:NH2	1:D:231:TRP:CE3	2.47	0.82
1:B:521:VAL:HG13	1:B:643:VAL:HG12	1.59	0.82
1:C:245:VAL:HG12	1:C:246:TYR:H	1.44	0.82
1:A:357:SER:HB3	1:A:453:THR:HB	1.60	0.82
1:D:473:THR:CG2	1:D:533:LEU:HD22	2.09	0.82
1:E:533:LEU:HD23	1:E:629:VAL:CG1	2.10	0.82
1:F:500:GLN:HB3	1:F:505:ILE:HG12	1.61	0.82
1:G:402:SER:HA	1:G:609:TYR:CG	2.14	0.82
1:D:217:THR:OG1	1:D:218:GLY:N	2.12	0.82
1:F:249:LEU:HG	1:F:253:VAL:O	1.78	0.82
1:F:521:VAL:HG13	1:F:643:VAL:HG12	1.61	0.82
1:G:170:ALA:O	1:G:172:GLU:N	2.11	0.82
1:E:217:THR:OG1	1:E:218:GLY:N	2.08	0.82
1:F:219:PHE:C	1:F:220:ARG:CG	2.45	0.82
1:F:246:TYR:HD1	1:F:258:VAL:CB	1.89	0.82
1:F:387:ILE:HD12	1:F:450:GLY:CA	2.08	0.82
1:B:148:PRO:HD3	1:B:188:TYR:CE2	2.15	0.82
1:H:153:LEU:CD2	1:H:162:HIS:ND1	2.43	0.82
1:B:42:ALA:O	1:B:95:ALA:HA	1.79	0.82
1:C:430:TRP:HB3	1:C:571:TYR:HD2	1.45	0.82
1:D:148:PRO:HD3	1:D:188:TYR:CE2	2.14	0.82
1:D:387:ILE:HG21	1:D:450:GLY:HA2	1.60	0.82
1:H:263:ASN:ND2	1:H:265:LEU:HB2	1.94	0.82
1:C:119:GLU:CB	1:C:121:PRO:HD2	2.09	0.82
1:G:153:LEU:CD2	1:G:162:HIS:ND1	2.43	0.82
1:A:231:TRP:CE3	1:D:236:ARG:NH2	2.48	0.82
1:B:430:TRP:HB3	1:B:571:TYR:HD2	1.44	0.82
1:E:651:GLN:HE21	1:F:492:ILE:HD13	1.43	0.82
1:B:540:LEU:CD2	1:B:621:LYS:NZ	2.42	0.82
1:D:358:GLY:O	1:D:359:LEU:HB2	1.80	0.82
1:E:42:ALA:O	1:E:95:ALA:HA	1.78	0.82
1:F:134:ARG:HB2	1:F:300:PHE:CE1	2.15	0.82
1:G:220:ARG:HH12	1:G:223:LEU:HD22	1.44	0.82
1:H:253:VAL:HB	1:H:255:PHE:CZ	2.15	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ASN:ND2	1:A:265:LEU:HB2	1.94	0.81
1:B:153:LEU:CD2	1:B:162:HIS:ND1	2.43	0.81
1:B:501:MET:HA	1:B:505:ILE:HD13	1.62	0.81
1:D:230:GLN:C	1:D:232:HIS:H	1.80	0.81
1:E:387:ILE:CD1	1:E:449:GLN:HG3	2.10	0.81
1:G:111:PHE:HZ	1:G:572:ARG:CG	1.90	0.81
1:G:179:CYS:HB2	1:G:181:GLU:CG	1.99	0.81
1:G:217:THR:OG1	1:G:218:GLY:N	2.12	0.81
1:G:473:THR:CG2	1:G:633:MET:HG3	2.10	0.81
1:H:262:PRO:HB3	1:H:409:SER:OG	1.80	0.81
1:A:170:ALA:O	1:A:172:GLU:N	2.13	0.81
1:A:230:GLN:C	1:A:232:HIS:H	1.81	0.81
1:A:249:LEU:HG	1:A:253:VAL:O	1.80	0.81
1:D:42:ALA:O	1:D:95:ALA:HA	1.80	0.81
1:A:533:LEU:CD2	1:A:629:VAL:CG1	2.57	0.81
1:D:153:LEU:CD2	1:D:162:HIS:ND1	2.44	0.81
1:F:42:ALA:O	1:F:95:ALA:HA	1.80	0.81
1:F:220:ARG:NH1	1:F:223:LEU:HD22	1.95	0.81
1:F:282:MET:CB	1:F:286:ARG:HG3	2.11	0.81
1:G:282:MET:CB	1:G:286:ARG:HG3	2.11	0.81
1:D:322:VAL:HG12	1:D:323:HIS:H	1.43	0.81
1:E:253:VAL:HB	1:E:255:PHE:CZ	2.15	0.81
1:C:42:ALA:O	1:C:95:ALA:HA	1.80	0.81
1:C:655:TRP:CD1	1:D:496:LYS:HB2	2.16	0.81
1:E:134:ARG:CA	1:E:300:PHE:HZ	1.94	0.81
1:E:434:TRP:CD1	1:E:435:GLN:N	2.48	0.81
1:B:170:ALA:O	1:B:172:GLU:N	2.14	0.81
1:B:272:LYS:HG2	1:B:273:LEU:N	1.93	0.81
1:D:170:ALA:O	1:D:172:GLU:N	2.14	0.81
1:E:423:TYR:CE2	1:E:425:HIS:HB2	2.16	0.81
1:H:423:TYR:CE2	1:H:425:HIS:HB2	2.15	0.81
1:A:493:ASP:HB3	1:A:514:TRP:CH2	2.16	0.81
1:B:249:LEU:HG	1:B:253:VAL:O	1.79	0.81
1:C:170:ALA:O	1:C:172:GLU:N	2.14	0.81
1:D:423:TYR:CE2	1:D:425:HIS:HB2	2.15	0.81
1:E:245:VAL:HG12	1:E:246:TYR:H	1.44	0.81
1:E:661:ALA:HB1	1:F:662:CYS:SG	2.20	0.81
1:F:423:TYR:CE2	1:F:425:HIS:HB2	2.16	0.81
1:H:434:TRP:HZ3	1:H:568:ARG:CG	1.94	0.81
1:C:651:GLN:HE21	1:D:492:ILE:HD13	1.46	0.81
1:D:475:GLU:HG2	1:D:636:MET:CE	2.10	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:282:MET:CB	1:E:286:ARG:HG3	2.11	0.81
1:E:547:LEU:HD22	1:E:611:GLN:HG2	1.63	0.81
1:E:571:TYR:CZ	1:E:590:MET:SD	2.73	0.81
1:B:179:CYS:HB2	1:B:181:GLU:CG	2.01	0.81
1:B:494:LEU:HD13	1:B:514:TRP:HB3	1.63	0.81
1:C:357:SER:HB3	1:C:453:THR:HB	1.63	0.81
1:H:220:ARG:HH12	1:H:223:LEU:HD22	1.46	0.81
1:H:249:LEU:HG	1:H:253:VAL:O	1.80	0.81
1:A:272:LYS:HG2	1:A:273:LEU:N	1.94	0.80
1:C:423:TYR:CE2	1:C:425:HIS:HB2	2.17	0.80
1:H:42:ALA:O	1:H:95:ALA:HA	1.80	0.80
1:H:148:PRO:HD3	1:H:188:TYR:CE2	2.15	0.80
1:A:153:LEU:CD2	1:A:162:HIS:ND1	2.44	0.80
1:A:423:TYR:CE2	1:A:425:HIS:HB2	2.16	0.80
1:B:423:TYR:CE2	1:B:425:HIS:HB2	2.16	0.80
1:C:249:LEU:HG	1:C:253:VAL:O	1.80	0.80
1:F:134:ARG:HB2	1:F:300:PHE:HE1	1.44	0.80
1:F:153:LEU:CD2	1:F:162:HIS:ND1	2.43	0.80
1:F:322:VAL:HG12	1:F:323:HIS:H	1.45	0.80
1:G:387:ILE:HD11	1:G:449:GLN:HG3	1.60	0.80
1:B:219:PHE:C	1:B:220:ARG:CG	2.44	0.80
1:C:494:LEU:HD12	1:C:514:TRP:HE3	1.46	0.80
1:F:111:PHE:CZ	1:F:572:ARG:HG3	2.16	0.80
1:F:217:THR:OG1	1:F:218:GLY:N	2.09	0.80
1:G:249:LEU:HG	1:G:253:VAL:O	1.80	0.80
1:G:423:TYR:CE2	1:G:425:HIS:HB2	2.16	0.80
1:B:26:PHE:CE2	1:B:181:GLU:CD	2.55	0.80
1:B:563:LEU:HD21	1:B:596:LEU:HB2	1.62	0.80
1:H:170:ALA:O	1:H:172:GLU:N	2.14	0.80
1:D:249:LEU:HG	1:D:253:VAL:O	1.82	0.80
1:D:570:LEU:HD23	1:D:590:MET:HG2	1.64	0.80
1:E:434:TRP:CZ3	1:E:568:ARG:HA	2.17	0.80
1:G:434:TRP:CD1	1:G:435:GLN:N	2.49	0.80
1:B:253:VAL:HB	1:B:255:PHE:CZ	2.16	0.80
1:F:497:TYR:CD2	1:F:497:TYR:O	2.35	0.80
1:G:282:MET:HB2	1:G:286:ARG:CG	2.12	0.80
1:G:322:VAL:HG12	1:G:323:HIS:H	1.47	0.80
1:A:282:MET:HB2	1:A:286:ARG:CG	2.12	0.80
1:E:246:TYR:HD1	1:E:258:VAL:CB	1.91	0.80
1:F:170:ALA:O	1:F:172:GLU:N	2.14	0.80
1:F:358:GLY:O	1:F:359:LEU:HB2	1.81	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:134:ARG:HA	1:G:300:PHE:CZ	2.17	0.80
1:G:148:PRO:HD3	1:G:188:TYR:CE2	2.16	0.80
1:C:433:ILE:HB	1:C:571:TYR:CZ	2.16	0.80
1:D:434:TRP:CD1	1:D:435:GLN:N	2.50	0.80
1:H:402:SER:HA	1:H:609:TYR:CD1	2.17	0.80
1:H:433:ILE:HB	1:H:571:TYR:CZ	2.17	0.80
1:A:282:MET:CB	1:A:286:ARG:HG3	2.11	0.79
1:C:570:LEU:HB3	1:C:590:MET:HE3	1.64	0.79
1:D:134:ARG:HA	1:D:300:PHE:CZ	2.17	0.79
1:E:26:PHE:CE2	1:E:181:GLU:CD	2.56	0.79
1:E:119:GLU:CB	1:E:121:PRO:HD2	2.12	0.79
1:G:42:ALA:O	1:G:95:ALA:HA	1.81	0.79
1:G:134:ARG:HA	1:G:300:PHE:HZ	1.45	0.79
1:A:579:ARG:HH22	1:D:580:ASP:HB3	1.47	0.79
1:B:245:VAL:HG12	1:B:246:TYR:H	1.47	0.79
1:D:263:ASN:ND2	1:D:265:LEU:HB2	1.95	0.79
1:D:282:MET:CB	1:D:286:ARG:HG3	2.12	0.79
1:H:473:THR:CG2	1:H:533:LEU:HD22	2.13	0.79
1:A:246:TYR:HD1	1:A:258:VAL:CB	1.89	0.79
1:A:655:TRP:NE1	1:B:496:LYS:HB2	1.95	0.79
1:E:358:GLY:O	1:E:359:LEU:HB2	1.81	0.79
1:E:658:LEU:HD12	1:F:658:LEU:HA	1.63	0.79
1:F:282:MET:HB2	1:F:286:ARG:CG	2.12	0.79
1:C:497:TYR:N	1:D:655:TRP:HZ2	1.80	0.79
1:E:263:ASN:ND2	1:E:265:LEU:HB2	1.98	0.79
1:F:357:SER:HB3	1:F:453:THR:HA	1.64	0.79
1:G:419:ARG:H	1:G:420:PRO:CD	1.95	0.79
1:B:220:ARG:NH1	1:B:223:LEU:HD22	1.98	0.79
1:C:422:THR:HB	1:C:585:GLY:HA3	1.62	0.79
1:C:547:LEU:HD13	1:C:615:THR:HG22	1.45	0.79
1:C:547:LEU:HD12	1:C:615:THR:HG22	1.61	0.79
1:D:438:ARG:HG2	1:D:564:GLU:HG3	1.63	0.79
1:A:358:GLY:O	1:A:359:LEU:HB2	1.80	0.79
1:B:220:ARG:HH12	1:B:223:LEU:HD22	1.46	0.79
1:C:134:ARG:HB2	1:C:300:PHE:HE1	1.46	0.79
1:F:119:GLU:CB	1:F:121:PRO:HD2	2.13	0.79
1:F:533:LEU:HD23	1:F:629:VAL:HG13	1.62	0.79
1:C:120:GLY:O	1:C:124:THR:N	2.14	0.79
1:C:570:LEU:HB3	1:C:590:MET:CE	2.12	0.79
1:G:220:ARG:NH1	1:G:223:LEU:HD22	1.95	0.79
1:H:235:VAL:HB	1:H:243:ILE:HA	1.65	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:HG12	1:A:323:HIS:H	1.47	0.79
1:B:322:VAL:HG12	1:B:323:HIS:H	1.47	0.79
1:B:441:LYS:HB2	1:B:560:LEU:CD2	2.12	0.79
1:C:246:TYR:HD1	1:C:258:VAL:CB	1.90	0.79
1:D:253:VAL:HB	1:D:255:PHE:CZ	2.18	0.79
1:F:533:LEU:HD23	1:F:629:VAL:CG1	2.13	0.79
1:G:358:GLY:O	1:G:359:LEU:HB2	1.82	0.79
1:A:434:TRP:HZ3	1:A:568:ARG:HG3	1.47	0.79
1:A:570:LEU:HD23	1:A:590:MET:HG2	1.64	0.79
1:B:422:THR:HB	1:B:585:GLY:CA	2.13	0.79
1:C:235:VAL:HB	1:C:243:ILE:HA	1.64	0.79
1:C:322:VAL:HG12	1:C:323:HIS:H	1.48	0.79
1:E:419:ARG:HA	1:E:587:SER:OG	1.81	0.79
1:H:219:PHE:C	1:H:220:ARG:CG	2.49	0.79
1:H:358:GLY:O	1:H:359:LEU:HB2	1.82	0.79
1:A:409:SER:CB	1:A:412:ILE:HD12	2.13	0.79
1:D:220:ARG:HH12	1:D:223:LEU:HD22	1.47	0.79
1:E:651:GLN:NE2	1:F:492:ILE:HG23	1.97	0.79
1:C:134:ARG:CA	1:C:300:PHE:HZ	1.96	0.78
1:C:358:GLY:O	1:C:359:LEU:HB2	1.81	0.78
1:D:245:VAL:HG12	1:D:246:TYR:H	1.47	0.78
1:D:637:ARG:O	1:D:641:LYS:HB2	1.81	0.78
1:E:134:ARG:HB2	1:E:300:PHE:CE1	2.17	0.78
1:G:409:SER:CB	1:G:412:ILE:HD12	2.13	0.78
1:D:219:PHE:C	1:D:220:ARG:CG	2.46	0.78
1:D:433:ILE:HB	1:D:571:TYR:CZ	2.19	0.78
1:E:494:LEU:HD12	1:E:514:TRP:HE3	1.46	0.78
1:F:434:TRP:HE3	1:F:568:ARG:HA	1.44	0.78
1:H:217:THR:OG1	1:H:218:GLY:N	2.08	0.78
1:B:282:MET:CB	1:B:286:ARG:HG3	2.14	0.78
1:C:220:ARG:HH12	1:C:223:LEU:HD22	1.47	0.78
1:D:119:GLU:HB3	1:D:121:PRO:HD2	1.66	0.78
1:D:660:ILE:HG22	1:D:661:ALA:H	1.49	0.78
1:E:120:GLY:O	1:E:124:THR:N	2.16	0.78
1:E:322:VAL:HG12	1:E:323:HIS:H	1.46	0.78
1:F:419:ARG:H	1:F:420:PRO:CD	1.97	0.78
1:C:119:GLU:HB3	1:C:121:PRO:HD2	1.64	0.78
1:D:120:GLY:O	1:D:124:THR:N	2.17	0.78
1:A:580:ASP:HB3	1:D:579:ARG:NH2	1.98	0.78
1:D:235:VAL:HB	1:D:243:ILE:HA	1.65	0.78
1:D:319:SER:OG	1:D:403:LEU:HB2	1.83	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:409:SER:CB	1:E:412:ILE:HD12	2.14	0.78
1:F:473:THR:CG2	1:F:533:LEU:HD22	2.04	0.78
1:G:394:LYS:HE3	1:G:609:TYR:O	1.83	0.78
1:H:26:PHE:CE2	1:H:181:GLU:OE1	2.37	0.78
1:G:245:VAL:HG12	1:G:246:TYR:H	1.48	0.78
1:C:282:MET:HB2	1:C:286:ARG:CG	2.13	0.78
1:F:253:VAL:HB	1:F:255:PHE:CZ	2.19	0.78
1:A:217:THR:OG1	1:A:218:GLY:N	2.12	0.78
1:B:434:TRP:CD1	1:B:435:GLN:N	2.51	0.78
1:B:571:TYR:CZ	1:B:590:MET:SD	2.77	0.78
1:F:359:LEU:HA	1:F:460:ARG:HH12	1.49	0.78
1:B:263:ASN:ND2	1:B:265:LEU:HB2	1.96	0.78
1:F:134:ARG:CA	1:F:300:PHE:HZ	1.93	0.78
1:H:434:TRP:CZ3	1:H:568:ARG:CA	2.64	0.78
1:C:282:MET:CB	1:C:286:ARG:HG3	2.13	0.77
1:D:547:LEU:CD1	1:D:615:THR:HG22	2.13	0.77
1:H:419:ARG:H	1:H:420:PRO:CD	1.97	0.77
1:E:422:THR:HB	1:E:585:GLY:C	2.03	0.77
1:G:120:GLY:O	1:G:124:THR:N	2.17	0.77
1:A:220:ARG:HH12	1:A:223:LEU:HD22	1.46	0.77
1:B:185:THR:HG23	1:B:187:GLN:CG	2.09	0.77
1:C:409:SER:CB	1:C:412:ILE:HD12	2.15	0.77
1:C:419:ARG:H	1:C:420:PRO:CD	1.97	0.77
1:G:219:PHE:C	1:G:220:ARG:CG	2.51	0.77
1:H:282:MET:HB2	1:H:286:ARG:CG	2.14	0.77
1:A:510:LEU:HD12	1:A:657:LEU:CD1	2.14	0.77
1:B:387:ILE:HD12	1:B:450:GLY:CA	2.14	0.77
1:D:434:TRP:HB3	1:D:571:TYR:HD1	1.43	0.77
1:D:660:ILE:CG2	1:D:661:ALA:N	2.48	0.77
1:H:219:PHE:O	1:H:220:ARG:HG3	1.84	0.77
1:A:533:LEU:CD2	1:A:629:VAL:HG13	2.15	0.77
1:B:419:ARG:H	1:B:420:PRO:CD	1.96	0.77
1:B:476:CYS:CB	1:B:636:MET:SD	2.72	0.77
1:C:547:LEU:CD1	1:C:615:THR:CG2	2.51	0.77
1:D:249:LEU:CD2	1:D:252:ALA:HA	2.15	0.77
1:F:249:LEU:CD2	1:F:252:ALA:HA	2.15	0.77
1:A:245:VAL:HG12	1:A:246:TYR:H	1.48	0.77
1:A:387:ILE:HD11	1:A:449:GLN:HG3	1.67	0.77
1:B:282:MET:HB2	1:B:286:ARG:CG	2.14	0.77
1:E:220:ARG:HH12	1:E:223:LEU:HD22	1.49	0.77
1:E:272:LYS:HB2	1:E:306:ILE:CG2	2.15	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:253:VAL:HB	1:G:255:PHE:CZ	2.20	0.77
1:B:119:GLU:CB	1:B:121:PRO:HD2	2.14	0.77
1:E:492:ILE:HG23	1:F:651:GLN:HE22	1.48	0.77
1:H:220:ARG:NH1	1:H:223:LEU:HD22	1.99	0.77
1:H:245:VAL:HG12	1:H:246:TYR:H	1.49	0.77
1:A:253:VAL:HB	1:A:255:PHE:CZ	2.20	0.77
1:A:529:GLU:HG3	1:A:633:MET:CE	2.14	0.77
1:F:529:GLU:HG3	1:F:633:MET:HE1	1.67	0.77
1:H:282:MET:CB	1:H:286:ARG:HG3	2.13	0.77
1:A:120:GLY:O	1:A:124:THR:N	2.18	0.77
1:C:134:ARG:HB2	1:C:300:PHE:CE1	2.19	0.77
1:C:434:TRP:HE3	1:C:568:ARG:HA	1.50	0.77
1:D:441:LYS:HD2	1:D:561:ASP:OD1	1.84	0.77
1:E:570:LEU:HB3	1:E:590:MET:CE	2.15	0.77
1:F:235:VAL:HB	1:F:243:ILE:HA	1.67	0.77
1:B:527:GLU:C	1:B:529:GLU:H	1.87	0.77
1:C:193:LEU:HB2	1:C:196:GLN:HE22	1.48	0.77
1:D:282:MET:HB2	1:D:286:ARG:CG	2.13	0.77
1:F:26:PHE:CZ	1:F:179:CYS:HB3	2.19	0.77
1:F:517:MET:HE3	1:F:647:GLN:OE1	1.85	0.77
1:H:118:LYS:CG	1:H:264:HIS:O	2.31	0.77
1:H:409:SER:CB	1:H:412:ILE:HD12	2.15	0.77
1:H:582:ARG:H	1:H:582:ARG:HD2	1.49	0.77
1:A:219:PHE:O	1:A:220:ARG:HG3	1.85	0.76
1:B:479:LEU:C	1:B:640:GLU:OE2	2.24	0.76
1:C:220:ARG:NH1	1:C:223:LEU:HD22	1.99	0.76
1:C:253:VAL:HB	1:C:255:PHE:CZ	2.20	0.76
1:C:582:ARG:H	1:C:582:ARG:HD2	1.50	0.76
1:D:433:ILE:HB	1:D:571:TYR:OH	1.84	0.76
1:D:536:LYS:HB3	1:D:625:LEU:CD1	2.16	0.76
1:F:245:VAL:HG12	1:F:246:TYR:H	1.48	0.76
1:G:402:SER:HA	1:G:609:TYR:CD1	2.20	0.76
1:C:107:TYR:O	1:C:110:GLN:N	2.18	0.76
1:C:185:THR:HG23	1:C:187:GLN:CG	2.08	0.76
1:D:515:ARG:HA	1:D:518:GLU:CD	2.04	0.76
1:E:220:ARG:NH1	1:E:223:LEU:HD22	1.99	0.76
1:E:282:MET:HB2	1:E:286:ARG:CG	2.11	0.76
1:F:272:LYS:HB2	1:F:306:ILE:CG2	2.15	0.76
1:F:409:SER:CB	1:F:412:ILE:HD12	2.14	0.76
1:A:235:VAL:HB	1:A:243:ILE:HA	1.66	0.76
1:A:419:ARG:H	1:A:420:PRO:CD	1.97	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:GLY:O	1:B:124:THR:N	2.18	0.76
1:C:434:TRP:CD1	1:C:435:GLN:N	2.54	0.76
1:G:272:LYS:HB2	1:G:306:ILE:CG2	2.16	0.76
1:G:359:LEU:HA	1:G:460:ARG:NH1	2.00	0.76
1:G:570:LEU:HB3	1:G:590:MET:CE	2.15	0.76
1:A:219:PHE:C	1:A:220:ARG:CG	2.49	0.76
1:A:220:ARG:NH1	1:A:223:LEU:HD22	2.00	0.76
1:A:422:THR:HB	1:A:585:GLY:HA2	1.64	0.76
1:B:409:SER:CB	1:B:412:ILE:HD12	2.15	0.76
1:C:272:LYS:HB2	1:C:306:ILE:CG2	2.15	0.76
1:C:515:ARG:HA	1:C:518:GLU:CD	2.04	0.76
1:H:193:LEU:HB2	1:H:196:GLN:HE22	1.49	0.76
1:B:235:VAL:HB	1:B:243:ILE:HA	1.67	0.76
1:B:358:GLY:O	1:B:359:LEU:HB2	1.83	0.76
1:C:485:PHE:CE2	1:D:485:PHE:CB	2.69	0.76
1:D:220:ARG:NH1	1:D:223:LEU:HD22	1.98	0.76
1:F:521:VAL:HG22	1:F:643:VAL:CG1	2.15	0.76
1:A:107:TYR:CD1	1:A:153:LEU:HD12	2.21	0.76
1:C:286:ARG:HA	1:C:290:THR:HG22	1.67	0.76
1:D:419:ARG:H	1:D:420:PRO:CD	1.97	0.76
1:D:430:TRP:HB3	1:D:571:TYR:CD2	2.17	0.76
1:E:515:ARG:HA	1:E:518:GLU:CD	2.06	0.76
1:F:119:GLU:HB3	1:F:121:PRO:HD2	1.68	0.76
1:G:235:VAL:HB	1:G:243:ILE:HA	1.68	0.76
1:G:434:TRP:HB3	1:G:571:TYR:HD1	1.49	0.76
1:A:316:ASN:O	1:A:388:PHE:O	2.04	0.76
1:C:434:TRP:HB3	1:C:571:TYR:HD1	1.44	0.76
1:D:272:LYS:HB2	1:D:306:ILE:CG2	2.16	0.76
1:D:570:LEU:HB3	1:D:590:MET:CE	2.15	0.76
1:E:655:TRP:HE1	1:F:496:LYS:HB2	0.67	0.76
1:E:661:ALA:O	1:F:661:ALA:O	2.04	0.76
1:F:563:LEU:HD21	1:F:596:LEU:HB2	1.68	0.76
1:G:119:GLU:CB	1:G:121:PRO:HD2	2.16	0.76
1:A:473:THR:HG21	1:A:533:LEU:CD2	2.14	0.76
1:C:573:ARG:HH22	1:D:573:ARG:HH12	1.31	0.76
1:C:573:ARG:NH2	1:D:573:ARG:HH12	1.84	0.76
1:D:185:THR:HG23	1:D:187:GLN:CG	2.07	0.76
1:E:419:ARG:H	1:E:420:PRO:CD	1.98	0.76
1:E:658:LEU:HA	1:F:658:LEU:CD1	2.16	0.76
1:A:186:LEU:O	1:A:188:TYR:N	2.18	0.76
1:B:476:CYS:HA	1:B:636:MET:SD	2.25	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:TYR:CD1	1:E:153:LEU:HD12	2.21	0.76
1:H:119:GLU:CB	1:H:121:PRO:HD2	2.16	0.76
1:B:515:ARG:HA	1:B:518:GLU:CD	2.06	0.75
1:C:26:PHE:CE2	1:C:181:GLU:CD	2.58	0.75
1:C:662:CYS:SG	1:D:661:ALA:HB1	2.27	0.75
1:E:249:LEU:CD2	1:E:252:ALA:HA	2.16	0.75
1:E:666:ARG:NH1	1:F:502:GLU:HG3	2.01	0.75
1:F:193:LEU:HD22	1:F:231:TRP:CD1	2.21	0.75
1:A:118:LYS:CG	1:A:264:HIS:O	2.32	0.75
1:A:434:TRP:CD1	1:A:435:GLN:N	2.53	0.75
1:A:476:CYS:HB2	1:A:636:MET:SD	2.26	0.75
1:F:327:VAL:HG11	1:F:367:LEU:CB	2.16	0.75
1:A:582:ARG:H	1:A:582:ARG:HD2	1.51	0.75
1:B:272:LYS:HB2	1:B:306:ILE:CG2	2.16	0.75
1:B:500:GLN:HB3	1:B:505:ILE:CG1	2.16	0.75
1:F:443:ASP:O	1:F:446:ARG:CB	2.34	0.75
1:F:515:ARG:HA	1:F:518:GLU:CD	2.07	0.75
1:F:582:ARG:H	1:F:582:ARG:HD2	1.50	0.75
1:B:394:LYS:CE	1:B:401:ILE:HA	2.17	0.75
1:E:119:GLU:HB3	1:E:121:PRO:HD2	1.69	0.75
1:E:582:ARG:H	1:E:582:ARG:HD2	1.52	0.75
1:H:322:VAL:HG12	1:H:323:HIS:H	1.52	0.75
1:A:434:TRP:CZ3	1:A:568:ARG:CA	2.68	0.75
1:B:134:ARG:HB2	1:B:300:PHE:HE1	1.52	0.75
1:B:434:TRP:HE3	1:B:568:ARG:HA	1.45	0.75
1:C:533:LEU:HD23	1:C:629:VAL:HG13	1.67	0.75
1:D:171:LYS:HG3	1:D:171:LYS:O	1.87	0.75
1:D:193:LEU:HD22	1:D:231:TRP:CD1	2.20	0.75
1:E:272:LYS:HB2	1:E:306:ILE:HG21	1.68	0.75
1:G:26:PHE:CZ	1:G:179:CYS:HB3	2.21	0.75
1:G:193:LEU:HB2	1:G:196:GLN:HE22	1.51	0.75
1:H:443:ASP:O	1:H:446:ARG:HB2	1.86	0.75
1:C:272:LYS:HB2	1:C:306:ILE:HG21	1.68	0.75
1:A:430:TRP:HB3	1:A:571:TYR:HD2	1.50	0.75
1:B:107:TYR:CD1	1:B:153:LEU:HD12	2.22	0.75
1:B:536:LYS:O	1:B:625:LEU:HD13	1.87	0.75
1:C:424:THR:OG1	1:C:425:HIS:ND1	2.17	0.75
1:D:409:SER:CB	1:D:412:ILE:HD12	2.16	0.75
1:D:582:ARG:H	1:D:582:ARG:HD2	1.50	0.75
1:F:107:TYR:O	1:F:110:GLN:N	2.20	0.75
1:F:434:TRP:CD1	1:F:435:GLN:N	2.54	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LYS:HZ2	1:A:33:ILE:HG21	1.51	0.75
1:A:515:ARG:HA	1:A:518:GLU:CD	2.07	0.75
1:A:588:ASN:CG	1:A:589:ASP:H	1.89	0.75
1:B:357:SER:HA	1:B:453:THR:HB	1.68	0.75
1:E:496:LYS:HB2	1:F:655:TRP:HE1	0.66	0.75
1:G:327:VAL:HG11	1:G:367:LEU:CB	2.16	0.75
1:G:582:ARG:H	1:G:582:ARG:HD2	1.49	0.75
1:A:272:LYS:HB2	1:A:306:ILE:CG2	2.17	0.75
1:B:394:LYS:HE2	1:B:401:ILE:CA	2.17	0.75
1:C:107:TYR:CD1	1:C:153:LEU:HD12	2.22	0.75
1:D:107:TYR:CD1	1:D:153:LEU:HD12	2.22	0.75
1:E:502:GLU:HG3	1:F:666:ARG:HH12	1.51	0.75
1:F:185:THR:HG23	1:F:187:GLN:CG	2.08	0.75
1:G:387:ILE:CD1	1:G:450:GLY:HA2	2.16	0.75
1:G:434:TRP:CZ3	1:G:568:ARG:CA	2.70	0.75
1:G:473:THR:HG21	1:G:533:LEU:CD2	2.14	0.75
1:H:327:VAL:HG11	1:H:367:LEU:CB	2.17	0.75
1:B:193:LEU:HB2	1:B:196:GLN:HE22	1.52	0.74
1:B:494:LEU:CD1	1:B:514:TRP:HB3	2.17	0.74
1:C:533:LEU:CD2	1:C:629:VAL:HG11	2.13	0.74
1:E:502:GLU:HG3	1:F:666:ARG:HH11	1.51	0.74
1:E:660:ILE:HG22	1:E:661:ALA:H	1.51	0.74
1:E:665:VAL:CG2	1:F:665:VAL:HG22	2.17	0.74
1:F:118:LYS:HG2	1:F:265:LEU:HA	1.69	0.74
1:H:107:TYR:CD1	1:H:153:LEU:HD12	2.22	0.74
1:A:107:TYR:O	1:A:110:GLN:N	2.20	0.74
1:A:327:VAL:HG11	1:A:367:LEU:CB	2.16	0.74
1:B:118:LYS:CG	1:B:264:HIS:O	2.34	0.74
1:B:582:ARG:H	1:B:582:ARG:HD2	1.51	0.74
1:C:654:LEU:CD1	1:D:655:TRP:CE3	2.69	0.74
1:D:660:ILE:CG2	1:D:661:ALA:H	2.00	0.74
1:E:235:VAL:HB	1:E:243:ILE:HA	1.68	0.74
1:E:503:PHE:O	1:E:505:ILE:HG13	1.86	0.74
1:F:517:MET:O	1:F:517:MET:HG2	1.87	0.74
1:F:521:VAL:HG22	1:F:643:VAL:HG13	1.67	0.74
1:F:660:ILE:CG2	1:F:661:ALA:N	2.51	0.74
1:H:412:ILE:HG23	1:H:433:ILE:HD12	1.69	0.74
1:H:570:LEU:HB3	1:H:590:MET:HE2	1.69	0.74
1:A:422:THR:HB	1:A:585:GLY:HA3	1.69	0.74
1:F:107:TYR:CD1	1:F:153:LEU:HD12	2.22	0.74
1:F:394:LYS:HG3	1:F:613:SER:HB2	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LYS:HZ2	1:B:33:ILE:HG21	1.52	0.74
1:C:217:THR:OG1	1:C:218:GLY:N	2.15	0.74
1:E:424:THR:OG1	1:E:425:HIS:ND1	2.19	0.74
1:E:660:ILE:CG2	1:E:661:ALA:N	2.50	0.74
1:H:588:ASN:CG	1:H:589:ASP:H	1.89	0.74
1:F:193:LEU:HB2	1:F:196:GLN:HE22	1.53	0.74
1:H:272:LYS:HB2	1:H:306:ILE:CG2	2.17	0.74
1:H:357:SER:HA	1:H:453:THR:HB	1.67	0.74
1:D:18:LYS:HZ2	1:D:33:ILE:HG21	1.52	0.74
1:E:28:TYR:O	1:E:44:LYS:HA	1.87	0.74
1:A:119:GLU:CB	1:A:121:PRO:HD2	2.16	0.74
1:C:316:ASN:O	1:C:388:PHE:O	2.06	0.74
1:D:26:PHE:HE2	1:D:181:GLU:OE1	1.69	0.74
1:D:107:TYR:O	1:D:110:GLN:N	2.20	0.74
1:D:186:LEU:O	1:D:188:TYR:N	2.20	0.74
1:D:193:LEU:HB2	1:D:196:GLN:HE22	1.53	0.74
1:G:316:ASN:O	1:G:388:PHE:O	2.06	0.74
1:H:387:ILE:CD1	1:H:449:GLN:HG3	2.06	0.74
1:B:286:ARG:HA	1:B:290:THR:HG22	1.70	0.74
1:B:540:LEU:HD11	1:B:621:LYS:HB3	1.69	0.74
1:D:588:ASN:CG	1:D:589:ASP:H	1.89	0.74
1:E:107:TYR:O	1:E:110:GLN:N	2.21	0.74
1:E:658:LEU:HA	1:F:658:LEU:HD12	1.69	0.74
1:A:517:MET:HG2	1:A:517:MET:O	1.88	0.74
1:C:18:LYS:HZ2	1:C:33:ILE:HG21	1.52	0.74
1:D:26:PHE:CE2	1:D:181:GLU:CD	2.61	0.74
1:H:120:GLY:O	1:H:124:THR:N	2.19	0.74
1:H:430:TRP:HB3	1:H:571:TYR:HD2	1.53	0.74
1:B:500:GLN:C	1:B:505:ILE:HG12	2.08	0.74
1:B:107:TYR:O	1:B:110:GLN:N	2.20	0.73
1:C:658:LEU:CD1	1:D:658:LEU:HA	2.17	0.73
1:E:143:HIS:HD2	1:E:145:ASP:O	1.71	0.73
1:A:193:LEU:HB2	1:A:196:GLN:HE22	1.52	0.73
1:A:529:GLU:HG3	1:A:633:MET:HE1	1.70	0.73
1:A:660:ILE:HG22	1:A:661:ALA:H	1.53	0.73
1:C:646:ARG:O	1:C:650:ARG:HG2	1.89	0.73
1:C:660:ILE:CG2	1:C:661:ALA:N	2.50	0.73
1:E:319:SER:OG	1:E:403:LEU:CB	2.35	0.73
1:F:143:HIS:HD2	1:F:145:ASP:O	1.70	0.73
1:F:387:ILE:HD11	1:F:449:GLN:HG3	1.69	0.73
1:G:389:LEU:HD11	1:G:454:SER:OG	1.87	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:451:GLN:CD	1:H:611:GLN:NE2	2.41	0.73
1:B:119:GLU:HB3	1:B:121:PRO:HD2	1.69	0.73
1:B:517:MET:O	1:B:517:MET:HG2	1.87	0.73
1:D:28:TYR:O	1:D:44:LYS:HA	1.89	0.73
1:F:430:TRP:CE3	1:F:574:LEU:HD22	2.23	0.73
1:F:570:LEU:HD23	1:F:590:MET:CG	2.16	0.73
1:G:185:THR:HG23	1:G:187:GLN:CG	2.08	0.73
1:G:249:LEU:CD2	1:G:252:ALA:HA	2.18	0.73
1:G:588:ASN:CG	1:G:589:ASP:H	1.91	0.73
1:H:570:LEU:HB3	1:H:590:MET:HE3	1.69	0.73
1:A:171:LYS:HG3	1:A:171:LYS:O	1.87	0.73
1:C:28:TYR:O	1:C:44:LYS:HA	1.89	0.73
1:D:438:ARG:HG2	1:D:564:GLU:CG	2.18	0.73
1:E:171:LYS:HG3	1:E:171:LYS:O	1.88	0.73
1:E:654:LEU:CD1	1:F:655:TRP:CZ3	2.70	0.73
1:H:119:GLU:HB3	1:H:121:PRO:HD2	1.71	0.73
1:A:134:ARG:HB2	1:A:300:PHE:HE1	1.53	0.73
1:A:424:THR:OG1	1:A:425:HIS:ND1	2.19	0.73
1:B:134:ARG:CA	1:B:300:PHE:HZ	2.01	0.73
1:B:186:LEU:O	1:B:188:TYR:N	2.22	0.73
1:B:249:LEU:CD2	1:B:252:ALA:HA	2.18	0.73
1:C:219:PHE:O	1:C:220:ARG:HG3	1.85	0.73
1:F:186:LEU:O	1:F:188:TYR:N	2.22	0.73
1:F:353:LEU:HB3	1:F:361:LEU:HD12	1.70	0.73
1:H:107:TYR:O	1:H:110:GLN:N	2.21	0.73
1:H:171:LYS:HG3	1:H:171:LYS:O	1.88	0.73
1:F:660:ILE:HG22	1:F:661:ALA:H	1.53	0.73
1:G:171:LYS:HG3	1:G:171:LYS:O	1.88	0.73
1:A:143:HIS:HD2	1:A:145:ASP:O	1.71	0.73
1:B:26:PHE:HE2	1:B:181:GLU:OE1	1.70	0.73
1:C:660:ILE:CG2	1:C:661:ALA:H	2.02	0.73
1:D:422:THR:HB	1:D:585:GLY:C	2.09	0.73
1:E:193:LEU:HB2	1:E:196:GLN:HE22	1.53	0.73
1:H:466:SER:O	1:H:541:GLN:NE2	2.21	0.73
1:A:28:TYR:O	1:A:44:LYS:HA	1.88	0.73
1:C:143:HIS:HD2	1:C:145:ASP:O	1.72	0.73
1:C:533:LEU:CD2	1:C:629:VAL:HG13	2.17	0.73
1:C:660:ILE:HG22	1:C:661:ALA:H	1.52	0.73
1:E:480:LYS:HE3	1:E:527:GLU:HB2	1.71	0.73
1:H:424:THR:OG1	1:H:425:HIS:ND1	2.18	0.73
1:C:517:MET:O	1:C:517:MET:HG2	1.87	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:LYS:CG	1:D:264:HIS:O	2.37	0.73
1:E:316:ASN:O	1:E:388:PHE:O	2.06	0.73
1:E:651:GLN:NE2	1:F:492:ILE:CG2	2.52	0.73
1:E:660:ILE:CG2	1:E:661:ALA:H	2.01	0.73
1:F:171:LYS:O	1:F:171:LYS:HG3	1.88	0.73
1:F:536:LYS:HB3	1:F:625:LEU:CD1	2.18	0.73
1:G:472:MET:HG2	1:G:633:MET:HB2	1.70	0.73
1:H:186:LEU:O	1:H:188:TYR:N	2.22	0.73
1:H:254:LYS:O	1:H:255:PHE:CD2	2.42	0.73
1:B:588:ASN:CG	1:B:589:ASP:H	1.91	0.73
1:C:485:PHE:CZ	1:D:485:PHE:HB2	2.23	0.73
1:C:666:ARG:HG3	1:D:503:PHE:CE1	2.24	0.73
1:E:254:LYS:C	1:E:255:PHE:CG	2.62	0.73
1:C:665:VAL:HG13	1:D:665:VAL:HG13	1.69	0.72
1:E:422:THR:HB	1:E:585:GLY:HA2	1.68	0.72
1:E:479:LEU:HD11	1:E:641:LYS:HG3	1.70	0.72
1:F:517:MET:CE	1:F:647:GLN:OE1	2.37	0.72
1:H:472:MET:SD	1:H:633:MET:HB2	2.30	0.72
1:A:660:ILE:CG2	1:A:661:ALA:N	2.51	0.72
1:D:143:HIS:HD2	1:D:145:ASP:O	1.71	0.72
1:E:18:LYS:HZ2	1:E:33:ILE:HD12	1.53	0.72
1:E:111:PHE:CZ	1:E:572:ARG:HG3	2.23	0.72
1:F:28:TYR:O	1:F:44:LYS:HA	1.88	0.72
1:F:387:ILE:CD1	1:F:450:GLY:CA	2.67	0.72
1:G:107:TYR:CD1	1:G:153:LEU:HD12	2.23	0.72
1:G:186:LEU:O	1:G:188:TYR:N	2.22	0.72
1:E:134:ARG:CA	1:E:300:PHE:CZ	2.72	0.72
1:E:430:TRP:HB3	1:E:571:TYR:HD2	1.52	0.72
1:H:286:ARG:HA	1:H:290:THR:HG22	1.72	0.72
1:A:353:LEU:HB3	1:A:361:LEU:HD12	1.71	0.72
1:B:327:VAL:HG11	1:B:367:LEU:CB	2.18	0.72
1:B:660:ILE:CG2	1:B:661:ALA:N	2.52	0.72
1:D:286:ARG:HA	1:D:290:THR:HG22	1.71	0.72
1:E:186:LEU:O	1:E:188:TYR:N	2.21	0.72
1:G:107:TYR:O	1:G:110:GLN:N	2.22	0.72
1:B:402:SER:HA	1:B:609:TYR:CD1	2.25	0.72
1:B:419:ARG:O	1:B:419:ARG:HG2	1.90	0.72
1:B:424:THR:OG1	1:B:425:HIS:ND1	2.18	0.72
1:B:660:ILE:HG22	1:B:661:ALA:H	1.55	0.72
1:C:286:ARG:HA	1:C:290:THR:CG2	2.20	0.72
1:F:120:GLY:O	1:F:124:THR:N	2.20	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ARG:HG2	1:A:286:ARG:NH1	2.05	0.72
1:F:412:ILE:HG23	1:F:433:ILE:HD12	1.72	0.72
1:G:119:GLU:HB3	1:G:121:PRO:HD2	1.72	0.72
1:G:143:HIS:HD2	1:G:145:ASP:O	1.73	0.72
1:B:28:TYR:O	1:B:44:LYS:HA	1.89	0.72
1:B:438:ARG:NH1	1:B:568:ARG:HH21	1.87	0.72
1:C:419:ARG:HG2	1:C:419:ARG:O	1.89	0.72
1:F:424:THR:OG1	1:F:425:HIS:ND1	2.19	0.72
1:H:143:HIS:HD2	1:H:145:ASP:O	1.73	0.72
1:H:419:ARG:HG2	1:H:419:ARG:O	1.88	0.72
1:A:263:ASN:HD21	1:A:265:LEU:CB	1.99	0.72
1:B:550:ASN:HD21	1:B:611:GLN:CG	2.01	0.72
1:C:422:THR:HB	1:C:585:GLY:C	2.09	0.72
1:C:480:LYS:NZ	1:C:527:GLU:HB2	2.04	0.72
1:D:412:ILE:HG23	1:D:433:ILE:HD12	1.71	0.72
1:E:588:ASN:CG	1:E:589:ASP:H	1.92	0.72
1:F:322:VAL:HG12	1:F:323:HIS:N	2.05	0.72
1:F:359:LEU:HA	1:F:460:ARG:NH1	2.04	0.72
1:C:419:ARG:HA	1:C:587:SER:CB	2.19	0.72
1:G:28:TYR:O	1:G:44:LYS:HA	1.88	0.72
1:A:286:ARG:HA	1:A:290:THR:HG22	1.72	0.72
1:A:337:LYS:HD3	1:A:348:GLU:HB3	1.72	0.72
1:F:434:TRP:HZ3	1:F:568:ARG:HG3	1.53	0.72
1:A:646:ARG:O	1:A:650:ARG:HG2	1.90	0.71
1:B:254:LYS:C	1:B:255:PHE:CG	2.64	0.71
1:C:654:LEU:HD23	1:D:654:LEU:HD21	1.66	0.71
1:A:433:ILE:CG2	1:A:571:TYR:OH	2.38	0.71
1:B:134:ARG:HB2	1:B:300:PHE:CE1	2.25	0.71
1:C:284:HIS:NE2	1:E:342:GLN:NE2	2.38	0.71
1:D:517:MET:HG2	1:D:517:MET:O	1.90	0.71
1:E:286:ARG:HA	1:E:290:THR:HG22	1.70	0.71
1:E:419:ARG:O	1:E:419:ARG:HG2	1.89	0.71
1:E:646:ARG:O	1:E:650:ARG:HG2	1.90	0.71
1:F:588:ASN:CG	1:F:589:ASP:H	1.93	0.71
1:H:28:TYR:O	1:H:44:LYS:HA	1.89	0.71
1:C:171:LYS:O	1:C:171:LYS:HG3	1.89	0.71
1:C:387:ILE:HD11	1:C:449:GLN:HG3	1.70	0.71
1:C:486:PHE:CE1	1:C:647:GLN:HB3	2.25	0.71
1:C:643:VAL:O	1:C:644:VAL:HG23	1.90	0.71
1:D:337:LYS:HD3	1:D:348:GLU:HB3	1.72	0.71
1:E:254:LYS:O	1:E:255:PHE:CD2	2.43	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:GLN:C	1:A:232:HIS:N	2.43	0.71
1:A:510:LEU:HD12	1:A:657:LEU:HD12	1.72	0.71
1:A:665:VAL:HG13	1:B:665:VAL:CG1	2.16	0.71
1:B:475:GLU:O	1:B:478:GLN:N	2.22	0.71
1:C:337:LYS:HD3	1:C:348:GLU:HB3	1.72	0.71
1:D:322:VAL:HG12	1:D:323:HIS:N	2.04	0.71
1:E:409:SER:HB2	1:E:412:ILE:HD12	1.72	0.71
1:H:249:LEU:CD2	1:H:252:ALA:HA	2.17	0.71
1:H:254:LYS:C	1:H:255:PHE:CG	2.64	0.71
1:H:434:TRP:CD1	1:H:434:TRP:C	2.64	0.71
1:B:171:LYS:HG3	1:B:171:LYS:O	1.89	0.71
1:B:272:LYS:HB2	1:B:306:ILE:HG21	1.72	0.71
1:F:272:LYS:HB2	1:F:306:ILE:HG21	1.70	0.71
1:G:322:VAL:HG12	1:G:323:HIS:N	2.06	0.71
1:H:185:THR:HG23	1:H:187:GLN:CG	2.11	0.71
1:B:26:PHE:HE2	1:B:181:GLU:CD	1.92	0.71
1:D:191:PRO:HG3	1:D:234:LYS:NZ	2.06	0.71
1:D:327:VAL:HG11	1:D:367:LEU:CB	2.19	0.71
1:D:646:ARG:O	1:D:650:ARG:HG2	1.89	0.71
1:F:118:LYS:CG	1:F:265:LEU:HA	2.20	0.71
1:G:337:LYS:HD3	1:G:348:GLU:HB3	1.71	0.71
1:G:341:GLN:OE1	1:G:347:PRO:HB3	1.89	0.71
1:H:248:ASP:C	1:H:248:ASP:OD1	2.29	0.71
1:B:494:LEU:CD1	1:B:514:TRP:HE3	2.00	0.71
1:B:646:ARG:O	1:B:650:ARG:HG2	1.90	0.71
1:C:412:ILE:HG23	1:C:433:ILE:HD12	1.73	0.71
1:C:503:PHE:H	1:C:505:ILE:HD11	1.56	0.71
1:D:272:LYS:HB2	1:D:306:ILE:HG21	1.72	0.71
1:E:185:THR:HG23	1:E:187:GLN:CG	2.07	0.71
1:E:417:PRO:O	1:E:418:LYS:HG3	1.91	0.71
1:G:286:ARG:HA	1:G:290:THR:HG22	1.72	0.71
1:H:337:LYS:HD3	1:H:348:GLU:HB3	1.71	0.71
1:A:322:VAL:HG12	1:A:323:HIS:N	2.06	0.71
1:B:115:CYS:HB2	1:B:435:GLN:HG3	1.72	0.71
1:B:402:SER:HA	1:B:609:TYR:CG	2.26	0.71
1:C:254:LYS:C	1:C:255:PHE:CG	2.62	0.71
1:D:353:LEU:HB3	1:D:361:LEU:HD12	1.71	0.71
1:D:547:LEU:HD13	1:D:615:THR:CG2	2.20	0.71
1:E:517:MET:O	1:E:517:MET:HG2	1.89	0.71
1:E:665:VAL:HG22	1:F:665:VAL:CG2	2.21	0.71
1:F:533:LEU:CD2	1:F:629:VAL:CG1	2.68	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:438:ARG:NH1	1:G:568:ARG:HH21	1.89	0.71
1:H:316:ASN:O	1:H:388:PHE:O	2.08	0.71
1:A:185:THR:HG23	1:A:187:GLN:CG	2.12	0.71
1:B:143:HIS:HD2	1:B:145:ASP:O	1.73	0.71
1:B:643:VAL:O	1:B:644:VAL:HG23	1.91	0.71
1:C:492:ILE:HG21	1:D:651:GLN:NE2	2.06	0.71
1:D:424:THR:OG1	1:D:425:HIS:ND1	2.17	0.71
1:G:272:LYS:HB2	1:G:306:ILE:HG21	1.72	0.71
1:G:353:LEU:HB3	1:G:361:LEU:HD12	1.71	0.71
1:H:134:ARG:CA	1:H:300:PHE:CZ	2.68	0.71
1:B:193:LEU:HD22	1:B:231:TRP:CD1	2.25	0.71
1:B:433:ILE:HB	1:B:571:TYR:CZ	2.26	0.71
1:B:444:CYS:C	1:B:446:ARG:H	1.94	0.71
1:F:286:ARG:HA	1:F:290:THR:HG22	1.73	0.71
1:A:249:LEU:CD2	1:A:252:ALA:HA	2.19	0.70
1:A:655:TRP:CZ3	1:B:654:LEU:HD12	2.26	0.70
1:B:412:ILE:HG23	1:B:433:ILE:HD12	1.73	0.70
1:B:479:LEU:HD12	1:B:640:GLU:HB3	1.72	0.70
1:C:179:CYS:CB	1:C:181:GLU:CG	2.66	0.70
1:B:253:VAL:HB	1:B:255:PHE:HZ	1.55	0.70
1:C:588:ASN:CG	1:C:589:ASP:H	1.92	0.70
1:D:419:ARG:HA	1:D:587:SER:OG	1.91	0.70
1:E:253:VAL:HB	1:E:255:PHE:HZ	1.53	0.70
1:F:337:LYS:HD3	1:F:348:GLU:HB3	1.73	0.70
1:F:646:ARG:O	1:F:650:ARG:HG2	1.91	0.70
1:G:409:SER:HB2	1:G:412:ILE:HD12	1.72	0.70
1:A:419:ARG:O	1:A:419:ARG:HG2	1.91	0.70
1:D:357:SER:HA	1:D:453:THR:HB	1.73	0.70
1:E:422:THR:HB	1:E:585:GLY:HA3	1.72	0.70
1:H:26:PHE:HZ	1:H:179:CYS:HB3	1.56	0.70
1:H:253:VAL:HB	1:H:255:PHE:HZ	1.55	0.70
1:A:409:SER:HB2	1:A:412:ILE:HD12	1.74	0.70
1:B:322:VAL:HG12	1:B:323:HIS:N	2.05	0.70
1:B:647:GLN:CD	1:B:647:GLN:N	2.44	0.70
1:C:497:TYR:HE2	1:C:511:LEU:HD22	1.56	0.70
1:E:503:PHE:H	1:E:505:ILE:HD11	1.55	0.70
1:E:480:LYS:CE	1:E:527:GLU:HB2	2.21	0.70
1:F:500:GLN:CB	1:F:505:ILE:HG12	2.21	0.70
1:G:130:SER:O	1:G:300:PHE:CE1	2.44	0.70
1:H:263:ASN:HD21	1:H:265:LEU:CB	1.99	0.70
1:H:341:GLN:OE1	1:H:347:PRO:HB3	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:PHE:CZ	1:A:179:CYS:HB3	2.27	0.70
1:D:286:ARG:HA	1:D:290:THR:CG2	2.22	0.70
1:F:263:ASN:HD21	1:F:265:LEU:CB	1.99	0.70
1:A:660:ILE:CG2	1:A:661:ALA:H	2.05	0.70
1:B:114:CYS:O	1:B:115:CYS:HB2	1.91	0.70
1:B:286:ARG:NH1	1:B:286:ARG:HG2	2.04	0.70
1:C:322:VAL:HG12	1:C:323:HIS:N	2.05	0.70
1:C:353:LEU:HB3	1:C:361:LEU:HD12	1.72	0.70
1:C:649:LYS:HA	1:C:652:GLN:HB2	1.73	0.70
1:D:187:GLN:CB	1:D:223:LEU:CD2	2.60	0.70
1:D:316:ASN:O	1:D:388:PHE:O	2.09	0.70
1:F:419:ARG:HG2	1:F:419:ARG:O	1.91	0.70
1:G:18:LYS:HZ2	1:G:33:ILE:HD12	1.55	0.70
1:H:18:LYS:HZ2	1:H:33:ILE:HD12	1.57	0.70
1:H:412:ILE:HG23	1:H:433:ILE:CD1	2.21	0.70
1:A:441:LYS:HB2	1:A:560:LEU:CD2	2.21	0.70
1:A:513:ALA:HB1	1:A:650:ARG:HH12	1.56	0.70
1:D:434:TRP:HE3	1:D:568:ARG:HA	1.52	0.70
1:E:337:LYS:HD3	1:E:348:GLU:HB3	1.72	0.70
1:G:434:TRP:CZ3	1:G:568:ARG:HG3	2.25	0.70
1:B:286:ARG:HA	1:B:290:THR:CG2	2.22	0.70
1:E:114:CYS:O	1:E:115:CYS:HB2	1.92	0.70
1:E:260:PRO:HG3	1:E:274:GLU:HG2	1.74	0.70
1:E:322:VAL:HG12	1:E:323:HIS:N	2.06	0.70
1:A:655:TRP:CZ3	1:B:654:LEU:CD1	2.75	0.70
1:C:263:ASN:HD21	1:C:265:LEU:CB	1.98	0.70
1:C:654:LEU:HD21	1:D:654:LEU:HD23	1.71	0.70
1:D:419:ARG:O	1:D:419:ARG:HG2	1.91	0.70
1:E:263:ASN:HD21	1:E:265:LEU:CB	2.02	0.70
1:G:571:TYR:CZ	1:G:590:MET:SD	2.85	0.70
1:B:33:ILE:HD11	1:B:40:GLN:CD	2.12	0.69
1:D:472:MET:SD	1:D:633:MET:HB2	2.31	0.69
1:E:248:ASP:OD1	1:E:248:ASP:C	2.30	0.69
1:E:286:ARG:HA	1:E:290:THR:CG2	2.21	0.69
1:G:412:ILE:HG23	1:G:433:ILE:HD12	1.74	0.69
1:A:118:LYS:HG2	1:A:265:LEU:HA	1.73	0.69
1:B:337:LYS:HD3	1:B:348:GLU:HB3	1.74	0.69
1:D:479:LEU:HD12	1:D:640:GLU:HB3	1.74	0.69
1:F:254:LYS:C	1:F:255:PHE:CG	2.65	0.69
1:H:272:LYS:HB2	1:H:306:ILE:HG21	1.72	0.69
1:A:412:ILE:HG23	1:A:433:ILE:HD12	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ASN:HD21	1:B:265:LEU:CB	2.01	0.69
1:E:33:ILE:HD11	1:E:40:GLN:CD	2.13	0.69
1:E:493:ASP:HB3	1:E:514:TRP:CH2	2.28	0.69
1:F:120:GLY:H	1:F:122:ILE:H	1.41	0.69
1:G:419:ARG:O	1:G:419:ARG:HG2	1.90	0.69
1:G:434:TRP:CD1	1:G:434:TRP:C	2.65	0.69
1:A:119:GLU:HB3	1:A:121:PRO:HD2	1.73	0.69
1:A:341:GLN:OE1	1:A:347:PRO:HB3	1.91	0.69
1:C:249:LEU:CD2	1:C:252:ALA:HA	2.18	0.69
1:D:422:THR:HG22	1:D:426:LEU:HD21	1.74	0.69
1:F:18:LYS:HZ2	1:F:33:ILE:HD12	1.57	0.69
1:F:230:GLN:C	1:F:232:HIS:N	2.44	0.69
1:H:115:CYS:HB2	1:H:435:GLN:HG3	1.74	0.69
1:B:16:GLU:HA	1:B:83:LEU:HD22	1.75	0.69
1:B:341:GLN:OE1	1:B:347:PRO:HB3	1.92	0.69
1:B:353:LEU:HB3	1:B:361:LEU:HD12	1.73	0.69
1:D:230:GLN:C	1:D:232:HIS:N	2.43	0.69
1:D:341:GLN:OE1	1:D:347:PRO:HB3	1.92	0.69
1:E:26:PHE:CE2	1:E:181:GLU:OE1	2.43	0.69
1:H:353:LEU:HB3	1:H:361:LEU:HD12	1.73	0.69
1:C:118:LYS:NZ	1:C:123:ARG:HH22	1.90	0.69
1:C:402:SER:HA	1:C:609:TYR:CG	2.27	0.69
1:D:350:GLU:HG2	1:D:391:ASP:HB2	1.75	0.69
1:E:62:ILE:HD12	1:E:94:LEU:HB2	1.74	0.69
1:E:497:TYR:HE2	1:E:511:LEU:HD22	1.53	0.69
1:H:33:ILE:HD11	1:H:40:GLN:CD	2.13	0.69
1:H:286:ARG:HA	1:H:290:THR:CG2	2.23	0.69
1:A:62:ILE:HD12	1:A:94:LEU:HB2	1.74	0.69
1:B:417:PRO:O	1:B:418:LYS:HG3	1.92	0.69
1:C:433:ILE:CG2	1:C:571:TYR:OH	2.40	0.69
1:F:409:SER:HB2	1:F:412:ILE:HD12	1.73	0.69
1:F:660:ILE:CG2	1:F:661:ALA:H	2.03	0.69
1:G:254:LYS:C	1:G:255:PHE:CG	2.66	0.69
1:A:660:ILE:C	1:A:662:CYS:H	1.96	0.69
1:B:434:TRP:CD1	1:B:434:TRP:C	2.65	0.69
1:B:521:VAL:CG1	1:B:643:VAL:HG12	2.22	0.69
1:C:33:ILE:HD11	1:C:40:GLN:CD	2.13	0.69
1:C:660:ILE:C	1:C:662:CYS:H	1.96	0.69
1:D:120:GLY:H	1:D:122:ILE:H	1.41	0.69
1:E:327:VAL:HG11	1:E:367:LEU:CB	2.21	0.69
1:F:179:CYS:CB	1:F:181:GLU:CG	2.67	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:341:GLN:OE1	1:F:347:PRO:HB3	1.93	0.69
1:F:496:LYS:O	1:F:499:GLU:HB2	1.93	0.69
1:H:62:ILE:HD12	1:H:94:LEU:HB2	1.74	0.69
1:H:419:ARG:N	1:H:420:PRO:HD3	2.03	0.69
1:A:134:ARG:HB2	1:A:300:PHE:CE1	2.27	0.69
1:B:120:GLY:H	1:B:122:ILE:H	1.40	0.69
1:B:438:ARG:HG2	1:B:564:GLU:CG	2.23	0.69
1:C:40:GLN:HB3	1:C:98:TYR:HD2	1.58	0.69
1:C:62:ILE:HD12	1:C:94:LEU:HB2	1.75	0.69
1:C:248:ASP:C	1:C:248:ASP:OD1	2.30	0.69
1:C:327:VAL:HG11	1:C:367:LEU:CB	2.21	0.69
1:D:16:GLU:HA	1:D:83:LEU:HD22	1.75	0.69
1:F:412:ILE:HG23	1:F:433:ILE:CD1	2.23	0.69
1:H:40:GLN:HB3	1:H:98:TYR:HD2	1.58	0.69
1:H:260:PRO:HB2	1:H:273:LEU:HD13	1.75	0.69
1:A:33:ILE:HD11	1:A:40:GLN:CD	2.13	0.69
1:A:254:LYS:C	1:A:255:PHE:CG	2.65	0.69
1:B:219:PHE:O	1:B:220:ARG:HG3	1.85	0.69
1:B:660:ILE:CG2	1:B:661:ALA:H	2.05	0.69
1:C:485:PHE:CD2	1:D:485:PHE:CD2	2.80	0.69
1:D:647:GLN:CD	1:D:647:GLN:N	2.46	0.69
1:E:40:GLN:HB3	1:E:98:TYR:HD2	1.58	0.69
1:E:478:GLN:HB2	1:F:478:GLN:HA	1.75	0.69
1:E:500:GLN:HB3	1:E:505:ILE:HG12	1.73	0.69
1:F:497:TYR:HE2	1:F:511:LEU:HD22	1.52	0.69
1:G:33:ILE:HD11	1:G:40:GLN:CD	2.13	0.69
1:H:143:HIS:CE1	1:H:167:LEU:HB2	2.28	0.69
1:B:62:ILE:HD12	1:B:94:LEU:HB2	1.74	0.68
1:B:496:LYS:O	1:B:499:GLU:HB2	1.94	0.68
1:C:186:LEU:O	1:C:188:TYR:N	2.24	0.68
1:C:496:LYS:O	1:C:499:GLU:HB2	1.93	0.68
1:D:254:LYS:C	1:D:255:PHE:CG	2.66	0.68
1:E:434:TRP:CD1	1:E:434:TRP:C	2.63	0.68
1:G:115:CYS:O	1:G:263:ASN:HA	1.93	0.68
1:A:272:LYS:HB2	1:A:306:ILE:HG21	1.73	0.68
1:D:319:SER:OG	1:D:403:LEU:CB	2.41	0.68
1:D:422:THR:HB	1:D:585:GLY:HA2	1.75	0.68
1:D:505:ILE:O	1:D:506:THR:O	2.10	0.68
1:E:120:GLY:H	1:E:122:ILE:H	1.39	0.68
1:H:319:SER:C	1:H:321:ARG:H	1.96	0.68
1:C:473:THR:HG21	1:C:533:LEU:HD21	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:ILE:HD13	1:D:651:GLN:NE2	2.04	0.68
1:D:26:PHE:HE2	1:D:181:GLU:CD	1.97	0.68
1:D:62:ILE:HD12	1:D:94:LEU:HB2	1.75	0.68
1:D:434:TRP:HZ3	1:D:568:ARG:CB	2.05	0.68
1:E:665:VAL:CG2	1:F:665:VAL:CG2	2.71	0.68
1:G:417:PRO:O	1:G:418:LYS:HG3	1.93	0.68
1:G:434:TRP:HZ3	1:G:568:ARG:CG	2.06	0.68
1:A:118:LYS:O	1:A:118:LYS:HG3	1.93	0.68
1:A:120:GLY:H	1:A:122:ILE:H	1.41	0.68
1:B:40:GLN:HB3	1:B:98:TYR:HD2	1.58	0.68
1:C:26:PHE:CE2	1:C:181:GLU:OE1	2.46	0.68
1:E:265:LEU:CD2	1:E:269:LEU:HB3	2.24	0.68
1:E:353:LEU:HB3	1:E:361:LEU:HD12	1.74	0.68
1:F:643:VAL:O	1:F:644:VAL:HG23	1.94	0.68
1:G:134:ARG:HB2	1:G:300:PHE:CE1	2.28	0.68
1:H:265:LEU:CD2	1:H:269:LEU:HB3	2.23	0.68
1:H:433:ILE:CG2	1:H:571:TYR:OH	2.42	0.68
1:A:286:ARG:HA	1:A:290:THR:CG2	2.24	0.68
1:A:517:MET:SD	1:A:650:ARG:CG	2.75	0.68
1:C:260:PRO:HB2	1:C:273:LEU:HD13	1.76	0.68
1:D:412:ILE:HG23	1:D:433:ILE:CD1	2.24	0.68
1:D:475:GLU:HG2	1:D:636:MET:HE3	1.75	0.68
1:E:16:GLU:HA	1:E:83:LEU:HD22	1.75	0.68
1:G:40:GLN:HB3	1:G:98:TYR:HD2	1.58	0.68
1:G:263:ASN:HD21	1:G:265:LEU:CB	1.99	0.68
1:A:16:GLU:HA	1:A:83:LEU:HD22	1.75	0.68
1:B:438:ARG:HG2	1:B:564:GLU:CD	2.13	0.68
1:C:114:CYS:O	1:C:115:CYS:HB2	1.93	0.68
1:C:549:ARG:O	1:C:550:ASN:HB2	1.93	0.68
1:E:191:PRO:HG3	1:E:234:LYS:NZ	2.08	0.68
1:E:486:PHE:HZ	1:E:517:MET:CE	2.05	0.68
1:F:16:GLU:HA	1:F:83:LEU:HD22	1.75	0.68
1:F:316:ASN:O	1:F:388:PHE:O	2.12	0.68
1:G:536:LYS:O	1:G:625:LEU:HD13	1.94	0.68
1:H:120:GLY:H	1:H:122:ILE:H	1.42	0.68
1:B:660:ILE:C	1:B:662:CYS:H	1.95	0.68
1:C:16:GLU:HA	1:C:83:LEU:HD22	1.76	0.68
1:C:286:ARG:NH1	1:C:286:ARG:HG2	2.08	0.68
1:D:409:SER:HB2	1:D:412:ILE:HD12	1.76	0.68
1:G:143:HIS:CE1	1:G:167:LEU:HB2	2.28	0.68
1:H:417:PRO:O	1:H:418:LYS:HG3	1.92	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:PRO:HG2	1:A:255:PHE:CE2	2.29	0.68
1:A:549:ARG:O	1:A:550:ASN:HB2	1.94	0.68
1:B:412:ILE:HG23	1:B:433:ILE:CD1	2.24	0.68
1:B:438:ARG:HG2	1:B:564:GLU:HG3	1.75	0.68
1:B:505:ILE:O	1:B:506:THR:O	2.11	0.68
1:D:419:ARG:N	1:D:420:PRO:HD3	2.04	0.68
1:D:494:LEU:HD12	1:D:514:TRP:CE3	2.22	0.68
1:F:62:ILE:HD12	1:F:94:LEU:HB2	1.74	0.68
1:F:417:PRO:O	1:F:418:LYS:HG3	1.93	0.68
1:H:394:LYS:HE2	1:H:401:ILE:HA	1.75	0.68
1:A:319:SER:C	1:A:321:ARG:H	1.96	0.68
1:B:434:TRP:HZ3	1:B:568:ARG:HG3	1.59	0.68
1:C:409:SER:HB2	1:C:412:ILE:HD12	1.74	0.68
1:C:417:PRO:O	1:C:418:LYS:HG3	1.93	0.68
1:C:647:GLN:CD	1:C:647:GLN:N	2.43	0.68
1:D:434:TRP:CD1	1:D:434:TRP:C	2.65	0.68
1:F:40:GLN:HB3	1:F:98:TYR:HD2	1.59	0.68
1:F:350:GLU:HG2	1:F:391:ASP:HB2	1.76	0.68
1:D:33:ILE:HD11	1:D:40:GLN:CD	2.14	0.68
1:D:286:ARG:HG2	1:D:286:ARG:NH1	2.08	0.68
1:D:479:LEU:HB3	1:D:640:GLU:OE2	1.94	0.68
1:D:643:VAL:O	1:D:644:VAL:HG23	1.94	0.68
1:F:434:TRP:HB3	1:F:571:TYR:HD1	1.51	0.68
1:F:434:TRP:CD1	1:F:434:TRP:C	2.67	0.68
1:G:16:GLU:HA	1:G:83:LEU:HD22	1.76	0.68
1:G:118:LYS:HG3	1:G:118:LYS:O	1.93	0.68
1:G:219:PHE:O	1:G:220:ARG:HG3	1.88	0.68
1:H:16:GLU:HA	1:H:83:LEU:HD22	1.74	0.68
1:H:115:CYS:CB	1:H:435:GLN:HG3	2.24	0.68
1:H:179:CYS:CB	1:H:181:GLU:CG	2.66	0.68
1:H:536:LYS:HB3	1:H:625:LEU:HD22	1.74	0.68
1:A:434:TRP:CD1	1:A:434:TRP:C	2.67	0.67
1:B:387:ILE:HD11	1:B:449:GLN:HG3	1.76	0.67
1:C:394:LYS:CG	1:C:613:SER:HB2	2.24	0.67
1:D:111:PHE:HZ	1:D:572:ARG:HG3	1.57	0.67
1:D:319:SER:C	1:D:321:ARG:H	1.97	0.67
1:E:286:ARG:NH1	1:E:286:ARG:HG2	2.09	0.67
1:E:643:VAL:O	1:E:644:VAL:HG23	1.93	0.67
1:F:254:LYS:O	1:F:255:PHE:CD2	2.47	0.67
1:G:475:GLU:CG	1:G:636:MET:CE	2.57	0.67
1:A:118:LYS:CG	1:A:265:LEU:HA	2.24	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:CA	1:A:300:PHE:HZ	2.06	0.67
1:A:318:VAL:O	1:A:320:GLY:N	2.27	0.67
1:B:254:LYS:O	1:B:255:PHE:CD2	2.46	0.67
1:D:219:PHE:O	1:D:220:ARG:HG3	1.82	0.67
1:E:647:GLN:CD	1:E:647:GLN:N	2.46	0.67
1:F:33:ILE:HD11	1:F:40:GLN:CD	2.13	0.67
1:F:319:SER:C	1:F:321:ARG:H	1.98	0.67
1:G:118:LYS:HG2	1:G:264:HIS:O	1.95	0.67
1:H:571:TYR:CE2	1:H:590:MET:HG3	2.29	0.67
1:B:571:TYR:CE2	1:B:590:MET:HG3	2.29	0.67
1:C:654:LEU:HD22	1:D:654:LEU:CD2	2.25	0.67
1:D:496:LYS:O	1:D:499:GLU:HB2	1.93	0.67
1:G:318:VAL:O	1:G:320:GLY:N	2.28	0.67
1:H:286:ARG:NH1	1:H:286:ARG:HG2	2.09	0.67
1:A:248:ASP:C	1:A:248:ASP:OD1	2.33	0.67
1:A:643:VAL:O	1:A:644:VAL:HG23	1.94	0.67
1:B:244:VAL:HG12	1:B:278:GLN:OE1	1.94	0.67
1:B:248:ASP:C	1:B:248:ASP:OD1	2.32	0.67
1:B:319:SER:C	1:B:321:ARG:H	1.98	0.67
1:B:479:LEU:O	1:B:640:GLU:OE2	2.13	0.67
1:D:417:PRO:O	1:D:418:LYS:HG3	1.93	0.67
1:F:248:ASP:C	1:F:248:ASP:OD1	2.33	0.67
1:C:253:VAL:HB	1:C:255:PHE:HZ	1.58	0.67
1:C:283:TRP:O	1:C:284:HIS:HB2	1.94	0.67
1:C:434:TRP:CD1	1:C:434:TRP:C	2.66	0.67
1:F:505:ILE:O	1:F:506:THR:O	2.13	0.67
1:A:505:ILE:O	1:A:506:THR:O	2.12	0.67
1:B:409:SER:HB2	1:B:412:ILE:HD12	1.76	0.67
1:C:412:ILE:HG23	1:C:433:ILE:CD1	2.24	0.67
1:D:418:LYS:O	1:D:419:ARG:HB2	1.95	0.67
1:D:438:ARG:CG	1:D:564:GLU:HG3	2.25	0.67
1:E:350:GLU:HG2	1:E:391:ASP:HB2	1.76	0.67
1:F:503:PHE:H	1:F:505:ILE:HD11	1.59	0.67
1:G:62:ILE:HD12	1:G:94:LEU:HB2	1.76	0.67
1:G:71:PRO:O	1:G:72:ASN:HB2	1.94	0.67
1:G:179:CYS:CB	1:G:181:GLU:CG	2.67	0.67
1:G:419:ARG:N	1:G:420:PRO:HD3	2.03	0.67
1:A:105:ARG:O	1:A:108:LEU:N	2.28	0.67
1:F:143:HIS:CE1	1:F:167:LEU:HB2	2.29	0.67
1:G:260:PRO:HB2	1:G:273:LEU:HD13	1.77	0.67
1:H:322:VAL:HG12	1:H:323:HIS:N	2.10	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:549:ARG:O	1:H:550:ASN:HB2	1.95	0.67
1:E:412:ILE:HG23	1:E:433:ILE:HD12	1.76	0.67
1:E:422:THR:HG22	1:E:426:LEU:HD21	1.77	0.67
1:G:262:PRO:HB3	1:G:409:SER:OG	1.94	0.67
1:G:286:ARG:HA	1:G:290:THR:CG2	2.24	0.67
1:G:319:SER:C	1:G:321:ARG:H	1.97	0.67
1:G:473:THR:HG22	1:G:633:MET:HG3	1.74	0.67
1:H:409:SER:HB2	1:H:412:ILE:HD12	1.74	0.67
1:H:419:ARG:HA	1:H:587:SER:OG	1.94	0.67
1:B:350:GLU:HG2	1:B:391:ASP:HB2	1.75	0.67
1:C:254:LYS:O	1:C:255:PHE:CD2	2.47	0.67
1:D:40:GLN:HB3	1:D:98:TYR:HD2	1.59	0.67
1:G:245:VAL:O	1:G:257:SER:O	2.13	0.67
1:G:265:LEU:CD2	1:G:269:LEU:HB3	2.25	0.67
1:B:260:PRO:HB2	1:B:273:LEU:HD13	1.78	0.67
1:C:118:LYS:HG2	1:C:265:LEU:HA	1.77	0.67
1:D:143:HIS:CE1	1:D:167:LEU:HB2	2.30	0.67
1:D:263:ASN:HD21	1:D:265:LEU:CB	1.99	0.67
1:E:263:ASN:ND2	1:E:265:LEU:H	1.93	0.67
1:F:286:ARG:NH1	1:F:286:ARG:HG2	2.09	0.67
1:G:105:ARG:O	1:G:108:LEU:N	2.28	0.67
1:G:114:CYS:O	1:G:115:CYS:HB2	1.95	0.67
1:G:549:ARG:O	1:G:550:ASN:HB2	1.95	0.67
1:A:462:ASN:HD21	1:A:540:LEU:HB2	1.60	0.66
1:C:319:SER:C	1:C:321:ARG:H	1.97	0.66
1:D:260:PRO:HB2	1:D:273:LEU:HD13	1.75	0.66
1:E:570:LEU:HB3	1:E:590:MET:HE3	1.76	0.66
1:G:248:ASP:C	1:G:248:ASP:OD1	2.33	0.66
1:A:143:HIS:CE1	1:A:167:LEU:HB2	2.30	0.66
1:C:658:LEU:HD12	1:D:658:LEU:HA	1.76	0.66
1:D:120:GLY:O	1:D:123:ARG:N	2.29	0.66
1:D:254:LYS:O	1:D:255:PHE:CD2	2.48	0.66
1:E:26:PHE:HE2	1:E:181:GLU:CD	1.97	0.66
1:F:260:PRO:HB2	1:F:273:LEU:HD13	1.78	0.66
1:G:191:PRO:HG3	1:G:234:LYS:NZ	2.10	0.66
1:A:254:LYS:O	1:A:255:PHE:CD2	2.49	0.66
1:A:496:LYS:O	1:A:499:GLU:HB2	1.96	0.66
1:B:402:SER:O	1:B:403:LEU:HB2	1.95	0.66
1:C:496:LYS:HB2	1:D:655:TRP:CD1	2.25	0.66
1:D:224:PRO:HG2	1:D:255:PHE:CE2	2.30	0.66
1:E:462:ASN:ND2	1:E:540:LEU:HB2	2.09	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:549:ARG:O	1:E:550:ASN:HB2	1.93	0.66
1:E:651:GLN:HE22	1:F:492:ILE:CG2	2.04	0.66
1:G:424:THR:OG1	1:G:425:HIS:ND1	2.20	0.66
1:G:609:TYR:O	1:G:612:LEU:HB3	1.95	0.66
1:B:143:HIS:CE1	1:B:167:LEU:HB2	2.30	0.66
1:B:316:ASN:O	1:B:388:PHE:O	2.13	0.66
1:C:263:ASN:ND2	1:C:265:LEU:H	1.94	0.66
1:C:505:ILE:O	1:C:506:THR:O	2.12	0.66
1:D:179:CYS:CB	1:D:181:GLU:CG	2.67	0.66
1:D:660:ILE:C	1:D:662:CYS:H	1.99	0.66
1:E:492:ILE:CG2	1:F:651:GLN:HE22	2.07	0.66
1:F:224:PRO:HG2	1:F:255:PHE:CE2	2.31	0.66
1:F:433:ILE:HB	1:F:571:TYR:CZ	2.29	0.66
1:G:254:LYS:O	1:G:255:PHE:CD2	2.48	0.66
1:H:118:LYS:NZ	1:H:123:ARG:HH22	1.94	0.66
1:A:114:CYS:O	1:A:115:CYS:HB2	1.95	0.66
1:B:118:LYS:NZ	1:B:123:ARG:HH22	1.93	0.66
1:C:115:CYS:HB2	1:C:435:GLN:HG3	1.77	0.66
1:C:208:PHE:HD2	1:C:211:LEU:HD23	1.61	0.66
1:C:514:TRP:O	1:C:518:GLU:N	2.28	0.66
1:D:549:ARG:O	1:D:550:ASN:HB2	1.94	0.66
1:B:626:SER:HB2	1:B:630:LYS:HE3	1.77	0.66
1:C:433:ILE:HB	1:C:571:TYR:OH	1.96	0.66
1:C:434:TRP:HZ3	1:C:568:ARG:HG3	1.60	0.66
1:E:118:LYS:CG	1:E:265:LEU:HA	2.26	0.66
1:E:319:SER:C	1:E:321:ARG:H	1.98	0.66
1:E:418:LYS:O	1:E:419:ARG:HB2	1.96	0.66
1:E:660:ILE:C	1:E:662:CYS:H	1.99	0.66
1:F:286:ARG:HA	1:F:290:THR:CG2	2.24	0.66
1:F:500:GLN:HB3	1:F:505:ILE:CG1	2.26	0.66
1:A:647:GLN:CD	1:A:647:GLN:N	2.47	0.66
1:B:179:CYS:CB	1:B:181:GLU:CG	2.69	0.66
1:B:475:GLU:O	1:B:476:CYS:C	2.32	0.66
1:C:402:SER:O	1:C:403:LEU:HB2	1.96	0.66
1:D:422:THR:HB	1:D:585:GLY:HA3	1.75	0.66
1:D:517:MET:HG3	1:D:646:ARG:HH11	1.60	0.66
1:E:118:LYS:NZ	1:E:123:ARG:HH22	1.94	0.66
1:F:357:SER:CA	1:F:453:THR:HB	2.25	0.66
1:G:134:ARG:CA	1:G:300:PHE:HZ	2.09	0.66
1:G:253:VAL:HB	1:G:255:PHE:HZ	1.59	0.66
1:G:286:ARG:HG2	1:G:286:ARG:NH1	2.08	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:VAL:HB	1:A:255:PHE:HZ	1.60	0.66
1:C:193:LEU:O	1:C:196:GLN:OE1	2.13	0.66
1:C:418:LYS:O	1:C:419:ARG:HB2	1.94	0.66
1:F:494:LEU:HD12	1:F:514:TRP:HE3	1.59	0.66
1:G:350:GLU:HG2	1:G:391:ASP:HB2	1.77	0.66
1:H:438:ARG:NH1	1:H:568:ARG:HH21	1.93	0.66
1:H:438:ARG:HG2	1:H:564:GLU:CD	2.16	0.66
1:B:475:GLU:C	1:B:477:GLU:N	2.48	0.66
1:C:626:SER:HB2	1:C:630:LYS:HE3	1.78	0.66
1:E:179:CYS:CB	1:E:181:GLU:CG	2.68	0.66
1:A:40:GLN:HB3	1:A:98:TYR:HD2	1.60	0.66
1:C:659:LYS:HG2	1:D:500:GLN:HE22	1.60	0.66
1:E:49:GLU:HA	1:E:55:ARG:HD3	1.78	0.66
1:F:549:ARG:O	1:F:550:ASN:HB2	1.94	0.66
1:H:224:PRO:HG3	1:H:428:ARG:HH22	1.61	0.66
1:B:245:VAL:O	1:B:257:SER:O	2.14	0.65
1:B:394:LYS:CD	1:B:401:ILE:HA	2.26	0.65
1:D:550:ASN:OD1	1:D:611:GLN:OE1	2.14	0.65
1:E:665:VAL:HG13	1:F:665:VAL:HG13	1.78	0.65
1:F:430:TRP:HB3	1:F:571:TYR:HD2	1.61	0.65
1:F:647:GLN:N	1:F:647:GLN:CD	2.47	0.65
1:F:660:ILE:C	1:F:662:CYS:H	1.99	0.65
1:G:49:GLU:HA	1:G:55:ARG:HD3	1.78	0.65
1:G:473:THR:CG2	1:G:533:LEU:HD22	2.22	0.65
1:A:260:PRO:HG3	1:A:274:GLU:HG2	1.79	0.65
1:A:418:LYS:O	1:A:419:ARG:HB2	1.95	0.65
1:A:422:THR:HG22	1:A:426:LEU:HD21	1.78	0.65
1:A:654:LEU:CD2	1:B:654:LEU:HD22	2.19	0.65
1:B:71:PRO:O	1:B:72:ASN:HB2	1.96	0.65
1:B:540:LEU:CD2	1:B:621:LYS:HZ2	2.09	0.65
1:C:71:PRO:O	1:C:72:ASN:HB2	1.95	0.65
1:D:105:ARG:O	1:D:108:LEU:N	2.29	0.65
1:E:153:LEU:CD2	1:E:162:HIS:HD1	2.08	0.65
1:E:230:GLN:C	1:E:232:HIS:N	2.44	0.65
1:E:283:TRP:O	1:E:284:HIS:HB2	1.94	0.65
1:F:418:LYS:O	1:F:419:ARG:HB2	1.95	0.65
1:H:49:GLU:HA	1:H:55:ARG:HD3	1.78	0.65
1:A:503:PHE:CD1	1:B:666:ARG:HB2	2.31	0.65
1:A:654:LEU:HD23	1:B:654:LEU:HD21	1.75	0.65
1:B:479:LEU:CB	1:B:640:GLU:OE2	2.36	0.65
1:G:120:GLY:H	1:G:122:ILE:H	1.44	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLU:HG2	1:A:83:LEU:HD13	1.79	0.65
1:A:265:LEU:CD2	1:A:269:LEU:HB3	2.27	0.65
1:B:286:ARG:HG2	1:B:286:ARG:HH11	1.60	0.65
1:C:244:VAL:HG12	1:C:278:GLN:OE1	1.97	0.65
1:C:245:VAL:O	1:C:257:SER:O	2.14	0.65
1:D:265:LEU:CD2	1:D:269:LEU:HB3	2.26	0.65
1:E:341:GLN:OE1	1:E:347:PRO:HB3	1.96	0.65
1:F:116:GLY:HA2	1:F:217:THR:O	1.95	0.65
1:F:419:ARG:N	1:F:420:PRO:HD3	2.03	0.65
1:F:422:THR:HB	1:F:585:GLY:HA2	1.77	0.65
1:H:107:TYR:HE1	1:H:153:LEU:HB2	1.61	0.65
1:H:260:PRO:HG3	1:H:274:GLU:HG2	1.77	0.65
1:C:571:TYR:CZ	1:C:590:MET:SD	2.90	0.65
1:D:644:VAL:CA	1:D:647:GLN:HE21	2.08	0.65
1:F:49:GLU:HA	1:F:55:ARG:HD3	1.78	0.65
1:G:387:ILE:HD12	1:G:450:GLY:HA2	1.79	0.65
1:G:533:LEU:CD2	1:G:629:VAL:HG13	2.25	0.65
1:A:260:PRO:HB2	1:A:273:LEU:HD13	1.79	0.65
1:C:26:PHE:HE2	1:C:181:GLU:CD	1.98	0.65
1:C:105:ARG:O	1:C:108:LEU:N	2.30	0.65
1:C:192:GLU:OE1	1:C:192:GLU:HA	1.96	0.65
1:C:503:PHE:O	1:C:505:ILE:HG13	1.97	0.65
1:E:412:ILE:HG23	1:E:433:ILE:CD1	2.26	0.65
1:E:486:PHE:CE1	1:E:647:GLN:HB3	2.31	0.65
1:E:505:ILE:O	1:E:506:THR:O	2.14	0.65
1:F:244:VAL:HG12	1:F:278:GLN:OE1	1.96	0.65
1:F:318:VAL:O	1:F:320:GLY:N	2.30	0.65
1:F:319:SER:OG	1:F:403:LEU:HB2	1.97	0.65
1:G:443:ASP:O	1:G:446:ARG:HB2	1.96	0.65
1:H:350:GLU:HG2	1:H:391:ASP:HB2	1.77	0.65
1:A:350:GLU:HG2	1:A:391:ASP:HB2	1.78	0.65
1:B:476:CYS:CA	1:B:636:MET:SD	2.84	0.65
1:D:118:LYS:HG3	1:D:118:LYS:O	1.96	0.65
1:E:143:HIS:CE1	1:E:167:LEU:HB2	2.30	0.65
1:F:114:CYS:O	1:F:115:CYS:HB2	1.95	0.65
1:G:571:TYR:CE2	1:G:590:MET:HG3	2.31	0.65
1:A:49:GLU:HA	1:A:55:ARG:HD3	1.79	0.65
1:A:434:TRP:HZ3	1:A:568:ARG:CG	2.09	0.65
1:C:193:LEU:HD22	1:C:231:TRP:CD1	2.32	0.65
1:D:253:VAL:HB	1:D:255:PHE:HZ	1.58	0.65
1:F:191:PRO:HG3	1:F:234:LYS:NZ	2.11	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:LYS:NZ	1:G:123:ARG:HH22	1.94	0.65
1:H:71:PRO:O	1:H:72:ASN:HB2	1.95	0.65
1:A:286:ARG:HG2	1:A:286:ARG:HH11	1.60	0.65
1:A:357:SER:HA	1:A:453:THR:HB	1.78	0.65
1:A:610:ASP:O	1:A:613:SER:HB3	1.96	0.65
1:B:224:PRO:HG2	1:B:255:PHE:CE2	2.32	0.65
1:B:422:THR:HB	1:B:585:GLY:HA3	1.78	0.65
1:B:514:TRP:O	1:B:518:GLU:N	2.29	0.65
1:B:549:ARG:O	1:B:550:ASN:HB2	1.96	0.65
1:C:318:VAL:O	1:C:320:GLY:N	2.29	0.65
1:C:434:TRP:HZ3	1:C:568:ARG:HA	1.60	0.65
1:D:114:CYS:O	1:D:115:CYS:HB2	1.96	0.65
1:D:441:LYS:HB2	1:D:560:LEU:HD21	1.78	0.65
1:E:486:PHE:HZ	1:E:517:MET:HE2	1.61	0.65
1:G:224:PRO:HG2	1:G:255:PHE:CE2	2.31	0.65
1:H:283:TRP:O	1:H:284:HIS:HB2	1.95	0.65
1:H:418:LYS:O	1:H:419:ARG:HB2	1.95	0.65
1:A:478:GLN:HB2	1:B:478:GLN:HB2	1.77	0.65
1:B:475:GLU:HG2	1:B:476:CYS:N	2.12	0.65
1:D:119:GLU:CB	1:D:121:PRO:CD	2.75	0.65
1:D:248:ASP:C	1:D:248:ASP:OD1	2.34	0.65
1:D:438:ARG:HG2	1:D:564:GLU:CD	2.17	0.65
1:D:610:ASP:O	1:D:613:SER:HB3	1.97	0.65
1:E:16:GLU:HG2	1:E:83:LEU:HD13	1.79	0.65
1:E:260:PRO:HB2	1:E:273:LEU:HD13	1.79	0.65
1:E:434:TRP:HB3	1:E:571:TYR:HD1	1.60	0.65
1:E:496:LYS:O	1:E:499:GLU:HB2	1.97	0.65
1:F:422:THR:HG22	1:F:426:LEU:HD21	1.78	0.65
1:H:193:LEU:O	1:H:196:GLN:OE1	2.14	0.65
1:A:193:LEU:HD22	1:A:231:TRP:CD1	2.32	0.64
1:A:417:PRO:O	1:A:418:LYS:HG3	1.96	0.64
1:A:438:ARG:HG2	1:A:564:GLU:CD	2.17	0.64
1:A:533:LEU:CD2	1:A:629:VAL:HG11	2.21	0.64
1:C:49:GLU:HA	1:C:55:ARG:HD3	1.78	0.64
1:C:384:GLY:O	1:C:385:ASP:HB2	1.96	0.64
1:D:387:ILE:HG21	1:D:450:GLY:CA	2.28	0.64
1:D:476:CYS:HA	1:D:636:MET:SD	2.38	0.64
1:D:497:TYR:HE2	1:D:511:LEU:HD22	1.59	0.64
1:E:244:VAL:HG12	1:E:278:GLN:OE1	1.97	0.64
1:F:222:PHE:CG	1:F:255:PHE:HB3	2.32	0.64
1:F:480:LYS:HZ1	1:F:527:GLU:HB2	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:402:SER:O	1:H:403:LEU:HB2	1.96	0.64
1:A:71:PRO:O	1:A:72:ASN:HB2	1.96	0.64
1:A:412:ILE:HG23	1:A:433:ILE:CD1	2.27	0.64
1:B:260:PRO:HG3	1:B:274:GLU:HG2	1.78	0.64
1:B:283:TRP:O	1:B:284:HIS:HB2	1.97	0.64
1:C:16:GLU:HG2	1:C:83:LEU:HD13	1.79	0.64
1:C:118:LYS:CG	1:C:265:LEU:HA	2.28	0.64
1:C:581:GLN:O	1:C:584:PRO:HD2	1.97	0.64
1:D:110:GLN:O	1:D:111:PHE:CB	2.37	0.64
1:D:318:VAL:O	1:D:320:GLY:N	2.30	0.64
1:E:654:LEU:HD12	1:F:655:TRP:CZ3	2.31	0.64
1:F:437:ILE:HG13	1:F:594:LEU:CD1	2.27	0.64
1:G:118:LYS:HG2	1:G:265:LEU:HA	1.77	0.64
1:G:260:PRO:HG3	1:G:274:GLU:HG2	1.78	0.64
1:H:318:VAL:O	1:H:320:GLY:N	2.30	0.64
1:B:118:LYS:HG3	1:B:118:LYS:O	1.96	0.64
1:E:120:GLY:O	1:E:123:ARG:N	2.31	0.64
1:F:118:LYS:NZ	1:F:123:ARG:HH22	1.95	0.64
1:F:479:LEU:HD11	1:F:641:LYS:HG3	1.79	0.64
1:G:581:GLN:O	1:G:584:PRO:HD2	1.98	0.64
1:A:514:TRP:O	1:A:518:GLU:N	2.30	0.64
1:D:444:CYS:C	1:D:446:ARG:H	2.01	0.64
1:E:118:LYS:HG2	1:E:265:LEU:HA	1.77	0.64
1:F:105:ARG:O	1:F:108:LEU:N	2.31	0.64
1:G:107:TYR:HE1	1:G:153:LEU:HB2	1.62	0.64
1:A:115:CYS:O	1:A:263:ASN:HA	1.98	0.64
1:B:246:TYR:CD1	1:B:258:VAL:CB	2.70	0.64
1:C:143:HIS:CE1	1:C:167:LEU:HB2	2.31	0.64
1:D:105:ARG:O	1:D:107:TYR:N	2.31	0.64
1:D:244:VAL:HG12	1:D:278:GLN:OE1	1.97	0.64
1:F:253:VAL:HB	1:F:255:PHE:HZ	1.60	0.64
1:F:644:VAL:CA	1:F:647:GLN:HE21	2.10	0.64
1:G:244:VAL:HG12	1:G:278:GLN:OE1	1.97	0.64
1:H:434:TRP:HZ3	1:H:568:ARG:CA	2.10	0.64
1:H:437:ILE:HG22	1:H:564:GLU:HB2	1.78	0.64
1:A:70:HIS:CD2	1:A:71:PRO:O	2.51	0.64
1:C:224:PRO:HG2	1:C:255:PHE:CE2	2.33	0.64
1:C:341:GLN:OE1	1:C:347:PRO:HB3	1.97	0.64
1:C:529:GLU:HG3	1:C:633:MET:CE	2.27	0.64
1:D:49:GLU:HA	1:D:55:ARG:HD3	1.78	0.64
1:D:387:ILE:HD11	1:D:449:GLN:CG	2.28	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:ILE:HD12	1:D:450:GLY:N	2.12	0.64
1:F:402:SER:O	1:F:403:LEU:HB2	1.96	0.64
1:G:16:GLU:HG2	1:G:83:LEU:HD13	1.79	0.64
1:G:418:LYS:O	1:G:419:ARG:HB2	1.95	0.64
1:H:105:ARG:O	1:H:108:LEU:N	2.31	0.64
1:H:171:LYS:HA	1:H:177:GLU:HA	1.80	0.64
1:A:118:LYS:NZ	1:A:123:ARG:HH22	1.96	0.64
1:A:193:LEU:O	1:A:196:GLN:OE1	2.16	0.64
1:A:433:ILE:HB	1:A:571:TYR:OH	1.97	0.64
1:A:503:PHE:HE1	1:B:666:ARG:HG3	1.62	0.64
1:A:547:LEU:HD12	1:A:615:THR:HG22	1.77	0.64
1:B:418:LYS:O	1:B:419:ARG:HB2	1.95	0.64
1:B:443:ASP:O	1:B:446:ARG:HB2	1.97	0.64
1:D:16:GLU:HG2	1:D:83:LEU:HD13	1.78	0.64
1:E:665:VAL:HG21	1:F:665:VAL:HG22	1.78	0.64
1:H:114:CYS:O	1:H:115:CYS:HB2	1.97	0.64
1:H:222:PHE:CG	1:H:255:PHE:HB3	2.33	0.64
1:H:422:THR:HG22	1:H:426:LEU:HD21	1.80	0.64
1:A:244:VAL:HG12	1:A:278:GLN:OE1	1.96	0.64
1:A:386:LEU:H	1:A:386:LEU:HD12	1.63	0.64
1:B:107:TYR:HE1	1:B:153:LEU:HB2	1.63	0.64
1:F:570:LEU:CB	1:F:590:MET:CE	2.75	0.64
1:B:384:GLY:O	1:B:385:ASP:HB2	1.97	0.64
1:B:387:ILE:CD1	1:B:450:GLY:CA	2.74	0.64
1:C:118:LYS:HG3	1:C:118:LYS:O	1.97	0.64
1:C:206:TRP:CD1	1:C:206:TRP:C	2.71	0.64
1:C:230:GLN:C	1:C:232:HIS:N	2.44	0.64
1:C:286:ARG:HG2	1:C:286:ARG:HH11	1.62	0.64
1:C:485:PHE:CE2	1:D:485:PHE:CG	2.85	0.64
1:D:245:VAL:O	1:D:257:SER:O	2.16	0.64
1:E:245:VAL:O	1:E:257:SER:O	2.15	0.64
1:F:260:PRO:HG3	1:F:274:GLU:HG2	1.79	0.64
1:H:193:LEU:CD2	1:H:231:TRP:CD1	2.80	0.64
1:B:644:VAL:CA	1:B:647:GLN:HE21	2.09	0.64
1:C:119:GLU:CB	1:C:121:PRO:CD	2.76	0.64
1:C:260:PRO:HG3	1:C:274:GLU:HG2	1.78	0.64
1:C:316:ASN:O	1:C:317:MET:HB2	1.98	0.64
1:D:111:PHE:CZ	1:D:572:ARG:HG3	2.33	0.64
1:D:350:GLU:HA	1:D:391:ASP:OD2	1.98	0.64
1:D:581:GLN:O	1:D:584:PRO:HD2	1.98	0.64
1:F:153:LEU:CD2	1:F:162:HIS:HD1	2.11	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:387:ILE:CD1	1:F:450:GLY:N	2.60	0.64
1:F:402:SER:HA	1:F:609:TYR:CG	2.33	0.64
1:G:334:GLN:HA	1:G:337:LYS:HB2	1.80	0.64
1:G:402:SER:O	1:G:403:LEU:HB2	1.98	0.64
1:B:49:GLU:HA	1:B:55:ARG:HD3	1.79	0.63
1:B:433:ILE:HB	1:B:571:TYR:OH	1.98	0.63
1:B:503:PHE:H	1:B:505:ILE:HD11	1.62	0.63
1:C:120:GLY:H	1:C:122:ILE:H	1.45	0.63
1:D:171:LYS:HA	1:D:177:GLU:HA	1.80	0.63
1:E:71:PRO:O	1:E:72:ASN:HB2	1.97	0.63
1:F:220:ARG:HH12	1:F:223:LEU:CD2	2.10	0.63
1:F:352:GLU:O	1:F:388:PHE:HA	1.99	0.63
1:F:626:SER:HB2	1:F:630:LYS:HE3	1.78	0.63
1:G:412:ILE:HG23	1:G:433:ILE:CD1	2.28	0.63
1:H:145:ASP:OD1	1:H:167:LEU:HD13	1.97	0.63
1:H:224:PRO:HG2	1:H:255:PHE:CE2	2.34	0.63
1:H:245:VAL:O	1:H:257:SER:O	2.16	0.63
1:B:16:GLU:HG2	1:B:83:LEU:HD13	1.79	0.63
1:B:408:GLU:O	1:B:409:SER:HB2	1.98	0.63
1:D:193:LEU:O	1:D:196:GLN:OE1	2.16	0.63
1:E:105:ARG:O	1:E:108:LEU:N	2.30	0.63
1:E:193:LEU:O	1:E:196:GLN:OE1	2.16	0.63
1:E:473:THR:CG2	1:E:533:LEU:CD2	2.70	0.63
1:E:514:TRP:O	1:E:518:GLU:N	2.31	0.63
1:G:111:PHE:CZ	1:G:572:ARG:CG	2.70	0.63
1:G:153:LEU:CD2	1:G:162:HIS:HD1	2.11	0.63
1:H:70:HIS:CD2	1:H:71:PRO:O	2.52	0.63
1:A:145:ASP:OD1	1:A:167:LEU:HD13	1.98	0.63
1:C:107:TYR:HE1	1:C:153:LEU:HB2	1.63	0.63
1:C:573:ARG:HH22	1:D:573:ARG:NH1	1.95	0.63
1:D:70:HIS:CD2	1:D:71:PRO:O	2.51	0.63
1:D:246:TYR:CD1	1:D:258:VAL:CB	2.70	0.63
1:D:434:TRP:CE3	1:D:568:ARG:CA	2.68	0.63
1:F:444:CYS:C	1:F:446:ARG:N	2.50	0.63
1:G:70:HIS:CD2	1:G:71:PRO:O	2.51	0.63
1:G:422:THR:HG22	1:G:426:LEU:HD21	1.80	0.63
1:H:444:CYS:C	1:H:446:ARG:H	2.02	0.63
1:A:105:ARG:O	1:A:107:TYR:N	2.31	0.63
1:B:70:HIS:CD2	1:B:71:PRO:O	2.52	0.63
1:B:120:GLY:HA2	1:B:123:ARG:H	1.63	0.63
1:G:220:ARG:HH12	1:G:223:LEU:CD2	2.12	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:PRO:HB3	1:B:409:SER:HG	1.62	0.63
1:B:265:LEU:CD2	1:B:269:LEU:HB3	2.27	0.63
1:B:389:LEU:HD11	1:B:454:SER:OG	1.99	0.63
1:D:222:PHE:CG	1:D:255:PHE:HB3	2.34	0.63
1:D:352:GLU:O	1:D:388:PHE:HA	1.99	0.63
1:D:402:SER:O	1:D:403:LEU:HB2	1.99	0.63
1:D:402:SER:HA	1:D:609:TYR:CG	2.32	0.63
1:D:408:GLU:O	1:D:409:SER:HB2	1.98	0.63
1:D:434:TRP:HB3	1:D:571:TYR:CE1	2.32	0.63
1:E:433:ILE:HB	1:E:571:TYR:CZ	2.33	0.63
1:F:262:PRO:HB3	1:F:409:SER:HG	1.60	0.63
1:F:581:GLN:O	1:F:584:PRO:HD2	1.98	0.63
1:G:316:ASN:O	1:G:317:MET:HB2	1.96	0.63
1:A:105:ARG:O	1:A:106:LYS:C	2.36	0.63
1:A:626:SER:HB2	1:A:630:LYS:HE3	1.81	0.63
1:A:651:GLN:NE2	1:B:492:ILE:HG23	2.14	0.63
1:C:265:LEU:CD2	1:C:269:LEU:HB3	2.28	0.63
1:D:208:PHE:HD2	1:D:211:LEU:HD23	1.62	0.63
1:D:260:PRO:HG3	1:D:274:GLU:HG2	1.80	0.63
1:D:438:ARG:NH1	1:D:568:ARG:HH21	1.96	0.63
1:G:120:GLY:O	1:G:123:ARG:N	2.32	0.63
1:H:16:GLU:HG2	1:H:83:LEU:HD13	1.79	0.63
1:A:150:ASN:ND2	1:A:167:LEU:HD12	2.11	0.63
1:A:384:GLY:O	1:A:385:ASP:HB2	1.96	0.63
1:B:350:GLU:HA	1:B:391:ASP:OD2	1.98	0.63
1:C:527:GLU:O	1:C:529:GLU:N	2.30	0.63
1:D:71:PRO:O	1:D:72:ASN:HB2	1.98	0.63
1:E:208:PHE:HD2	1:E:211:LEU:HD23	1.63	0.63
1:E:318:VAL:O	1:E:320:GLY:N	2.31	0.63
1:E:581:GLN:O	1:E:584:PRO:HD2	1.98	0.63
1:F:286:ARG:HG2	1:F:286:ARG:HH11	1.64	0.63
1:H:244:VAL:HG12	1:H:278:GLN:OE1	1.99	0.63
1:H:387:ILE:HG21	1:H:450:GLY:CA	2.25	0.63
1:A:357:SER:CB	1:A:453:THR:HB	2.29	0.63
1:A:438:ARG:NH1	1:A:568:ARG:HH21	1.97	0.63
1:A:665:VAL:HG11	1:B:665:VAL:HG22	1.80	0.63
1:B:120:GLY:O	1:B:123:ARG:N	2.32	0.63
1:C:70:HIS:CD2	1:C:71:PRO:O	2.52	0.63
1:C:145:ASP:OD1	1:C:167:LEU:HD13	1.99	0.63
1:C:644:VAL:CA	1:C:647:GLN:HE21	2.10	0.63
1:C:666:ARG:HG3	1:D:503:PHE:HE1	1.64	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:626:SER:HB2	1:E:630:LYS:HE3	1.81	0.63
1:E:644:VAL:CA	1:E:647:GLN:HE21	2.11	0.63
1:F:71:PRO:O	1:F:72:ASN:HB2	1.98	0.63
1:F:118:LYS:HG3	1:F:118:LYS:O	1.99	0.63
1:G:434:TRP:HZ3	1:G:568:ARG:CA	2.11	0.63
1:A:581:GLN:O	1:A:584:PRO:HD2	1.99	0.63
1:B:192:GLU:OE1	1:B:192:GLU:HA	1.99	0.63
1:B:430:TRP:HB3	1:B:571:TYR:CD2	2.30	0.63
1:C:350:GLU:HG2	1:C:391:ASP:HB2	1.79	0.63
1:D:107:TYR:HE1	1:D:153:LEU:HB2	1.64	0.63
1:D:286:ARG:HG2	1:D:286:ARG:HH11	1.64	0.63
1:E:345:GLY:O	1:E:347:PRO:HD3	1.99	0.63
1:F:265:LEU:CD2	1:F:269:LEU:HB3	2.28	0.63
1:F:319:SER:CB	1:F:403:LEU:HB2	2.29	0.63
1:G:134:ARG:HB2	1:G:300:PHE:HE1	1.62	0.63
1:G:230:GLN:C	1:G:232:HIS:N	2.44	0.63
1:A:419:ARG:HA	1:A:587:SER:OG	1.98	0.62
1:A:430:TRP:CE3	1:A:574:LEU:HD22	2.34	0.62
1:D:260:PRO:CB	1:D:273:LEU:HD13	2.30	0.62
1:E:222:PHE:CG	1:E:255:PHE:HB3	2.34	0.62
1:F:171:LYS:HA	1:F:177:GLU:HA	1.81	0.62
1:F:514:TRP:O	1:F:518:GLU:N	2.29	0.62
1:A:644:VAL:CA	1:A:647:GLN:HE21	2.10	0.62
1:B:105:ARG:O	1:B:106:LYS:C	2.38	0.62
1:E:70:HIS:CD2	1:E:71:PRO:O	2.52	0.62
1:E:386:LEU:HD12	1:E:386:LEU:H	1.63	0.62
1:E:517:MET:CE	1:E:647:GLN:OE1	2.47	0.62
1:G:263:ASN:ND2	1:G:265:LEU:H	1.97	0.62
1:H:316:ASN:O	1:H:317:MET:HB2	1.99	0.62
1:A:150:ASN:OD1	1:A:150:ASN:N	2.32	0.62
1:A:494:LEU:HD12	1:A:514:TRP:HE3	1.63	0.62
1:C:500:GLN:HB3	1:C:505:ILE:HG12	1.81	0.62
1:D:143:HIS:CD2	1:D:145:ASP:O	2.51	0.62
1:D:192:GLU:HA	1:D:192:GLU:OE1	1.98	0.62
1:E:350:GLU:HA	1:E:391:ASP:OD2	1.99	0.62
1:E:478:GLN:HA	1:F:478:GLN:HB2	1.81	0.62
1:F:70:HIS:CD2	1:F:71:PRO:O	2.52	0.62
1:G:30:LEU:HD13	1:G:32:TRP:HE1	1.65	0.62
1:G:610:ASP:O	1:G:613:SER:HB3	1.99	0.62
1:H:394:LYS:HG2	1:H:401:ILE:N	2.12	0.62
1:H:581:GLN:O	1:H:584:PRO:HD2	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:626:SER:HB2	1:H:630:LYS:HE3	1.79	0.62
1:C:260:PRO:CB	1:C:273:LEU:HD13	2.29	0.62
1:E:387:ILE:HD12	1:E:450:GLY:N	2.14	0.62
1:F:143:HIS:CD2	1:F:145:ASP:O	2.51	0.62
1:G:150:ASN:OD1	1:G:150:ASN:N	2.32	0.62
1:G:283:TRP:O	1:G:284:HIS:HB2	1.99	0.62
1:H:63:GLN:O	1:H:67:LYS:HB2	1.99	0.62
1:B:134:ARG:CA	1:B:300:PHE:CZ	2.80	0.62
1:C:419:ARG:NH1	1:C:588:ASN:HA	2.14	0.62
1:D:105:ARG:O	1:D:106:LYS:C	2.38	0.62
1:D:186:LEU:HD23	1:D:227:GLN:HG2	1.81	0.62
1:E:547:LEU:HD22	1:E:611:GLN:CG	2.28	0.62
1:F:447:LEU:HD12	1:F:605:VAL:CG2	2.28	0.62
1:G:17:MET:HA	1:G:33:ILE:O	2.00	0.62
1:G:387:ILE:HD13	1:G:450:GLY:HA2	1.79	0.62
1:G:419:ARG:HA	1:G:587:SER:OG	2.00	0.62
1:A:208:PHE:HD2	1:A:211:LEU:HD23	1.65	0.62
1:A:263:ASN:ND2	1:A:265:LEU:H	1.96	0.62
1:B:581:GLN:O	1:B:584:PRO:HD2	2.00	0.62
1:D:119:GLU:HB2	1:D:121:PRO:CD	2.29	0.62
1:E:107:TYR:HE1	1:E:153:LEU:HB2	1.64	0.62
1:F:192:GLU:OE1	1:F:192:GLU:HA	1.98	0.62
1:H:208:PHE:HD2	1:H:211:LEU:HD23	1.63	0.62
1:A:222:PHE:CG	1:A:255:PHE:HB3	2.35	0.62
1:B:222:PHE:CG	1:B:255:PHE:HB3	2.35	0.62
1:B:359:LEU:HA	1:B:460:ARG:HH12	1.64	0.62
1:D:386:LEU:H	1:D:386:LEU:HD12	1.62	0.62
1:E:286:ARG:HG2	1:E:286:ARG:HH11	1.64	0.62
1:F:16:GLU:HG2	1:F:83:LEU:HD13	1.80	0.62
1:F:150:ASN:ND2	1:F:167:LEU:HD12	2.14	0.62
1:G:103:ASP:HB3	1:G:106:LYS:HG3	1.81	0.62
1:G:563:LEU:HD21	1:G:596:LEU:HB2	1.81	0.62
1:B:276:TRP:CE3	1:B:277:LEU:HD23	2.34	0.62
1:B:501:MET:C	1:B:505:ILE:HD11	2.20	0.62
1:C:105:ARG:O	1:C:106:LYS:C	2.38	0.62
1:D:190:ALA:HB2	1:D:206:TRP:CG	2.35	0.62
1:D:480:LYS:NZ	1:D:527:GLU:HB2	2.15	0.62
1:E:192:GLU:OE1	1:E:192:GLU:HA	2.00	0.62
1:E:206:TRP:CD1	1:E:206:TRP:C	2.73	0.62
1:F:134:ARG:CA	1:F:300:PHE:CZ	2.75	0.62
1:G:580:ASP:HA	1:G:582:ARG:NH1	2.15	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ARG:O	1:B:108:LEU:N	2.32	0.62
1:B:193:LEU:O	1:B:196:GLN:OE1	2.17	0.62
1:B:441:LYS:HB2	1:B:560:LEU:HD22	1.81	0.62
1:C:105:ARG:O	1:C:107:TYR:N	2.32	0.62
1:C:422:THR:CB	1:C:585:GLY:C	2.67	0.62
1:C:422:THR:HG22	1:C:426:LEU:HD21	1.81	0.62
1:E:402:SER:HA	1:E:609:TYR:CG	2.35	0.62
1:F:30:LEU:HD13	1:F:32:TRP:HE1	1.65	0.62
1:F:368:THR:HA	1:F:371:VAL:CG2	2.30	0.62
1:H:153:LEU:CD2	1:H:162:HIS:HD1	2.12	0.62
1:A:426:LEU:HB2	1:A:574:LEU:HD21	1.82	0.62
1:A:580:ASP:HA	1:A:582:ARG:NH1	2.15	0.62
1:B:318:VAL:O	1:B:320:GLY:N	2.32	0.62
1:D:480:LYS:CE	1:D:527:GLU:HB2	2.30	0.62
1:D:514:TRP:O	1:D:518:GLU:N	2.30	0.62
1:E:150:ASN:ND2	1:E:167:LEU:HD12	2.14	0.62
1:F:105:ARG:O	1:F:106:LYS:C	2.38	0.62
1:F:105:ARG:O	1:F:107:TYR:N	2.33	0.62
1:G:386:LEU:H	1:G:386:LEU:HD12	1.62	0.62
1:H:72:ASN:O	1:H:163:LYS:HA	2.00	0.62
1:H:334:GLN:HA	1:H:337:LYS:HB2	1.82	0.62
1:H:384:GLY:O	1:H:385:ASP:HB2	2.00	0.62
1:A:107:TYR:HE1	1:A:153:LEU:HB2	1.63	0.61
1:A:179:CYS:CB	1:A:181:GLU:CG	2.67	0.61
1:A:192:GLU:HA	1:A:192:GLU:OE1	1.99	0.61
1:A:224:PRO:HG2	1:A:255:PHE:HE2	1.64	0.61
1:A:345:GLY:O	1:A:347:PRO:HD3	2.00	0.61
1:A:434:TRP:CZ3	1:A:568:ARG:HG3	2.31	0.61
1:A:434:TRP:HZ3	1:A:568:ARG:CA	2.09	0.61
1:B:143:HIS:CD2	1:B:145:ASP:O	2.53	0.61
1:D:118:LYS:NZ	1:D:123:ARG:HH22	1.96	0.61
1:G:150:ASN:ND2	1:G:167:LEU:HD12	2.13	0.61
1:H:17:MET:HA	1:H:33:ILE:O	2.00	0.61
1:H:103:ASP:HB3	1:H:106:LYS:HG3	1.82	0.61
1:H:118:LYS:HG3	1:H:118:LYS:O	1.99	0.61
1:A:527:GLU:C	1:A:529:GLU:H	2.02	0.61
1:A:571:TYR:CZ	1:A:590:MET:SD	2.93	0.61
1:A:651:GLN:HE22	1:B:492:ILE:HG23	1.65	0.61
1:B:72:ASN:O	1:B:163:LYS:HA	2.00	0.61
1:B:263:ASN:ND2	1:B:265:LEU:H	1.96	0.61
1:C:580:ASP:HA	1:C:582:ARG:NH1	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:ASN:ND2	1:D:265:LEU:H	1.98	0.61
1:E:198:LYS:C	1:E:200:THR:H	2.04	0.61
1:F:208:PHE:HD2	1:F:211:LEU:HD23	1.64	0.61
1:H:263:ASN:ND2	1:H:265:LEU:H	1.98	0.61
1:H:386:LEU:H	1:H:386:LEU:HD12	1.64	0.61
1:A:153:LEU:CD2	1:A:162:HIS:HD1	2.14	0.61
1:A:434:TRP:HZ3	1:A:568:ARG:HA	1.54	0.61
1:B:171:LYS:HA	1:B:177:GLU:HA	1.82	0.61
1:C:441:LYS:HB2	1:C:560:LEU:CD2	2.29	0.61
1:C:660:ILE:HG23	1:C:661:ALA:N	2.15	0.61
1:D:150:ASN:OD1	1:D:150:ASN:N	2.33	0.61
1:E:116:GLY:HA2	1:E:217:THR:O	2.00	0.61
1:F:63:GLN:O	1:F:67:LYS:HB2	2.00	0.61
1:F:146:LEU:HA	1:F:150:ASN:HD21	1.65	0.61
1:H:260:PRO:CB	1:H:273:LEU:HD13	2.29	0.61
1:A:17:MET:HA	1:A:33:ILE:O	2.00	0.61
1:A:143:HIS:CD2	1:A:145:ASP:O	2.52	0.61
1:A:350:GLU:HA	1:A:391:ASP:OD2	1.99	0.61
1:D:334:GLN:HA	1:D:337:LYS:HB2	1.81	0.61
1:E:105:ARG:O	1:E:107:TYR:N	2.33	0.61
1:E:150:ASN:OD1	1:E:150:ASN:N	2.34	0.61
1:E:224:PRO:HG2	1:E:255:PHE:CE2	2.36	0.61
1:F:416:ASP:CG	1:F:417:PRO:HD3	2.21	0.61
1:H:286:ARG:HG2	1:H:286:ARG:HH11	1.64	0.61
1:H:408:GLU:O	1:H:409:SER:HB2	1.99	0.61
1:A:665:VAL:CG1	1:B:665:VAL:HG22	2.30	0.61
1:B:422:THR:HG22	1:B:426:LEU:HD21	1.81	0.61
1:B:441:LYS:HD2	1:B:561:ASP:OD1	2.01	0.61
1:C:386:LEU:H	1:C:386:LEU:HD12	1.65	0.61
1:D:283:TRP:O	1:D:284:HIS:HB2	2.01	0.61
1:F:345:GLY:O	1:F:347:PRO:HD3	2.00	0.61
1:F:386:LEU:H	1:F:386:LEU:HD12	1.64	0.61
1:F:567:ALA:HA	1:F:590:MET:HE1	1.82	0.61
1:F:660:ILE:HG23	1:F:661:ALA:N	2.15	0.61
1:G:145:ASP:OD1	1:G:167:LEU:HD13	2.01	0.61
1:G:193:LEU:O	1:G:196:GLN:OE1	2.18	0.61
1:G:408:GLU:O	1:G:409:SER:HB2	2.00	0.61
1:A:63:GLN:O	1:A:67:LYS:HB2	2.01	0.61
1:A:245:VAL:O	1:A:257:SER:O	2.18	0.61
1:A:334:GLN:HA	1:A:337:LYS:HB2	1.82	0.61
1:A:402:SER:O	1:A:403:LEU:HB2	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:PHE:HD2	1:B:211:LEU:HD23	1.65	0.61
1:C:191:PRO:HG3	1:C:234:LYS:NZ	2.16	0.61
1:C:408:GLU:O	1:C:409:SER:HB2	2.00	0.61
1:D:384:GLY:O	1:D:385:ASP:HB2	1.99	0.61
1:E:105:ARG:HG2	1:E:109:ASN:HD21	1.66	0.61
1:E:271:GLY:HA2	1:E:275:ARG:HH21	1.66	0.61
1:E:402:SER:O	1:E:403:LEU:HB2	2.01	0.61
1:G:222:PHE:CG	1:G:255:PHE:HB3	2.35	0.61
1:A:120:GLY:O	1:A:123:ARG:N	2.33	0.61
1:A:438:ARG:HG2	1:A:564:GLU:CG	2.30	0.61
1:A:492:ILE:HD13	1:B:651:GLN:HE21	1.66	0.61
1:A:658:LEU:HA	1:B:658:LEU:CD1	2.31	0.61
1:B:17:MET:HA	1:B:33:ILE:O	1.99	0.61
1:B:26:PHE:CE2	1:B:181:GLU:OE1	2.53	0.61
1:C:120:GLY:O	1:C:123:ARG:N	2.33	0.61
1:E:43:ILE:HA	1:E:94:LEU:O	2.00	0.61
1:E:105:ARG:O	1:E:106:LYS:C	2.38	0.61
1:E:118:LYS:HG3	1:E:118:LYS:O	2.00	0.61
1:E:408:GLU:O	1:E:409:SER:HB2	2.01	0.61
1:E:422:THR:CB	1:E:585:GLY:C	2.69	0.61
1:E:462:ASN:ND2	1:E:540:LEU:CB	2.63	0.61
1:F:17:MET:HA	1:F:33:ILE:O	2.00	0.61
1:F:107:TYR:HE1	1:F:153:LEU:HB2	1.64	0.61
1:G:316:ASN:O	1:G:317:MET:CB	2.49	0.61
1:A:283:TRP:O	1:A:284:HIS:HB2	2.00	0.61
1:A:316:ASN:O	1:A:317:MET:HB2	1.99	0.61
1:B:153:LEU:CD2	1:B:162:HIS:HD1	2.12	0.61
1:C:30:LEU:HD13	1:C:32:TRP:HE1	1.66	0.61
1:C:72:ASN:O	1:C:163:LYS:HA	2.01	0.61
1:C:373:ASP:C	1:C:374:CYS:SG	2.79	0.61
1:D:660:ILE:HG23	1:D:661:ALA:N	2.14	0.61
1:E:547:LEU:HD12	1:E:615:THR:CG2	2.04	0.61
1:H:359:LEU:HA	1:H:460:ARG:HH12	1.66	0.61
1:H:422:THR:HB	1:H:585:GLY:HA3	1.81	0.61
1:A:408:GLU:O	1:A:409:SER:HB2	2.01	0.61
1:B:345:GLY:O	1:B:347:PRO:HD3	2.01	0.61
1:B:386:LEU:HD12	1:B:386:LEU:H	1.65	0.61
1:E:334:GLN:HA	1:E:337:LYS:HB2	1.83	0.61
1:E:500:GLN:CB	1:E:505:ILE:HG12	2.30	0.61
1:F:563:LEU:HD23	1:F:597:ALA:HB2	1.83	0.61
1:F:580:ASP:HA	1:F:582:ARG:NH1	2.16	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:SER:HB3	1:A:453:THR:CB	2.31	0.61
1:B:105:ARG:O	1:B:107:TYR:N	2.34	0.61
1:B:352:GLU:O	1:B:388:PHE:HA	2.00	0.61
1:B:434:TRP:HB3	1:B:571:TYR:CE1	2.36	0.61
1:B:570:LEU:HD23	1:B:590:MET:HG2	1.81	0.61
1:C:143:HIS:CD2	1:C:145:ASP:O	2.53	0.61
1:E:17:MET:HA	1:E:33:ILE:O	2.01	0.61
1:E:384:GLY:O	1:E:385:ASP:HB2	2.00	0.61
1:E:402:SER:HA	1:E:609:TYR:CD1	2.36	0.61
1:F:437:ILE:HG13	1:F:594:LEU:HD12	1.81	0.61
1:G:105:ARG:HG2	1:G:109:ASN:HD21	1.66	0.61
1:G:206:TRP:C	1:G:206:TRP:CD1	2.74	0.61
1:H:120:GLY:HA2	1:H:123:ARG:HB2	1.83	0.61
1:H:192:GLU:OE1	1:H:192:GLU:HA	2.00	0.61
1:B:120:GLY:HA2	1:B:123:ARG:HB2	1.83	0.60
1:B:637:ARG:O	1:B:641:LYS:N	2.28	0.60
1:C:153:LEU:CD2	1:C:162:HIS:HD1	2.10	0.60
1:D:153:LEU:CD2	1:D:162:HIS:HD1	2.13	0.60
1:D:387:ILE:HD12	1:D:450:GLY:HA2	1.82	0.60
1:E:119:GLU:CB	1:E:121:PRO:CD	2.80	0.60
1:F:26:PHE:HE2	1:F:181:GLU:OE1	1.84	0.60
1:F:271:GLY:HA2	1:F:275:ARG:HH21	1.65	0.60
1:F:423:TYR:CD2	1:F:424:THR:HG23	2.35	0.60
1:F:434:TRP:CZ3	1:F:568:ARG:CA	2.77	0.60
1:G:409:SER:HB3	1:G:412:ILE:HD12	1.83	0.60
1:G:444:CYS:C	1:G:446:ARG:H	2.04	0.60
1:G:626:SER:HB2	1:G:630:LYS:HE3	1.80	0.60
1:H:143:HIS:CD2	1:H:145:ASP:O	2.54	0.60
1:A:644:VAL:O	1:A:644:VAL:HG12	2.01	0.60
1:C:651:GLN:HE22	1:D:492:ILE:CG2	1.98	0.60
1:C:654:LEU:HD11	1:D:655:TRP:HE3	1.64	0.60
1:D:145:ASP:OD1	1:D:167:LEU:HD13	2.00	0.60
1:D:345:GLY:O	1:D:347:PRO:HD3	2.00	0.60
1:D:626:SER:HB2	1:D:630:LYS:HE3	1.81	0.60
1:E:492:ILE:CG2	1:F:651:GLN:NE2	2.63	0.60
1:E:580:ASP:HA	1:E:582:ARG:NH1	2.16	0.60
1:F:145:ASP:OD1	1:F:167:LEU:HD13	2.01	0.60
1:G:260:PRO:CB	1:G:273:LEU:HD13	2.31	0.60
1:G:438:ARG:HG2	1:G:564:GLU:CD	2.20	0.60
1:H:368:THR:HA	1:H:371:VAL:CG2	2.31	0.60
1:H:580:ASP:HA	1:H:582:ARG:NH1	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LYS:HA	1:A:177:GLU:HA	1.83	0.60
1:A:500:GLN:HE22	1:B:659:LYS:HG2	1.65	0.60
1:B:220:ARG:HH12	1:B:223:LEU:CD2	2.14	0.60
1:C:333:LEU:HD11	1:C:353:LEU:HD13	1.83	0.60
1:D:434:TRP:HZ3	1:D:568:ARG:HG3	1.66	0.60
1:D:503:PHE:H	1:D:505:ILE:HD11	1.66	0.60
1:E:115:CYS:HB2	1:E:435:GLN:HG3	1.83	0.60
1:E:434:TRP:HE3	1:E:568:ARG:HA	1.62	0.60
1:F:18:LYS:HZ2	1:F:33:ILE:HG21	1.66	0.60
1:F:120:GLY:O	1:F:123:ARG:N	2.35	0.60
1:F:120:GLY:HA2	1:F:123:ARG:H	1.67	0.60
1:C:222:PHE:CG	1:C:255:PHE:HB3	2.36	0.60
1:D:220:ARG:HH12	1:D:223:LEU:CD2	2.14	0.60
1:E:117:LEU:O	1:E:119:GLU:HG2	2.00	0.60
1:E:462:ASN:HD21	1:E:540:LEU:CB	2.13	0.60
1:E:527:GLU:O	1:E:529:GLU:N	2.35	0.60
1:F:193:LEU:O	1:F:196:GLN:OE1	2.18	0.60
1:G:146:LEU:HA	1:G:150:ASN:HD21	1.67	0.60
1:H:18:LYS:HZ2	1:H:33:ILE:HG21	1.64	0.60
1:H:43:ILE:HA	1:H:94:LEU:O	2.01	0.60
1:H:416:ASP:CG	1:H:417:PRO:HD3	2.22	0.60
1:A:72:ASN:O	1:A:163:LYS:HA	2.01	0.60
1:A:83:LEU:HD21	1:A:86:LEU:HD11	1.83	0.60
1:A:220:ARG:HH12	1:A:223:LEU:CD2	2.15	0.60
1:B:30:LEU:HD13	1:B:32:TRP:HE1	1.67	0.60
1:B:419:ARG:N	1:B:420:PRO:HD3	2.03	0.60
1:C:17:MET:HA	1:C:33:ILE:O	2.01	0.60
1:C:171:LYS:HA	1:C:177:GLU:HA	1.82	0.60
1:D:30:LEU:HD13	1:D:32:TRP:HE1	1.66	0.60
1:D:43:ILE:HA	1:D:94:LEU:O	2.01	0.60
1:D:146:LEU:HA	1:D:150:ASN:HD21	1.66	0.60
1:E:265:LEU:HD21	1:E:269:LEU:HB3	1.83	0.60
1:E:473:THR:CG2	1:E:533:LEU:HD22	2.26	0.60
1:F:110:GLN:O	1:F:111:PHE:CB	2.34	0.60
1:F:120:GLY:HA2	1:F:123:ARG:HB2	1.84	0.60
1:F:245:VAL:O	1:F:257:SER:O	2.19	0.60
1:F:384:GLY:O	1:F:385:ASP:HB2	2.01	0.60
1:F:441:LYS:HB2	1:F:560:LEU:CD2	2.32	0.60
1:F:527:GLU:O	1:F:529:GLU:N	2.35	0.60
1:H:387:ILE:CD1	1:H:450:GLY:N	2.64	0.60
1:B:334:GLN:HA	1:B:337:LYS:HB2	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:ASN:ND2	1:C:265:LEU:N	2.49	0.60
1:E:570:LEU:HB3	1:E:590:MET:HE2	1.83	0.60
1:G:208:PHE:HD2	1:G:211:LEU:HD23	1.66	0.60
1:H:451:GLN:CD	1:H:611:GLN:HE22	2.03	0.60
1:A:222:PHE:CZ	1:A:225:ASN:HB2	2.37	0.60
1:A:409:SER:HB3	1:A:412:ILE:HD12	1.82	0.60
1:B:50:LEU:H	1:B:55:ARG:HD3	1.67	0.60
1:D:224:PRO:HG2	1:D:255:PHE:HE2	1.66	0.60
1:E:30:LEU:HD13	1:E:32:TRP:HE1	1.66	0.60
1:E:143:HIS:CD2	1:E:145:ASP:O	2.52	0.60
1:E:145:ASP:OD1	1:E:167:LEU:HD13	2.01	0.60
1:E:517:MET:HE3	1:E:647:GLN:OE1	2.01	0.60
1:E:644:VAL:O	1:E:644:VAL:HG12	2.02	0.60
1:F:333:LEU:HD11	1:F:353:LEU:HD13	1.82	0.60
1:G:68:LEU:HB3	1:G:135:TYR:HE2	1.66	0.60
1:H:230:GLN:C	1:H:232:HIS:N	2.44	0.60
1:H:352:GLU:O	1:H:388:PHE:HA	2.02	0.60
1:H:570:LEU:HD23	1:H:590:MET:HG2	1.82	0.60
1:B:503:PHE:O	1:B:505:ILE:HG13	2.02	0.60
1:C:63:GLN:O	1:C:67:LYS:HB2	2.02	0.60
1:C:150:ASN:OD1	1:C:150:ASN:N	2.31	0.60
1:D:387:ILE:CD1	1:D:450:GLY:N	2.65	0.60
1:D:580:ASP:HA	1:D:582:ARG:NH1	2.16	0.60
1:E:63:GLN:O	1:E:67:LYS:HB2	2.01	0.60
1:E:120:GLY:HA2	1:E:123:ARG:H	1.65	0.60
1:F:115:CYS:O	1:F:263:ASN:HA	2.01	0.60
1:F:493:ASP:HB3	1:F:514:TRP:CH2	2.36	0.60
1:F:587:SER:OG	1:F:588:ASN:N	2.34	0.60
1:A:419:ARG:N	1:A:420:PRO:HD3	2.04	0.60
1:C:246:TYR:CD1	1:C:258:VAL:CB	2.71	0.60
1:C:422:THR:CB	1:C:585:GLY:CA	2.69	0.60
1:C:497:TYR:HB2	1:D:655:TRP:CH2	2.37	0.60
1:C:502:GLU:HG3	1:D:666:ARG:HH11	1.64	0.60
1:F:119:GLU:CB	1:F:121:PRO:CD	2.80	0.60
1:F:224:PRO:HG2	1:F:255:PHE:HE2	1.67	0.60
1:F:283:TRP:O	1:F:284:HIS:HB2	2.01	0.60
1:F:408:GLU:O	1:F:409:SER:HB2	2.01	0.60
1:G:105:ARG:O	1:G:107:TYR:N	2.35	0.60
1:H:182:PHE:CE1	1:H:194:LEU:HD22	2.36	0.60
1:H:220:ARG:HH12	1:H:223:LEU:CD2	2.14	0.60
1:H:271:GLY:HA2	1:H:275:ARG:HH21	1.65	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:GLN:O	1:B:67:LYS:HB2	2.01	0.60
1:B:230:GLN:C	1:B:232:HIS:N	2.43	0.60
1:B:260:PRO:CB	1:B:273:LEU:HD13	2.32	0.60
1:D:17:MET:HA	1:D:33:ILE:O	2.01	0.60
1:D:63:GLN:O	1:D:67:LYS:HB2	2.01	0.60
1:D:103:ASP:HB3	1:D:106:LYS:HG3	1.84	0.60
1:D:316:ASN:O	1:D:317:MET:HB2	2.00	0.60
1:E:171:LYS:HA	1:E:177:GLU:HA	1.82	0.60
1:F:503:PHE:C	1:F:505:ILE:H	2.05	0.60
1:G:286:ARG:HG2	1:G:286:ARG:HH11	1.64	0.60
1:H:206:TRP:CD1	1:H:206:TRP:C	2.74	0.60
1:B:271:GLY:HA2	1:B:275:ARG:HH21	1.67	0.59
1:C:43:ILE:HA	1:C:94:LEU:O	2.02	0.59
1:C:473:THR:CG2	1:C:533:LEU:HD22	2.27	0.59
1:C:632:VAL:C	1:C:633:MET:SD	2.81	0.59
1:D:333:LEU:HD11	1:D:353:LEU:HD13	1.84	0.59
1:D:500:GLN:HB3	1:D:505:ILE:HG12	1.84	0.59
1:G:192:GLU:OE1	1:G:192:GLU:HA	2.02	0.59
1:G:198:LYS:C	1:G:200:THR:H	2.05	0.59
1:G:271:GLY:HA2	1:G:275:ARG:HH21	1.67	0.59
1:G:352:GLU:O	1:G:388:PHE:HA	2.02	0.59
1:H:409:SER:HB3	1:H:412:ILE:HD12	1.84	0.59
1:H:423:TYR:CD2	1:H:424:THR:HG23	2.37	0.59
1:A:182:PHE:CE1	1:A:194:LEU:HD22	2.37	0.59
1:B:105:ARG:HG2	1:B:109:ASN:HD21	1.66	0.59
1:B:434:TRP:HZ3	1:B:568:ARG:CB	2.15	0.59
1:C:119:GLU:HB2	1:C:121:PRO:CD	2.32	0.59
1:C:134:ARG:CA	1:C:300:PHE:CZ	2.76	0.59
1:C:150:ASN:ND2	1:C:167:LEU:HD12	2.13	0.59
1:C:496:LYS:CB	1:D:655:TRP:NE1	2.09	0.59
1:D:319:SER:O	1:D:321:ARG:N	2.35	0.59
1:D:416:ASP:CG	1:D:417:PRO:HD3	2.22	0.59
1:E:219:PHE:O	1:E:220:ARG:HG3	1.88	0.59
1:E:222:PHE:CZ	1:E:225:ASN:HB2	2.38	0.59
1:F:206:TRP:CD1	1:F:206:TRP:C	2.76	0.59
1:F:260:PRO:CB	1:F:273:LEU:HD13	2.32	0.59
1:A:246:TYR:CD1	1:A:258:VAL:CB	2.70	0.59
1:B:103:ASP:HB3	1:B:106:LYS:HG3	1.85	0.59
1:B:150:ASN:OD1	1:B:150:ASN:N	2.35	0.59
1:B:150:ASN:ND2	1:B:167:LEU:HD12	2.15	0.59
1:B:423:TYR:CD2	1:B:424:THR:HG23	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:ASN:O	1:C:317:MET:CB	2.50	0.59
1:C:476:CYS:HB2	1:C:636:MET:SD	2.42	0.59
1:C:485:PHE:CE1	1:D:485:PHE:CD1	2.90	0.59
1:D:531:GLN:O	1:D:535:ASP:N	2.34	0.59
1:D:632:VAL:C	1:D:633:MET:SD	2.81	0.59
1:E:319:SER:CB	1:E:403:LEU:HB2	2.31	0.59
1:E:472:MET:HG3	1:E:472:MET:O	2.03	0.59
1:G:276:TRP:CE3	1:G:277:LEU:HD23	2.37	0.59
1:G:394:LYS:HD2	1:G:613:SER:HB2	1.82	0.59
1:H:134:ARG:HD2	1:H:300:PHE:CE1	2.37	0.59
1:H:193:LEU:HD22	1:H:231:TRP:NE1	2.16	0.59
1:H:276:TRP:CE3	1:H:277:LEU:HD23	2.37	0.59
1:A:146:LEU:HA	1:A:150:ASN:HD21	1.67	0.59
1:A:276:TRP:CE3	1:A:277:LEU:HD23	2.37	0.59
1:A:531:GLN:O	1:A:535:ASP:N	2.35	0.59
1:B:146:LEU:HA	1:B:150:ASN:HD21	1.67	0.59
1:C:50:LEU:H	1:C:55:ARG:HD3	1.68	0.59
1:D:182:PHE:CE1	1:D:194:LEU:HD22	2.38	0.59
1:D:409:SER:HB3	1:D:412:ILE:HD12	1.84	0.59
1:D:433:ILE:CB	1:D:571:TYR:OH	2.49	0.59
1:E:50:LEU:H	1:E:55:ARG:HD3	1.68	0.59
1:G:171:LYS:HA	1:G:177:GLU:HA	1.83	0.59
1:G:350:GLU:HA	1:G:391:ASP:OD2	2.02	0.59
1:H:30:LEU:HD13	1:H:32:TRP:HE1	1.67	0.59
1:H:316:ASN:O	1:H:317:MET:CB	2.50	0.59
1:A:333:LEU:HD11	1:A:353:LEU:HD13	1.85	0.59
1:B:119:GLU:CB	1:B:121:PRO:CD	2.80	0.59
1:D:83:LEU:HD21	1:D:86:LEU:HD11	1.85	0.59
1:E:103:ASP:HB3	1:E:106:LYS:HG3	1.83	0.59
1:E:570:LEU:HD23	1:E:590:MET:HG2	1.83	0.59
1:E:660:ILE:HG23	1:E:661:ALA:N	2.15	0.59
1:F:105:ARG:HG2	1:F:109:ASN:HD21	1.67	0.59
1:F:319:SER:OG	1:F:403:LEU:CB	2.50	0.59
1:F:334:GLN:HA	1:F:337:LYS:HB2	1.84	0.59
1:F:387:ILE:HG21	1:F:450:GLY:CA	2.29	0.59
1:H:150:ASN:ND2	1:H:167:LEU:HD12	2.15	0.59
1:A:30:LEU:HD13	1:A:32:TRP:HE1	1.65	0.59
1:A:285:GLN:NE2	1:A:286:ARG:HH12	2.00	0.59
1:B:540:LEU:HD22	1:B:621:LYS:NZ	2.17	0.59
1:E:116:GLY:N	1:E:217:THR:O	2.36	0.59
1:E:497:TYR:O	1:E:497:TYR:HD2	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:GLN:O	1:G:67:LYS:HB2	2.02	0.59
1:G:120:GLY:HA2	1:G:123:ARG:HB2	1.85	0.59
1:G:200:THR:O	1:G:201:VAL:C	2.41	0.59
1:G:416:ASP:CG	1:G:417:PRO:HD3	2.23	0.59
1:H:265:LEU:HD21	1:H:269:LEU:HB3	1.85	0.59
1:A:43:ILE:HA	1:A:94:LEU:O	2.01	0.59
1:A:352:GLU:O	1:A:388:PHE:HA	2.03	0.59
1:A:423:TYR:CD2	1:A:424:THR:HG23	2.37	0.59
1:B:416:ASP:CG	1:B:417:PRO:HD3	2.23	0.59
1:B:580:ASP:HA	1:B:582:ARG:NH1	2.17	0.59
1:C:644:VAL:O	1:C:644:VAL:HG12	2.03	0.59
1:D:191:PRO:HG3	1:D:234:LYS:HZ2	1.67	0.59
1:D:394:LYS:HE3	1:D:609:TYR:C	2.22	0.59
1:D:433:ILE:CG2	1:D:571:TYR:OH	2.50	0.59
1:F:434:TRP:HZ3	1:F:568:ARG:HA	1.58	0.59
1:F:531:GLN:O	1:F:535:ASP:N	2.36	0.59
1:G:368:THR:HA	1:G:371:VAL:CG2	2.32	0.59
1:G:384:GLY:O	1:G:385:ASP:HB2	2.00	0.59
1:H:587:SER:OG	1:H:588:ASN:N	2.35	0.59
1:A:368:THR:HA	1:A:371:VAL:CG2	2.32	0.59
1:A:497:TYR:O	1:A:497:TYR:HD2	1.85	0.59
1:B:409:SER:HB3	1:B:412:ILE:HD12	1.82	0.59
1:B:501:MET:CA	1:B:505:ILE:HD13	2.33	0.59
1:C:462:ASN:HD21	1:C:540:LEU:CB	2.13	0.59
1:D:319:SER:CB	1:D:403:LEU:HB2	2.32	0.59
1:G:434:TRP:HZ3	1:G:568:ARG:HA	1.57	0.59
1:B:182:PHE:CE1	1:B:194:LEU:HD22	2.37	0.59
1:C:249:LEU:O	1:C:250:THR:HG23	2.03	0.59
1:D:50:LEU:H	1:D:55:ARG:HD3	1.68	0.59
1:E:423:TYR:CD2	1:E:424:THR:HG23	2.38	0.59
1:G:83:LEU:HD21	1:G:86:LEU:HD11	1.84	0.59
1:G:222:PHE:CZ	1:G:225:ASN:HB2	2.38	0.59
1:G:345:GLY:O	1:G:347:PRO:HD3	2.02	0.59
1:H:105:ARG:O	1:H:107:TYR:N	2.36	0.59
1:H:119:GLU:CB	1:H:121:PRO:CD	2.81	0.59
1:A:243:ILE:N	1:A:245:VAL:HG23	2.17	0.59
1:A:271:GLY:HA2	1:A:275:ARG:HH21	1.68	0.59
1:A:478:GLN:CG	1:A:479:LEU:N	2.66	0.59
1:B:145:ASP:OD1	1:B:167:LEU:HD13	2.02	0.59
1:B:500:GLN:O	1:B:505:ILE:HG21	2.03	0.59
1:C:200:THR:O	1:C:201:VAL:C	2.41	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:521:VAL:HG13	1:D:643:VAL:HG12	1.85	0.59
1:E:83:LEU:HD21	1:E:86:LEU:HD11	1.85	0.59
1:E:105:ARG:HG3	1:E:105:ARG:HH11	1.68	0.59
1:E:182:PHE:CE1	1:E:194:LEU:HD22	2.38	0.59
1:F:50:LEU:H	1:F:55:ARG:HD3	1.68	0.59
1:G:333:LEU:HD11	1:G:353:LEU:HD13	1.84	0.59
1:A:117:LEU:O	1:A:119:GLU:HG2	2.03	0.58
1:A:319:SER:O	1:A:321:ARG:N	2.34	0.58
1:A:660:ILE:HG23	1:A:661:ALA:N	2.18	0.58
1:B:333:LEU:HD11	1:B:353:LEU:HD13	1.84	0.58
1:B:394:LYS:HD3	1:B:401:ILE:HA	1.84	0.58
1:C:345:GLY:O	1:C:347:PRO:HD3	2.03	0.58
1:C:416:ASP:CG	1:C:417:PRO:HD3	2.22	0.58
1:C:426:LEU:HB2	1:C:574:LEU:HD21	1.83	0.58
1:D:271:GLY:HA2	1:D:275:ARG:HH21	1.67	0.58
1:E:146:LEU:HA	1:E:150:ASN:HD21	1.67	0.58
1:E:416:ASP:CG	1:E:417:PRO:HD3	2.23	0.58
1:E:655:TRP:CZ3	1:F:654:LEU:CD1	2.85	0.58
1:F:409:SER:HB3	1:F:412:ILE:HD12	1.85	0.58
1:F:521:VAL:CG1	1:F:643:VAL:HG12	2.31	0.58
1:G:246:TYR:CD1	1:G:258:VAL:CB	2.70	0.58
1:H:105:ARG:HG2	1:H:109:ASN:HD21	1.67	0.58
1:H:243:ILE:N	1:H:245:VAL:HG23	2.18	0.58
1:A:120:GLY:HA2	1:A:123:ARG:HB2	1.85	0.58
1:C:83:LEU:HD21	1:C:86:LEU:HD11	1.84	0.58
1:C:362:ASN:C	1:C:364:ALA:H	2.07	0.58
1:D:131:SER:O	1:D:134:ARG:HB3	2.03	0.58
1:E:352:GLU:O	1:E:388:PHE:HA	2.02	0.58
1:E:571:TYR:CE2	1:E:590:MET:HG3	2.38	0.58
1:F:43:ILE:HA	1:F:94:LEU:O	2.03	0.58
1:G:243:ILE:N	1:G:245:VAL:HG23	2.18	0.58
1:B:610:ASP:O	1:B:613:SER:HB3	2.03	0.58
1:H:120:GLY:O	1:H:123:ARG:N	2.36	0.58
1:H:422:THR:HB	1:H:585:GLY:C	2.22	0.58
1:A:455:MET:HE2	1:A:455:MET:O	2.03	0.58
1:B:83:LEU:HD21	1:B:86:LEU:HD11	1.85	0.58
1:B:521:VAL:HG13	1:B:643:VAL:HG11	1.83	0.58
1:C:222:PHE:CZ	1:C:225:ASN:HB2	2.39	0.58
1:C:352:GLU:O	1:C:388:PHE:HA	2.02	0.58
1:E:191:PRO:HG3	1:E:234:LYS:HZ3	1.69	0.58
1:E:260:PRO:CG	1:E:274:GLU:HG2	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:263:ASN:ND2	1:F:265:LEU:H	2.01	0.58
1:F:484:ASP:C	1:F:486:PHE:N	2.56	0.58
1:G:531:GLN:O	1:G:535:ASP:N	2.36	0.58
1:A:206:TRP:CD1	1:A:206:TRP:C	2.76	0.58
1:A:504:GLY:N	1:B:662:CYS:SG	2.77	0.58
1:C:423:TYR:CD2	1:C:424:THR:HG23	2.38	0.58
1:D:222:PHE:CZ	1:D:225:ASN:HB2	2.37	0.58
1:D:316:ASN:O	1:D:317:MET:CB	2.51	0.58
1:E:119:GLU:HB2	1:E:121:PRO:CD	2.34	0.58
1:E:419:ARG:N	1:E:420:PRO:HD3	2.04	0.58
1:F:480:LYS:CE	1:F:527:GLU:HB2	2.33	0.58
1:G:43:ILE:HA	1:G:94:LEU:O	2.02	0.58
1:H:246:TYR:CD1	1:H:258:VAL:CB	2.70	0.58
1:A:50:LEU:H	1:A:55:ARG:HD3	1.68	0.58
1:A:222:PHE:CD2	1:A:255:PHE:CD2	2.92	0.58
1:B:43:ILE:HA	1:B:94:LEU:O	2.03	0.58
1:B:183:VAL:HG12	1:B:184:GLY:N	2.19	0.58
1:B:206:TRP:C	1:B:206:TRP:CD1	2.77	0.58
1:B:387:ILE:HG21	1:B:450:GLY:CA	2.31	0.58
1:B:480:LYS:NZ	1:B:527:GLU:HB2	2.19	0.58
1:B:484:ASP:C	1:B:486:PHE:N	2.56	0.58
1:B:531:GLN:O	1:B:535:ASP:N	2.36	0.58
1:C:350:GLU:HA	1:C:391:ASP:OD2	2.03	0.58
1:D:387:ILE:CD1	1:D:449:GLN:HG3	2.32	0.58
1:E:131:SER:O	1:E:134:ARG:HB3	2.03	0.58
1:E:183:VAL:HG12	1:E:184:GLY:N	2.19	0.58
1:E:357:SER:HA	1:E:453:THR:HB	1.85	0.58
1:E:368:THR:HA	1:E:371:VAL:CG2	2.31	0.58
1:F:220:ARG:NH1	1:F:223:LEU:CD2	2.65	0.58
1:A:120:GLY:HA2	1:A:123:ARG:H	1.68	0.58
1:A:416:ASP:CG	1:A:417:PRO:HD3	2.24	0.58
1:D:120:GLY:HA2	1:D:123:ARG:HB2	1.85	0.58
1:D:437:ILE:HG13	1:D:594:LEU:HD12	1.85	0.58
1:E:72:ASN:H	1:E:163:LYS:HE2	1.67	0.58
1:E:243:ILE:N	1:E:245:VAL:HG23	2.19	0.58
1:E:394:LYS:CG	1:E:613:SER:HB2	2.32	0.58
1:E:500:GLN:HB3	1:E:505:ILE:CG1	2.33	0.58
1:G:315:MET:HB3	1:G:387:ILE:HA	1.85	0.58
1:H:350:GLU:HA	1:H:391:ASP:OD2	2.03	0.58
1:B:434:TRP:CZ3	1:B:568:ARG:HG3	2.39	0.58
1:C:116:GLY:N	1:C:217:THR:O	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:570:LEU:HD23	1:C:590:MET:HG2	1.86	0.58
1:C:587:SER:OG	1:C:588:ASN:N	2.31	0.58
1:E:263:ASN:ND2	1:E:265:LEU:N	2.51	0.58
1:E:654:LEU:HD21	1:F:654:LEU:HD23	1.86	0.58
1:E:659:LYS:HG2	1:F:500:GLN:HE22	1.68	0.58
1:F:249:LEU:HD23	1:F:252:ALA:CA	2.24	0.58
1:G:118:LYS:CG	1:G:265:LEU:HA	2.33	0.58
1:G:247:ASP:HB2	1:G:255:PHE:O	2.04	0.58
1:G:265:LEU:HD23	1:G:269:LEU:HB3	1.85	0.58
1:G:441:LYS:HB2	1:G:560:LEU:CD2	2.34	0.58
1:H:222:PHE:CZ	1:H:225:ASN:HB2	2.38	0.58
1:H:285:GLN:NE2	1:H:286:ARG:HH12	2.02	0.58
1:A:260:PRO:CB	1:A:273:LEU:HD13	2.33	0.58
1:B:191:PRO:HG3	1:B:234:LYS:NZ	2.19	0.58
1:B:570:LEU:HB3	1:B:590:MET:CE	2.34	0.58
1:D:276:TRP:CE3	1:D:277:LEU:HD23	2.39	0.58
1:E:220:ARG:HH12	1:E:223:LEU:CD2	2.17	0.58
1:E:249:LEU:O	1:E:250:THR:HG23	2.04	0.58
1:F:434:TRP:HZ3	1:F:568:ARG:CG	2.17	0.58
1:G:182:PHE:CE1	1:G:194:LEU:HD22	2.39	0.58
1:G:587:SER:OG	1:G:588:ASN:N	2.37	0.58
1:H:387:ILE:HD12	1:H:450:GLY:HA2	1.84	0.58
1:H:582:ARG:H	1:H:582:ARG:CD	2.17	0.58
1:A:580:ASP:HB3	1:D:579:ARG:HH22	1.69	0.58
1:C:146:LEU:HA	1:C:150:ASN:HD21	1.69	0.58
1:C:387:ILE:HD12	1:C:450:GLY:HA2	1.84	0.58
1:C:531:GLN:O	1:C:535:ASP:N	2.36	0.58
1:E:409:SER:HB3	1:E:412:ILE:HD12	1.85	0.58
1:F:276:TRP:CE3	1:F:277:LEU:HD23	2.38	0.58
1:F:433:ILE:CG2	1:F:571:TYR:OH	2.52	0.58
1:G:220:ARG:NH1	1:G:223:LEU:CD2	2.67	0.58
1:A:263:ASN:ND2	1:A:265:LEU:N	2.52	0.57
1:A:480:LYS:NZ	1:A:527:GLU:HB2	2.19	0.57
1:B:222:PHE:CZ	1:B:225:ASN:HB2	2.38	0.57
1:B:434:TRP:HZ3	1:B:568:ARG:CG	2.17	0.57
1:B:478:GLN:CG	1:B:479:LEU:N	2.66	0.57
1:B:587:SER:OG	1:B:588:ASN:N	2.35	0.57
1:C:220:ARG:HH12	1:C:223:LEU:CD2	2.16	0.57
1:C:409:SER:HB3	1:C:412:ILE:HD12	1.84	0.57
1:C:478:GLN:CG	1:C:479:LEU:N	2.67	0.57
1:D:476:CYS:HB2	1:D:636:MET:SD	2.43	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:527:GLU:HG2	1:E:530:VAL:HG13	1.86	0.57
1:F:222:PHE:CD2	1:F:255:PHE:CD2	2.91	0.57
1:G:119:GLU:CB	1:G:121:PRO:CD	2.82	0.57
1:H:105:ARG:O	1:H:106:LYS:C	2.42	0.57
1:H:146:LEU:HA	1:H:150:ASN:HD21	1.68	0.57
1:H:437:ILE:CG2	1:H:564:GLU:HB2	2.34	0.57
1:H:472:MET:HG3	1:H:472:MET:O	2.04	0.57
1:A:437:ILE:HG13	1:A:594:LEU:HD12	1.86	0.57
1:A:484:ASP:C	1:A:486:PHE:N	2.56	0.57
1:B:660:ILE:HG23	1:B:661:ALA:N	2.18	0.57
1:C:116:GLY:HA2	1:C:217:THR:O	2.04	0.57
1:C:118:LYS:HD3	1:C:265:LEU:HD12	1.85	0.57
1:D:213:PHE:O	1:D:216:ILE:N	2.37	0.57
1:D:434:TRP:HZ3	1:D:568:ARG:CG	2.16	0.57
1:E:426:LEU:HB2	1:E:574:LEU:HD21	1.85	0.57
1:G:120:GLY:HA2	1:G:123:ARG:H	1.69	0.57
1:G:171:LYS:HD2	1:G:177:GLU:HG2	1.85	0.57
1:G:249:LEU:O	1:G:250:THR:HG23	2.05	0.57
1:G:362:ASN:C	1:G:364:ALA:H	2.06	0.57
1:H:265:LEU:HD23	1:H:269:LEU:HB3	1.85	0.57
1:H:362:ASN:C	1:H:364:ALA:H	2.07	0.57
1:H:447:LEU:HD12	1:H:605:VAL:HG22	1.85	0.57
1:B:115:CYS:CB	1:B:435:GLN:HG3	2.33	0.57
1:B:644:VAL:HG12	1:B:644:VAL:O	2.03	0.57
1:C:492:ILE:CD1	1:D:651:GLN:HE21	2.10	0.57
1:C:661:ALA:O	1:D:661:ALA:O	2.21	0.57
1:D:105:ARG:HH11	1:D:105:ARG:HG3	1.69	0.57
1:D:285:GLN:NE2	1:D:286:ARG:HH12	2.01	0.57
1:D:362:ASN:C	1:D:364:ALA:H	2.07	0.57
1:E:107:TYR:HD1	1:E:153:LEU:HD12	1.69	0.57
1:E:666:ARG:HH11	1:F:502:GLU:HG3	1.68	0.57
1:F:118:LYS:HD3	1:F:265:LEU:HD12	1.85	0.57
1:F:637:ARG:O	1:F:641:LYS:N	2.31	0.57
1:G:143:HIS:CD2	1:G:145:ASP:O	2.54	0.57
1:H:315:MET:HB3	1:H:387:ILE:HA	1.85	0.57
1:A:30:LEU:HD13	1:A:32:TRP:NE1	2.19	0.57
1:A:105:ARG:HG2	1:A:109:ASN:HD21	1.67	0.57
1:A:316:ASN:O	1:A:317:MET:CB	2.51	0.57
1:A:651:GLN:NE2	1:B:492:ILE:CG2	2.67	0.57
1:B:315:MET:HB3	1:B:387:ILE:HA	1.85	0.57
1:B:478:GLN:HE21	1:B:479:LEU:HD23	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ARG:HH11	1:C:105:ARG:HG3	1.68	0.57
1:C:276:TRP:CE3	1:C:277:LEU:HD23	2.39	0.57
1:C:655:TRP:NE1	1:D:496:LYS:CB	2.45	0.57
1:C:666:ARG:HD2	1:D:503:PHE:CD1	2.39	0.57
1:D:115:CYS:SG	1:D:432:GLN:HA	2.45	0.57
1:D:120:GLY:HA2	1:D:123:ARG:H	1.70	0.57
1:D:423:TYR:CD2	1:D:424:THR:HG23	2.38	0.57
1:E:492:ILE:HG23	1:F:651:GLN:NE2	2.17	0.57
1:F:83:LEU:HD21	1:F:86:LEU:HD11	1.85	0.57
1:F:134:ARG:HD2	1:F:300:PHE:CE1	2.39	0.57
1:G:30:LEU:HD13	1:G:32:TRP:NE1	2.20	0.57
1:H:83:LEU:HD21	1:H:86:LEU:HD11	1.85	0.57
1:H:120:GLY:HA2	1:H:123:ARG:H	1.68	0.57
1:H:274:GLU:O	1:H:278:GLN:HB2	2.05	0.57
1:A:315:MET:HB3	1:A:387:ILE:HA	1.86	0.57
1:C:224:PRO:HG2	1:C:255:PHE:HE2	1.67	0.57
1:C:484:ASP:C	1:C:486:PHE:N	2.56	0.57
1:D:171:LYS:HD2	1:D:177:GLU:HG2	1.87	0.57
1:D:438:ARG:HG2	1:D:564:GLU:OE1	2.05	0.57
1:E:229:VAL:HG13	1:H:229:VAL:CG1	2.29	0.57
1:E:316:ASN:O	1:E:317:MET:HB2	2.04	0.57
1:E:632:VAL:C	1:E:633:MET:SD	2.83	0.57
1:G:105:ARG:O	1:G:106:LYS:C	2.40	0.57
1:A:115:CYS:HB2	1:A:435:GLN:HG3	1.85	0.57
1:A:119:GLU:CB	1:A:121:PRO:CD	2.81	0.57
1:A:200:THR:O	1:A:201:VAL:C	2.43	0.57
1:A:563:LEU:HD23	1:A:597:ALA:HB2	1.85	0.57
1:B:105:ARG:HH11	1:B:105:ARG:HG3	1.69	0.57
1:C:120:GLY:HA2	1:C:123:ARG:H	1.69	0.57
1:C:472:MET:O	1:C:472:MET:HG3	2.04	0.57
1:E:480:LYS:HZ2	1:E:525:GLY:C	2.08	0.57
1:H:107:TYR:HA	1:H:110:GLN:HB2	1.86	0.57
1:A:119:GLU:HB2	1:A:121:PRO:CD	2.35	0.57
1:B:198:LYS:C	1:B:200:THR:H	2.08	0.57
1:B:480:LYS:CE	1:B:527:GLU:HB2	2.35	0.57
1:C:120:GLY:HA2	1:C:123:ARG:HB2	1.85	0.57
1:E:115:CYS:O	1:E:263:ASN:HA	2.05	0.57
1:E:473:THR:CG2	1:E:533:LEU:HD21	2.33	0.57
1:F:434:TRP:HZ3	1:F:568:ARG:CA	2.16	0.57
1:F:478:GLN:CG	1:F:479:LEU:N	2.67	0.57
1:G:117:LEU:O	1:G:119:GLU:HG2	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:SER:O	1:C:321:ARG:N	2.34	0.57
1:C:338:SER:OG	1:E:284:HIS:HE1	1.88	0.57
1:D:536:LYS:O	1:D:625:LEU:CD1	2.45	0.57
1:D:570:LEU:HD23	1:D:590:MET:CG	2.32	0.57
1:E:189:LEU:CG	1:E:190:ALA:N	2.64	0.57
1:E:262:PRO:HB3	1:E:409:SER:HG	1.69	0.57
1:E:434:TRP:HZ3	1:E:568:ARG:HG3	1.68	0.57
1:F:350:GLU:HA	1:F:391:ASP:OD2	2.04	0.57
1:G:285:GLN:NE2	1:G:286:ARG:HH12	2.02	0.57
1:B:319:SER:O	1:B:321:ARG:N	2.34	0.57
1:B:387:ILE:CD1	1:B:450:GLY:N	2.68	0.57
1:B:438:ARG:HG2	1:B:564:GLU:OE1	2.05	0.57
1:C:271:GLY:HA2	1:C:275:ARG:HH21	1.70	0.57
1:D:387:ILE:HD12	1:D:450:GLY:CA	2.35	0.57
1:D:478:GLN:CG	1:D:479:LEU:N	2.68	0.57
1:E:274:GLU:O	1:E:278:GLN:HB2	2.05	0.57
1:F:362:ASN:C	1:F:364:ALA:H	2.08	0.57
1:G:50:LEU:H	1:G:55:ARG:HD3	1.70	0.57
1:H:50:LEU:H	1:H:55:ARG:HD3	1.69	0.57
1:H:171:LYS:HD2	1:H:177:GLU:HG2	1.86	0.57
1:A:103:ASP:HB3	1:A:106:LYS:HG3	1.87	0.57
1:A:231:TRP:HE3	1:D:236:ARG:NH2	1.98	0.57
1:A:265:LEU:HD23	1:A:269:LEU:HB3	1.86	0.57
1:A:373:ASP:C	1:A:374:CYS:SG	2.83	0.57
1:B:118:LYS:HG2	1:B:265:LEU:HA	1.87	0.57
1:B:285:GLN:NE2	1:B:286:ARG:HH12	2.03	0.57
1:B:490:ILE:HG23	1:B:490:ILE:O	2.04	0.57
1:B:540:LEU:CD2	1:B:621:LYS:HZ1	2.18	0.57
1:D:386:LEU:H	1:D:386:LEU:CD1	2.18	0.57
1:E:120:GLY:HA2	1:E:123:ARG:HB2	1.87	0.57
1:E:333:LEU:HD11	1:E:353:LEU:HD13	1.86	0.57
1:F:243:ILE:N	1:F:245:VAL:HG23	2.19	0.57
1:F:249:LEU:O	1:F:250:THR:HG23	2.05	0.57
1:F:517:MET:SD	1:F:650:ARG:HG3	2.45	0.57
1:G:108:LEU:HD21	1:G:215:CYS:SG	2.45	0.57
1:G:130:SER:O	1:G:300:PHE:HE1	1.88	0.57
1:H:131:SER:O	1:H:134:ARG:HB3	2.05	0.57
1:H:333:LEU:HD11	1:H:353:LEU:HD13	1.87	0.57
1:A:247:ASP:HB2	1:A:255:PHE:O	2.06	0.56
1:A:570:LEU:HD23	1:A:590:MET:CG	2.34	0.56
1:B:362:ASN:C	1:B:364:ALA:H	2.07	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:GLN:NE2	1:C:429:VAL:HG11	2.20	0.56
1:D:533:LEU:CD2	1:D:629:VAL:HG13	2.35	0.56
1:E:655:TRP:NE1	1:F:496:LYS:CB	2.37	0.56
1:F:434:TRP:CZ3	1:F:568:ARG:HG3	2.39	0.56
1:H:107:TYR:HD1	1:H:153:LEU:HD12	1.70	0.56
1:H:570:LEU:CB	1:H:590:MET:HE2	2.35	0.56
1:A:189:LEU:CG	1:A:190:ALA:N	2.64	0.56
1:A:249:LEU:HA	1:A:253:VAL:O	2.05	0.56
1:B:368:THR:HA	1:B:371:VAL:CG2	2.32	0.56
1:C:103:ASP:HB3	1:C:106:LYS:HG3	1.87	0.56
1:C:107:TYR:O	1:C:110:GLN:CB	2.53	0.56
1:C:111:PHE:HZ	1:C:572:ARG:CG	2.08	0.56
1:C:117:LEU:O	1:C:119:GLU:HG2	2.04	0.56
1:C:497:TYR:O	1:C:497:TYR:HD2	1.83	0.56
1:C:536:LYS:HB3	1:C:625:LEU:CD1	2.14	0.56
1:D:249:LEU:HD23	1:D:252:ALA:CA	2.24	0.56
1:E:587:SER:OG	1:E:588:ASN:N	2.34	0.56
1:F:125:LEU:HD21	1:F:215:CYS:SG	2.45	0.56
1:F:182:PHE:CE1	1:F:194:LEU:HD22	2.40	0.56
1:F:213:PHE:O	1:F:216:ILE:N	2.38	0.56
1:F:490:ILE:O	1:F:490:ILE:HG23	2.05	0.56
1:G:249:LEU:HA	1:G:253:VAL:O	2.05	0.56
1:G:423:TYR:CD2	1:G:424:THR:HG23	2.40	0.56
1:A:540:LEU:HD11	1:A:622:ALA:HB2	1.86	0.56
1:B:224:PRO:HG2	1:B:255:PHE:HE2	1.69	0.56
1:C:105:ARG:HG2	1:C:109:ASN:HD21	1.70	0.56
1:C:107:TYR:HD1	1:C:153:LEU:HD12	1.70	0.56
1:C:183:VAL:HG12	1:C:184:GLY:N	2.20	0.56
1:C:222:PHE:CD2	1:C:224:PRO:O	2.59	0.56
1:C:243:ILE:N	1:C:245:VAL:HG23	2.20	0.56
1:C:373:ASP:CG	1:C:374:CYS:SG	2.83	0.56
1:C:451:GLN:CD	1:C:611:GLN:NE2	2.59	0.56
1:D:30:LEU:HD13	1:D:32:TRP:NE1	2.21	0.56
1:D:105:ARG:HG2	1:D:109:ASN:HD21	1.69	0.56
1:D:198:LYS:HG2	1:D:284:HIS:HA	1.87	0.56
1:D:315:MET:HB3	1:D:387:ILE:HA	1.86	0.56
1:E:260:PRO:CB	1:E:273:LEU:HD13	2.35	0.56
1:E:362:ASN:C	1:E:364:ALA:H	2.09	0.56
1:E:478:GLN:HE21	1:E:479:LEU:HD23	1.70	0.56
1:E:490:ILE:HG23	1:E:490:ILE:O	2.03	0.56
1:E:531:GLN:O	1:E:535:ASP:N	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:30:LEU:HD13	1:F:32:TRP:NE1	2.20	0.56
1:F:247:ASP:HB2	1:F:255:PHE:O	2.05	0.56
1:F:319:SER:O	1:F:321:ARG:N	2.35	0.56
1:F:422:THR:HB	1:F:585:GLY:HA3	1.84	0.56
1:F:472:MET:SD	1:F:633:MET:HB2	2.45	0.56
1:F:536:LYS:O	1:F:625:LEU:HD13	2.05	0.56
1:G:274:GLU:O	1:G:278:GLN:HB2	2.05	0.56
1:H:249:LEU:HD23	1:H:252:ALA:CA	2.27	0.56
1:B:171:LYS:HD2	1:B:177:GLU:HG2	1.88	0.56
1:B:262:PRO:CB	1:B:409:SER:OG	2.45	0.56
1:B:451:GLN:NE2	1:B:608:ILE:O	2.38	0.56
1:B:472:MET:HG3	1:B:472:MET:O	2.05	0.56
1:C:222:PHE:CD2	1:C:255:PHE:CD2	2.93	0.56
1:C:430:TRP:CE3	1:C:574:LEU:HD22	2.40	0.56
1:C:433:ILE:CB	1:C:571:TYR:OH	2.53	0.56
1:C:582:ARG:H	1:C:582:ARG:CD	2.19	0.56
1:D:222:PHE:CD2	1:D:255:PHE:CD2	2.93	0.56
1:D:262:PRO:HB3	1:D:409:SER:HG	1.65	0.56
1:E:171:LYS:HD2	1:E:177:GLU:HG2	1.88	0.56
1:F:389:LEU:HD11	1:F:454:SER:OG	2.05	0.56
1:G:224:PRO:HG2	1:G:255:PHE:HE2	1.68	0.56
1:A:249:LEU:HD23	1:A:252:ALA:CA	2.27	0.56
1:A:249:LEU:O	1:A:250:THR:HG23	2.05	0.56
1:A:438:ARG:HG2	1:A:564:GLU:HG3	1.86	0.56
1:A:527:GLU:C	1:A:529:GLU:N	2.55	0.56
1:B:107:TYR:HA	1:B:110:GLN:HB2	1.87	0.56
1:C:107:TYR:HA	1:C:110:GLN:HB2	1.87	0.56
1:C:485:PHE:CE2	1:D:485:PHE:HB2	2.37	0.56
1:C:496:LYS:HB2	1:D:655:TRP:HE1	0.43	0.56
1:D:540:LEU:CD1	1:D:622:ALA:HB2	2.36	0.56
1:E:107:TYR:HA	1:E:110:GLN:HB2	1.88	0.56
1:H:531:GLN:O	1:H:535:ASP:N	2.35	0.56
1:A:28:TYR:HD2	1:A:45:GLN:HE21	1.54	0.56
1:A:183:VAL:HG12	1:A:184:GLY:N	2.20	0.56
1:B:200:THR:O	1:B:201:VAL:C	2.43	0.56
1:B:521:VAL:CG1	1:B:643:VAL:CG1	2.78	0.56
1:B:632:VAL:C	1:B:633:MET:SD	2.84	0.56
1:C:265:LEU:HD21	1:C:269:LEU:HB3	1.87	0.56
1:D:198:LYS:C	1:D:200:THR:H	2.08	0.56
1:D:357:SER:HB3	1:D:453:THR:HB	1.86	0.56
1:E:30:LEU:HD13	1:E:32:TRP:NE1	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:ILE:HG23	1:E:94:LEU:HD13	1.87	0.56
1:E:480:LYS:NZ	1:E:525:GLY:C	2.59	0.56
1:E:521:VAL:HA	1:E:524:CYS:HG	1.67	0.56
1:F:119:GLU:HB2	1:F:121:PRO:CD	2.36	0.56
1:G:472:MET:CG	1:G:633:MET:HB2	2.35	0.56
1:G:473:THR:HG21	1:G:629:VAL:HG13	1.87	0.56
1:A:171:LYS:HD2	1:A:177:GLU:HG2	1.86	0.56
1:B:119:GLU:HB2	1:B:121:PRO:CD	2.35	0.56
1:C:540:LEU:HD12	1:C:622:ALA:HB2	1.87	0.56
1:D:200:THR:O	1:D:201:VAL:C	2.42	0.56
1:D:368:THR:HA	1:D:371:VAL:CG2	2.32	0.56
1:G:105:ARG:HH11	1:G:105:ARG:HG3	1.70	0.56
1:G:190:ALA:HB3	1:G:203:VAL:HG22	1.88	0.56
1:G:263:ASN:ND2	1:G:265:LEU:N	2.53	0.56
1:H:224:PRO:HG2	1:H:255:PHE:HE2	1.70	0.56
1:H:387:ILE:HD12	1:H:450:GLY:N	2.21	0.56
1:B:222:PHE:CD2	1:B:224:PRO:O	2.59	0.56
1:B:249:LEU:HD23	1:B:252:ALA:CA	2.28	0.56
1:B:626:SER:OG	1:B:627:PRO:HD3	2.05	0.56
1:C:263:ASN:HD21	1:C:265:LEU:N	2.02	0.56
1:C:263:ASN:HD21	1:C:265:LEU:H	1.53	0.56
1:C:430:TRP:HB3	1:C:571:TYR:CD2	2.33	0.56
1:C:547:LEU:HD13	1:C:615:THR:HG23	1.82	0.56
1:D:503:PHE:O	1:D:505:ILE:HG13	2.06	0.56
1:E:276:TRP:CE3	1:E:277:LEU:HD23	2.40	0.56
1:F:144:ARG:HD2	1:F:171:LYS:CB	2.36	0.56
1:F:171:LYS:HD2	1:F:177:GLU:HG2	1.86	0.56
1:G:430:TRP:HB3	1:G:571:TYR:HD2	1.71	0.56
1:A:362:ASN:C	1:A:364:ALA:H	2.09	0.56
1:B:362:ASN:O	1:B:364:ALA:N	2.39	0.56
1:B:429:VAL:HG12	1:B:430:TRP:HD1	1.70	0.56
1:C:626:SER:OG	1:C:627:PRO:HD3	2.06	0.56
1:D:274:GLU:O	1:D:278:GLN:HB2	2.06	0.56
1:D:484:ASP:C	1:D:486:PHE:N	2.58	0.56
1:D:626:SER:OG	1:D:627:PRO:HD3	2.06	0.56
1:E:315:MET:HB3	1:E:387:ILE:HA	1.88	0.56
1:F:107:TYR:HD1	1:F:153:LEU:HD12	1.70	0.56
1:F:131:SER:O	1:F:134:ARG:HB3	2.05	0.56
1:F:274:GLU:O	1:F:278:GLN:HB2	2.06	0.56
1:F:316:ASN:O	1:F:317:MET:HB2	2.06	0.56
1:G:18:LYS:HZ2	1:G:33:ILE:HG21	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104:LEU:HB3	1:H:148:PRO:O	2.05	0.56
1:H:117:LEU:O	1:H:119:GLU:HG2	2.05	0.56
1:H:200:THR:O	1:H:201:VAL:C	2.44	0.56
1:A:433:ILE:CB	1:A:571:TYR:OH	2.53	0.56
1:A:437:ILE:HG22	1:A:564:GLU:HB2	1.88	0.56
1:B:62:ILE:HG23	1:B:94:LEU:HD13	1.88	0.56
1:B:320:GLY:O	1:B:321:ARG:C	2.45	0.56
1:C:171:LYS:HD2	1:C:177:GLU:HG2	1.87	0.56
1:C:274:GLU:O	1:C:278:GLN:HB2	2.06	0.56
1:C:315:MET:HB3	1:C:387:ILE:HA	1.88	0.56
1:C:350:GLU:OE2	1:C:391:ASP:O	2.23	0.56
1:D:134:ARG:HB2	1:D:300:PHE:HE1	1.69	0.56
1:D:222:PHE:CD2	1:D:224:PRO:O	2.59	0.56
1:D:480:LYS:HE3	1:D:527:GLU:HB2	1.88	0.56
1:E:655:TRP:CD1	1:F:496:LYS:HB2	2.37	0.56
1:E:665:VAL:HG22	1:F:665:VAL:HG21	1.88	0.56
1:F:429:VAL:HG12	1:F:430:TRP:HD1	1.69	0.56
1:G:222:PHE:CD2	1:G:255:PHE:CD2	2.94	0.56
1:G:319:SER:O	1:G:321:ARG:N	2.35	0.56
1:G:359:LEU:CA	1:G:460:ARG:HH12	2.11	0.56
1:H:433:ILE:HG21	1:H:571:TYR:OH	2.05	0.56
1:A:116:GLY:N	1:A:217:THR:O	2.39	0.55
1:A:131:SER:O	1:A:134:ARG:HB3	2.06	0.55
1:A:429:VAL:HG12	1:A:430:TRP:HD1	1.72	0.55
1:A:547:LEU:CD1	1:A:615:THR:CG2	2.54	0.55
1:A:587:SER:OG	1:A:588:ASN:N	2.38	0.55
1:B:316:ASN:O	1:B:317:MET:HB2	2.05	0.55
1:C:485:PHE:CD2	1:D:485:PHE:CG	2.94	0.55
1:D:26:PHE:CE2	1:D:181:GLU:OE1	2.55	0.55
1:E:478:GLN:CG	1:E:479:LEU:N	2.69	0.55
1:F:219:PHE:O	1:F:220:ARG:HG3	1.85	0.55
1:F:517:MET:HG3	1:F:646:ARG:NH1	2.13	0.55
1:G:386:LEU:H	1:G:386:LEU:CD1	2.20	0.55
1:G:419:ARG:NH1	1:G:588:ASN:HA	2.21	0.55
1:H:220:ARG:CB	1:H:221:PRO:HD2	2.35	0.55
1:B:89:ASN:HB3	1:B:91:LEU:H	1.72	0.55
1:B:220:ARG:NH1	1:B:223:LEU:CD2	2.70	0.55
1:B:263:ASN:ND2	1:B:265:LEU:N	2.54	0.55
1:C:131:SER:O	1:C:134:ARG:HB3	2.06	0.55
1:C:262:PRO:HB3	1:C:409:SER:HG	1.69	0.55
1:C:334:GLN:HA	1:C:337:LYS:HB2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:ARG:CA	1:C:587:SER:OG	2.51	0.55
1:C:455:MET:HE1	1:C:547:LEU:HB2	1.87	0.55
1:D:183:VAL:HG12	1:D:184:GLY:N	2.21	0.55
1:D:220:ARG:CB	1:D:221:PRO:HD2	2.37	0.55
1:D:263:ASN:ND2	1:D:265:LEU:N	2.54	0.55
1:D:265:LEU:HD21	1:D:269:LEU:HB3	1.87	0.55
1:D:320:GLY:O	1:D:321:ARG:C	2.45	0.55
1:D:499:GLU:C	1:D:500:GLN:HE21	2.10	0.55
1:E:576:GLU:OE2	1:F:573:ARG:NH2	2.40	0.55
1:F:582:ARG:H	1:F:582:ARG:CD	2.19	0.55
1:G:107:TYR:HD1	1:G:153:LEU:HD12	1.71	0.55
1:G:220:ARG:CB	1:G:221:PRO:HD2	2.37	0.55
1:H:222:PHE:CD2	1:H:224:PRO:O	2.60	0.55
1:A:116:GLY:HA2	1:A:217:THR:O	2.07	0.55
1:A:386:LEU:H	1:A:386:LEU:CD1	2.19	0.55
1:A:478:GLN:HE21	1:A:479:LEU:HD23	1.71	0.55
1:B:28:TYR:HD2	1:B:45:GLN:HE21	1.53	0.55
1:B:316:ASN:O	1:B:317:MET:CB	2.55	0.55
1:C:368:THR:HA	1:C:371:VAL:CG2	2.31	0.55
1:C:502:GLU:HG3	1:D:666:ARG:HH12	1.70	0.55
1:D:490:ILE:HG23	1:D:490:ILE:O	2.06	0.55
1:D:517:MET:HG3	1:D:646:ARG:NH1	2.21	0.55
1:E:503:PHE:C	1:E:505:ILE:H	2.09	0.55
1:G:429:VAL:HG12	1:G:430:TRP:HD1	1.69	0.55
1:G:570:LEU:HD23	1:G:590:MET:HG2	1.87	0.55
1:H:105:ARG:HG3	1:H:105:ARG:HH11	1.71	0.55
1:H:183:VAL:HG12	1:H:184:GLY:N	2.21	0.55
1:H:191:PRO:HG3	1:H:234:LYS:NZ	2.22	0.55
1:H:260:PRO:CG	1:H:274:GLU:HG2	2.36	0.55
1:A:198:LYS:C	1:A:200:THR:H	2.10	0.55
1:A:236:ARG:NH2	1:D:231:TRP:HE3	1.98	0.55
1:B:274:GLU:O	1:B:278:GLN:HB2	2.06	0.55
1:C:249:LEU:HD23	1:C:252:ALA:CA	2.27	0.55
1:C:362:ASN:O	1:C:364:ALA:N	2.40	0.55
1:D:150:ASN:ND2	1:D:167:LEU:HD12	2.16	0.55
1:D:472:MET:HG3	1:D:472:MET:O	2.06	0.55
1:F:315:MET:HB3	1:F:387:ILE:HA	1.87	0.55
1:F:387:ILE:HG22	1:F:388:PHE:H	1.71	0.55
1:H:30:LEU:HD13	1:H:32:TRP:NE1	2.22	0.55
1:A:120:GLY:N	1:A:122:ILE:H	2.05	0.55
1:A:632:VAL:C	1:A:633:MET:SD	2.85	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:LEU:HB3	1:B:590:MET:HE3	1.88	0.55
1:C:30:LEU:HD13	1:C:32:TRP:NE1	2.20	0.55
1:C:182:PHE:CE1	1:C:194:LEU:HD22	2.41	0.55
1:C:641:LYS:HB3	1:C:645:ARG:NH2	2.16	0.55
1:D:206:TRP:CD1	1:D:206:TRP:C	2.78	0.55
1:D:249:LEU:O	1:D:250:THR:HG23	2.07	0.55
1:D:422:THR:CB	1:D:585:GLY:C	2.74	0.55
1:E:187:GLN:CB	1:E:223:LEU:CD2	2.71	0.55
1:E:200:THR:O	1:E:201:VAL:C	2.45	0.55
1:E:265:LEU:HD23	1:E:269:LEU:HB3	1.88	0.55
1:F:104:LEU:HB3	1:F:148:PRO:O	2.07	0.55
1:F:285:GLN:NE2	1:F:286:ARG:HH12	2.04	0.55
1:G:433:ILE:HB	1:G:571:TYR:CZ	2.42	0.55
1:H:249:LEU:O	1:H:250:THR:HG23	2.06	0.55
1:H:430:TRP:CE3	1:H:574:LEU:HD22	2.42	0.55
1:A:134:ARG:CA	1:A:300:PHE:CZ	2.84	0.55
1:A:422:THR:HB	1:A:585:GLY:C	2.27	0.55
1:B:107:TYR:O	1:B:110:GLN:CB	2.55	0.55
1:B:144:ARG:HD2	1:B:171:LYS:CB	2.36	0.55
1:C:89:ASN:HB3	1:C:91:LEU:H	1.72	0.55
1:C:235:VAL:CB	1:C:243:ILE:HA	2.36	0.55
1:C:260:PRO:CG	1:C:274:GLU:HG2	2.37	0.55
1:C:478:GLN:HE21	1:C:479:LEU:HD23	1.71	0.55
1:D:243:ILE:N	1:D:245:VAL:HG23	2.22	0.55
1:F:472:MET:O	1:F:472:MET:HG3	2.07	0.55
1:F:478:GLN:HE21	1:F:479:LEU:HD23	1.72	0.55
1:G:107:TYR:HA	1:G:110:GLN:HB2	1.89	0.55
1:H:263:ASN:ND2	1:H:265:LEU:N	2.54	0.55
1:H:345:GLY:O	1:H:347:PRO:HD3	2.06	0.55
1:H:387:ILE:HD12	1:H:450:GLY:CA	2.37	0.55
1:A:62:ILE:HG23	1:A:94:LEU:HD13	1.89	0.55
1:A:191:PRO:HG3	1:A:234:LYS:NZ	2.21	0.55
1:B:30:LEU:HD13	1:B:32:TRP:NE1	2.21	0.55
1:B:497:TYR:CE2	1:B:511:LEU:HD22	2.42	0.55
1:B:660:ILE:O	1:B:662:CYS:N	2.40	0.55
1:C:28:TYR:HD2	1:C:45:GLN:HE21	1.53	0.55
1:C:478:GLN:OE1	1:D:481:ALA:CB	2.55	0.55
1:C:490:ILE:HG23	1:C:490:ILE:O	2.07	0.55
1:C:633:MET:SD	1:C:633:MET:N	2.80	0.55
1:C:647:GLN:CA	1:C:647:GLN:OE1	2.55	0.55
1:D:157:PRO:HD2	1:D:161:ILE:HD11	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:ASP:O	1:D:446:ARG:HB2	2.05	0.55
1:D:478:GLN:HE21	1:D:479:LEU:HD23	1.72	0.55
1:E:89:ASN:HB3	1:E:91:LEU:H	1.72	0.55
1:E:107:TYR:O	1:E:110:GLN:CB	2.54	0.55
1:E:224:PRO:HG2	1:E:255:PHE:HE2	1.71	0.55
1:E:297:VAL:HB	1:E:301:GLN:H	1.72	0.55
1:F:222:PHE:CZ	1:F:225:ASN:HB2	2.40	0.55
1:F:644:VAL:O	1:F:644:VAL:HG12	2.07	0.55
1:H:247:ASP:HB2	1:H:255:PHE:O	2.07	0.55
1:H:282:MET:HA	1:H:282:MET:HE2	1.88	0.55
1:H:449:GLN:OE1	1:H:449:GLN:HA	2.06	0.55
1:A:507:SER:C	1:A:509:LYS:H	2.10	0.55
1:A:570:LEU:HB3	1:A:590:MET:HE2	1.86	0.55
1:B:120:GLY:N	1:B:122:ILE:H	2.05	0.55
1:B:131:SER:O	1:B:134:ARG:HB3	2.07	0.55
1:B:243:ILE:N	1:B:245:VAL:HG23	2.21	0.55
1:B:433:ILE:CG2	1:B:571:TYR:OH	2.55	0.55
1:C:499:GLU:C	1:C:500:GLN:HE21	2.10	0.55
1:E:285:GLN:NE2	1:E:286:ARG:HH12	2.05	0.55
1:E:386:LEU:H	1:E:386:LEU:CD1	2.20	0.55
1:E:626:SER:OG	1:E:627:PRO:HD3	2.07	0.55
1:F:103:ASP:HB3	1:F:106:LYS:HG3	1.89	0.55
1:G:104:LEU:HB3	1:G:148:PRO:O	2.07	0.55
1:H:28:TYR:HD2	1:H:45:GLN:HE21	1.54	0.55
1:A:100:GLU:H	1:A:154:GLN:HG3	1.72	0.55
1:A:100:GLU:N	1:A:154:GLN:HG3	2.21	0.55
1:A:220:ARG:CB	1:A:221:PRO:HD2	2.36	0.55
1:A:521:VAL:HA	1:A:524:CYS:HG	1.69	0.55
1:B:107:TYR:HD1	1:B:153:LEU:HD12	1.70	0.55
1:B:120:GLY:CA	1:B:123:ARG:H	2.19	0.55
1:B:157:PRO:HD2	1:B:161:ILE:HD11	1.88	0.55
1:C:529:GLU:HG3	1:C:633:MET:HE1	1.89	0.55
1:C:651:GLN:NE2	1:D:492:ILE:HG21	2.20	0.55
1:D:362:ASN:O	1:D:364:ALA:N	2.40	0.55
1:D:448:LEU:HD23	1:D:608:ILE:HG12	1.88	0.55
1:E:373:ASP:C	1:E:374:CYS:SG	2.85	0.55
1:E:430:TRP:CE3	1:E:574:LEU:HD22	2.42	0.55
1:F:107:TYR:HA	1:F:110:GLN:HB2	1.89	0.55
1:F:265:LEU:HD23	1:F:269:LEU:HB3	1.88	0.55
1:F:316:ASN:O	1:F:317:MET:CB	2.55	0.55
1:F:320:GLY:O	1:F:321:ARG:C	2.44	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:131:SER:O	1:G:134:ARG:HB3	2.07	0.55
1:G:144:ARG:HD2	1:G:171:LYS:CB	2.37	0.55
1:B:438:ARG:CG	1:B:564:GLU:HG3	2.35	0.55
1:D:265:LEU:HD23	1:D:269:LEU:HB3	1.87	0.55
1:D:527:GLU:O	1:D:529:GLU:N	2.40	0.55
1:E:18:LYS:HZ2	1:E:33:ILE:HG21	1.72	0.55
1:E:193:LEU:HD22	1:E:231:TRP:CD1	2.41	0.55
1:E:247:ASP:HB2	1:E:255:PHE:O	2.06	0.55
1:F:28:TYR:HD2	1:F:45:GLN:HE21	1.54	0.55
1:G:89:ASN:HB3	1:G:91:LEU:H	1.72	0.55
1:H:222:PHE:CD2	1:H:255:PHE:CD2	2.94	0.55
1:H:265:LEU:HD23	1:H:269:LEU:CB	2.37	0.55
1:H:426:LEU:HB2	1:H:574:LEU:HD21	1.88	0.55
1:H:429:VAL:HG12	1:H:430:TRP:HD1	1.72	0.55
1:B:499:GLU:C	1:B:500:GLN:HE21	2.10	0.54
1:B:616:VAL:HG13	1:B:619:LYS:HD2	1.88	0.54
1:D:350:GLU:OE2	1:D:391:ASP:O	2.26	0.54
1:E:28:TYR:HD2	1:E:45:GLN:HE21	1.54	0.54
1:F:148:PRO:HD3	1:F:188:TYR:CZ	2.42	0.54
1:F:200:THR:O	1:F:201:VAL:C	2.44	0.54
1:G:183:VAL:HG12	1:G:184:GLY:N	2.20	0.54
1:G:632:VAL:C	1:G:633:MET:SD	2.86	0.54
1:H:89:ASN:HB3	1:H:91:LEU:H	1.72	0.54
1:H:119:GLU:HB2	1:H:121:PRO:CD	2.36	0.54
1:H:386:LEU:H	1:H:386:LEU:CD1	2.20	0.54
1:H:564:GLU:OE2	1:H:568:ARG:NH2	2.41	0.54
1:A:235:VAL:CB	1:A:243:ILE:HA	2.37	0.54
1:B:249:LEU:O	1:B:250:THR:HG23	2.06	0.54
1:B:265:LEU:HD21	1:B:269:LEU:HB3	1.89	0.54
1:C:26:PHE:CE2	1:C:179:CYS:HB3	2.40	0.54
1:C:224:PRO:HG3	1:C:428:ARG:HH22	1.73	0.54
1:C:434:TRP:CZ3	1:C:568:ARG:CA	2.82	0.54
1:C:658:LEU:HA	1:D:658:LEU:HD12	1.90	0.54
1:C:666:ARG:CG	1:D:503:PHE:CE1	2.90	0.54
1:D:107:TYR:HD1	1:D:153:LEU:HD12	1.69	0.54
1:D:475:GLU:CD	1:D:636:MET:HE1	2.28	0.54
1:F:632:VAL:C	1:F:633:MET:SD	2.86	0.54
1:A:274:GLU:O	1:A:278:GLN:HB2	2.07	0.54
1:A:327:VAL:CG1	1:A:367:LEU:HB2	2.31	0.54
1:B:297:VAL:HB	1:B:301:GLN:H	1.72	0.54
1:C:157:PRO:HD2	1:C:161:ILE:HD11	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:660:ILE:O	1:C:662:CYS:N	2.40	0.54
1:D:220:ARG:NH1	1:D:223:LEU:CD2	2.69	0.54
1:D:514:TRP:O	1:D:518:GLU:HG3	2.06	0.54
1:D:587:SER:OG	1:D:588:ASN:N	2.36	0.54
1:E:148:PRO:HD3	1:E:188:TYR:CZ	2.42	0.54
1:E:263:ASN:HD21	1:E:265:LEU:N	2.05	0.54
1:E:373:ASP:CG	1:E:374:CYS:SG	2.85	0.54
1:E:449:GLN:OE1	1:E:449:GLN:HA	2.08	0.54
1:E:540:LEU:HD12	1:E:622:ALA:HB2	1.81	0.54
1:F:386:LEU:H	1:F:386:LEU:CD1	2.20	0.54
1:G:626:SER:OG	1:G:627:PRO:HD3	2.07	0.54
1:H:150:ASN:OD1	1:H:150:ASN:N	2.33	0.54
1:H:157:PRO:HD2	1:H:161:ILE:HD11	1.89	0.54
1:H:626:SER:OG	1:H:627:PRO:HD3	2.07	0.54
1:A:105:ARG:HH11	1:A:105:ARG:HG3	1.71	0.54
1:A:570:LEU:CB	1:A:590:MET:CE	2.78	0.54
1:B:260:PRO:CG	1:B:274:GLU:HG2	2.37	0.54
1:C:637:ARG:O	1:C:641:LYS:HB2	2.08	0.54
1:D:536:LYS:HB3	1:D:625:LEU:CD2	2.37	0.54
1:E:222:PHE:CD2	1:E:224:PRO:O	2.61	0.54
1:E:494:LEU:HD21	1:E:518:GLU:OE2	2.06	0.54
1:E:536:LYS:HB3	1:E:625:LEU:CD1	2.15	0.54
1:F:246:TYR:CD1	1:F:258:VAL:CB	2.71	0.54
1:F:521:VAL:HG13	1:F:643:VAL:CG1	2.36	0.54
1:F:616:VAL:HG13	1:F:619:LYS:HD2	1.90	0.54
1:G:362:ASN:O	1:G:364:ALA:N	2.40	0.54
1:H:144:ARG:HD2	1:H:171:LYS:CB	2.38	0.54
1:H:449:GLN:NE2	1:H:453:THR:HG22	2.22	0.54
1:A:104:LEU:HB3	1:A:148:PRO:O	2.07	0.54
1:A:510:LEU:HD12	1:A:657:LEU:HD13	1.88	0.54
1:C:144:ARG:HD2	1:C:171:LYS:CB	2.38	0.54
1:C:486:PHE:HZ	1:C:517:MET:HE2	1.72	0.54
1:C:497:TYR:HB2	1:D:655:TRP:HH2	1.72	0.54
1:E:144:ARG:HD2	1:E:171:LYS:CB	2.38	0.54
1:E:484:ASP:C	1:E:486:PHE:N	2.58	0.54
1:E:507:SER:C	1:E:509:LYS:H	2.11	0.54
1:F:89:ASN:HB3	1:F:91:LEU:H	1.73	0.54
1:F:107:TYR:O	1:F:110:GLN:CB	2.55	0.54
1:F:394:LYS:HE2	1:F:401:ILE:HA	1.88	0.54
1:G:265:LEU:HD21	1:G:269:LEU:HB3	1.88	0.54
1:H:362:ASN:O	1:H:364:ALA:N	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:O	1:B:119:GLU:HG2	2.07	0.54
1:B:501:MET:CA	1:B:505:ILE:CD1	2.85	0.54
1:B:641:LYS:HB3	1:B:645:ARG:NH2	2.13	0.54
1:C:297:VAL:HB	1:C:301:GLN:H	1.72	0.54
1:C:386:LEU:H	1:C:386:LEU:CD1	2.21	0.54
1:C:419:ARG:N	1:C:420:PRO:HD3	2.04	0.54
1:D:104:LEU:HB3	1:D:148:PRO:O	2.08	0.54
1:D:426:LEU:HB2	1:D:574:LEU:HD21	1.89	0.54
1:D:429:VAL:HG12	1:D:430:TRP:HD1	1.72	0.54
1:E:89:ASN:C	1:E:91:LEU:H	2.11	0.54
1:F:566:GLN:HG2	1:F:593:LEU:HD11	1.90	0.54
1:F:641:LYS:HB3	1:F:645:ARG:NH2	2.15	0.54
1:G:28:TYR:HD2	1:G:45:GLN:HE21	1.54	0.54
1:G:119:GLU:HB2	1:G:121:PRO:CD	2.38	0.54
1:H:297:VAL:HB	1:H:301:GLN:H	1.73	0.54
1:A:26:PHE:CE2	1:A:181:GLU:CD	2.81	0.54
1:A:68:LEU:HB3	1:A:135:TYR:HE2	1.72	0.54
1:A:433:ILE:HG21	1:A:571:TYR:OH	2.08	0.54
1:B:521:VAL:HG21	1:B:646:ARG:HD2	1.90	0.54
1:C:419:ARG:HA	1:C:587:SER:HB3	1.90	0.54
1:C:429:VAL:O	1:C:433:ILE:HG12	2.08	0.54
1:D:117:LEU:O	1:D:119:GLU:HG2	2.07	0.54
1:D:430:TRP:CB	1:D:571:TYR:CD2	2.90	0.54
1:E:387:ILE:HD11	1:E:449:GLN:CB	2.37	0.54
1:G:327:VAL:CG1	1:G:367:LEU:HB2	2.31	0.54
1:H:62:ILE:HG23	1:H:94:LEU:HD13	1.89	0.54
1:H:458:LEU:CD1	1:H:544:SER:HB2	2.37	0.54
1:H:571:TYR:CE2	1:H:590:MET:CG	2.91	0.54
1:A:260:PRO:CG	1:A:274:GLU:HG2	2.38	0.54
1:C:148:PRO:HD3	1:C:188:TYR:CZ	2.42	0.54
1:D:614:LYS:O	1:D:617:VAL:HB	2.07	0.54
1:E:233:GLY:C	1:E:235:VAL:H	2.12	0.54
1:G:71:PRO:O	1:G:72:ASN:CB	2.55	0.54
1:A:472:MET:HG3	1:A:472:MET:O	2.08	0.54
1:A:626:SER:OG	1:A:627:PRO:HD3	2.07	0.54
1:B:233:GLY:C	1:B:235:VAL:H	2.12	0.54
1:B:245:VAL:HG12	1:B:246:TYR:N	2.22	0.54
1:B:582:ARG:H	1:B:582:ARG:CD	2.20	0.54
1:C:71:PRO:O	1:C:72:ASN:CB	2.56	0.54
1:C:277:LEU:C	1:C:279:CYS:H	2.11	0.54
1:D:32:TRP:CD1	1:D:43:ILE:HD13	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:ARG:CA	1:D:300:PHE:HZ	2.17	0.54
1:D:144:ARG:HD2	1:D:171:LYS:CB	2.37	0.54
1:F:115:CYS:HB2	1:F:435:GLN:HG3	1.89	0.54
1:F:183:VAL:HG12	1:F:184:GLY:N	2.23	0.54
1:F:263:ASN:ND2	1:F:265:LEU:N	2.56	0.54
1:F:447:LEU:HD12	1:F:605:VAL:HG22	1.89	0.54
1:H:212:ALA:O	1:H:213:PHE:C	2.45	0.54
1:A:434:TRP:HZ3	1:A:568:ARG:CB	2.21	0.54
1:B:118:LYS:CG	1:B:265:LEU:HA	2.38	0.54
1:B:235:VAL:CB	1:B:243:ILE:HA	2.38	0.54
1:B:449:GLN:OE1	1:B:449:GLN:HA	2.07	0.54
1:B:614:LYS:O	1:B:617:VAL:HB	2.09	0.54
1:C:89:ASN:C	1:C:91:LEU:H	2.11	0.54
1:E:118:LYS:HD3	1:E:265:LEU:HD12	1.90	0.54
1:E:263:ASN:HD21	1:E:265:LEU:H	1.54	0.54
1:E:316:ASN:O	1:E:317:MET:CB	2.55	0.54
1:E:387:ILE:HG21	1:E:450:GLY:HA2	1.89	0.54
1:E:514:TRP:O	1:E:518:GLU:HG3	2.07	0.54
1:E:616:VAL:HG13	1:E:619:LYS:HD2	1.90	0.54
1:G:260:PRO:CG	1:G:274:GLU:HG2	2.38	0.54
1:G:263:ASN:HD21	1:G:265:LEU:N	2.06	0.54
1:G:430:TRP:CZ3	1:G:574:LEU:HD13	2.43	0.54
1:H:249:LEU:HA	1:H:253:VAL:O	2.07	0.54
1:B:357:SER:HB3	1:B:453:THR:HA	1.90	0.53
1:B:475:GLU:O	1:B:477:GLU:N	2.41	0.53
1:C:500:GLN:CB	1:C:505:ILE:HG12	2.38	0.53
1:D:190:ALA:HB2	1:D:206:TRP:CD1	2.43	0.53
1:E:157:PRO:HD2	1:E:161:ILE:HD11	1.90	0.53
1:E:319:SER:O	1:E:321:ARG:N	2.35	0.53
1:E:350:GLU:OE2	1:E:391:ASP:O	2.26	0.53
1:G:187:GLN:HB3	1:G:223:LEU:HD22	1.81	0.53
1:H:118:LYS:CG	1:H:265:LEU:HA	2.39	0.53
1:H:235:VAL:CB	1:H:243:ILE:HA	2.35	0.53
1:A:660:ILE:O	1:A:662:CYS:N	2.40	0.53
1:B:249:LEU:HA	1:B:253:VAL:O	2.08	0.53
1:D:62:ILE:HG23	1:D:94:LEU:HD13	1.89	0.53
1:D:107:TYR:O	1:D:110:GLN:CB	2.57	0.53
1:D:500:GLN:CB	1:D:505:ILE:HG12	2.38	0.53
1:E:415:GLN:NE2	1:E:429:VAL:HG11	2.23	0.53
1:E:641:LYS:HB3	1:E:645:ARG:NH2	2.13	0.53
1:F:327:VAL:CG1	1:F:367:LEU:HB2	2.32	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:362:ASN:O	1:F:364:ALA:N	2.41	0.53
1:F:514:TRP:O	1:F:518:GLU:HG3	2.08	0.53
1:G:282:MET:HE2	1:G:282:MET:HA	1.91	0.53
1:G:438:ARG:HG2	1:G:564:GLU:CG	2.38	0.53
1:G:449:GLN:NE2	1:G:453:THR:HG22	2.23	0.53
1:G:472:MET:HG3	1:G:472:MET:O	2.08	0.53
1:A:144:ARG:HD2	1:A:171:LYS:CB	2.38	0.53
1:A:582:ARG:H	1:A:582:ARG:CD	2.20	0.53
1:B:359:LEU:HA	1:B:460:ARG:NH1	2.23	0.53
1:B:480:LYS:HE3	1:B:527:GLU:HB2	1.89	0.53
1:B:649:LYS:HA	1:B:652:GLN:CB	2.39	0.53
1:C:62:ILE:HG23	1:C:94:LEU:HD13	1.89	0.53
1:C:616:VAL:HG13	1:C:619:LYS:HD2	1.90	0.53
1:D:415:GLN:NE2	1:D:429:VAL:HG11	2.22	0.53
1:D:616:VAL:HG13	1:D:619:LYS:HD2	1.90	0.53
1:E:222:PHE:CD2	1:E:255:PHE:CD2	2.96	0.53
1:E:582:ARG:H	1:E:582:ARG:CD	2.20	0.53
1:E:658:LEU:CD1	1:F:658:LEU:HD12	2.33	0.53
1:F:105:ARG:HH11	1:F:105:ARG:HG3	1.74	0.53
1:F:272:LYS:HG3	1:F:276:TRP:HB2	1.90	0.53
1:G:118:LYS:HB2	1:G:265:LEU:HD12	1.90	0.53
1:G:449:GLN:OE1	1:G:449:GLN:HA	2.07	0.53
1:H:89:ASN:C	1:H:91:LEU:H	2.12	0.53
1:A:89:ASN:HB3	1:A:91:LEU:HB2	1.91	0.53
1:A:107:TYR:O	1:A:110:GLN:CB	2.57	0.53
1:A:107:TYR:HA	1:A:110:GLN:HB2	1.90	0.53
1:A:119:GLU:HB2	1:A:121:PRO:HB2	1.90	0.53
1:A:245:VAL:HG12	1:A:246:TYR:N	2.22	0.53
1:A:490:ILE:O	1:A:490:ILE:HG23	2.08	0.53
1:B:220:ARG:CB	1:B:221:PRO:HD2	2.39	0.53
1:B:222:PHE:CD2	1:B:255:PHE:CD2	2.96	0.53
1:C:104:LEU:HB3	1:C:148:PRO:O	2.09	0.53
1:C:496:LYS:C	1:D:655:TRP:HZ2	2.11	0.53
1:D:68:LEU:HB3	1:D:135:TYR:HE2	1.73	0.53
1:D:644:VAL:O	1:D:644:VAL:HG12	2.08	0.53
1:E:118:LYS:NZ	1:E:123:ARG:HH12	2.06	0.53
1:E:235:VAL:CB	1:E:243:ILE:HA	2.38	0.53
1:E:564:GLU:OE2	1:E:568:ARG:NH2	2.41	0.53
1:H:319:SER:O	1:H:321:ARG:N	2.35	0.53
1:H:472:MET:SD	1:H:633:MET:CB	2.96	0.53
1:A:71:PRO:O	1:A:72:ASN:CB	2.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ASN:HB3	1:A:91:LEU:H	1.72	0.53
1:B:494:LEU:CD1	1:B:514:TRP:CB	2.85	0.53
1:B:656:ASN:C	1:B:656:ASN:OD1	2.46	0.53
1:C:89:ASN:HB3	1:C:91:LEU:HB2	1.90	0.53
1:D:647:GLN:OE1	1:D:647:GLN:CA	2.57	0.53
1:E:265:LEU:HD23	1:E:269:LEU:CB	2.38	0.53
1:E:282:MET:HE2	1:E:282:MET:HA	1.90	0.53
1:E:429:VAL:HG12	1:E:430:TRP:HD1	1.73	0.53
1:F:32:TRP:CD1	1:F:43:ILE:HD13	2.43	0.53
1:F:157:PRO:HD2	1:F:161:ILE:HD11	1.89	0.53
1:F:226:TRP:CD1	1:F:227:GLN:HB3	2.44	0.53
1:F:260:PRO:CG	1:F:274:GLU:HG2	2.38	0.53
1:F:626:SER:OG	1:F:627:PRO:HD3	2.09	0.53
1:G:373:ASP:C	1:G:374:CYS:SG	2.87	0.53
1:H:118:LYS:HG2	1:H:265:LEU:HA	1.89	0.53
1:H:190:ALA:HB2	1:H:206:TRP:CG	2.44	0.53
1:A:265:LEU:HD21	1:A:269:LEU:HB3	1.90	0.53
1:A:297:VAL:HB	1:A:301:GLN:H	1.74	0.53
1:B:113:ASN:HA	1:B:116:GLY:O	2.09	0.53
1:B:226:TRP:CD1	1:B:227:GLN:HB3	2.44	0.53
1:B:263:ASN:HD21	1:B:265:LEU:H	1.56	0.53
1:C:348:GLU:H	1:C:348:GLU:CD	2.11	0.53
1:C:507:SER:C	1:C:509:LYS:H	2.12	0.53
1:D:115:CYS:HB2	1:D:435:GLN:HG3	1.90	0.53
1:D:125:LEU:HD21	1:D:215:CYS:SG	2.49	0.53
1:D:644:VAL:HA	1:D:647:GLN:NE2	2.18	0.53
1:E:362:ASN:O	1:E:364:ALA:N	2.42	0.53
1:E:511:LEU:HG	1:E:515:ARG:CZ	2.38	0.53
1:F:499:GLU:C	1:F:500:GLN:HE21	2.12	0.53
1:G:249:LEU:HD23	1:G:252:ALA:CA	2.27	0.53
1:G:387:ILE:HG22	1:G:388:PHE:H	1.72	0.53
1:G:564:GLU:OE2	1:G:568:ARG:NH2	2.41	0.53
1:H:32:TRP:CD1	1:H:43:ILE:HD13	2.43	0.53
1:A:157:PRO:HD2	1:A:161:ILE:HD11	1.90	0.53
1:B:229:VAL:CG1	1:C:229:VAL:HG13	2.32	0.53
1:B:277:LEU:C	1:B:279:CYS:H	2.12	0.53
1:B:373:ASP:C	1:B:374:CYS:SG	2.87	0.53
1:C:308:SER:O	1:C:309:LEU:HB2	2.09	0.53
1:C:402:SER:HA	1:C:609:TYR:CD1	2.43	0.53
1:D:28:TYR:HD2	1:D:45:GLN:HE21	1.54	0.53
1:D:308:SER:O	1:D:309:LEU: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:641:LYS:HB3	1:D:645:ARG:NH2	2.13	0.53
1:E:226:TRP:CD1	1:E:227:GLN:HB3	2.44	0.53
1:E:387:ILE:CD1	1:E:450:GLY:N	2.71	0.53
1:F:150:ASN:OD1	1:F:150:ASN:N	2.39	0.53
1:F:317:MET:CE	1:F:609:TYR:CZ	2.92	0.53
1:F:642:ILE:HG12	1:F:645:ARG:CZ	2.39	0.53
1:A:148:PRO:HD3	1:A:188:TYR:CZ	2.43	0.53
1:A:213:PHE:O	1:A:216:ILE:N	2.42	0.53
1:A:263:ASN:HD21	1:A:265:LEU:N	2.06	0.53
1:A:616:VAL:HG13	1:A:619:LYS:HD2	1.91	0.53
1:B:71:PRO:O	1:B:72:ASN:CB	2.57	0.53
1:B:265:LEU:HD23	1:B:269:LEU:HB3	1.89	0.53
1:C:32:TRP:CD1	1:C:43:ILE:HD13	2.44	0.53
1:C:109:ASN:O	1:C:111:PHE:N	2.42	0.53
1:C:282:MET:HA	1:C:282:MET:HE2	1.90	0.53
1:C:285:GLN:NE2	1:C:286:ARG:HH12	2.05	0.53
1:C:433:ILE:HG21	1:C:571:TYR:OH	2.08	0.53
1:D:189:LEU:CG	1:D:190:ALA:N	2.66	0.53
1:D:233:GLY:C	1:D:235:VAL:H	2.11	0.53
1:E:107:TYR:CE1	1:E:153:LEU:HD12	2.44	0.53
1:E:118:LYS:CB	1:E:264:HIS:O	2.57	0.53
1:E:249:LEU:HD23	1:E:252:ALA:CA	2.26	0.53
1:E:433:ILE:CG2	1:E:571:TYR:OH	2.56	0.53
1:E:493:ASP:HB3	1:E:514:TRP:CZ3	2.44	0.53
1:E:633:MET:SD	1:E:633:MET:N	2.82	0.53
1:E:653:GLU:HA	1:E:656:ASN:HB3	1.91	0.53
1:F:444:CYS:O	1:F:446:ARG:N	2.41	0.53
1:F:449:GLN:NE2	1:F:453:THR:HG22	2.24	0.53
1:F:614:LYS:O	1:F:617:VAL:HB	2.09	0.53
1:G:107:TYR:O	1:G:110:GLN:CB	2.56	0.53
1:G:116:GLY:N	1:G:217:THR:O	2.42	0.53
1:G:582:ARG:H	1:G:582:ARG:CD	2.18	0.53
1:H:107:TYR:O	1:H:110:GLN:CB	2.56	0.53
1:H:433:ILE:HB	1:H:571:TYR:OH	2.09	0.53
1:H:614:LYS:O	1:H:617:VAL:HB	2.09	0.53
1:A:362:ASN:O	1:A:364:ALA:N	2.42	0.53
1:A:499:GLU:C	1:A:500:GLN:HE21	2.12	0.53
1:B:32:TRP:CD1	1:B:43:ILE:HD13	2.44	0.53
1:D:107:TYR:HA	1:D:110:GLN:HB2	1.90	0.53
1:D:394:LYS:HG3	1:D:613:SER:HB2	1.90	0.53
1:D:434:TRP:CZ3	1:D:568:ARG:HG3	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:LEU:HB3	1:E:148:PRO:O	2.09	0.53
1:E:116:GLY:CA	1:E:217:THR:O	2.57	0.53
1:E:416:ASP:OD1	1:E:416:ASP:N	2.40	0.53
1:F:62:ILE:HG23	1:F:94:LEU:HD13	1.90	0.53
1:F:137:HIS:ND1	1:F:201:VAL:HG13	2.24	0.53
1:H:153:LEU:HD23	1:H:162:HIS:CB	2.39	0.53
1:H:387:ILE:HG22	1:H:388:PHE:H	1.73	0.53
1:A:373:ASP:CG	1:A:374:CYS:SG	2.88	0.53
1:A:438:ARG:HG2	1:A:564:GLU:OE1	2.08	0.53
1:B:357:SER:CA	1:B:453:THR:HB	2.36	0.53
1:B:473:THR:CG2	1:B:533:LEU:HD22	2.31	0.53
1:C:198:LYS:C	1:C:200:THR:H	2.12	0.53
1:C:449:GLN:HA	1:C:449:GLN:OE1	2.07	0.53
1:D:120:GLY:CA	1:D:123:ARG:H	2.22	0.53
1:D:260:PRO:CG	1:D:274:GLU:HG2	2.39	0.53
1:E:430:TRP:HB3	1:E:571:TYR:CD2	2.39	0.53
1:F:119:GLU:HB2	1:F:121:PRO:HB2	1.91	0.53
1:F:146:LEU:HB3	1:F:207:SER:HB2	1.91	0.53
1:F:387:ILE:HD13	1:F:450:GLY:HA2	1.89	0.53
1:G:157:PRO:HD2	1:G:161:ILE:HD11	1.90	0.53
1:A:285:GLN:HE21	1:A:286:ARG:HH12	1.57	0.52
1:D:148:PRO:HD3	1:D:188:TYR:CZ	2.44	0.52
1:D:536:LYS:HB3	1:D:625:LEU:HD22	1.90	0.52
1:E:123:ARG:HD2	1:E:374:CYS:SG	2.50	0.52
1:E:220:ARG:NH1	1:E:223:LEU:CD2	2.71	0.52
1:E:245:VAL:HG12	1:E:246:TYR:N	2.20	0.52
1:E:320:GLY:O	1:E:321:ARG:C	2.47	0.52
1:E:348:GLU:H	1:E:348:GLU:CD	2.11	0.52
1:E:642:ILE:HG12	1:E:645:ARG:NH1	2.24	0.52
1:F:72:ASN:H	1:F:163:LYS:HE2	1.73	0.52
1:F:449:GLN:OE1	1:F:449:GLN:HA	2.09	0.52
1:G:272:LYS:HG3	1:G:276:TRP:HB2	1.91	0.52
1:A:641:LYS:HB3	1:A:645:ARG:NH2	2.12	0.52
1:B:109:ASN:O	1:B:111:PHE:N	2.42	0.52
1:C:485:PHE:CZ	1:D:485:PHE:CB	2.91	0.52
1:C:614:LYS:O	1:C:617:VAL:HB	2.10	0.52
1:D:26:PHE:CE2	1:D:179:CYS:HB3	2.41	0.52
1:E:540:LEU:HD13	1:E:622:ALA:HB2	1.82	0.52
1:F:116:GLY:CA	1:F:217:THR:O	2.57	0.52
1:F:120:GLY:N	1:F:122:ILE:H	2.06	0.52
1:F:265:LEU:HD21	1:F:269:LEU:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:415:GLN:NE2	1:F:429:VAL:HG11	2.24	0.52
1:G:70:HIS:NE2	1:G:131:SER:O	2.43	0.52
1:G:213:PHE:O	1:G:216:ILE:N	2.42	0.52
1:H:313:SER:HA	1:H:324:THR:HA	1.90	0.52
1:A:89:ASN:C	1:A:91:LEU:H	2.12	0.52
1:A:308:SER:O	1:A:309:LEU:HB2	2.10	0.52
1:A:654:LEU:HD11	1:B:655:TRP:CE3	2.44	0.52
1:B:89:ASN:C	1:B:91:LEU:H	2.12	0.52
1:B:213:PHE:O	1:B:216:ILE:N	2.42	0.52
1:B:226:TRP:HD1	1:B:227:GLN:H	1.41	0.52
1:C:226:TRP:CD1	1:C:227:GLN:HB3	2.44	0.52
1:C:247:ASP:HB2	1:C:255:PHE:O	2.08	0.52
1:C:462:ASN:ND2	1:C:540:LEU:CB	2.71	0.52
1:D:89:ASN:HB3	1:D:91:LEU:H	1.74	0.52
1:D:633:MET:SD	1:D:633:MET:N	2.82	0.52
1:E:89:ASN:HB3	1:E:91:LEU:HB2	1.92	0.52
1:E:260:PRO:CD	1:E:274:GLU:HG2	2.39	0.52
1:F:409:SER:HB2	1:F:412:ILE:CD1	2.39	0.52
1:G:533:LEU:HD23	1:G:629:VAL:HG13	1.91	0.52
1:A:277:LEU:C	1:A:279:CYS:H	2.13	0.52
1:B:153:LEU:HD23	1:B:162:HIS:CB	2.40	0.52
1:B:540:LEU:HD22	1:B:621:LYS:HZ1	1.74	0.52
1:B:642:ILE:HG12	1:B:645:ARG:CZ	2.40	0.52
1:C:165:ILE:HG12	1:C:166:ASP:H	1.74	0.52
1:C:213:PHE:O	1:C:216:ILE:N	2.41	0.52
1:C:233:GLY:C	1:C:235:VAL:H	2.12	0.52
1:D:89:ASN:HB3	1:D:91:LEU:HB2	1.91	0.52
1:D:107:TYR:CE1	1:D:153:LEU:HD12	2.44	0.52
1:D:521:VAL:HG13	1:D:643:VAL:CG1	2.40	0.52
1:E:145:ASP:OD2	1:E:167:LEU:HD13	2.09	0.52
1:E:529:GLU:HG3	1:E:633:MET:CE	2.39	0.52
1:F:308:SER:O	1:F:309:LEU:HB2	2.09	0.52
1:F:647:GLN:OE1	1:F:647:GLN:CA	2.58	0.52
1:G:320:GLY:O	1:G:321:ARG:C	2.47	0.52
1:H:148:PRO:HD3	1:H:188:TYR:CZ	2.45	0.52
1:A:107:TYR:CE1	1:A:153:LEU:HD12	2.44	0.52
1:A:107:TYR:HD1	1:A:153:LEU:HD12	1.68	0.52
1:A:348:GLU:CD	1:A:348:GLU:H	2.13	0.52
1:C:521:VAL:HA	1:C:524:CYS:HG	1.72	0.52
1:D:660:ILE:O	1:D:662:CYS:N	2.42	0.52
1:E:120:GLY:CA	1:E:123:ARG:H	2.21	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:449:GLN:NE2	1:E:453:THR:HG22	2.25	0.52
1:E:499:GLU:C	1:E:500:GLN:HE21	2.13	0.52
1:F:180:THR:HG22	1:F:180:THR:O	2.10	0.52
1:F:222:PHE:CD2	1:F:224:PRO:O	2.63	0.52
1:F:426:LEU:HB3	1:F:430:TRP:CD1	2.45	0.52
1:G:180:THR:O	1:G:180:THR:HG22	2.10	0.52
1:G:226:TRP:CD1	1:G:227:GLN:HB3	2.45	0.52
1:H:193:LEU:CB	1:H:196:GLN:HE22	2.22	0.52
1:H:434:TRP:HZ3	1:H:568:ARG:CB	2.22	0.52
1:A:32:TRP:CD1	1:A:43:ILE:HD13	2.44	0.52
1:A:221:PRO:O	1:A:222:PHE:HB3	2.09	0.52
1:A:387:ILE:HD11	1:A:449:GLN:CG	2.39	0.52
1:A:387:ILE:HG22	1:A:388:PHE:H	1.74	0.52
1:A:517:MET:CE	1:A:650:ARG:HG3	2.39	0.52
1:A:642:ILE:HG12	1:A:645:ARG:NH1	2.25	0.52
1:B:104:LEU:HB3	1:B:148:PRO:O	2.10	0.52
1:B:387:ILE:HG22	1:B:388:PHE:H	1.74	0.52
1:B:647:GLN:OE1	1:B:647:GLN:CA	2.57	0.52
1:C:409:SER:HB2	1:C:412:ILE:CD1	2.40	0.52
1:C:494:LEU:HD21	1:C:518:GLU:OE2	2.09	0.52
1:C:653:GLU:HA	1:C:656:ASN:HB3	1.90	0.52
1:D:109:ASN:O	1:D:111:PHE:N	2.43	0.52
1:D:534:VAL:HG13	1:D:535:ASP:N	2.24	0.52
1:G:415:GLN:NE2	1:G:429:VAL:HG11	2.24	0.52
1:H:71:PRO:O	1:H:72:ASN:CB	2.57	0.52
1:A:213:PHE:C	1:A:213:PHE:CD2	2.83	0.52
1:A:222:PHE:CD2	1:A:224:PRO:O	2.63	0.52
1:A:265:LEU:HD23	1:A:269:LEU:CB	2.40	0.52
1:B:145:ASP:OD2	1:B:167:LEU:HD13	2.09	0.52
1:C:107:TYR:CE1	1:C:153:LEU:HD12	2.44	0.52
1:C:272:LYS:HG2	1:C:273:LEU:CA	2.40	0.52
1:D:165:ILE:HG12	1:D:166:ASP:H	1.74	0.52
1:D:475:GLU:HG2	1:D:636:MET:HE1	1.88	0.52
1:D:531:GLN:HA	1:D:534:VAL:HG12	1.91	0.52
1:E:220:ARG:CB	1:E:221:PRO:HD2	2.39	0.52
1:F:117:LEU:O	1:F:119:GLU:HG2	2.10	0.52
1:F:153:LEU:HD23	1:F:162:HIS:CB	2.40	0.52
1:F:656:ASN:C	1:F:656:ASN:OD1	2.48	0.52
1:G:68:LEU:HB3	1:G:135:TYR:CE2	2.45	0.52
1:G:145:ASP:OD2	1:G:167:LEU:HD13	2.10	0.52
1:H:632:VAL:C	1:H:633:MET:SD	2.88	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:TYR:CE1	1:B:153:LEU:HD12	2.45	0.52
1:B:263:ASN:HD21	1:B:265:LEU:N	2.06	0.52
1:B:494:LEU:HD22	1:B:518:GLU:OE2	2.07	0.52
1:B:540:LEU:HD11	1:B:621:LYS:CB	2.39	0.52
1:C:245:VAL:HG12	1:C:246:TYR:N	2.20	0.52
1:D:180:THR:O	1:D:180:THR:HG22	2.10	0.52
1:D:245:VAL:HG12	1:D:246:TYR:N	2.22	0.52
1:D:570:LEU:HD23	1:D:590:MET:CE	2.40	0.52
1:H:394:LYS:CE	1:H:401:ILE:HA	2.40	0.52
1:H:409:SER:HB2	1:H:412:ILE:CD1	2.40	0.52
1:H:540:LEU:HD21	1:H:621:LYS:HB3	1.91	0.52
1:A:145:ASP:OD2	1:A:167:LEU:HD13	2.09	0.52
1:A:373:ASP:OD1	1:A:374:CYS:N	2.43	0.52
1:A:437:ILE:HG13	1:A:594:LEU:CD1	2.39	0.52
1:A:534:VAL:HG13	1:A:535:ASP:N	2.24	0.52
1:C:118:LYS:NZ	1:C:123:ARG:HH12	2.08	0.52
1:C:368:THR:O	1:C:368:THR:HG22	2.10	0.52
1:E:165:ILE:HG12	1:E:166:ASP:H	1.75	0.52
1:E:249:LEU:HD23	1:E:253:VAL:H	1.75	0.52
1:E:322:VAL:HG21	1:E:446:ARG:NH1	2.24	0.52
1:F:571:TYR:CZ	1:F:590:MET:SD	3.03	0.52
1:G:32:TRP:CD1	1:G:43:ILE:HD13	2.45	0.52
1:G:437:ILE:HG22	1:G:564:GLU:HB2	1.92	0.52
1:H:145:ASP:OD2	1:H:167:LEU:HD13	2.10	0.52
1:A:429:VAL:O	1:A:433:ILE:HG12	2.10	0.52
1:B:415:GLN:NE2	1:B:429:VAL:HG11	2.25	0.52
1:B:507:SER:C	1:B:509:LYS:H	2.13	0.52
1:C:514:TRP:O	1:C:518:GLU:HG3	2.10	0.52
1:C:531:GLN:HA	1:C:534:VAL:HG12	1.92	0.52
1:D:115:CYS:O	1:D:263:ASN:HA	2.09	0.52
1:D:221:PRO:O	1:D:222:PHE:HB3	2.09	0.52
1:D:507:SER:C	1:D:509:LYS:H	2.14	0.52
1:E:534:VAL:HG13	1:E:535:ASP:N	2.25	0.52
1:F:120:GLY:CA	1:F:123:ARG:H	2.22	0.52
1:F:233:GLY:C	1:F:235:VAL:H	2.13	0.52
1:F:438:ARG:NH1	1:F:568:ARG:HH21	2.08	0.52
1:F:529:GLU:HG3	1:F:633:MET:CE	2.39	0.52
1:G:285:GLN:HE21	1:G:286:ARG:HH12	1.58	0.52
1:H:226:TRP:CD1	1:H:227:GLN:HB3	2.45	0.52
1:H:248:ASP:OD1	1:H:248:ASP:O	2.28	0.52
1:A:120:GLY:CA	1:A:123:ARG:H	2.23	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ILE:HG12	1:A:166:ASP:H	1.75	0.51
1:A:527:GLU:HG2	1:A:530:VAL:HG13	1.92	0.51
1:A:642:ILE:HG12	1:A:645:ARG:CZ	2.40	0.51
1:A:653:GLU:HA	1:A:656:ASN:HB3	1.92	0.51
1:B:180:THR:O	1:B:180:THR:HG22	2.10	0.51
1:C:434:TRP:HZ3	1:C:568:ARG:CA	2.21	0.51
1:D:89:ASN:C	1:D:91:LEU:H	2.13	0.51
1:D:387:ILE:HG22	1:D:388:PHE:H	1.74	0.51
1:D:412:ILE:HG12	1:D:433:ILE:CD1	2.40	0.51
1:D:582:ARG:H	1:D:582:ARG:CD	2.19	0.51
1:E:115:CYS:SG	1:E:432:GLN:HA	2.50	0.51
1:F:89:ASN:C	1:F:91:LEU:H	2.11	0.51
1:F:117:LEU:O	1:F:122:ILE:HD11	2.09	0.51
1:F:245:VAL:HG12	1:F:246:TYR:N	2.22	0.51
1:F:426:LEU:HB2	1:F:574:LEU:HD21	1.90	0.51
1:G:62:ILE:HG23	1:G:94:LEU:HD13	1.92	0.51
1:G:89:ASN:C	1:G:91:LEU:H	2.12	0.51
1:G:433:ILE:CG2	1:G:571:TYR:OH	2.57	0.51
1:G:534:VAL:HG13	1:G:535:ASP:N	2.25	0.51
1:A:26:PHE:HE2	1:A:181:GLU:CD	2.13	0.51
1:A:614:LYS:O	1:A:617:VAL:HB	2.10	0.51
1:C:286:ARG:O	1:C:290:THR:HG21	2.10	0.51
1:C:373:ASP:OD1	1:C:374:CYS:N	2.42	0.51
1:C:580:ASP:HA	1:C:582:ARG:HH11	1.75	0.51
1:D:153:LEU:HD23	1:D:162:HIS:CB	2.40	0.51
1:E:71:PRO:O	1:E:72:ASN:CB	2.58	0.51
1:E:119:GLU:HB2	1:E:121:PRO:HB2	1.92	0.51
1:F:107:TYR:CE1	1:F:153:LEU:HD12	2.45	0.51
1:F:297:VAL:HB	1:F:301:GLN:H	1.75	0.51
1:F:348:GLU:CD	1:F:348:GLU:H	2.12	0.51
1:G:153:LEU:HD23	1:G:162:HIS:CB	2.40	0.51
1:G:322:VAL:CG1	1:G:323:HIS:H	2.21	0.51
1:G:339:TRP:HA	1:G:342:GLN:CB	2.34	0.51
1:G:341:GLN:O	1:G:345:GLY:N	2.43	0.51
1:H:119:GLU:HB2	1:H:121:PRO:HB2	1.91	0.51
1:H:220:ARG:HB3	1:H:221:PRO:HD2	1.92	0.51
1:H:447:LEU:HD12	1:H:605:VAL:CG2	2.40	0.51
1:H:632:VAL:HG12	1:H:633:MET:HE1	1.91	0.51
1:A:409:SER:HB2	1:A:412:ILE:CD1	2.39	0.51
1:A:478:GLN:HG3	1:A:479:LEU:N	2.25	0.51
1:B:350:GLU:OE2	1:B:391:ASP:O	2.29	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:TRP:O	1:B:518:GLU:HG3	2.10	0.51
1:B:547:LEU:O	1:B:550:ASN:ND2	2.44	0.51
1:C:145:ASP:OD2	1:C:167:LEU:HD13	2.10	0.51
1:C:265:LEU:HD23	1:C:269:LEU:HB3	1.93	0.51
1:C:322:VAL:CG1	1:C:323:HIS:H	2.21	0.51
1:C:387:ILE:HG22	1:C:388:PHE:H	1.76	0.51
1:C:462:ASN:ND2	1:C:540:LEU:HB2	2.19	0.51
1:D:193:LEU:CB	1:D:196:GLN:HE22	2.23	0.51
1:D:224:PRO:HG3	1:D:428:ARG:HH22	1.75	0.51
1:D:235:VAL:CB	1:D:243:ILE:HA	2.37	0.51
1:D:282:MET:HE2	1:D:282:MET:HA	1.91	0.51
1:D:402:SER:HA	1:D:609:TYR:CD1	2.45	0.51
1:D:642:ILE:HG12	1:D:645:ARG:CZ	2.40	0.51
1:E:272:LYS:HG2	1:E:273:LEU:CA	2.40	0.51
1:G:72:ASN:O	1:G:163:LYS:HA	2.11	0.51
1:G:134:ARG:CA	1:G:300:PHE:CZ	2.86	0.51
1:G:297:VAL:HB	1:G:301:GLN:H	1.75	0.51
1:H:348:GLU:H	1:H:348:GLU:CD	2.13	0.51
1:A:113:ASN:HA	1:A:116:GLY:O	2.10	0.51
1:A:263:ASN:HD21	1:A:265:LEU:H	1.57	0.51
1:A:282:MET:HE2	1:A:282:MET:HA	1.91	0.51
1:A:320:GLY:O	1:A:321:ARG:C	2.48	0.51
1:A:580:ASP:CB	1:D:579:ARG:NH2	2.71	0.51
1:B:89:ASN:HB3	1:B:91:LEU:HB2	1.92	0.51
1:B:285:GLN:HE21	1:B:286:ARG:HH12	1.59	0.51
1:B:285:GLN:HG2	1:B:285:GLN:O	2.11	0.51
1:B:327:VAL:CG1	1:B:367:LEU:HB2	2.34	0.51
1:B:442:GLU:HB3	1:B:446:ARG:HH21	1.75	0.51
1:C:511:LEU:HG	1:C:515:ARG:CZ	2.40	0.51
1:D:263:ASN:HD21	1:D:265:LEU:N	2.07	0.51
1:D:297:VAL:HB	1:D:301:GLN:H	1.74	0.51
1:D:449:GLN:OE1	1:D:449:GLN:HA	2.09	0.51
1:E:357:SER:HB3	1:E:453:THR:HB	1.93	0.51
1:E:571:TYR:OH	1:E:590:MET:SD	2.69	0.51
1:E:642:ILE:HG12	1:E:645:ARG:CZ	2.40	0.51
1:F:119:GLU:HB3	1:F:121:PRO:CD	2.40	0.51
1:F:220:ARG:CB	1:F:221:PRO:HD2	2.41	0.51
1:F:303:LEU:O	1:F:307:LEU:HB2	2.11	0.51
1:G:100:GLU:H	1:G:154:GLN:HG3	1.74	0.51
1:H:547:LEU:O	1:H:550:ASN:ND2	2.44	0.51
1:A:120:GLY:C	1:A:122:ILE:N	2.63	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:ASP:HA	1:A:582:ARG:HH11	1.75	0.51
1:B:348:GLU:H	1:B:348:GLU:CD	2.14	0.51
1:B:386:LEU:H	1:B:386:LEU:CD1	2.22	0.51
1:B:550:ASN:HD21	1:B:611:GLN:HG3	1.74	0.51
1:B:642:ILE:HG12	1:B:645:ARG:NH1	2.25	0.51
1:C:107:TYR:C	1:C:110:GLN:H	2.12	0.51
1:C:134:ARG:HD2	1:C:300:PHE:CE1	2.45	0.51
1:C:249:LEU:HA	1:C:253:VAL:O	2.11	0.51
1:C:320:GLY:O	1:C:321:ARG:C	2.48	0.51
1:C:429:VAL:HG12	1:C:430:TRP:HD1	1.75	0.51
1:D:272:LYS:HG3	1:D:276:TRP:HB2	1.93	0.51
1:E:246:TYR:CD1	1:E:258:VAL:CB	2.72	0.51
1:E:249:LEU:HA	1:E:253:VAL:O	2.11	0.51
1:F:118:LYS:CD	1:F:265:LEU:HA	2.39	0.51
1:F:213:PHE:C	1:F:213:PHE:CD2	2.84	0.51
1:F:373:ASP:CG	1:F:374:CYS:SG	2.89	0.51
1:F:642:ILE:HG12	1:F:645:ARG:NH1	2.25	0.51
1:G:265:LEU:HD23	1:G:269:LEU:CB	2.40	0.51
1:H:145:ASP:CG	1:H:167:LEU:HD13	2.31	0.51
1:H:534:VAL:HG13	1:H:535:ASP:N	2.26	0.51
1:B:107:TYR:O	1:B:110:GLN:HB2	2.11	0.51
1:C:547:LEU:HD22	1:C:611:GLN:HG2	1.93	0.51
1:D:191:PRO:HG3	1:D:234:LYS:HZ3	1.76	0.51
1:D:368:THR:O	1:D:368:THR:HG22	2.11	0.51
1:E:32:TRP:CD1	1:E:43:ILE:HD13	2.46	0.51
1:F:107:TYR:O	1:F:110:GLN:HB2	2.11	0.51
1:F:107:TYR:C	1:F:110:GLN:H	2.13	0.51
1:F:145:ASP:OD2	1:F:167:LEU:HD13	2.11	0.51
1:F:507:SER:C	1:F:509:LYS:H	2.13	0.51
1:G:120:GLY:CA	1:G:123:ARG:H	2.23	0.51
1:G:148:PRO:HD3	1:G:188:TYR:CZ	2.45	0.51
1:G:165:ILE:HG12	1:G:166:ASP:H	1.74	0.51
1:A:153:LEU:HD23	1:A:162:HIS:CB	2.40	0.51
1:A:350:GLU:OE2	1:A:391:ASP:O	2.28	0.51
1:A:357:SER:CA	1:A:453:THR:HB	2.41	0.51
1:A:415:GLN:NE2	1:A:429:VAL:HG11	2.26	0.51
1:A:449:GLN:NE2	1:A:453:THR:HG22	2.25	0.51
1:A:449:GLN:OE1	1:A:449:GLN:HA	2.10	0.51
1:A:531:GLN:O	1:A:535:ASP:HB3	2.11	0.51
1:A:570:LEU:CB	1:A:590:MET:HE2	2.39	0.51
1:D:120:GLY:C	1:D:122:ILE:N	2.63	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:ASP:HB2	1:D:255:PHE:O	2.11	0.51
1:D:426:LEU:HB3	1:D:430:TRP:CD1	2.46	0.51
1:F:564:GLU:OE2	1:F:568:ARG:NH2	2.44	0.51
1:G:245:VAL:HG12	1:G:246:TYR:N	2.22	0.51
1:G:429:VAL:O	1:G:433:ILE:HG12	2.10	0.51
1:G:434:TRP:HZ3	1:G:568:ARG:CB	2.24	0.51
1:A:119:GLU:HB2	1:A:121:PRO:CB	2.41	0.51
1:A:226:TRP:CD1	1:A:227:GLN:HB3	2.45	0.51
1:A:440:LEU:HD12	1:A:597:ALA:O	2.10	0.51
1:A:647:GLN:OE1	1:A:647:GLN:CA	2.58	0.51
1:B:148:PRO:HD3	1:B:188:TYR:CZ	2.45	0.51
1:B:286:ARG:O	1:B:290:THR:HG21	2.11	0.51
1:B:313:SER:HA	1:B:324:THR:HA	1.93	0.51
1:B:571:TYR:OH	1:B:590:MET:SD	2.64	0.51
1:C:511:LEU:HD21	1:C:515:ARG:NH2	2.26	0.51
1:D:341:GLN:O	1:D:345:GLY:N	2.44	0.51
1:D:632:VAL:HG12	1:D:633:MET:HE1	1.93	0.51
1:E:254:LYS:N	1:E:255:PHE:CE1	2.79	0.51
1:E:387:ILE:HG22	1:E:388:PHE:H	1.76	0.51
1:F:226:TRP:CG	1:F:227:GLN:N	2.59	0.51
1:F:322:VAL:CG1	1:F:323:HIS:H	2.20	0.51
1:F:534:VAL:HG13	1:F:535:ASP:N	2.25	0.51
1:G:100:GLU:N	1:G:154:GLN:HG3	2.26	0.51
1:G:222:PHE:CD2	1:G:224:PRO:O	2.63	0.51
1:A:272:LYS:HG3	1:A:276:TRP:HB2	1.93	0.51
1:A:531:GLN:HA	1:A:534:VAL:HG12	1.92	0.51
1:B:497:TYR:O	1:B:497:TYR:HD2	1.85	0.51
1:C:153:LEU:HD23	1:C:162:HIS:CB	2.40	0.51
1:C:656:ASN:C	1:C:656:ASN:OD1	2.48	0.51
1:D:249:LEU:HA	1:D:253:VAL:O	2.11	0.51
1:D:444:CYS:O	1:D:446:ARG:N	2.44	0.51
1:D:479:LEU:HD12	1:D:640:GLU:CB	2.40	0.51
1:D:588:ASN:OD1	1:D:589:ASP:N	2.44	0.51
1:D:642:ILE:HG12	1:D:645:ARG:NH1	2.25	0.51
1:E:409:SER:HB2	1:E:412:ILE:CD1	2.38	0.51
1:E:580:ASP:HA	1:E:582:ARG:HH11	1.76	0.51
1:E:647:GLN:OE1	1:E:647:GLN:CA	2.58	0.51
1:F:71:PRO:O	1:F:72:ASN:CB	2.58	0.51
1:F:429:VAL:O	1:F:433:ILE:HG12	2.10	0.51
1:F:529:GLU:O	1:F:533:LEU:HG	2.10	0.51
1:G:119:GLU:HB2	1:G:121:PRO:HB2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:387:ILE:CD1	1:G:450:GLY:CA	2.87	0.51
1:G:426:LEU:HB3	1:G:430:TRP:CD1	2.45	0.51
1:G:633:MET:SD	1:G:633:MET:N	2.84	0.51
1:H:165:ILE:HG12	1:H:166:ASP:H	1.76	0.51
1:H:440:LEU:HD12	1:H:597:ALA:O	2.11	0.51
1:H:451:GLN:OE1	1:H:611:GLN:NE2	2.44	0.51
1:H:547:LEU:HD13	1:H:615:THR:HG22	1.93	0.51
1:A:109:ASN:O	1:A:111:PHE:N	2.44	0.51
1:A:220:ARG:NH1	1:A:223:LEU:CD2	2.71	0.51
1:A:313:SER:HA	1:A:324:THR:HA	1.92	0.51
1:B:531:GLN:O	1:B:535:ASP:HB3	2.11	0.51
1:C:107:TYR:O	1:C:110:GLN:HB2	2.10	0.51
1:C:116:GLY:CA	1:C:217:THR:O	2.59	0.51
1:C:449:GLN:NE2	1:C:453:THR:HG22	2.26	0.51
1:C:534:VAL:HG13	1:C:535:ASP:N	2.25	0.51
1:D:189:LEU:HD12	1:D:207:SER:HB3	1.93	0.51
1:D:265:LEU:HD23	1:D:269:LEU:CB	2.41	0.51
1:D:422:THR:HG21	1:D:586:ASP:C	2.30	0.51
1:E:107:TYR:O	1:E:110:GLN:HB2	2.10	0.51
1:E:649:LYS:HA	1:E:652:GLN:HB2	1.92	0.51
1:F:226:TRP:HD1	1:F:227:GLN:N	2.04	0.51
1:F:368:THR:O	1:F:368:THR:HG22	2.11	0.51
1:G:26:PHE:CE2	1:G:181:GLU:CD	2.84	0.51
1:G:89:ASN:HB3	1:G:91:LEU:HB2	1.92	0.51
1:G:409:SER:HB2	1:G:412:ILE:CD1	2.38	0.51
1:H:320:GLY:O	1:H:321:ARG:C	2.49	0.51
1:A:18:LYS:NZ	1:A:33:ILE:HD12	2.27	0.50
1:A:233:GLY:C	1:A:235:VAL:H	2.14	0.50
1:A:588:ASN:OD1	1:A:589:ASP:N	2.43	0.50
1:B:409:SER:HB2	1:B:412:ILE:CD1	2.40	0.50
1:B:449:GLN:NE2	1:B:453:THR:HG22	2.26	0.50
1:B:521:VAL:HA	1:B:524:CYS:HG	1.75	0.50
1:B:660:ILE:C	1:B:662:CYS:N	2.65	0.50
1:C:303:LEU:O	1:C:307:LEU:HB2	2.11	0.50
1:C:437:ILE:HG22	1:C:564:GLU:HB2	1.92	0.50
1:C:666:ARG:HD2	1:D:503:PHE:HD1	1.75	0.50
1:D:226:TRP:CD1	1:D:227:GLN:HB3	2.45	0.50
1:D:475:GLU:CG	1:D:636:MET:CE	2.85	0.50
1:E:368:THR:HG22	1:E:368:THR:O	2.11	0.50
1:F:350:GLU:OE2	1:F:391:ASP:O	2.29	0.50
1:G:121:PRO:HA	1:G:124:THR:OG1	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:89:ASN:HB3	1:H:91:LEU:HB2	1.93	0.50
1:H:308:SER:O	1:H:309:LEU:HB2	2.12	0.50
1:A:107:TYR:C	1:A:110:GLN:H	2.14	0.50
1:A:118:LYS:HD3	1:A:265:LEU:HD12	1.94	0.50
1:B:221:PRO:O	1:B:222:PHE:HB3	2.11	0.50
1:D:116:GLY:HA2	1:D:217:THR:O	2.12	0.50
1:D:117:LEU:O	1:D:122:ILE:HD11	2.11	0.50
1:D:285:GLN:HE21	1:D:286:ARG:HH12	1.57	0.50
1:D:476:CYS:CA	1:D:636:MET:SD	2.98	0.50
1:E:118:LYS:CD	1:E:265:LEU:HA	2.42	0.50
1:E:153:LEU:HD23	1:E:162:HIS:CB	2.40	0.50
1:E:213:PHE:O	1:E:216:ILE:N	2.43	0.50
1:E:480:LYS:NZ	1:E:527:GLU:HB2	2.27	0.50
1:F:60:LEU:HD21	1:F:175:GLN:HB3	1.91	0.50
1:F:361:LEU:HD11	1:F:386:LEU:HD23	1.94	0.50
1:G:107:TYR:CE1	1:G:153:LEU:HD12	2.46	0.50
1:G:270:ALA:HB1	1:G:274:GLU:OE2	2.12	0.50
1:G:580:ASP:HA	1:G:582:ARG:HH11	1.75	0.50
1:H:260:PRO:CD	1:H:274:GLU:HG2	2.41	0.50
1:H:633:MET:SD	1:H:633:MET:N	2.84	0.50
1:A:547:LEU:O	1:A:550:ASN:ND2	2.45	0.50
1:A:655:TRP:CE3	1:B:654:LEU:HD12	2.35	0.50
1:B:110:GLN:O	1:B:111:PHE:CB	2.37	0.50
1:B:193:LEU:CB	1:B:196:GLN:HE22	2.23	0.50
1:B:441:LYS:HB2	1:B:560:LEU:HD21	1.93	0.50
1:C:180:THR:HG22	1:C:180:THR:O	2.11	0.50
1:D:547:LEU:HD12	1:D:615:THR:HG22	1.93	0.50
1:E:180:THR:O	1:E:180:THR:HG22	2.12	0.50
1:E:494:LEU:CD2	1:E:518:GLU:OE2	2.59	0.50
1:G:193:LEU:HD22	1:G:231:TRP:CD1	2.47	0.50
1:G:263:ASN:HD21	1:G:265:LEU:H	1.57	0.50
1:G:531:GLN:O	1:G:535:ASP:HB3	2.12	0.50
1:H:213:PHE:O	1:H:216:ILE:N	2.45	0.50
1:H:233:GLY:C	1:H:235:VAL:H	2.14	0.50
1:H:303:LEU:O	1:H:307:LEU:HB2	2.10	0.50
1:H:394:LYS:HE2	1:H:401:ILE:CA	2.40	0.50
1:A:33:ILE:HG22	1:A:34:HIS:C	2.31	0.50
1:A:145:ASP:CG	1:A:167:LEU:HD13	2.32	0.50
1:A:220:ARG:HB3	1:A:221:PRO:HD2	1.92	0.50
1:B:159:ARG:HD3	1:B:375:THR:HG21	1.93	0.50
1:B:272:LYS:HG3	1:B:276:TRP:HB2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:ARG:HA	1:B:587:SER:OG	2.11	0.50
1:C:113:ASN:HA	1:C:116:GLY:O	2.12	0.50
1:C:119:GLU:HB2	1:C:121:PRO:HB2	1.93	0.50
1:C:285:GLN:O	1:C:285:GLN:HG2	2.12	0.50
1:C:473:THR:CG2	1:C:533:LEU:CD2	2.80	0.50
1:C:529:GLU:O	1:C:533:LEU:HG	2.11	0.50
1:C:564:GLU:OE2	1:C:568:ARG:NH2	2.43	0.50
1:D:18:LYS:NZ	1:D:33:ILE:HD12	2.27	0.50
1:D:119:GLU:HB2	1:D:121:PRO:HB2	1.94	0.50
1:D:134:ARG:HB2	1:D:300:PHE:CE1	2.46	0.50
1:D:529:GLU:O	1:D:533:LEU:HG	2.12	0.50
1:D:656:ASN:C	1:D:656:ASN:OD1	2.49	0.50
1:F:221:PRO:O	1:F:222:PHE:HB3	2.11	0.50
1:F:235:VAL:CB	1:F:243:ILE:HA	2.38	0.50
1:F:497:TYR:O	1:F:497:TYR:HD2	1.91	0.50
1:G:26:PHE:HE2	1:G:181:GLU:OE1	1.95	0.50
1:G:529:GLU:O	1:G:533:LEU:HG	2.11	0.50
1:G:614:LYS:O	1:G:617:VAL:HB	2.11	0.50
1:H:226:TRP:HB3	1:H:229:VAL:CG2	2.42	0.50
1:H:359:LEU:HA	1:H:460:ARG:NH1	2.25	0.50
1:H:402:SER:HB3	1:H:609:TYR:HB2	1.94	0.50
1:H:434:TRP:CZ3	1:H:568:ARG:CG	2.82	0.50
1:H:609:TYR:O	1:H:612:LEU:HB3	2.12	0.50
1:A:447:LEU:HD13	1:A:609:TYR:HE1	1.75	0.50
1:B:107:TYR:C	1:B:110:GLN:H	2.13	0.50
1:B:500:GLN:CA	1:B:505:ILE:HG12	2.41	0.50
1:B:511:LEU:HG	1:B:515:ARG:CZ	2.42	0.50
1:B:547:LEU:HD11	1:B:614:LYS:HB3	1.81	0.50
1:C:260:PRO:CD	1:C:274:GLU:HG2	2.41	0.50
1:C:412:ILE:HG12	1:C:433:ILE:CD1	2.42	0.50
1:E:486:PHE:CZ	1:E:517:MET:HE2	2.44	0.50
1:F:89:ASN:HB3	1:F:91:LEU:HB2	1.91	0.50
1:F:113:ASN:HA	1:F:116:GLY:O	2.12	0.50
1:F:120:GLY:C	1:F:122:ILE:N	2.65	0.50
1:F:248:ASP:OD1	1:F:248:ASP:O	2.30	0.50
1:F:412:ILE:HG12	1:F:433:ILE:CD1	2.41	0.50
1:F:437:ILE:CG1	1:F:594:LEU:HD12	2.41	0.50
1:G:616:VAL:HG13	1:G:619:LYS:HD2	1.93	0.50
1:H:107:TYR:CE1	1:H:153:LEU:HD12	2.45	0.50
1:H:254:LYS:N	1:H:255:PHE:CE1	2.80	0.50
1:H:415:GLN:NE2	1:H:429:VAL:HG11	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LYS:NZ	1:A:123:ARG:HH12	2.10	0.50
1:A:479:LEU:HD11	1:A:641:LYS:HG3	1.92	0.50
1:A:514:TRP:O	1:A:518:GLU:HG3	2.11	0.50
1:B:444:CYS:C	1:B:446:ARG:N	2.63	0.50
1:C:485:PHE:CD1	1:D:485:PHE:CD1	3.00	0.50
1:D:107:TYR:O	1:D:110:GLN:HB2	2.12	0.50
1:D:222:PHE:CE2	1:D:224:PRO:O	2.64	0.50
1:E:285:GLN:HG2	1:E:285:GLN:O	2.12	0.50
1:F:109:ASN:O	1:F:111:PHE:N	2.45	0.50
1:F:660:ILE:O	1:F:662:CYS:N	2.45	0.50
1:G:308:SER:O	1:G:309:LEU:HB2	2.12	0.50
1:G:313:SER:HA	1:G:324:THR:HA	1.92	0.50
1:H:109:ASN:O	1:H:111:PHE:N	2.45	0.50
1:H:180:THR:HG22	1:H:180:THR:O	2.11	0.50
1:H:189:LEU:HD12	1:H:207:SER:HB3	1.94	0.50
1:B:487:ARG:HH21	1:B:522:GLU:HA	1.77	0.50
1:C:120:GLY:CA	1:C:123:ARG:H	2.24	0.50
1:C:265:LEU:HD23	1:C:269:LEU:CB	2.42	0.50
1:C:327:VAL:CG1	1:C:367:LEU:HB2	2.36	0.50
1:D:437:ILE:HG13	1:D:594:LEU:CD1	2.41	0.50
1:D:441:LYS:CB	1:D:560:LEU:HD21	2.42	0.50
1:D:564:GLU:OE2	1:D:568:ARG:NH2	2.44	0.50
1:E:134:ARG:HD2	1:E:300:PHE:CE1	2.46	0.50
1:F:26:PHE:CE2	1:F:181:GLU:CD	2.85	0.50
1:F:26:PHE:CE2	1:F:179:CYS:HB3	2.47	0.50
1:F:72:ASN:O	1:F:163:LYS:HA	2.12	0.50
1:F:317:MET:HE1	1:F:609:TYR:CZ	2.46	0.50
1:F:339:TRP:HA	1:F:342:GLN:CB	2.35	0.50
1:F:534:VAL:CG1	1:F:535:ASP:N	2.75	0.50
1:G:186:LEU:HD23	1:G:227:GLN:HG2	1.94	0.50
1:G:191:PRO:HG3	1:G:234:LYS:HZ3	1.75	0.50
1:G:277:LEU:C	1:G:279:CYS:H	2.14	0.50
1:A:286:ARG:O	1:A:290:THR:HG21	2.12	0.50
1:A:387:ILE:HD12	1:A:450:GLY:HA2	1.94	0.50
1:B:247:ASP:HB2	1:B:255:PHE:O	2.11	0.50
1:B:265:LEU:HD23	1:B:269:LEU:CB	2.42	0.50
1:B:368:THR:HG22	1:B:368:THR:O	2.12	0.50
1:B:389:LEU:HD12	1:B:389:LEU:N	2.26	0.50
1:C:18:LYS:NZ	1:C:33:ILE:HD12	2.26	0.50
1:C:418:LYS:O	1:C:419:ARG:CB	2.60	0.50
1:C:459:LEU:CD1	1:C:548:GLN:HB3	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:547:LEU:O	1:C:550:ASN:ND2	2.44	0.50
1:C:649:LYS:HA	1:C:652:GLN:CB	2.41	0.50
1:D:429:VAL:O	1:D:433:ILE:HG12	2.11	0.50
1:D:493:ASP:HB3	1:D:514:TRP:CH2	2.47	0.50
1:E:221:PRO:O	1:E:222:PHE:HB3	2.11	0.50
1:E:272:LYS:HG3	1:E:276:TRP:HB2	1.94	0.50
1:E:308:SER:O	1:E:309:LEU:HB2	2.10	0.50
1:F:216:ILE:HG21	1:F:273:LEU:HD12	1.94	0.50
1:F:373:ASP:C	1:F:374:CYS:SG	2.90	0.50
1:F:531:GLN:HA	1:F:534:VAL:HG12	1.92	0.50
1:G:220:ARG:HB3	1:G:221:PRO:HD2	1.93	0.50
1:G:361:LEU:HD11	1:G:386:LEU:HD23	1.94	0.50
1:A:341:GLN:O	1:A:345:GLY:N	2.45	0.50
1:A:588:ASN:CG	1:A:589:ASP:N	2.63	0.50
1:B:26:PHE:HZ	1:B:179:CYS:HB3	1.73	0.50
1:B:260:PRO:CD	1:B:274:GLU:HG2	2.42	0.50
1:C:361:LEU:HD11	1:C:386:LEU:HD23	1.94	0.50
1:D:33:ILE:HG22	1:D:34:HIS:C	2.32	0.50
1:D:71:PRO:O	1:D:72:ASN:CB	2.59	0.50
1:D:107:TYR:C	1:D:110:GLN:H	2.14	0.50
1:D:313:SER:HA	1:D:324:THR:HA	1.94	0.50
1:D:594:LEU:O	1:D:598:ILE:HG13	2.12	0.50
1:E:120:GLY:N	1:E:122:ILE:H	2.06	0.50
1:E:426:LEU:HB3	1:E:430:TRP:CD1	2.47	0.50
1:E:534:VAL:CG1	1:E:535:ASP:N	2.75	0.50
1:G:368:THR:O	1:G:368:THR:HG22	2.11	0.50
1:G:547:LEU:O	1:G:550:ASN:ND2	2.44	0.50
1:H:272:LYS:HG3	1:H:276:TRP:HB2	1.93	0.50
1:H:277:LEU:C	1:H:279:CYS:H	2.15	0.50
1:H:390:PHE:HZ	1:H:612:LEU:HD11	1.77	0.50
1:A:269:LEU:HD22	1:A:272:LYS:HE3	1.94	0.49
1:A:534:VAL:CG1	1:A:535:ASP:N	2.74	0.49
1:C:115:CYS:O	1:C:263:ASN:HA	2.12	0.49
1:C:115:CYS:CB	1:C:435:GLN:HG3	2.42	0.49
1:C:313:SER:HA	1:C:324:THR:HA	1.92	0.49
1:C:573:ARG:HH12	1:D:573:ARG:CZ	2.15	0.49
1:D:113:ASN:HA	1:D:116:GLY:O	2.12	0.49
1:D:226:TRP:HB3	1:D:229:VAL:CG2	2.41	0.49
1:E:107:TYR:C	1:E:110:GLN:H	2.14	0.49
1:E:120:GLY:C	1:E:122:ILE:N	2.65	0.49
1:E:303:LEU:O	1:E:307:LEU:HB2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:226:TRP:HB3	1:F:229:VAL:CG2	2.41	0.49
1:F:249:LEU:HD23	1:F:253:VAL:H	1.76	0.49
1:F:265:LEU:HD23	1:F:269:LEU:CB	2.42	0.49
1:F:282:MET:HE2	1:F:282:MET:HA	1.94	0.49
1:F:341:GLN:O	1:F:345:GLY:N	2.45	0.49
1:G:33:ILE:HG22	1:G:34:HIS:C	2.32	0.49
1:G:233:GLY:C	1:G:235:VAL:H	2.16	0.49
1:G:286:ARG:O	1:G:290:THR:HG21	2.12	0.49
1:G:443:ASP:O	1:G:446:ARG:CB	2.59	0.49
1:G:534:VAL:CG1	1:G:535:ASP:N	2.75	0.49
1:H:272:LYS:HG2	1:H:273:LEU:CA	2.42	0.49
1:A:107:TYR:O	1:A:110:GLN:HB2	2.12	0.49
1:A:361:LEU:HD11	1:A:386:LEU:HD23	1.94	0.49
1:B:116:GLY:N	1:B:217:THR:O	2.45	0.49
1:B:165:ILE:HG12	1:B:166:ASP:H	1.78	0.49
1:B:303:LEU:O	1:B:307:LEU:HB2	2.13	0.49
1:B:433:ILE:HG21	1:B:590:MET:O	2.11	0.49
1:B:534:VAL:HG13	1:B:535:ASP:N	2.25	0.49
1:C:115:CYS:SG	1:C:432:GLN:HA	2.52	0.49
1:C:117:LEU:O	1:C:122:ILE:HD11	2.12	0.49
1:C:119:GLU:HB3	1:C:121:PRO:CD	2.37	0.49
1:C:434:TRP:HZ3	1:C:568:ARG:CG	2.24	0.49
1:C:517:MET:SD	1:C:650:ARG:HG3	2.52	0.49
1:C:570:LEU:HB3	1:C:590:MET:HE2	1.91	0.49
1:D:262:PRO:HB3	1:D:409:SER:CB	2.41	0.49
1:D:303:LEU:O	1:D:307:LEU:HB2	2.12	0.49
1:D:390:PHE:CZ	1:D:612:LEU:HD11	2.46	0.49
1:D:534:VAL:CG1	1:D:535:ASP:N	2.74	0.49
1:E:109:ASN:O	1:E:111:PHE:N	2.45	0.49
1:E:187:GLN:HB3	1:E:223:LEU:HD22	1.86	0.49
1:E:423:TYR:O	1:E:425:HIS:N	2.45	0.49
1:F:116:GLY:N	1:F:217:THR:O	2.44	0.49
1:F:394:LYS:CG	1:F:613:SER:HB2	2.42	0.49
1:F:402:SER:HA	1:F:609:TYR:CD1	2.47	0.49
1:G:190:ALA:HB2	1:G:206:TRP:CG	2.47	0.49
1:H:120:GLY:C	1:H:122:ILE:N	2.66	0.49
1:H:190:ALA:HB2	1:H:206:TRP:CD1	2.46	0.49
1:H:588:ASN:OD1	1:H:589:ASP:N	2.44	0.49
1:B:115:CYS:SG	1:B:432:GLN:HA	2.51	0.49
1:B:226:TRP:HB3	1:B:229:VAL:CG2	2.42	0.49
1:B:531:GLN:HA	1:B:534:VAL:HG12	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:ASN:OD1	1:B:589:ASP:N	2.44	0.49
1:C:583:THR:HB	1:C:584:PRO:CD	2.42	0.49
1:C:654:LEU:CD2	1:D:654:LEU:HD22	2.36	0.49
1:D:348:GLU:CD	1:D:348:GLU:H	2.14	0.49
1:D:580:ASP:HA	1:D:582:ARG:HH11	1.76	0.49
1:E:33:ILE:HG22	1:E:34:HIS:C	2.33	0.49
1:E:153:LEU:HD22	1:E:162:HIS:HD1	1.78	0.49
1:F:277:LEU:C	1:F:279:CYS:H	2.16	0.49
1:F:531:GLN:O	1:F:535:ASP:HB3	2.12	0.49
1:F:580:ASP:HA	1:F:582:ARG:HH11	1.76	0.49
1:G:107:TYR:O	1:G:110:GLN:HB2	2.12	0.49
1:G:109:ASN:O	1:G:111:PHE:N	2.45	0.49
1:G:125:LEU:CA	1:G:162:HIS:NE2	2.70	0.49
1:G:348:GLU:CD	1:G:348:GLU:H	2.14	0.49
1:G:443:ASP:O	1:G:446:ARG:N	2.45	0.49
1:G:588:ASN:OD1	1:G:589:ASP:N	2.45	0.49
1:H:113:ASN:HA	1:H:116:GLY:O	2.12	0.49
1:A:368:THR:O	1:A:368:THR:HG22	2.11	0.49
1:A:426:LEU:HB3	1:A:430:TRP:CD1	2.47	0.49
1:A:441:LYS:HD2	1:A:561:ASP:OD1	2.13	0.49
1:A:573:ARG:HH22	1:B:572:ARG:HD3	1.77	0.49
1:B:130:SER:O	1:B:300:PHE:CE1	2.66	0.49
1:B:373:ASP:OD1	1:B:374:CYS:N	2.45	0.49
1:C:272:LYS:HG3	1:C:276:TRP:HB2	1.93	0.49
1:D:119:GLU:HB2	1:D:121:PRO:CB	2.43	0.49
1:D:285:GLN:O	1:D:285:GLN:HG2	2.12	0.49
1:D:394:LYS:CG	1:D:613:SER:HB2	2.42	0.49
1:D:588:ASN:CG	1:D:589:ASP:N	2.62	0.49
1:E:118:LYS:HD3	1:E:265:LEU:HA	1.94	0.49
1:E:419:ARG:NH1	1:E:588:ASN:HA	2.27	0.49
1:E:531:GLN:HA	1:E:534:VAL:HG12	1.93	0.49
1:E:547:LEU:O	1:E:550:ASN:ND2	2.45	0.49
1:F:18:LYS:NZ	1:F:33:ILE:HD12	2.26	0.49
1:F:33:ILE:HG22	1:F:34:HIS:C	2.32	0.49
1:F:313:SER:HA	1:F:324:THR:HA	1.93	0.49
1:F:478:GLN:HG3	1:F:479:LEU:N	2.26	0.49
1:H:120:GLY:N	1:H:122:ILE:H	2.08	0.49
1:H:120:GLY:CA	1:H:123:ARG:H	2.25	0.49
1:A:226:TRP:HB3	1:A:229:VAL:CG2	2.42	0.49
1:A:319:SER:C	1:A:321:ARG:N	2.65	0.49
1:A:493:ASP:HB3	1:A:514:TRP:HH2	1.74	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:ASN:C	1:A:656:ASN:OD1	2.50	0.49
1:C:33:ILE:HG22	1:C:34:HIS:C	2.32	0.49
1:C:212:ALA:O	1:C:213:PHE:C	2.51	0.49
1:C:254:LYS:N	1:C:255:PHE:CE1	2.80	0.49
1:C:387:ILE:HD11	1:C:449:GLN:CG	2.42	0.49
1:C:426:LEU:HB3	1:C:430:TRP:CD1	2.47	0.49
1:D:72:ASN:O	1:D:163:LYS:HA	2.12	0.49
1:D:145:ASP:OD2	1:D:167:LEU:HD13	2.12	0.49
1:D:531:GLN:O	1:D:535:ASP:HB3	2.12	0.49
1:F:260:PRO:CD	1:F:274:GLU:HG2	2.43	0.49
1:G:116:GLY:CA	1:G:216:ILE:O	2.60	0.49
1:G:285:GLN:HG2	1:G:285:GLN:O	2.12	0.49
1:G:303:LEU:O	1:G:307:LEU:HB2	2.13	0.49
1:H:118:LYS:NZ	1:H:123:ARG:HH12	2.10	0.49
1:H:263:ASN:HD21	1:H:265:LEU:H	1.60	0.49
1:H:434:TRP:HE3	1:H:568:ARG:CA	2.08	0.49
1:H:531:GLN:HA	1:H:534:VAL:HG12	1.94	0.49
1:A:180:THR:O	1:A:180:THR:HG22	2.13	0.49
1:A:193:LEU:CB	1:A:196:GLN:HE22	2.24	0.49
1:A:270:ALA:HB1	1:A:274:GLU:OE2	2.13	0.49
1:A:303:LEU:O	1:A:307:LEU:HB2	2.12	0.49
1:A:564:GLU:OE2	1:A:568:ARG:NH2	2.45	0.49
1:A:633:MET:SD	1:A:633:MET:N	2.85	0.49
1:C:118:LYS:CB	1:C:264:HIS:O	2.59	0.49
1:C:220:ARG:CB	1:C:221:PRO:HD2	2.42	0.49
1:C:642:ILE:HG12	1:C:645:ARG:CZ	2.42	0.49
1:D:478:GLN:HG3	1:D:479:LEU:N	2.28	0.49
1:E:119:GLU:HB3	1:E:121:PRO:CD	2.42	0.49
1:E:216:ILE:HG21	1:E:273:LEU:CD1	2.43	0.49
1:E:494:LEU:HD12	1:E:514:TRP:CE3	2.37	0.49
1:E:511:LEU:HD21	1:E:515:ARG:NH2	2.27	0.49
1:G:120:GLY:N	1:G:122:ILE:H	2.08	0.49
1:G:235:VAL:CB	1:G:243:ILE:HA	2.39	0.49
1:G:269:LEU:HD22	1:G:272:LYS:HE3	1.94	0.49
1:H:119:GLU:HB2	1:H:121:PRO:CB	2.43	0.49
1:H:412:ILE:HG12	1:H:433:ILE:CD1	2.42	0.49
1:A:246:TYR:HB2	1:A:256:SER:HB3	1.94	0.49
1:A:285:GLN:O	1:A:285:GLN:HG2	2.12	0.49
1:A:583:THR:HB	1:A:584:PRO:CD	2.43	0.49
1:B:72:ASN:O	1:B:164:ILE:HG22	2.13	0.49
1:B:189:LEU:HD12	1:B:207:SER:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:TRP:HA	1:B:342:GLN:CB	2.36	0.49
1:C:119:GLU:HB2	1:C:121:PRO:CB	2.43	0.49
1:C:342:GLN:NE2	1:E:284:HIS:NE2	2.59	0.49
1:C:478:GLN:HG3	1:C:479:LEU:N	2.27	0.49
1:C:655:TRP:CZ2	1:D:497:TYR:HB2	2.48	0.49
1:C:660:ILE:C	1:C:662:CYS:N	2.65	0.49
1:C:665:VAL:HG21	1:D:665:VAL:HG22	1.95	0.49
1:D:263:ASN:HD21	1:D:265:LEU:H	1.58	0.49
1:D:276:TRP:CZ2	1:D:280:MET:HG3	2.47	0.49
1:E:193:LEU:CB	1:E:196:GLN:HE22	2.25	0.49
1:E:550:ASN:OD1	1:E:611:GLN:OE1	2.30	0.49
1:F:118:LYS:HD3	1:F:265:LEU:HA	1.95	0.49
1:F:263:ASN:HD21	1:F:265:LEU:N	2.10	0.49
1:G:198:LYS:C	1:G:200:THR:N	2.66	0.49
1:G:226:TRP:HB3	1:G:229:VAL:CG2	2.42	0.49
1:G:276:TRP:CZ2	1:G:280:MET:HG3	2.47	0.49
1:G:416:ASP:OD1	1:G:416:ASP:N	2.41	0.49
1:G:583:THR:HB	1:G:584:PRO:CD	2.43	0.49
1:H:245:VAL:HG12	1:H:246:TYR:N	2.24	0.49
1:H:269:LEU:HD22	1:H:272:LYS:HE3	1.95	0.49
1:H:285:GLN:HE21	1:H:286:ARG:HH12	1.58	0.49
1:H:423:TYR:O	1:H:425:HIS:N	2.45	0.49
1:A:322:VAL:CG1	1:A:323:HIS:H	2.21	0.49
1:A:571:TYR:CE2	1:A:590:MET:HG3	2.48	0.49
1:A:662:CYS:SG	1:B:661:ALA:HB1	2.53	0.49
1:B:190:ALA:HB2	1:B:206:TRP:CG	2.48	0.49
1:C:153:LEU:HD22	1:C:162:HIS:HD1	1.78	0.49
1:C:643:VAL:O	1:C:644:VAL:CG2	2.59	0.49
1:C:655:TRP:CE3	1:D:654:LEU:HD12	2.47	0.49
1:C:665:VAL:CG2	1:D:665:VAL:HG22	2.43	0.49
1:E:146:LEU:HB3	1:E:207:SER:HB2	1.95	0.49
1:E:186:LEU:HD23	1:E:227:GLN:HG2	1.94	0.49
1:E:269:LEU:HD22	1:E:272:LYS:HE3	1.95	0.49
1:F:486:PHE:CE1	1:F:647:GLN:HB3	2.48	0.49
1:F:566:GLN:HG2	1:F:593:LEU:CD1	2.42	0.49
1:G:213:PHE:C	1:G:213:PHE:CD2	2.86	0.49
1:G:594:LEU:O	1:G:598:ILE:HG13	2.13	0.49
1:H:249:LEU:HD23	1:H:253:VAL:H	1.77	0.49
1:H:390:PHE:CZ	1:H:612:LEU:HD11	2.48	0.49
1:A:492:ILE:HG23	1:B:651:GLN:HE22	1.77	0.49
1:C:118:LYS:HD3	1:C:265:LEU:HA	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:LYS:CD	1:C:265:LEU:HA	2.42	0.49
1:C:216:ILE:HG21	1:C:273:LEU:HD12	1.95	0.49
1:C:423:TYR:O	1:C:425:HIS:N	2.45	0.49
1:D:322:VAL:CG1	1:D:323:HIS:H	2.17	0.49
1:D:418:LYS:O	1:D:419:ARG:CB	2.61	0.49
1:D:497:TYR:O	1:D:497:TYR:HD2	1.85	0.49
1:E:277:LEU:C	1:E:279:CYS:H	2.15	0.49
1:E:660:ILE:O	1:E:662:CYS:N	2.45	0.49
1:F:493:ASP:HB3	1:F:514:TRP:CZ3	2.48	0.49
1:G:438:ARG:HH11	1:G:568:ARG:HH21	1.57	0.49
1:G:531:GLN:HA	1:G:534:VAL:HG12	1.94	0.49
1:H:263:ASN:HD21	1:H:265:LEU:N	2.09	0.49
1:B:18:LYS:NZ	1:B:33:ILE:HD12	2.27	0.49
1:B:222:PHE:HD2	1:B:224:PRO:HD2	1.78	0.49
1:B:341:GLN:O	1:B:345:GLY:N	2.45	0.49
1:B:434:TRP:CE3	1:B:568:ARG:CA	2.68	0.49
1:B:583:THR:HB	1:B:584:PRO:CD	2.43	0.49
1:B:644:VAL:HA	1:B:647:GLN:NE2	2.19	0.49
1:B:653:GLU:HA	1:B:656:ASN:HB3	1.95	0.49
1:C:534:VAL:CG1	1:C:535:ASP:N	2.75	0.49
1:C:646:ARG:HG3	1:C:647:GLN:CD	2.30	0.49
1:E:270:ALA:HB1	1:E:274:GLU:OE2	2.13	0.49
1:E:469:LYS:NZ	1:E:630:LYS:HE2	2.28	0.49
1:E:529:GLU:O	1:E:533:LEU:HG	2.13	0.49
1:E:531:GLN:O	1:E:535:ASP:HB3	2.13	0.49
1:G:422:THR:HB	1:G:585:GLY:CA	2.42	0.49
1:H:588:ASN:CG	1:H:589:ASP:N	2.63	0.49
1:B:145:ASP:CG	1:B:167:LEU:HD13	2.33	0.48
1:B:308:SER:O	1:B:309:LEU:HB2	2.12	0.48
1:B:478:GLN:HG3	1:B:479:LEU:N	2.27	0.48
1:B:529:GLU:O	1:B:533:LEU:HG	2.12	0.48
1:B:534:VAL:CG1	1:B:535:ASP:N	2.75	0.48
1:C:42:ALA:HB3	1:C:96:MET:HB2	1.95	0.48
1:C:145:ASP:CG	1:C:167:LEU:HD13	2.32	0.48
1:C:281:LEU:O	1:C:282:MET:HG2	2.12	0.48
1:D:249:LEU:HD23	1:D:253:VAL:H	1.78	0.48
1:D:527:GLU:HG2	1:D:530:VAL:HG13	1.95	0.48
1:E:234:LYS:O	1:E:235:VAL:O	2.31	0.48
1:E:651:GLN:NE2	1:F:492:ILE:HG21	2.26	0.48
1:E:656:ASN:C	1:E:656:ASN:OD1	2.50	0.48
1:F:119:GLU:HB2	1:F:121:PRO:CB	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:LEU:HA	1:F:253:VAL:O	2.13	0.48
1:G:107:TYR:C	1:G:110:GLN:H	2.15	0.48
1:H:220:ARG:NH1	1:H:223:LEU:CD2	2.70	0.48
1:H:350:GLU:OE2	1:H:391:ASP:O	2.30	0.48
1:H:534:VAL:CG1	1:H:535:ASP:N	2.76	0.48
1:A:16:GLU:HG2	1:A:83:LEU:CD1	2.43	0.48
1:A:441:LYS:HB2	1:A:560:LEU:HD22	1.93	0.48
1:A:654:LEU:HD23	1:A:654:LEU:C	2.33	0.48
1:B:120:GLY:C	1:B:122:ILE:N	2.64	0.48
1:B:319:SER:C	1:B:321:ARG:N	2.66	0.48
1:B:422:THR:HB	1:B:585:GLY:C	2.34	0.48
1:C:120:GLY:N	1:C:122:ILE:H	2.11	0.48
1:C:387:ILE:HD12	1:C:450:GLY:CA	2.44	0.48
1:C:531:GLN:O	1:C:535:ASP:HB3	2.13	0.48
1:D:444:CYS:C	1:D:446:ARG:N	2.66	0.48
1:E:517:MET:SD	1:E:650:ARG:HG3	2.52	0.48
1:F:272:LYS:HG2	1:F:273:LEU:CA	2.41	0.48
1:G:113:ASN:HA	1:G:116:GLY:O	2.12	0.48
1:G:120:GLY:C	1:G:122:ILE:N	2.66	0.48
1:G:145:ASP:CG	1:G:167:LEU:HD13	2.33	0.48
1:G:588:ASN:CG	1:G:589:ASP:N	2.65	0.48
1:H:444:CYS:O	1:H:446:ARG:N	2.46	0.48
1:H:529:GLU:O	1:H:533:LEU:HG	2.12	0.48
1:B:440:LEU:HD12	1:B:597:ALA:O	2.14	0.48
1:B:633:MET:SD	1:B:633:MET:N	2.86	0.48
1:C:220:ARG:NH1	1:C:223:LEU:CD2	2.71	0.48
1:C:226:TRP:CG	1:C:227:GLN:N	2.62	0.48
1:C:319:SER:C	1:C:321:ARG:N	2.66	0.48
1:C:341:GLN:O	1:C:345:GLY:N	2.47	0.48
1:E:145:ASP:CG	1:E:167:LEU:HD13	2.33	0.48
1:E:373:ASP:OD1	1:E:374:CYS:N	2.46	0.48
1:E:492:ILE:HG21	1:F:651:GLN:NE2	2.27	0.48
1:E:545:VAL:HA	1:E:548:GLN:HG2	1.95	0.48
1:E:654:LEU:HD23	1:F:654:LEU:HD21	1.85	0.48
1:F:319:SER:C	1:F:321:ARG:N	2.66	0.48
1:G:216:ILE:HG21	1:G:273:LEU:HD12	1.96	0.48
1:G:359:LEU:CA	1:G:460:ARG:NH1	2.71	0.48
1:G:389:LEU:HD12	1:G:389:LEU:N	2.28	0.48
1:G:444:CYS:C	1:G:446:ARG:N	2.66	0.48
1:H:137:HIS:ND1	1:H:201:VAL:HG13	2.28	0.48
1:A:430:TRP:HB3	1:A:571:TYR:CD2	2.40	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LYS:NZ	1:B:123:ARG:HH12	2.11	0.48
1:B:213:PHE:C	1:B:213:PHE:CD2	2.86	0.48
1:B:270:ALA:HB1	1:B:274:GLU:OE2	2.13	0.48
1:B:517:MET:CE	1:B:650:ARG:HG3	2.43	0.48
1:C:30:LEU:HB2	1:C:43:ILE:HB	1.96	0.48
1:C:386:LEU:HD12	1:C:386:LEU:N	2.29	0.48
1:D:216:ILE:HG21	1:D:273:LEU:HD12	1.94	0.48
1:D:653:GLU:HA	1:D:656:ASN:HB3	1.95	0.48
1:E:119:GLU:HB2	1:E:121:PRO:CB	2.43	0.48
1:E:226:TRP:HB3	1:E:229:VAL:CG2	2.43	0.48
1:E:422:THR:HG22	1:E:426:LEU:HD11	1.96	0.48
1:E:583:THR:HB	1:E:584:PRO:CD	2.43	0.48
1:G:116:GLY:HA3	1:G:216:ILE:O	2.14	0.48
1:G:402:SER:HB3	1:G:609:TYR:HB2	1.94	0.48
1:G:472:MET:HG2	1:G:633:MET:CB	2.40	0.48
1:H:107:TYR:C	1:H:110:GLN:H	2.15	0.48
1:H:286:ARG:O	1:H:290:THR:HG21	2.13	0.48
1:A:418:LYS:HB3	1:A:420:PRO:HD3	1.95	0.48
1:A:658:LEU:HA	1:B:658:LEU:HD12	1.95	0.48
1:B:144:ARG:HD2	1:B:171:LYS:HB3	1.95	0.48
1:B:437:ILE:HG22	1:B:564:GLU:HB2	1.96	0.48
1:B:580:ASP:HA	1:B:582:ARG:HH11	1.77	0.48
1:C:249:LEU:HD23	1:C:253:VAL:H	1.78	0.48
1:C:485:PHE:CD1	1:D:485:PHE:CE1	3.02	0.48
1:C:647:GLN:OE1	1:C:647:GLN:HA	2.14	0.48
1:D:102:GLY:O	1:D:152:VAL:HA	2.14	0.48
1:D:409:SER:HB2	1:D:412:ILE:CD1	2.41	0.48
1:D:423:TYR:O	1:D:425:HIS:N	2.46	0.48
1:D:426:LEU:O	1:D:430:TRP:N	2.42	0.48
1:D:434:TRP:CZ3	1:D:568:ARG:CB	2.91	0.48
1:E:72:ASN:O	1:E:163:LYS:HA	2.14	0.48
1:E:313:SER:HA	1:E:324:THR:HA	1.94	0.48
1:F:285:GLN:HE21	1:F:286:ARG:HH12	1.60	0.48
1:F:418:LYS:HB3	1:F:420:PRO:HD3	1.95	0.48
1:A:105:ARG:HG2	1:A:109:ASN:ND2	2.29	0.48
1:B:33:ILE:HG22	1:B:34:HIS:C	2.34	0.48
1:B:248:ASP:OD1	1:B:248:ASP:O	2.31	0.48
1:B:276:TRP:CZ2	1:B:280:MET:HG3	2.49	0.48
1:B:511:LEU:HD21	1:B:515:ARG:NH2	2.29	0.48
1:B:540:LEU:CD2	1:B:621:LYS:CE	2.91	0.48
1:B:643:VAL:O	1:B:644:VAL:CG2	2.60	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:ASP:OD1	1:C:248:ASP:O	2.30	0.48
1:C:449:GLN:O	1:C:450:GLY:C	2.51	0.48
1:C:522:GLU:C	1:C:523:LEU:HG	2.33	0.48
1:D:220:ARG:HB3	1:D:221:PRO:HD2	1.95	0.48
1:D:361:LEU:HD11	1:D:386:LEU:HD23	1.96	0.48
1:D:394:LYS:HE3	1:D:609:TYR:O	2.14	0.48
1:E:130:SER:O	1:E:300:PHE:CE1	2.65	0.48
1:E:190:ALA:HB2	1:E:206:TRP:CG	2.47	0.48
1:E:655:TRP:CZ3	1:F:654:LEU:HD12	2.47	0.48
1:F:276:TRP:CZ2	1:F:280:MET:HG3	2.49	0.48
1:F:547:LEU:O	1:F:550:ASN:ND2	2.47	0.48
1:F:653:GLU:HA	1:F:656:ASN:HB3	1.94	0.48
1:G:18:LYS:NZ	1:G:33:ILE:HD12	2.27	0.48
1:G:118:LYS:CG	1:G:264:HIS:O	2.62	0.48
1:A:216:ILE:HG21	1:A:273:LEU:HD12	1.96	0.48
1:A:418:LYS:O	1:A:419:ARG:CB	2.61	0.48
1:A:660:ILE:C	1:A:662:CYS:N	2.65	0.48
1:B:276:TRP:CE3	1:B:277:LEU:CD2	2.96	0.48
1:B:373:ASP:CG	1:B:374:CYS:SG	2.92	0.48
1:B:426:LEU:HB3	1:B:430:TRP:CD1	2.49	0.48
1:B:448:LEU:HD23	1:B:608:ILE:HG12	1.95	0.48
1:C:221:PRO:O	1:C:222:PHE:HB3	2.12	0.48
1:C:387:ILE:HD12	1:C:450:GLY:N	2.28	0.48
1:C:485:PHE:CE2	1:D:485:PHE:HB3	2.49	0.48
1:D:319:SER:C	1:D:321:ARG:N	2.66	0.48
1:D:494:LEU:HD21	1:D:518:GLU:OE2	2.14	0.48
1:E:42:ALA:HB3	1:E:96:MET:HB2	1.96	0.48
1:E:198:LYS:HG2	1:E:284:HIS:HA	1.96	0.48
1:E:220:ARG:HB3	1:E:221:PRO:HD2	1.95	0.48
1:E:322:VAL:HG21	1:E:446:ARG:HH12	1.78	0.48
1:E:418:LYS:O	1:E:419:ARG:CB	2.62	0.48
1:F:115:CYS:SG	1:F:432:GLN:HA	2.54	0.48
1:F:191:PRO:HG3	1:F:234:LYS:HZ3	1.77	0.48
1:F:435:GLN:O	1:F:439:ALA:N	2.46	0.48
1:F:637:ARG:O	1:F:641:LYS:HB2	2.12	0.48
1:G:272:LYS:HG2	1:G:273:LEU:CA	2.44	0.48
1:H:107:TYR:O	1:H:110:GLN:HB2	2.13	0.48
1:H:373:ASP:C	1:H:374:CYS:SG	2.92	0.48
1:H:438:ARG:HH11	1:H:568:ARG:HH21	1.59	0.48
1:A:479:LEU:HD12	1:A:640:GLU:CB	2.26	0.48
1:A:655:TRP:CH2	1:B:497:TYR:HB2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:LEU:HD22	1:B:272:LYS:HE3	1.96	0.48
1:B:650:ARG:HD3	1:B:650:ARG:HA	1.64	0.48
1:B:654:LEU:C	1:B:654:LEU:HD23	2.34	0.48
1:C:285:GLN:HE21	1:C:286:ARG:HH12	1.62	0.48
1:C:339:TRP:HA	1:C:342:GLN:CB	2.37	0.48
1:D:272:LYS:HG2	1:D:273:LEU:CA	2.43	0.48
1:D:500:GLN:HB3	1:D:505:ILE:CG1	2.44	0.48
1:D:547:LEU:O	1:D:550:ASN:ND2	2.46	0.48
1:E:569:ASP:HB3	1:E:573:ARG:HD3	1.95	0.48
1:E:614:LYS:O	1:E:617:VAL:HB	2.13	0.48
1:F:285:GLN:O	1:F:285:GLN:HG2	2.13	0.48
1:F:317:MET:HE3	1:F:609:TYR:CE2	2.49	0.48
1:H:616:VAL:HG13	1:H:619:LYS:HD2	1.95	0.48
1:H:632:VAL:CG1	1:H:633:MET:HE1	2.44	0.48
1:A:119:GLU:HB3	1:A:121:PRO:CD	2.44	0.48
1:A:513:ALA:HB1	1:A:650:ARG:NH1	2.26	0.48
1:A:522:GLU:C	1:A:523:LEU:HG	2.33	0.48
1:A:536:LYS:HD3	1:A:625:LEU:HD22	1.95	0.48
1:B:433:ILE:CB	1:B:571:TYR:OH	2.61	0.48
1:B:480:LYS:HE2	1:B:640:GLU:OE1	2.13	0.48
1:D:120:GLY:N	1:D:122:ILE:H	2.07	0.48
1:D:212:ALA:O	1:D:213:PHE:C	2.52	0.48
1:D:437:ILE:HG22	1:D:564:GLU:HB2	1.94	0.48
1:E:105:ARG:HG2	1:E:109:ASN:ND2	2.29	0.48
1:E:210:THR:O	1:E:211:LEU:C	2.52	0.48
1:E:327:VAL:CG1	1:E:367:LEU:HB2	2.36	0.48
1:E:422:THR:HG21	1:E:586:ASP:C	2.34	0.48
1:E:581:GLN:O	1:E:582:ARG:C	2.53	0.48
1:E:643:VAL:O	1:E:644:VAL:CG2	2.61	0.48
1:E:650:ARG:HD3	1:E:650:ARG:HA	1.63	0.48
1:E:654:LEU:HD11	1:F:655:TRP:HE3	1.60	0.48
1:F:118:LYS:NZ	1:F:123:ARG:HH12	2.10	0.48
1:F:473:THR:CG2	1:F:533:LEU:CD2	2.80	0.48
1:F:650:ARG:HD3	1:F:650:ARG:HA	1.66	0.48
1:H:84:GLN:HB3	1:H:85:LYS:H	1.50	0.48
1:H:437:ILE:HG22	1:H:564:GLU:CB	2.43	0.48
1:A:389:LEU:N	1:A:389:LEU:HD12	2.29	0.48
1:B:16:GLU:HG2	1:B:83:LEU:CD1	2.44	0.48
1:B:412:ILE:HG12	1:B:433:ILE:CD1	2.44	0.48
1:B:423:TYR:O	1:B:425:HIS:N	2.47	0.48
1:C:500:GLN:HE22	1:D:659:LYS:HG2	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:594:LEU:O	1:C:598:ILE:HG13	2.14	0.48
1:D:124:THR:OG1	1:D:162:HIS:HE1	1.97	0.48
1:D:210:THR:O	1:D:211:LEU:C	2.52	0.48
1:D:286:ARG:O	1:D:290:THR:HG21	2.13	0.48
1:E:125:LEU:HD21	1:E:215:CYS:SG	2.54	0.48
1:E:248:ASP:OD1	1:E:248:ASP:O	2.31	0.48
1:E:665:VAL:HG21	1:F:665:VAL:CG2	2.40	0.48
1:F:16:GLU:HG2	1:F:83:LEU:CD1	2.44	0.48
1:G:42:ALA:HB3	1:G:96:MET:HB2	1.96	0.48
1:G:386:LEU:HD12	1:G:386:LEU:N	2.27	0.48
1:H:426:LEU:HB3	1:H:430:TRP:CD1	2.49	0.48
1:A:249:LEU:HB3	1:A:250:THR:H	1.39	0.47
1:A:430:TRP:CZ3	1:A:574:LEU:HD13	2.49	0.47
1:B:191:PRO:HG3	1:B:234:LYS:HZ2	1.78	0.47
1:B:249:LEU:HD23	1:B:253:VAL:H	1.77	0.47
1:B:649:LYS:HA	1:B:652:GLN:HB2	1.94	0.47
1:C:105:ARG:HG3	1:C:105:ARG:NH1	2.29	0.47
1:C:581:GLN:O	1:C:582:ARG:C	2.52	0.47
1:C:658:LEU:HA	1:D:658:LEU:CD1	2.44	0.47
1:D:119:GLU:HB3	1:D:121:PRO:CD	2.39	0.47
1:E:118:LYS:HG2	1:E:264:HIS:C	2.28	0.47
1:E:213:PHE:CD2	1:E:213:PHE:C	2.87	0.47
1:F:511:LEU:HG	1:F:515:ARG:CZ	2.43	0.47
1:F:588:ASN:CG	1:F:589:ASP:N	2.66	0.47
1:H:33:ILE:HG22	1:H:34:HIS:C	2.34	0.47
1:H:130:SER:O	1:H:300:PHE:CE1	2.66	0.47
1:H:394:LYS:CD	1:H:401:ILE:HA	2.44	0.47
1:H:434:TRP:CB	1:H:571:TYR:CD1	2.80	0.47
1:H:455:MET:O	1:H:455:MET:HE3	2.14	0.47
1:A:260:PRO:CD	1:A:274:GLU:HG2	2.44	0.47
1:A:272:LYS:HG2	1:A:273:LEU:CA	2.44	0.47
1:A:386:LEU:HD12	1:A:386:LEU:N	2.28	0.47
1:A:423:TYR:O	1:A:425:HIS:N	2.47	0.47
1:A:529:GLU:O	1:A:533:LEU:HG	2.14	0.47
1:B:254:LYS:N	1:B:255:PHE:CE1	2.82	0.47
1:B:272:LYS:HG2	1:B:273:LEU:CA	2.43	0.47
1:B:402:SER:O	1:B:403:LEU:CB	2.61	0.47
1:B:545:VAL:HA	1:B:548:GLN:HG2	1.96	0.47
1:C:297:VAL:HG23	1:C:301:GLN:HE21	1.80	0.47
1:C:389:LEU:N	1:C:389:LEU:HD12	2.29	0.47
1:C:480:LYS:NZ	1:C:525:GLY:C	2.67	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:449:GLN:NE2	1:D:453:THR:HG22	2.29	0.47
1:D:449:GLN:O	1:D:450:GLY:C	2.53	0.47
1:E:530:VAL:CA	1:E:533:LEU:HD12	2.30	0.47
1:F:260:PRO:HB3	1:F:273:LEU:HD22	1.96	0.47
1:F:263:ASN:HD21	1:F:265:LEU:H	1.62	0.47
1:F:423:TYR:O	1:F:425:HIS:N	2.47	0.47
1:F:426:LEU:O	1:F:430:TRP:N	2.41	0.47
1:H:18:LYS:NZ	1:H:33:ILE:HD12	2.26	0.47
1:H:341:GLN:O	1:H:345:GLY:N	2.47	0.47
1:H:571:TYR:OH	1:H:590:MET:SD	2.72	0.47
1:H:580:ASP:HA	1:H:582:ARG:HH11	1.76	0.47
1:H:583:THR:HB	1:H:584:PRO:CD	2.44	0.47
1:A:503:PHE:CE1	1:B:666:ARG:HG3	2.45	0.47
1:A:545:VAL:HA	1:A:548:GLN:HG2	1.96	0.47
1:B:222:PHE:CE2	1:B:224:PRO:O	2.67	0.47
1:B:435:GLN:O	1:B:439:ALA:N	2.46	0.47
1:C:563:LEU:HD23	1:C:597:ALA:HB2	1.96	0.47
1:D:171:LYS:O	1:D:171:LYS:CG	2.59	0.47
1:D:260:PRO:CD	1:D:274:GLU:HG2	2.44	0.47
1:D:451:GLN:NE2	1:D:608:ILE:O	2.47	0.47
1:E:198:LYS:C	1:E:200:THR:N	2.68	0.47
1:E:322:VAL:CG1	1:E:323:HIS:H	2.21	0.47
1:E:469:LYS:NZ	1:E:630:LYS:CE	2.77	0.47
1:F:430:TRP:HZ2	1:F:586:ASP:O	1.97	0.47
1:F:511:LEU:HD21	1:F:515:ARG:NH2	2.29	0.47
1:G:248:ASP:OD1	1:G:248:ASP:O	2.32	0.47
1:G:390:PHE:N	1:G:390:PHE:CD1	2.83	0.47
1:G:545:VAL:HA	1:G:548:GLN:HG2	1.96	0.47
1:H:253:VAL:HB	1:H:255:PHE:CE1	2.50	0.47
1:H:418:LYS:HB3	1:H:420:PRO:HD3	1.95	0.47
1:H:429:VAL:O	1:H:433:ILE:HG12	2.13	0.47
1:H:430:TRP:HB3	1:H:571:TYR:CD2	2.42	0.47
1:A:102:GLY:O	1:A:152:VAL:HA	2.14	0.47
1:A:116:GLY:CA	1:A:217:THR:O	2.62	0.47
1:A:276:TRP:CZ2	1:A:280:MET:HG3	2.49	0.47
1:A:511:LEU:HG	1:A:515:ARG:CZ	2.44	0.47
1:B:105:ARG:HG2	1:B:109:ASN:ND2	2.30	0.47
1:B:119:GLU:HB2	1:B:121:PRO:HB2	1.95	0.47
1:B:125:LEU:CA	1:B:162:HIS:NE2	2.70	0.47
1:B:581:GLN:O	1:B:582:ARG:C	2.52	0.47
1:C:16:GLU:HG2	1:C:83:LEU:CD1	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:GLY:O	1:C:152:VAL:HA	2.14	0.47
1:C:247:ASP:HB3	1:C:248:ASP:H	1.51	0.47
1:C:441:LYS:HB2	1:C:560:LEU:HD22	1.96	0.47
1:C:642:ILE:HG12	1:C:645:ARG:NH1	2.29	0.47
1:D:145:ASP:CG	1:D:167:LEU:HD13	2.34	0.47
1:D:213:PHE:C	1:D:213:PHE:CD2	2.88	0.47
1:D:418:LYS:HB3	1:D:420:PRO:HD3	1.97	0.47
1:D:530:VAL:CA	1:D:533:LEU:HD12	2.30	0.47
1:D:583:THR:HB	1:D:584:PRO:CD	2.44	0.47
1:E:281:LEU:O	1:E:282:MET:HG2	2.14	0.47
1:E:436:THR:O	1:E:440:LEU:HG	2.14	0.47
1:F:30:LEU:HB2	1:F:43:ILE:HB	1.95	0.47
1:F:165:ILE:HG12	1:F:166:ASP:H	1.78	0.47
1:F:229:VAL:CG1	1:G:229:VAL:HG13	2.27	0.47
1:F:389:LEU:CD2	1:F:612:LEU:HD21	2.45	0.47
1:F:438:ARG:HG2	1:F:564:GLU:CD	2.35	0.47
1:G:189:LEU:HA	1:G:189:LEU:HD12	1.66	0.47
1:H:412:ILE:O	1:H:415:GLN:HB2	2.15	0.47
1:H:438:ARG:HG2	1:H:564:GLU:OE1	2.14	0.47
1:A:117:LEU:O	1:A:122:ILE:HD11	2.14	0.47
1:B:30:LEU:HB2	1:B:43:ILE:HB	1.96	0.47
1:B:121:PRO:HA	1:B:124:THR:OG1	2.14	0.47
1:B:133:LEU:O	1:B:134:ARG:C	2.53	0.47
1:B:540:LEU:HD22	1:B:621:LYS:CE	2.44	0.47
1:C:222:PHE:CE2	1:C:224:PRO:O	2.66	0.47
1:C:402:SER:O	1:C:403:LEU:CB	2.62	0.47
1:D:277:LEU:C	1:D:279:CYS:H	2.16	0.47
1:D:386:LEU:HD12	1:D:386:LEU:N	2.27	0.47
1:E:113:ASN:HA	1:E:116:GLY:O	2.13	0.47
1:E:588:ASN:OD1	1:E:589:ASP:N	2.47	0.47
1:G:144:ARG:HD2	1:G:171:LYS:HB3	1.96	0.47
1:G:426:LEU:O	1:G:430:TRP:N	2.43	0.47
1:G:438:ARG:HG2	1:G:564:GLU:HG3	1.96	0.47
1:H:74:VAL:HG21	1:H:165:ILE:HA	1.96	0.47
1:H:222:PHE:CE2	1:H:224:PRO:O	2.67	0.47
1:H:339:TRP:HA	1:H:342:GLN:CB	2.36	0.47
1:H:373:ASP:CG	1:H:374:CYS:SG	2.93	0.47
1:A:189:LEU:HD12	1:A:207:SER:HB3	1.95	0.47
1:B:220:ARG:HB3	1:B:221:PRO:HD2	1.97	0.47
1:B:357:SER:HB3	1:B:453:THR:HB	1.97	0.47
1:C:226:TRP:HB3	1:C:229:VAL:CG2	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ALA:HB1	1:C:274:GLU:OE2	2.14	0.47
1:D:373:ASP:CG	1:D:374:CYS:SG	2.93	0.47
1:E:286:ARG:O	1:E:290:THR:HG21	2.14	0.47
1:E:297:VAL:HG23	1:E:301:GLN:HE21	1.79	0.47
1:E:429:VAL:O	1:E:433:ILE:HG12	2.15	0.47
1:F:144:ARG:HD2	1:F:171:LYS:HB3	1.95	0.47
1:F:145:ASP:CG	1:F:167:LEU:HD13	2.33	0.47
1:G:438:ARG:HG2	1:G:564:GLU:OE1	2.15	0.47
1:H:386:LEU:HD12	1:H:386:LEU:N	2.29	0.47
1:A:189:LEU:HD12	1:A:189:LEU:HA	1.65	0.47
1:B:249:LEU:HB3	1:B:250:THR:H	1.38	0.47
1:B:282:MET:HE2	1:B:282:MET:HA	1.97	0.47
1:B:322:VAL:CG1	1:B:323:HIS:H	2.22	0.47
1:B:418:LYS:HB3	1:B:420:PRO:HD3	1.96	0.47
1:B:444:CYS:O	1:B:446:ARG:N	2.47	0.47
1:C:144:ARG:HD2	1:C:171:LYS:HB3	1.97	0.47
1:C:434:TRP:CZ3	1:C:568:ARG:HG3	2.46	0.47
1:C:494:LEU:CD2	1:C:518:GLU:OE2	2.63	0.47
1:C:659:LYS:CG	1:D:500:GLN:HE22	2.26	0.47
1:D:248:ASP:OD1	1:D:248:ASP:O	2.33	0.47
1:D:350:GLU:CG	1:D:391:ASP:HB2	2.44	0.47
1:D:570:LEU:CB	1:D:590:MET:CE	2.91	0.47
1:D:647:GLN:OE1	1:D:647:GLN:HA	2.15	0.47
1:E:16:GLU:HG2	1:E:83:LEU:CD1	2.44	0.47
1:E:30:LEU:HB2	1:E:43:ILE:HB	1.96	0.47
1:E:285:GLN:HE21	1:E:286:ARG:HH12	1.62	0.47
1:E:341:GLN:O	1:E:345:GLY:N	2.48	0.47
1:E:361:LEU:HD11	1:E:386:LEU:HD23	1.96	0.47
1:E:386:LEU:HD12	1:E:386:LEU:N	2.27	0.47
1:E:419:ARG:HA	1:E:587:SER:CB	2.45	0.47
1:E:570:LEU:CB	1:E:590:MET:HE2	2.45	0.47
1:F:373:ASP:OD1	1:F:374:CYS:N	2.47	0.47
1:F:633:MET:SD	1:F:633:MET:N	2.87	0.47
1:G:72:ASN:O	1:G:164:ILE:HG22	2.15	0.47
1:G:153:LEU:HD23	1:G:162:HIS:HB3	1.97	0.47
1:G:221:PRO:O	1:G:222:PHE:HB3	2.14	0.47
1:G:276:TRP:CE3	1:G:277:LEU:CD2	2.98	0.47
1:G:402:SER:O	1:G:403:LEU:CB	2.63	0.47
1:G:632:VAL:HG12	1:G:633:MET:HE1	1.95	0.47
1:H:64:ILE:HG12	1:H:172:GLU:OE1	2.15	0.47
1:H:72:ASN:H	1:H:163:LYS:HE2	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:121:PRO:HA	1:H:124:THR:OG1	2.15	0.47
1:H:270:ALA:HB1	1:H:274:GLU:OE2	2.14	0.47
1:H:285:GLN:HG2	1:H:285:GLN:O	2.15	0.47
1:H:531:GLN:O	1:H:535:ASP:HB3	2.13	0.47
1:A:30:LEU:HB2	1:A:43:ILE:HB	1.96	0.47
1:A:115:CYS:SG	1:A:432:GLN:HA	2.54	0.47
1:A:249:LEU:HD23	1:A:253:VAL:H	1.80	0.47
1:B:117:LEU:O	1:B:122:ILE:HD11	2.15	0.47
1:B:212:ALA:O	1:B:213:PHE:C	2.53	0.47
1:C:297:VAL:HG23	1:C:301:GLN:NE2	2.30	0.47
1:C:500:GLN:HB3	1:C:505:ILE:CG1	2.44	0.47
1:D:373:ASP:OD1	1:D:374:CYS:N	2.48	0.47
1:D:447:LEU:HD13	1:D:609:TYR:HE1	1.80	0.47
1:D:570:LEU:CD2	1:D:590:MET:HE2	2.45	0.47
1:E:418:LYS:HB3	1:E:420:PRO:HD3	1.96	0.47
1:F:193:LEU:CB	1:F:196:GLN:HE22	2.24	0.47
1:F:594:LEU:O	1:F:598:ILE:HG13	2.14	0.47
1:G:105:ARG:HG2	1:G:109:ASN:ND2	2.29	0.47
1:G:119:GLU:HB2	1:G:121:PRO:CB	2.45	0.47
1:G:359:LEU:N	1:G:460:ARG:NH1	2.62	0.47
1:G:418:LYS:O	1:G:419:ARG:CB	2.62	0.47
1:H:189:LEU:HD12	1:H:189:LEU:HA	1.68	0.47
1:H:402:SER:O	1:H:403:LEU:CB	2.62	0.47
1:H:433:ILE:CB	1:H:571:TYR:OH	2.63	0.47
1:H:536:LYS:HB3	1:H:625:LEU:CD2	2.44	0.47
1:A:42:ALA:HB3	1:A:96:MET:HB2	1.96	0.47
1:A:115:CYS:CB	1:A:435:GLN:HG3	2.45	0.47
1:B:486:PHE:CE1	1:B:647:GLN:HB3	2.50	0.47
1:B:564:GLU:OE2	1:B:568:ARG:NH2	2.47	0.47
1:C:130:SER:O	1:C:300:PHE:CE1	2.68	0.47
1:C:570:LEU:HD23	1:C:590:MET:CE	2.44	0.47
1:D:479:LEU:O	1:D:640:GLU:OE2	2.32	0.47
1:E:212:ALA:O	1:E:213:PHE:C	2.53	0.47
1:E:222:PHE:CE2	1:E:224:PRO:O	2.68	0.47
1:E:387:ILE:HD11	1:E:449:GLN:HB3	1.96	0.47
1:F:286:ARG:O	1:F:290:THR:HG21	2.14	0.47
1:F:588:ASN:OD1	1:F:589:ASP:N	2.47	0.47
1:F:654:LEU:HD23	1:F:654:LEU:C	2.35	0.47
1:G:373:ASP:OD1	1:G:374:CYS:N	2.48	0.47
1:H:276:TRP:CZ2	1:H:280:MET:HG3	2.50	0.47
1:H:368:THR:HG22	1:H:368:THR:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:594:LEU:O	1:H:598:ILE:HG13	2.15	0.47
1:A:110:GLN:O	1:A:111:PHE:CB	2.36	0.47
1:A:216:ILE:HG21	1:A:273:LEU:CD1	2.45	0.47
1:A:319:SER:OG	1:A:403:LEU:HB2	2.14	0.47
1:A:422:THR:HG22	1:A:426:LEU:HD11	1.96	0.47
1:B:102:GLY:O	1:B:152:VAL:HA	2.14	0.47
1:B:120:GLY:CA	1:B:123:ARG:HB2	2.44	0.47
1:C:213:PHE:C	1:C:213:PHE:CD2	2.88	0.47
1:C:644:VAL:HA	1:C:647:GLN:NE2	2.19	0.47
1:C:654:LEU:CD1	1:D:655:TRP:CZ3	2.98	0.47
1:D:545:VAL:HA	1:D:548:GLN:HG2	1.97	0.47
1:F:210:THR:O	1:F:211:LEU:C	2.53	0.47
1:F:213:PHE:HD2	1:F:214:GLU:N	2.13	0.47
1:F:386:LEU:HD12	1:F:386:LEU:N	2.28	0.47
1:F:387:ILE:HD12	1:F:450:GLY:N	2.27	0.47
1:F:583:THR:HB	1:F:584:PRO:CD	2.44	0.47
1:G:30:LEU:HB2	1:G:43:ILE:HB	1.95	0.47
1:G:216:ILE:HG21	1:G:273:LEU:CD1	2.45	0.47
1:G:260:PRO:CD	1:G:274:GLU:HG2	2.45	0.47
1:G:387:ILE:HD12	1:G:450:GLY:CA	2.44	0.47
1:G:419:ARG:HA	1:G:587:SER:CB	2.45	0.47
1:G:423:TYR:O	1:G:425:HIS:N	2.48	0.47
1:G:449:GLN:NE2	1:G:453:THR:CG2	2.78	0.47
1:H:30:LEU:HB2	1:H:43:ILE:HB	1.97	0.47
1:H:276:TRP:CE3	1:H:277:LEU:CD2	2.98	0.47
1:H:418:LYS:O	1:H:419:ARG:CB	2.61	0.47
1:H:530:VAL:CA	1:H:533:LEU:HD12	2.31	0.47
1:A:390:PHE:N	1:A:390:PHE:CD1	2.83	0.46
1:B:118:LYS:HD3	1:B:265:LEU:HD12	1.98	0.46
1:B:119:GLU:HB2	1:B:121:PRO:CB	2.45	0.46
1:C:120:GLY:C	1:C:122:ILE:N	2.69	0.46
1:D:327:VAL:CG1	1:D:367:LEU:HB2	2.34	0.46
1:D:389:LEU:N	1:D:389:LEU:HD12	2.30	0.46
1:D:511:LEU:HG	1:D:515:ARG:CZ	2.45	0.46
1:E:291:ASP:HA	1:E:292:PRO:HD3	1.82	0.46
1:F:189:LEU:CG	1:F:190:ALA:N	2.66	0.46
1:F:296:ASN:ND2	1:F:302:ALA:HB2	2.30	0.46
1:F:402:SER:O	1:F:403:LEU:CB	2.62	0.46
1:F:430:TRP:CZ3	1:F:574:LEU:HD13	2.51	0.46
1:F:475:GLU:HG2	1:F:636:MET:CE	2.45	0.46
1:F:478:GLN:O	1:F:482:LYS:HB3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:111:PHE:CE2	1:H:572:ARG:HG3	2.47	0.46
1:H:153:LEU:HD22	1:H:162:HIS:HD1	1.80	0.46
1:H:222:PHE:HD2	1:H:224:PRO:HD2	1.80	0.46
1:H:389:LEU:HD12	1:H:389:LEU:N	2.30	0.46
1:A:231:TRP:HZ3	1:D:232:HIS:NE2	2.14	0.46
1:A:394:LYS:HG3	1:A:613:SER:HB2	1.96	0.46
1:B:386:LEU:HD12	1:B:386:LEU:N	2.30	0.46
1:C:357:SER:CB	1:C:453:THR:HB	2.41	0.46
1:D:30:LEU:HB2	1:D:43:ILE:HB	1.97	0.46
1:D:118:LYS:HB3	1:D:264:HIS:CD2	2.50	0.46
1:D:144:ARG:HD2	1:D:171:LYS:HB3	1.97	0.46
1:D:390:PHE:N	1:D:390:PHE:CD1	2.84	0.46
1:E:125:LEU:CA	1:E:162:HIS:NE2	2.72	0.46
1:E:522:GLU:C	1:E:523:LEU:HG	2.35	0.46
1:F:130:SER:O	1:F:300:PHE:CE1	2.68	0.46
1:F:564:GLU:HG2	1:F:564:GLU:O	2.15	0.46
1:G:102:GLY:O	1:G:152:VAL:HA	2.16	0.46
1:G:189:LEU:HD12	1:G:207:SER:HB3	1.97	0.46
1:G:296:ASN:ND2	1:G:302:ALA:HB2	2.31	0.46
1:G:581:GLN:O	1:G:582:ARG:C	2.53	0.46
1:H:221:PRO:O	1:H:222:PHE:HB3	2.15	0.46
1:A:226:TRP:CG	1:A:227:GLN:N	2.65	0.46
1:A:447:LEU:HD13	1:A:609:TYR:CE1	2.50	0.46
1:A:517:MET:HE1	1:A:647:GLN:OE1	2.16	0.46
1:A:540:LEU:HD12	1:A:622:ALA:HB2	1.93	0.46
1:A:643:VAL:O	1:A:644:VAL:CG2	2.62	0.46
1:B:115:CYS:O	1:B:263:ASN:HA	2.15	0.46
1:B:390:PHE:N	1:B:390:PHE:CD1	2.83	0.46
1:B:467:LYS:HD3	1:B:467:LYS:HA	1.75	0.46
1:B:646:ARG:HG3	1:B:647:GLN:CD	2.33	0.46
1:C:503:PHE:C	1:C:505:ILE:H	2.17	0.46
1:D:422:THR:HG22	1:D:426:LEU:HD11	1.97	0.46
1:D:478:GLN:O	1:D:482:LYS:HB3	2.15	0.46
1:D:581:GLN:O	1:D:582:ARG:C	2.53	0.46
1:D:643:VAL:O	1:D:644:VAL:CG2	2.62	0.46
1:E:594:LEU:O	1:E:598:ILE:HG13	2.15	0.46
1:F:390:PHE:N	1:F:390:PHE:CD1	2.83	0.46
1:F:416:ASP:OD1	1:F:416:ASP:N	2.39	0.46
1:G:281:LEU:O	1:G:282:MET:HG2	2.15	0.46
1:G:412:ILE:O	1:G:415:GLN:HB2	2.15	0.46
1:H:234:LYS:O	1:H:235:VAL:O	2.33	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:357:SER:HB3	1:H:453:THR:HA	1.97	0.46
1:A:118:LYS:CB	1:A:264:HIS:O	2.64	0.46
1:A:276:TRP:CE3	1:A:277:LEU:CD2	2.98	0.46
1:A:475:GLU:O	1:A:478:GLN:HG2	2.15	0.46
1:C:189:LEU:HD12	1:C:189:LEU:HA	1.67	0.46
1:C:418:LYS:HB3	1:C:420:PRO:HD3	1.97	0.46
1:C:545:VAL:HA	1:C:548:GLN:HG2	1.96	0.46
1:C:610:ASP:O	1:C:613:SER:HB3	2.15	0.46
1:D:146:LEU:HB3	1:D:207:SER:HB2	1.97	0.46
1:D:270:ALA:HB1	1:D:274:GLU:OE2	2.16	0.46
1:D:373:ASP:C	1:D:374:CYS:SG	2.93	0.46
1:D:500:GLN:C	1:D:505:ILE:HG12	2.36	0.46
1:D:533:LEU:HD23	1:D:629:VAL:HG13	1.97	0.46
1:E:222:PHE:HD2	1:E:224:PRO:HD2	1.80	0.46
1:E:350:GLU:CG	1:E:391:ASP:HB2	2.45	0.46
1:E:412:ILE:O	1:E:415:GLN:HB2	2.16	0.46
1:E:666:ARG:HG3	1:F:503:PHE:HE1	1.81	0.46
1:F:102:GLY:O	1:F:152:VAL:HA	2.15	0.46
1:F:191:PRO:HG3	1:F:234:LYS:HZ2	1.79	0.46
1:F:216:ILE:HG21	1:F:273:LEU:CD1	2.46	0.46
1:F:412:ILE:O	1:F:415:GLN:HB2	2.16	0.46
1:G:249:LEU:HD23	1:G:253:VAL:H	1.80	0.46
1:H:42:ALA:HB3	1:H:96:MET:HB2	1.97	0.46
1:H:102:GLY:O	1:H:152:VAL:HA	2.15	0.46
1:H:144:ARG:HD2	1:H:171:LYS:HB3	1.96	0.46
1:H:571:TYR:CE2	1:H:590:MET:SD	3.07	0.46
1:A:118:LYS:CD	1:A:265:LEU:HA	2.45	0.46
1:A:497:TYR:CE2	1:A:511:LEU:HD22	2.50	0.46
1:B:361:LEU:HD11	1:B:386:LEU:HD23	1.97	0.46
1:B:449:GLN:O	1:B:450:GLY:C	2.52	0.46
1:C:281:LEU:C	1:C:282:MET:HG2	2.36	0.46
1:C:422:THR:HG22	1:C:426:LEU:HD11	1.97	0.46
1:C:438:ARG:HG2	1:C:564:GLU:HG3	1.98	0.46
1:C:506:THR:HG22	1:C:507:SER:H	1.81	0.46
1:D:55:ARG:HE	1:D:55:ARG:HB2	1.53	0.46
1:D:475:GLU:CG	1:D:636:MET:HE1	2.45	0.46
1:D:506:THR:HG22	1:D:507:SER:H	1.80	0.46
1:D:569:ASP:HB3	1:D:573:ARG:HD3	1.98	0.46
1:E:144:ARG:HD2	1:E:171:LYS:HB3	1.97	0.46
1:E:216:ILE:HG21	1:E:273:LEU:HD12	1.96	0.46
1:E:547:LEU:CD1	1:E:615:THR:HG21	2.04	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:444:CYS:O	1:F:447:LEU:N	2.47	0.46
1:F:522:GLU:C	1:F:523:LEU:HG	2.35	0.46
1:G:418:LYS:HB3	1:G:420:PRO:HD3	1.96	0.46
1:H:105:ARG:HG2	1:H:109:ASN:ND2	2.30	0.46
1:H:118:LYS:CB	1:H:264:HIS:O	2.63	0.46
1:H:119:GLU:HB3	1:H:121:PRO:CD	2.42	0.46
1:H:614:LYS:HD3	1:H:614:LYS:HA	1.80	0.46
1:A:412:ILE:O	1:A:415:GLN:HB2	2.15	0.46
1:B:74:VAL:HG21	1:B:165:ILE:HA	1.98	0.46
1:B:105:ARG:HG3	1:B:105:ARG:NH1	2.31	0.46
1:B:153:LEU:HD22	1:B:162:HIS:HD1	1.81	0.46
1:B:479:LEU:HB3	1:B:640:GLU:CD	2.29	0.46
1:C:133:LEU:O	1:C:134:ARG:C	2.53	0.46
1:C:137:HIS:ND1	1:C:201:VAL:HG13	2.31	0.46
1:C:226:TRP:HD1	1:C:227:GLN:N	2.03	0.46
1:C:235:VAL:CG1	1:C:243:ILE:N	2.71	0.46
1:C:412:ILE:O	1:C:415:GLN:HB2	2.16	0.46
1:C:588:ASN:OD1	1:C:589:ASP:N	2.48	0.46
1:D:16:GLU:HG2	1:D:83:LEU:CD1	2.43	0.46
1:D:187:GLN:HB3	1:D:223:LEU:HD22	1.79	0.46
1:E:186:LEU:C	1:E:188:TYR:H	2.19	0.46
1:E:222:PHE:HB3	1:E:255:PHE:HB3	1.98	0.46
1:E:644:VAL:HA	1:E:647:GLN:NE2	2.20	0.46
1:F:220:ARG:HB3	1:F:221:PRO:HD2	1.97	0.46
1:F:438:ARG:HG2	1:F:564:GLU:HG3	1.98	0.46
1:F:449:GLN:NE2	1:F:453:THR:CG2	2.79	0.46
1:F:643:VAL:O	1:F:644:VAL:CG2	2.62	0.46
1:G:412:ILE:HG12	1:G:433:ILE:CD1	2.46	0.46
1:G:455:MET:HE3	1:G:455:MET:HB2	1.83	0.46
1:H:208:PHE:O	1:H:211:LEU:HB3	2.15	0.46
1:H:281:LEU:O	1:H:282:MET:HG2	2.16	0.46
1:H:327:VAL:CG1	1:H:367:LEU:HB2	2.32	0.46
1:H:449:GLN:NE2	1:H:453:THR:CG2	2.78	0.46
1:A:581:GLN:O	1:A:582:ARG:C	2.54	0.46
1:C:276:TRP:CE3	1:C:277:LEU:CD2	2.98	0.46
1:C:358:GLY:O	1:C:359:LEU:CB	2.60	0.46
1:C:422:THR:CB	1:C:585:GLY:HA3	2.40	0.46
1:D:408:GLU:HA	1:D:408:GLU:OE2	2.16	0.46
1:D:522:GLU:C	1:D:523:LEU:HG	2.35	0.46
1:E:21:LEU:HD12	1:E:29:VAL:HG12	1.98	0.46
1:E:72:ASN:O	1:E:164:ILE:HG22	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:GLY:O	1:E:152:VAL:HA	2.15	0.46
1:E:265:LEU:CD2	1:E:269:LEU:CB	2.94	0.46
1:E:322:VAL:CG2	1:E:446:ARG:NH1	2.77	0.46
1:E:452:ARG:HD2	1:E:550:ASN:ND2	2.30	0.46
1:E:646:ARG:HG3	1:E:647:GLN:CD	2.31	0.46
1:E:647:GLN:OE1	1:E:647:GLN:HA	2.16	0.46
1:F:581:GLN:O	1:F:582:ARG:C	2.53	0.46
1:G:16:GLU:HG2	1:G:83:LEU:CD1	2.44	0.46
1:G:422:THR:HG22	1:G:426:LEU:HD11	1.97	0.46
1:H:74:VAL:CG2	1:H:165:ILE:HA	2.46	0.46
1:H:250:THR:C	1:H:251:GLY:O	2.54	0.46
1:H:322:VAL:CG1	1:H:323:HIS:H	2.25	0.46
1:H:390:PHE:CD1	1:H:390:PHE:N	2.83	0.46
1:H:581:GLN:O	1:H:582:ARG:C	2.53	0.46
1:A:594:LEU:O	1:A:598:ILE:HG13	2.16	0.46
1:A:658:LEU:HD12	1:B:658:LEU:CD1	2.33	0.46
1:B:269:LEU:C	1:B:271:GLY:N	2.68	0.46
1:B:418:LYS:O	1:B:419:ARG:CB	2.61	0.46
1:C:55:ARG:HE	1:C:55:ARG:HB2	1.54	0.46
1:C:193:LEU:CB	1:C:196:GLN:HE22	2.21	0.46
1:C:216:ILE:HG21	1:C:273:LEU:CD1	2.46	0.46
1:C:480:LYS:HE3	1:C:527:GLU:CB	2.39	0.46
1:C:497:TYR:CA	1:D:655:TRP:HZ2	2.29	0.46
1:D:153:LEU:HD22	1:D:162:HIS:HD1	1.81	0.46
1:D:412:ILE:O	1:D:415:GLN:HB2	2.15	0.46
1:E:478:GLN:HG3	1:E:479:LEU:N	2.30	0.46
1:E:533:LEU:CD2	1:E:629:VAL:CG1	2.88	0.46
1:F:193:LEU:CD2	1:F:231:TRP:CD1	2.97	0.46
1:F:647:GLN:OE1	1:F:647:GLN:HA	2.15	0.46
1:G:105:ARG:CZ	1:G:149:GLU:OE2	2.64	0.46
1:G:564:GLU:O	1:G:564:GLU:HG2	2.16	0.46
1:G:571:TYR:CE2	1:G:590:MET:CG	2.98	0.46
1:H:117:LEU:O	1:H:122:ILE:HD11	2.14	0.46
1:H:216:ILE:HG21	1:H:273:LEU:HD12	1.96	0.46
1:A:144:ARG:HD2	1:A:171:LYS:HB3	1.97	0.46
1:A:644:VAL:HA	1:A:647:GLN:NE2	2.20	0.46
1:B:540:LEU:HD21	1:B:621:LYS:HD2	1.97	0.46
1:B:647:GLN:OE1	1:B:647:GLN:HA	2.15	0.46
1:C:125:LEU:HD21	1:C:215:CYS:SG	2.56	0.46
1:C:467:LYS:HD3	1:C:467:LYS:HA	1.76	0.46
1:C:569:ASP:HB3	1:C:573:ARG:HD3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:SER:O	1:D:403:LEU:CB	2.64	0.46
1:E:105:ARG:CZ	1:E:149:GLU:OE2	2.64	0.46
1:E:246:TYR:HB2	1:E:256:SER:HB3	1.98	0.46
1:E:572:ARG:HD3	1:F:573:ARG:HH22	1.80	0.46
1:E:660:ILE:C	1:E:662:CYS:N	2.68	0.46
1:F:433:ILE:HG23	1:F:594:LEU:HD22	1.97	0.46
1:F:447:LEU:HD12	1:F:605:VAL:HG21	1.98	0.46
1:G:26:PHE:HE2	1:G:181:GLU:CD	2.19	0.46
1:G:81:ASP:HA	1:G:84:GLN:HE21	1.81	0.46
1:G:210:THR:N	1:G:281:LEU:HD11	2.31	0.46
1:G:359:LEU:H	1:G:460:ARG:NH1	2.14	0.46
1:G:475:GLU:OE2	1:G:637:ARG:CG	2.58	0.46
1:H:296:ASN:ND2	1:H:302:ALA:HB2	2.30	0.46
1:H:323:HIS:HB3	1:H:325:TYR:CE1	2.51	0.46
1:A:125:LEU:HD21	1:A:215:CYS:SG	2.56	0.46
1:A:651:GLN:HE22	1:B:492:ILE:CG2	2.25	0.46
1:B:246:TYR:HB2	1:B:256:SER:HB3	1.98	0.46
1:B:522:GLU:C	1:B:523:LEU:HG	2.36	0.46
1:B:651:GLN:O	1:B:652:GLN:C	2.55	0.46
1:C:269:LEU:HD22	1:C:272:LYS:HE3	1.97	0.46
1:C:484:ASP:C	1:C:486:PHE:H	2.20	0.46
1:C:573:ARG:NH1	1:D:573:ARG:NH2	2.10	0.46
1:D:125:LEU:CA	1:D:162:HIS:NE2	2.71	0.46
1:E:412:ILE:O	1:E:416:ASP:OD1	2.34	0.46
1:E:614:LYS:HA	1:E:614:LYS:HD3	1.81	0.46
1:E:662:CYS:SG	1:F:661:ALA:CB	2.97	0.46
1:F:153:LEU:HD23	1:F:162:HIS:HB3	1.98	0.46
1:F:269:LEU:HD22	1:F:272:LYS:HE3	1.97	0.46
1:F:276:TRP:CE3	1:F:277:LEU:CD2	2.99	0.46
1:G:212:ALA:O	1:G:213:PHE:C	2.54	0.46
1:G:323:HIS:HB3	1:G:325:TYR:CE1	2.51	0.46
1:G:373:ASP:CG	1:G:374:CYS:SG	2.94	0.46
1:G:563:LEU:HD23	1:G:597:ALA:HB2	1.97	0.46
1:H:16:GLU:HG2	1:H:83:LEU:CD1	2.44	0.46
1:H:216:ILE:HG21	1:H:273:LEU:CD1	2.45	0.46
1:A:316:ASN:N	1:A:321:ARG:O	2.49	0.45
1:B:540:LEU:HD21	1:B:621:LYS:HZ2	1.80	0.45
1:C:105:ARG:HG2	1:C:109:ASN:ND2	2.31	0.45
1:C:246:TYR:HB2	1:C:256:SER:HB3	1.98	0.45
1:C:316:ASN:N	1:C:321:ARG:O	2.49	0.45
1:E:469:LYS:NZ	1:E:630:LYS:HD3	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:469:LYS:HD2	1:E:630:LYS:HG2	1.98	0.45
1:E:666:ARG:HG3	1:F:503:PHE:CE1	2.51	0.45
1:F:222:PHE:HB3	1:F:255:PHE:HB3	1.98	0.45
1:F:246:TYR:HB2	1:F:256:SER:HB3	1.98	0.45
1:F:419:ARG:NH1	1:F:588:ASN:HA	2.32	0.45
1:H:72:ASN:O	1:H:164:ILE:HG22	2.16	0.45
1:H:133:LEU:O	1:H:134:ARG:C	2.54	0.45
1:H:361:LEU:HD11	1:H:386:LEU:HD23	1.98	0.45
1:A:140:ARG:NH2	1:A:174:ASP:OD2	2.50	0.45
1:A:247:ASP:HB3	1:A:248:ASP:H	1.49	0.45
1:A:449:GLN:O	1:A:450:GLY:C	2.54	0.45
1:B:42:ALA:HB3	1:B:96:MET:HB2	1.97	0.45
1:B:296:ASN:ND2	1:B:302:ALA:HB2	2.31	0.45
1:B:563:LEU:HD23	1:B:597:ALA:HB2	1.98	0.45
1:B:564:GLU:O	1:B:564:GLU:HG2	2.16	0.45
1:C:222:PHE:HD2	1:C:224:PRO:HD2	1.81	0.45
1:C:440:LEU:HD12	1:C:597:ALA:O	2.17	0.45
1:D:260:PRO:HB3	1:D:273:LEU:HD22	1.98	0.45
1:E:50:LEU:H	1:E:55:ARG:CD	2.29	0.45
1:E:118:LYS:HZ1	1:E:123:ARG:HH12	1.63	0.45
1:E:449:GLN:O	1:E:450:GLY:C	2.55	0.45
1:F:105:ARG:HG2	1:F:109:ASN:ND2	2.30	0.45
1:G:193:LEU:CB	1:G:196:GLN:HE22	2.24	0.45
1:H:135:TYR:O	1:H:139:ASN:ND2	2.48	0.45
1:H:198:LYS:HG2	1:H:284:HIS:HA	1.98	0.45
1:H:569:ASP:HB3	1:H:573:ARG:HD3	1.97	0.45
1:A:186:LEU:C	1:A:188:TYR:H	2.19	0.45
1:A:248:ASP:OD1	1:A:248:ASP:O	2.34	0.45
1:A:560:LEU:HD12	1:A:601:PHE:HB2	1.98	0.45
1:B:81:ASP:HA	1:B:84:GLN:HE21	1.82	0.45
1:B:116:GLY:HA2	1:B:217:THR:O	2.17	0.45
1:B:350:GLU:CG	1:B:391:ASP:HB2	2.44	0.45
1:B:448:LEU:HB2	1:B:608:ILE:HD11	1.97	0.45
1:C:191:PRO:HG3	1:C:234:LYS:HZ2	1.80	0.45
1:C:225:ASN:OD1	1:C:229:VAL:HG12	2.15	0.45
1:D:235:VAL:CG1	1:D:243:ILE:N	2.71	0.45
1:D:416:ASP:HB3	1:D:591:VAL:HG13	1.98	0.45
1:E:224:PRO:HG3	1:E:428:ARG:HH22	1.81	0.45
1:E:249:LEU:HB3	1:E:250:THR:H	1.39	0.45
1:E:323:HIS:HB3	1:E:325:TYR:CE1	2.52	0.45
1:E:422:THR:HG22	1:E:426:LEU:CD2	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:497:TYR:CD2	1:E:511:LEU:HD22	2.48	0.45
1:F:120:GLY:CA	1:F:123:ARG:HB2	2.47	0.45
1:F:148:PRO:HD2	1:F:149:GLU:OE2	2.16	0.45
1:F:418:LYS:O	1:F:419:ARG:CB	2.61	0.45
1:G:312:LEU:O	1:G:324:THR:HG23	2.17	0.45
1:H:422:THR:HG22	1:H:426:LEU:HD11	1.98	0.45
1:A:222:PHE:CE2	1:A:224:PRO:O	2.70	0.45
1:A:402:SER:HB2	1:A:403:LEU:H	1.67	0.45
1:A:506:THR:HG22	1:A:507:SER:H	1.80	0.45
1:A:647:GLN:OE1	1:A:647:GLN:HA	2.16	0.45
1:A:665:VAL:HG22	1:B:665:VAL:HG21	1.97	0.45
1:B:322:VAL:CG1	1:B:323:HIS:N	2.76	0.45
1:B:416:ASP:OD1	1:B:416:ASP:N	2.39	0.45
1:B:426:LEU:O	1:B:430:TRP:N	2.45	0.45
1:B:443:ASP:O	1:B:446:ARG:CB	2.65	0.45
1:C:272:LYS:O	1:C:273:LEU:C	2.55	0.45
1:C:284:HIS:HE1	1:E:338:SER:OG	1.99	0.45
1:C:530:VAL:CA	1:C:533:LEU:HD12	2.30	0.45
1:C:571:TYR:CE2	1:C:590:MET:HG3	2.52	0.45
1:D:140:ARG:NH2	1:D:174:ASP:OD2	2.49	0.45
1:D:216:ILE:HG21	1:D:273:LEU:CD1	2.46	0.45
1:D:249:LEU:HB3	1:D:250:THR:H	1.37	0.45
1:E:412:ILE:HG12	1:E:433:ILE:CD1	2.46	0.45
1:E:458:LEU:CD1	1:E:544:SER:HB3	2.47	0.45
1:F:135:TYR:O	1:F:139:ASN:ND2	2.47	0.45
1:F:412:ILE:O	1:F:416:ASP:OD1	2.34	0.45
1:F:433:ILE:HG21	1:F:571:TYR:OH	2.15	0.45
1:F:436:THR:O	1:F:440:LEU:HG	2.15	0.45
1:F:521:VAL:HA	1:F:524:CYS:HG	1.76	0.45
1:H:118:LYS:HD3	1:H:265:LEU:HD12	1.97	0.45
1:H:153:LEU:HD23	1:H:162:HIS:HB3	1.97	0.45
1:A:133:LEU:O	1:A:134:ARG:C	2.54	0.45
1:A:212:ALA:O	1:A:213:PHE:C	2.55	0.45
1:A:296:ASN:ND2	1:A:302:ALA:HB2	2.30	0.45
1:A:402:SER:HA	1:A:609:TYR:CG	2.51	0.45
1:A:412:ILE:HG12	1:A:433:ILE:CD1	2.45	0.45
1:A:646:ARG:HG3	1:A:647:GLN:CD	2.32	0.45
1:D:42:ALA:HB3	1:D:96:MET:HB2	1.97	0.45
1:D:297:VAL:HG23	1:D:301:GLN:HE21	1.82	0.45
1:D:402:SER:HB3	1:D:609:TYR:HB2	1.99	0.45
1:D:479:LEU:C	1:D:640:GLU:OE2	2.55	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:486:PHE:HZ	1:D:517:MET:HE1	1.81	0.45
1:D:660:ILE:C	1:D:662:CYS:N	2.67	0.45
1:E:117:LEU:O	1:E:122:ILE:HD11	2.16	0.45
1:E:462:ASN:ND2	1:E:540:LEU:HB3	2.31	0.45
1:F:470:ASN:HD22	1:F:470:ASN:N	2.15	0.45
1:F:506:THR:HG22	1:F:507:SER:H	1.81	0.45
1:G:133:LEU:O	1:G:134:ARG:C	2.54	0.45
1:G:350:GLU:OE2	1:G:391:ASP:O	2.33	0.45
1:G:569:ASP:HB3	1:G:573:ARG:HD3	1.98	0.45
1:H:81:ASP:HA	1:H:84:GLN:HE21	1.81	0.45
1:H:191:PRO:HG3	1:H:234:LYS:HZ3	1.81	0.45
1:H:235:VAL:CG1	1:H:243:ILE:N	2.73	0.45
1:H:373:ASP:OD1	1:H:374:CYS:N	2.49	0.45
1:A:134:ARG:HD2	1:A:300:PHE:CE1	2.52	0.45
1:A:438:ARG:CG	1:A:564:GLU:HG3	2.46	0.45
1:B:102:GLY:CA	1:B:152:VAL:HG13	2.47	0.45
1:B:134:ARG:HD2	1:B:300:PHE:CE1	2.52	0.45
1:B:484:ASP:C	1:B:486:PHE:H	2.20	0.45
1:C:72:ASN:H	1:C:163:LYS:HE2	1.82	0.45
1:C:220:ARG:HB3	1:C:221:PRO:HD2	1.98	0.45
1:D:84:GLN:HB3	1:D:85:LYS:H	1.50	0.45
1:D:189:LEU:HD12	1:D:189:LEU:HA	1.63	0.45
1:D:213:PHE:O	1:D:214:GLU:C	2.54	0.45
1:D:276:TRP:CE3	1:D:277:LEU:CD2	3.00	0.45
1:D:475:GLU:O	1:D:478:GLN:HG2	2.17	0.45
1:E:103:ASP:O	1:E:105:ARG:N	2.50	0.45
1:E:115:CYS:CB	1:E:435:GLN:HG3	2.46	0.45
1:F:153:LEU:HD22	1:F:162:HIS:HD1	1.81	0.45
1:F:270:ALA:HB1	1:F:274:GLU:OE2	2.16	0.45
1:F:545:VAL:HA	1:F:548:GLN:HG2	1.99	0.45
1:G:234:LYS:O	1:G:235:VAL:O	2.35	0.45
1:G:300:PHE:O	1:G:301:GLN:C	2.55	0.45
1:H:125:LEU:HD21	1:H:215:CYS:SG	2.56	0.45
1:H:297:VAL:HG23	1:H:301:GLN:NE2	2.32	0.45
1:A:105:ARG:CZ	1:A:149:GLU:OE2	2.65	0.45
1:A:130:SER:O	1:A:300:PHE:CE1	2.69	0.45
1:A:254:LYS:N	1:A:255:PHE:CE1	2.85	0.45
1:A:409:SER:CB	1:A:412:ILE:CD1	2.92	0.45
1:B:119:GLU:HB3	1:B:121:PRO:CD	2.41	0.45
1:B:297:VAL:HG23	1:B:301:GLN:HE21	1.82	0.45
1:B:408:GLU:HA	1:B:408:GLU:OE2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:LYS:HB3	1:B:419:ARG:H	1.67	0.45
1:B:500:GLN:HB2	1:B:505:ILE:HG23	1.98	0.45
1:B:501:MET:HA	1:B:505:ILE:CD1	2.39	0.45
1:C:654:LEU:HD22	1:D:654:LEU:HD21	1.74	0.45
1:D:260:PRO:HB2	1:D:273:LEU:CD1	2.45	0.45
1:E:632:VAL:HB	1:E:633:MET:HE2	1.99	0.45
1:F:103:ASP:O	1:F:105:ARG:N	2.50	0.45
1:F:449:GLN:O	1:F:450:GLY:C	2.54	0.45
1:F:642:ILE:C	1:F:644:VAL:H	2.20	0.45
1:G:297:VAL:HG23	1:G:301:GLN:HE21	1.81	0.45
1:H:26:PHE:CE2	1:H:181:GLU:CG	2.99	0.45
1:H:102:GLY:CA	1:H:152:VAL:HG13	2.47	0.45
1:H:426:LEU:O	1:H:430:TRP:N	2.43	0.45
1:A:81:ASP:HA	1:A:84:GLN:HE21	1.82	0.45
1:B:21:LEU:HD12	1:B:29:VAL:HG12	1.99	0.45
1:B:276:TRP:HE3	1:B:277:LEU:HD23	1.81	0.45
1:B:300:PHE:O	1:B:301:GLN:C	2.55	0.45
1:B:422:THR:HG22	1:B:426:LEU:HD11	1.98	0.45
1:B:430:TRP:CE3	1:B:574:LEU:HD22	2.50	0.45
1:B:470:ASN:HD22	1:B:470:ASN:N	2.14	0.45
1:B:528:ARG:HA	1:B:530:VAL:HG22	1.99	0.45
1:C:110:GLN:O	1:C:111:PHE:CB	2.33	0.45
1:C:373:ASP:O	1:C:374:CYS:CB	2.65	0.45
1:D:135:TYR:O	1:D:139:ASN:ND2	2.49	0.45
1:E:191:PRO:HG3	1:E:234:LYS:HZ2	1.82	0.45
1:E:253:VAL:HB	1:E:255:PHE:CE1	2.52	0.45
1:E:276:TRP:CE3	1:E:277:LEU:CD2	3.00	0.45
1:E:276:TRP:CZ2	1:E:280:MET:HG3	2.52	0.45
1:E:297:VAL:HG23	1:E:301:GLN:NE2	2.31	0.45
1:E:517:MET:HE1	1:E:647:GLN:OE1	2.15	0.45
1:G:111:PHE:HE2	1:G:572:ARG:HE	1.64	0.45
1:G:124:THR:O	1:G:127:SER:N	2.48	0.45
1:G:206:TRP:CD1	1:G:207:SER:N	2.85	0.45
1:H:21:LEU:HD12	1:H:29:VAL:HG12	1.99	0.45
1:H:297:VAL:HG23	1:H:301:GLN:HE21	1.81	0.45
1:A:118:LYS:HD3	1:A:265:LEU:HA	1.99	0.45
1:A:222:PHE:HB2	1:A:255:PHE:HD2	1.82	0.45
1:A:291:ASP:HA	1:A:292:PRO:HD3	1.83	0.45
1:A:402:SER:O	1:A:403:LEU:CB	2.64	0.45
1:A:566:GLN:HG2	1:A:593:LEU:HD11	1.99	0.45
1:B:153:LEU:HD23	1:B:162:HIS:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:VAL:O	1:B:433:ILE:HG12	2.17	0.45
1:B:569:ASP:HB3	1:B:573:ARG:HD3	1.99	0.45
1:C:222:PHE:HB3	1:C:255:PHE:HB3	1.99	0.45
1:C:485:PHE:CZ	1:D:485:PHE:CG	3.04	0.45
1:D:120:GLY:CA	1:D:123:ARG:HB2	2.47	0.45
1:D:134:ARG:CA	1:D:300:PHE:CZ	2.97	0.45
1:D:246:TYR:HB2	1:D:256:SER:HB3	1.97	0.45
1:D:488:SER:O	1:D:492:ILE:HG22	2.17	0.45
1:E:661:ALA:CB	1:F:662:CYS:SG	2.99	0.45
1:F:42:ALA:HB3	1:F:96:MET:HB2	1.98	0.45
1:F:50:LEU:H	1:F:55:ARG:CD	2.30	0.45
1:F:222:PHE:CE2	1:F:224:PRO:O	2.70	0.45
1:F:443:ASP:O	1:F:446:ARG:N	2.50	0.45
1:G:84:GLN:HB3	1:G:85:LYS:H	1.51	0.45
1:G:137:HIS:ND1	1:G:201:VAL:HG13	2.32	0.45
1:H:70:HIS:HB2	1:H:135:TYR:CD2	2.52	0.45
1:H:105:ARG:CZ	1:H:149:GLU:OE2	2.65	0.45
1:A:494:LEU:HD12	1:A:514:TRP:CE3	2.48	0.45
1:A:510:LEU:HB2	1:A:657:LEU:HD13	1.99	0.45
1:A:569:ASP:HB3	1:A:573:ARG:HD3	1.98	0.45
1:B:412:ILE:O	1:B:415:GLN:HB2	2.17	0.45
1:B:530:VAL:CA	1:B:533:LEU:HD12	2.32	0.45
1:C:21:LEU:HD12	1:C:29:VAL:HG12	1.99	0.45
1:C:588:ASN:CG	1:C:589:ASP:N	2.66	0.45
1:D:422:THR:HG22	1:D:426:LEU:CD2	2.44	0.45
1:D:430:TRP:HA	1:D:571:TYR:CE2	2.52	0.45
1:D:521:VAL:HA	1:D:524:CYS:HG	1.75	0.45
1:E:118:LYS:CB	1:E:264:HIS:C	2.85	0.45
1:E:124:THR:O	1:E:127:SER:N	2.50	0.45
1:E:319:SER:C	1:E:321:ARG:N	2.67	0.45
1:E:478:GLN:O	1:E:482:LYS:HB3	2.15	0.45
1:E:494:LEU:HD13	1:E:514:TRP:HB3	1.99	0.45
1:E:665:VAL:HG22	1:F:665:VAL:CG1	2.47	0.45
1:F:121:PRO:HA	1:F:124:THR:OG1	2.17	0.45
1:F:317:MET:HE3	1:F:609:TYR:CZ	2.52	0.45
1:F:644:VAL:HA	1:F:647:GLN:NE2	2.20	0.45
1:G:18:LYS:HD2	1:G:33:ILE:HB	1.99	0.45
1:G:246:TYR:HB2	1:G:256:SER:HB3	1.99	0.45
1:H:467:LYS:HD3	1:H:467:LYS:HA	1.74	0.45
1:H:583:THR:O	1:H:584:PRO:C	2.56	0.45
1:A:213:PHE:HD2	1:A:214:GLU:N	2.15	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:MET:CE	1:A:647:GLN:OE1	2.65	0.44
1:B:105:ARG:CZ	1:B:149:GLU:OE2	2.66	0.44
1:B:233:GLY:O	1:B:235:VAL:N	2.50	0.44
1:B:323:HIS:HB3	1:B:325:TYR:CE1	2.52	0.44
1:B:436:THR:O	1:B:440:LEU:HG	2.17	0.44
1:C:18:LYS:HD2	1:C:33:ILE:HB	1.98	0.44
1:C:206:TRP:CD1	1:C:207:SER:N	2.85	0.44
1:C:654:LEU:HD23	1:C:654:LEU:C	2.38	0.44
1:D:100:GLU:H	1:D:154:GLN:HG3	1.82	0.44
1:D:222:PHE:CE2	1:D:225:ASN:CB	2.89	0.44
1:D:435:GLN:O	1:D:439:ALA:N	2.50	0.44
1:E:573:ARG:HH12	1:F:573:ARG:HH12	1.65	0.44
1:E:588:ASN:CG	1:E:589:ASP:N	2.66	0.44
1:F:81:ASP:HA	1:F:84:GLN:HE21	1.82	0.44
1:F:422:THR:HG22	1:F:426:LEU:HD11	1.98	0.44
1:G:249:LEU:HB3	1:G:250:THR:H	1.39	0.44
1:H:409:SER:CB	1:H:412:ILE:CD1	2.93	0.44
1:H:419:ARG:HA	1:H:587:SER:CB	2.47	0.44
1:A:422:THR:CB	1:A:585:GLY:C	2.84	0.44
1:B:234:LYS:O	1:B:235:VAL:O	2.35	0.44
1:C:272:LYS:HG2	1:C:273:LEU:HA	1.99	0.44
1:C:387:ILE:CD1	1:C:450:GLY:N	2.80	0.44
1:D:18:LYS:HD2	1:D:33:ILE:HB	1.99	0.44
1:D:296:ASN:ND2	1:D:302:ALA:HB2	2.32	0.44
1:D:475:GLU:CG	1:D:636:MET:HE3	2.45	0.44
1:E:189:LEU:HD12	1:E:207:SER:HB3	1.99	0.44
1:E:281:LEU:C	1:E:282:MET:HG2	2.38	0.44
1:E:527:GLU:C	1:E:529:GLU:N	2.69	0.44
1:E:536:LYS:CG	1:E:625:LEU:HD13	2.47	0.44
1:E:564:GLU:O	1:E:564:GLU:HG2	2.18	0.44
1:F:193:LEU:HD22	1:F:231:TRP:NE1	2.32	0.44
1:F:291:ASP:HA	1:F:292:PRO:HD3	1.81	0.44
1:F:484:ASP:O	1:F:485:PHE:C	2.55	0.44
1:G:117:LEU:O	1:G:122:ILE:HD11	2.16	0.44
1:G:222:PHE:CE2	1:G:224:PRO:O	2.70	0.44
1:G:272:LYS:O	1:G:273:LEU:C	2.55	0.44
1:H:18:LYS:HD2	1:H:33:ILE:HB	1.99	0.44
1:H:105:ARG:HG3	1:H:105:ARG:NH1	2.33	0.44
1:H:222:PHE:HB3	1:H:255:PHE:HB3	1.99	0.44
1:H:319:SER:C	1:H:321:ARG:N	2.65	0.44
1:A:26:PHE:HE2	1:A:181:GLU:OE1	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:SER:HB3	1:A:537:MET:HE1	1.98	0.44
1:B:434:TRP:CZ3	1:B:568:ARG:CB	2.97	0.44
1:C:153:LEU:HD23	1:C:162:HIS:HB3	2.00	0.44
1:C:234:LYS:O	1:C:235:VAL:O	2.35	0.44
1:C:361:LEU:HD23	1:C:361:LEU:HA	1.87	0.44
1:D:269:LEU:HD22	1:D:272:LYS:HE3	1.99	0.44
1:D:642:ILE:C	1:D:644:VAL:H	2.20	0.44
1:E:316:ASN:N	1:E:321:ARG:O	2.50	0.44
1:E:492:ILE:HD13	1:F:651:GLN:NE2	2.22	0.44
1:E:665:VAL:CG2	1:F:665:VAL:HG21	2.45	0.44
1:F:389:LEU:N	1:F:389:LEU:HD12	2.32	0.44
1:F:530:VAL:CA	1:F:533:LEU:HD12	2.30	0.44
1:G:260:PRO:HB2	1:G:273:LEU:CD1	2.47	0.44
1:H:213:PHE:C	1:H:213:PHE:CD2	2.90	0.44
1:H:272:LYS:O	1:H:273:LEU:C	2.55	0.44
1:A:102:GLY:CA	1:A:152:VAL:HG13	2.47	0.44
1:A:153:LEU:HD23	1:A:162:HIS:HB3	1.98	0.44
1:A:153:LEU:HD22	1:A:162:HIS:HD1	1.83	0.44
1:A:455:MET:O	1:A:455:MET:CE	2.65	0.44
1:B:412:ILE:O	1:B:416:ASP:OD1	2.36	0.44
1:B:506:THR:HG22	1:B:507:SER:H	1.82	0.44
1:C:140:ARG:NH2	1:C:174:ASP:OD2	2.51	0.44
1:C:390:PHE:N	1:C:390:PHE:CD1	2.85	0.44
1:C:484:ASP:O	1:C:485:PHE:C	2.55	0.44
1:C:496:LYS:C	1:D:655:TRP:CZ2	2.91	0.44
1:D:100:GLU:N	1:D:154:GLN:HG3	2.31	0.44
1:D:105:ARG:CZ	1:D:149:GLU:OE2	2.66	0.44
1:D:153:LEU:HD23	1:D:162:HIS:HB3	1.99	0.44
1:D:222:PHE:HD2	1:D:224:PRO:HD2	1.83	0.44
1:D:254:LYS:N	1:D:255:PHE:CE1	2.85	0.44
1:E:654:LEU:HD23	1:E:654:LEU:C	2.38	0.44
1:F:430:TRP:HB3	1:F:571:TYR:CD2	2.47	0.44
1:G:307:LEU:O	1:G:307:LEU:HD23	2.18	0.44
1:H:422:THR:HB	1:H:585:GLY:HA2	1.96	0.44
1:H:436:THR:O	1:H:440:LEU:HG	2.17	0.44
1:H:444:CYS:C	1:H:446:ARG:N	2.69	0.44
1:A:21:LEU:HD12	1:A:29:VAL:HG12	1.99	0.44
1:A:222:PHE:HB3	1:A:255:PHE:HB3	1.99	0.44
1:A:234:LYS:O	1:A:235:VAL:O	2.36	0.44
1:A:269:LEU:C	1:A:271:GLY:N	2.68	0.44
1:B:118:LYS:CG	1:B:118:LYS:O	2.64	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:LEU:O	1:C:430:TRP:N	2.43	0.44
1:D:81:ASP:HA	1:D:84:GLN:HE21	1.83	0.44
1:D:436:THR:O	1:D:440:LEU:HG	2.17	0.44
1:D:654:LEU:HD23	1:D:654:LEU:C	2.38	0.44
1:E:104:LEU:N	1:E:151:ILE:O	2.35	0.44
1:E:482:LYS:C	1:E:484:ASP:N	2.71	0.44
1:F:140:ARG:NH2	1:F:174:ASP:OD2	2.50	0.44
1:F:297:VAL:HG23	1:F:301:GLN:HE21	1.82	0.44
1:F:467:LYS:HA	1:F:467:LYS:HD3	1.75	0.44
1:G:105:ARG:HG3	1:G:105:ARG:NH1	2.33	0.44
1:G:120:GLY:CA	1:G:123:ARG:HB2	2.47	0.44
1:G:319:SER:C	1:G:321:ARG:N	2.66	0.44
1:H:271:GLY:HA2	1:H:275:ARG:NH2	2.32	0.44
1:H:312:LEU:HA	1:H:312:LEU:HD23	1.53	0.44
1:H:316:ASN:O	1:H:317:MET:HG2	2.18	0.44
1:H:545:VAL:HA	1:H:548:GLN:HG2	1.98	0.44
1:A:148:PRO:HD2	1:A:149:GLU:OE2	2.18	0.44
1:A:190:ALA:HB2	1:A:206:TRP:CG	2.53	0.44
1:A:312:LEU:O	1:A:324:THR:HG23	2.18	0.44
1:A:579:ARG:HA	1:A:582:ARG:NH2	2.33	0.44
1:B:102:GLY:HA3	1:B:152:VAL:HG13	1.99	0.44
1:B:185:THR:CG2	1:B:187:GLN:CG	2.81	0.44
1:B:515:ARG:HA	1:B:518:GLU:OE2	2.18	0.44
1:C:72:ASN:O	1:C:164:ILE:HG22	2.18	0.44
1:C:124:THR:O	1:C:127:SER:N	2.50	0.44
1:C:346:ILE:HG23	1:C:346:ILE:O	2.18	0.44
1:C:394:LYS:HE3	1:C:609:TYR:O	2.17	0.44
1:C:438:ARG:HG2	1:C:564:GLU:OE1	2.18	0.44
1:C:459:LEU:HD12	1:C:548:GLN:HB3	2.00	0.44
1:D:253:VAL:HB	1:D:255:PHE:CE1	2.53	0.44
1:D:297:VAL:HG23	1:D:301:GLN:NE2	2.33	0.44
1:D:438:ARG:CG	1:D:564:GLU:CG	2.90	0.44
1:D:579:ARG:HA	1:D:582:ARG:NH2	2.33	0.44
1:F:21:LEU:HD12	1:F:29:VAL:HG12	1.99	0.44
1:F:187:GLN:CB	1:F:223:LEU:CD2	2.76	0.44
1:F:480:LYS:HE3	1:F:527:GLU:HB2	1.99	0.44
1:G:191:PRO:HG3	1:G:234:LYS:HZ2	1.80	0.44
1:G:254:LYS:N	1:G:255:PHE:CE1	2.86	0.44
1:G:260:PRO:HB3	1:G:273:LEU:HD22	1.99	0.44
1:H:412:ILE:HG12	1:H:433:ILE:HD13	1.99	0.44
1:A:118:LYS:CG	1:A:118:LYS:O	2.63	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:TRP:HD1	1:A:227:GLN:N	2.08	0.44
1:A:339:TRP:HA	1:A:342:GLN:CB	2.36	0.44
1:A:350:GLU:CG	1:A:391:ASP:HB2	2.47	0.44
1:B:124:THR:O	1:B:127:SER:N	2.51	0.44
1:B:437:ILE:HG13	1:B:594:LEU:HD12	1.99	0.44
1:B:642:ILE:C	1:B:644:VAL:H	2.21	0.44
1:C:120:GLY:CA	1:C:123:ARG:HB2	2.47	0.44
1:C:493:ASP:HB3	1:C:514:TRP:CH2	2.52	0.44
1:C:547:LEU:HD22	1:C:611:GLN:CG	2.48	0.44
1:C:650:ARG:HA	1:C:650:ARG:HD3	1.70	0.44
1:C:651:GLN:HE21	1:D:492:ILE:CG2	2.23	0.44
1:E:189:LEU:HD12	1:E:189:LEU:HA	1.66	0.44
1:E:312:LEU:O	1:E:324:THR:HG23	2.17	0.44
1:E:449:GLN:NE2	1:E:453:THR:CG2	2.81	0.44
1:F:222:PHE:HD2	1:F:224:PRO:HD2	1.82	0.44
1:F:253:VAL:HB	1:F:255:PHE:CE1	2.53	0.44
1:F:569:ASP:HB3	1:F:573:ARG:HD3	1.98	0.44
1:G:312:LEU:HD23	1:G:312:LEU:HA	1.49	0.44
1:G:387:ILE:HD13	1:G:450:GLY:CA	2.47	0.44
1:H:73:VAL:HB	1:H:164:ILE:HG23	1.99	0.44
1:H:134:ARG:CB	1:H:300:PHE:CE1	2.91	0.44
1:H:387:ILE:CD1	1:H:450:GLY:HA2	2.47	0.44
1:A:103:ASP:O	1:A:105:ARG:N	2.50	0.44
1:A:210:THR:O	1:A:211:LEU:C	2.57	0.44
1:A:286:ARG:CG	1:A:286:ARG:HH11	2.30	0.44
1:A:511:LEU:HD21	1:A:515:ARG:NH2	2.32	0.44
1:B:73:VAL:HB	1:B:164:ILE:HG23	2.00	0.44
1:C:121:PRO:HA	1:C:124:THR:OG1	2.18	0.44
1:C:249:LEU:HB3	1:C:250:THR:H	1.42	0.44
1:C:269:LEU:C	1:C:271:GLY:N	2.68	0.44
1:C:494:LEU:HD12	1:C:514:TRP:CE3	2.38	0.44
1:D:186:LEU:C	1:D:188:TYR:H	2.19	0.44
1:D:222:PHE:HB3	1:D:255:PHE:HB3	1.99	0.44
1:D:412:ILE:HG12	1:D:433:ILE:HD13	1.99	0.44
1:E:81:ASP:HA	1:E:84:GLN:HE21	1.82	0.44
1:E:195:GLU:O	1:E:196:GLN:HB2	2.18	0.44
1:E:300:PHE:O	1:E:301:GLN:C	2.55	0.44
1:E:389:LEU:HD12	1:E:389:LEU:N	2.32	0.44
1:E:475:GLU:HG2	1:E:636:MET:HE1	2.00	0.44
1:E:500:GLN:C	1:E:505:ILE:HG12	2.38	0.44
1:F:18:LYS:HD2	1:F:33:ILE:HB	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:118:LYS:HZ1	1:F:123:ARG:HH12	1.66	0.44
1:F:212:ALA:O	1:F:213:PHE:C	2.56	0.44
1:F:300:PHE:O	1:F:301:GLN:C	2.56	0.44
1:F:486:PHE:HZ	1:F:517:MET:CE	2.30	0.44
1:G:222:PHE:HD2	1:G:224:PRO:HD2	1.83	0.44
1:G:362:ASN:C	1:G:364:ALA:N	2.71	0.44
1:H:143:HIS:NE2	1:H:167:LEU:HB2	2.33	0.44
1:A:16:GLU:HB3	1:A:17:MET:H	1.71	0.44
1:A:18:LYS:HD2	1:A:33:ILE:HB	2.00	0.44
1:A:528:ARG:HA	1:A:530:VAL:HG22	2.00	0.44
1:B:18:LYS:HD2	1:B:33:ILE:HB	2.00	0.44
1:B:297:VAL:HG23	1:B:301:GLN:NE2	2.33	0.44
1:B:479:LEU:HD12	1:B:640:GLU:CB	2.45	0.44
1:B:649:LYS:HA	1:B:652:GLN:HB3	2.00	0.44
1:C:195:GLU:O	1:C:196:GLN:HB2	2.18	0.44
1:C:284:HIS:NE2	1:E:342:GLN:CD	2.71	0.44
1:D:105:ARG:HG2	1:D:109:ASN:ND2	2.32	0.44
1:D:134:ARG:HD2	1:D:300:PHE:CE1	2.53	0.44
1:D:448:LEU:HB2	1:D:608:ILE:HD11	1.99	0.44
1:F:84:GLN:HB3	1:F:85:LYS:H	1.50	0.44
1:F:225:ASN:OD1	1:F:229:VAL:HG12	2.18	0.44
1:F:316:ASN:O	1:F:317:MET:HG2	2.18	0.44
1:G:103:ASP:O	1:G:105:ARG:N	2.51	0.44
1:G:222:PHE:HB3	1:G:255:PHE:HB3	2.00	0.44
1:H:68:LEU:HD11	1:H:141:ILE:HD12	1.98	0.44
1:H:120:GLY:CA	1:H:123:ARG:HB2	2.47	0.44
1:H:261:THR:HB	1:H:262:PRO:HD2	2.00	0.44
1:H:316:ASN:N	1:H:321:ARG:O	2.51	0.44
1:H:434:TRP:CZ3	1:H:568:ARG:CB	2.99	0.44
1:H:560:LEU:CD1	1:H:601:PHE:HB2	2.48	0.44
1:A:607:LEU:HD23	1:A:607:LEU:HA	1.88	0.43
1:B:216:ILE:HG21	1:B:273:LEU:CD1	2.48	0.43
1:B:438:ARG:HH11	1:B:568:ARG:HH21	1.63	0.43
1:C:105:ARG:CZ	1:C:149:GLU:OE2	2.65	0.43
1:C:118:LYS:CG	1:C:118:LYS:O	2.65	0.43
1:C:323:HIS:HB3	1:C:325:TYR:CE1	2.53	0.43
1:C:333:LEU:O	1:C:336:LEU:N	2.51	0.43
1:D:133:LEU:O	1:D:134:ARG:C	2.56	0.43
1:D:323:HIS:HB3	1:D:325:TYR:CE1	2.52	0.43
1:D:339:TRP:HA	1:D:342:GLN:CB	2.38	0.43
1:D:362:ASN:C	1:D:364:ALA:N	2.71	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:297:VAL:HG23	1:F:301:GLN:NE2	2.33	0.43
1:F:434:TRP:HZ3	1:F:568:ARG:CB	2.30	0.43
1:F:438:ARG:HG2	1:F:564:GLU:CG	2.48	0.43
1:H:171:LYS:O	1:H:171:LYS:CG	2.60	0.43
1:H:233:GLY:O	1:H:235:VAL:N	2.52	0.43
1:H:362:ASN:C	1:H:364:ALA:N	2.71	0.43
1:A:105:ARG:HG3	1:A:105:ARG:NH1	2.33	0.43
1:A:451:GLN:CD	1:A:611:GLN:NE2	2.71	0.43
1:A:462:ASN:HD21	1:A:540:LEU:CB	2.29	0.43
1:A:484:ASP:C	1:A:486:PHE:H	2.20	0.43
1:B:84:GLN:HB3	1:B:85:LYS:H	1.50	0.43
1:B:216:ILE:HG21	1:B:273:LEU:HD12	1.99	0.43
1:B:571:TYR:CE2	1:B:590:MET:CG	3.00	0.43
1:C:81:ASP:HA	1:C:84:GLN:HE21	1.83	0.43
1:C:338:SER:OG	1:C:339:TRP:N	2.52	0.43
1:C:350:GLU:CG	1:C:391:ASP:HB2	2.48	0.43
1:C:422:THR:OG1	1:C:585:GLY:C	2.56	0.43
1:D:50:LEU:H	1:D:55:ARG:CD	2.30	0.43
1:D:57:ARG:NE	1:D:177:GLU:O	2.51	0.43
1:D:233:GLY:O	1:D:235:VAL:N	2.49	0.43
1:D:502:GLU:OE1	1:D:502:GLU:N	2.51	0.43
1:E:153:LEU:HD23	1:E:162:HIS:HB3	1.99	0.43
1:E:247:ASP:HB3	1:E:248:ASP:H	1.52	0.43
1:E:358:GLY:O	1:E:359:LEU:CB	2.60	0.43
1:F:269:LEU:C	1:F:271:GLY:N	2.71	0.43
1:F:441:LYS:HD2	1:F:561:ASP:OD1	2.19	0.43
1:G:143:HIS:NE2	1:G:167:LEU:HB2	2.34	0.43
1:G:144:ARG:HD2	1:G:171:LYS:HB2	2.00	0.43
1:G:297:VAL:HG23	1:G:301:GLN:NE2	2.33	0.43
1:G:430:TRP:CD2	1:G:574:LEU:HD22	2.53	0.43
1:G:449:GLN:O	1:G:450:GLY:C	2.56	0.43
1:H:212:ALA:O	1:H:215:CYS:N	2.51	0.43
1:H:281:LEU:C	1:H:282:MET:HG2	2.38	0.43
1:H:470:ASN:HD22	1:H:470:ASN:N	2.16	0.43
1:A:102:GLY:HA3	1:A:152:VAL:HG13	1.99	0.43
1:A:121:PRO:HA	1:A:124:THR:OG1	2.19	0.43
1:A:260:PRO:HB3	1:A:273:LEU:HD22	2.00	0.43
1:A:316:ASN:O	1:A:317:MET:HG2	2.18	0.43
1:B:74:VAL:CG2	1:B:165:ILE:HA	2.48	0.43
1:B:250:THR:C	1:B:251:GLY:O	2.54	0.43
1:B:281:LEU:O	1:B:282:MET:HE3	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:ASN:O	1:C:141:ILE:HG13	2.18	0.43
1:C:276:TRP:CZ2	1:C:280:MET:HG3	2.53	0.43
1:C:422:THR:OG1	1:C:585:GLY:O	2.36	0.43
1:C:438:ARG:HG2	1:C:564:GLU:CD	2.38	0.43
1:D:268:ILE:HD12	1:D:268:ILE:HA	1.86	0.43
1:D:394:LYS:HB2	1:D:613:SER:HB2	2.00	0.43
1:D:412:ILE:O	1:D:416:ASP:OD1	2.36	0.43
1:D:470:ASN:HD22	1:D:470:ASN:N	2.16	0.43
1:D:528:ARG:HA	1:D:530:VAL:HG22	2.00	0.43
1:E:117:LEU:O	1:E:117:LEU:HG	2.18	0.43
1:E:408:GLU:OE2	1:E:408:GLU:HA	2.18	0.43
1:F:171:LYS:O	1:F:171:LYS:CG	2.60	0.43
1:G:470:ASN:HD22	1:G:470:ASN:N	2.16	0.43
1:H:110:GLN:O	1:H:111:PHE:CB	2.34	0.43
1:H:408:GLU:OE2	1:H:408:GLU:HA	2.18	0.43
1:H:579:ARG:HA	1:H:582:ARG:NH2	2.33	0.43
1:A:222:PHE:HD2	1:A:224:PRO:HD2	1.83	0.43
1:A:276:TRP:HE3	1:A:277:LEU:HD23	1.83	0.43
1:A:435:GLN:O	1:A:439:ALA:N	2.50	0.43
1:A:470:ASN:HD22	1:A:470:ASN:N	2.16	0.43
1:B:19:GLU:HB3	1:B:20:ARG:H	1.66	0.43
1:B:272:LYS:O	1:B:273:LEU:C	2.56	0.43
1:B:362:ASN:C	1:B:364:ALA:N	2.71	0.43
1:C:583:THR:O	1:C:584:PRO:C	2.57	0.43
1:C:642:ILE:C	1:C:644:VAL:H	2.21	0.43
1:C:655:TRP:HZ2	1:D:497:TYR:HB2	1.82	0.43
1:D:19:GLU:HB3	1:D:20:ARG:H	1.65	0.43
1:D:21:LEU:HD12	1:D:29:VAL:HG12	2.00	0.43
1:D:116:GLY:N	1:D:217:THR:O	2.50	0.43
1:D:226:TRP:HD1	1:D:227:GLN:N	2.06	0.43
1:D:281:LEU:O	1:D:282:MET:HG2	2.19	0.43
1:D:394:LYS:CB	1:D:613:SER:HB2	2.48	0.43
1:D:430:TRP:C	1:D:571:TYR:CD2	2.92	0.43
1:D:503:PHE:C	1:D:505:ILE:H	2.21	0.43
1:E:18:LYS:NZ	1:E:33:ILE:HD12	2.27	0.43
1:E:55:ARG:HE	1:E:55:ARG:HB2	1.54	0.43
1:E:133:LEU:O	1:E:134:ARG:C	2.56	0.43
1:E:137:HIS:ND1	1:E:201:VAL:HG13	2.33	0.43
1:E:394:LYS:HE3	1:E:609:TYR:O	2.19	0.43
1:E:433:ILE:HB	1:E:571:TYR:OH	2.18	0.43
1:E:505:ILE:HG13	1:E:505:ILE:H	1.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:LEU:O	1:F:282:MET:HG2	2.17	0.43
1:F:317:MET:HA	1:F:609:TYR:OH	2.19	0.43
1:G:412:ILE:O	1:G:416:ASP:OD1	2.36	0.43
1:G:414:LEU:O	1:G:418:LYS:HB2	2.19	0.43
1:G:533:LEU:O	1:G:537:MET:HG2	2.18	0.43
1:G:581:GLN:H	1:G:582:ARG:HD2	1.83	0.43
1:H:50:LEU:H	1:H:55:ARG:CD	2.31	0.43
1:H:146:LEU:HB3	1:H:207:SER:HB2	2.00	0.43
1:H:430:TRP:CB	1:H:571:TYR:HD2	2.29	0.43
1:A:281:LEU:O	1:A:282:MET:HG2	2.18	0.43
1:A:323:HIS:HB3	1:A:325:TYR:CE1	2.53	0.43
1:B:189:LEU:CG	1:B:190:ALA:N	2.65	0.43
1:B:253:VAL:HB	1:B:255:PHE:CE1	2.52	0.43
1:C:478:GLN:O	1:C:482:LYS:HB3	2.19	0.43
1:C:654:LEU:HD22	1:D:654:LEU:HD22	2.00	0.43
1:D:346:ILE:HG23	1:D:346:ILE:O	2.18	0.43
1:D:480:LYS:NZ	1:D:640:GLU:OE1	2.49	0.43
1:D:511:LEU:HD21	1:D:515:ARG:NH2	2.34	0.43
1:D:533:LEU:O	1:D:537:MET:HG2	2.19	0.43
1:D:581:GLN:H	1:D:582:ARG:HD2	1.84	0.43
1:E:144:ARG:HD2	1:E:171:LYS:HB2	2.01	0.43
1:E:319:SER:OG	1:E:403:LEU:HB3	2.17	0.43
1:E:490:ILE:O	1:E:490:ILE:CG2	2.67	0.43
1:E:642:ILE:C	1:E:644:VAL:H	2.22	0.43
1:F:125:LEU:HD12	1:F:129:ILE:HG12	2.00	0.43
1:G:346:ILE:HG23	1:G:346:ILE:O	2.18	0.43
1:H:246:TYR:CE1	1:H:258:VAL:HB	2.45	0.43
1:H:300:PHE:O	1:H:301:GLN:C	2.57	0.43
1:A:300:PHE:O	1:A:301:GLN:C	2.56	0.43
1:A:412:ILE:O	1:A:416:ASP:OD1	2.37	0.43
1:A:502:GLU:OE1	1:A:502:GLU:N	2.51	0.43
1:A:505:ILE:O	1:A:505:ILE:HG22	2.18	0.43
1:B:646:ARG:CG	1:B:647:GLN:NE2	2.54	0.43
1:C:25:GLY:O	1:C:181:GLU:HG3	2.19	0.43
1:C:478:GLN:OE1	1:D:481:ALA:HB3	2.19	0.43
1:C:486:PHE:HZ	1:C:517:MET:CE	2.31	0.43
1:C:581:GLN:H	1:C:582:ARG:HD2	1.83	0.43
1:D:494:LEU:HD13	1:D:514:TRP:HB3	2.01	0.43
1:E:208:PHE:O	1:E:211:LEU:HB3	2.19	0.43
1:E:269:LEU:C	1:E:271:GLY:N	2.70	0.43
1:E:312:LEU:HA	1:E:312:LEU:HD23	1.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:506:THR:HG22	1:E:507:SER:H	1.82	0.43
1:E:579:ARG:HA	1:E:582:ARG:NH2	2.34	0.43
1:F:412:ILE:HG12	1:F:433:ILE:HD13	2.01	0.43
1:F:607:LEU:HD23	1:F:607:LEU:HA	1.85	0.43
1:H:249:LEU:HB3	1:H:250:THR:H	1.35	0.43
1:H:437:ILE:HG13	1:H:594:LEU:HD12	2.01	0.43
1:B:307:LEU:O	1:B:307:LEU:HD23	2.19	0.43
1:B:312:LEU:HA	1:B:312:LEU:HD23	1.50	0.43
1:C:148:PRO:HG3	1:C:188:TYR:OH	2.18	0.43
1:C:254:LYS:O	1:C:255:PHE:CG	2.72	0.43
1:C:408:GLU:HA	1:C:408:GLU:OE2	2.17	0.43
1:C:480:LYS:HZ2	1:C:525:GLY:C	2.21	0.43
1:C:505:ILE:HG13	1:C:505:ILE:H	1.56	0.43
1:C:607:LEU:HD23	1:C:607:LEU:HA	1.85	0.43
1:C:659:LYS:CD	1:D:500:GLN:HE22	2.32	0.43
1:D:261:THR:HB	1:D:262:PRO:HD2	2.01	0.43
1:D:300:PHE:O	1:D:301:GLN:C	2.57	0.43
1:E:233:GLY:O	1:E:235:VAL:N	2.49	0.43
1:E:319:SER:HB3	1:E:402:SER:O	2.19	0.43
1:E:571:TYR:CE2	1:E:590:MET:CG	3.00	0.43
1:F:422:THR:HG22	1:F:426:LEU:CD2	2.47	0.43
1:F:614:LYS:HA	1:F:614:LYS:HD3	1.75	0.43
1:H:455:MET:HE3	1:H:455:MET:HB2	1.82	0.43
1:A:233:GLY:O	1:A:235:VAL:N	2.51	0.43
1:A:467:LYS:HD3	1:A:467:LYS:HA	1.75	0.43
1:B:118:LYS:CB	1:B:264:HIS:O	2.66	0.43
1:C:18:LYS:HZ2	1:C:33:ILE:HD12	1.83	0.43
1:C:110:GLN:HB3	1:C:113:ASN:ND2	2.34	0.43
1:C:296:ASN:ND2	1:C:302:ALA:HB2	2.34	0.43
1:C:579:ARG:HA	1:C:582:ARG:NH2	2.34	0.43
1:C:651:GLN:O	1:C:652:GLN:C	2.57	0.43
1:C:655:TRP:CD1	1:D:496:LYS:CB	2.95	0.43
1:D:115:CYS:CB	1:D:435:GLN:HG3	2.48	0.43
1:D:208:PHE:O	1:D:211:LEU:HB3	2.19	0.43
1:D:226:TRP:CG	1:D:227:GLN:N	2.61	0.43
1:D:276:TRP:CE2	1:D:280:MET:HG3	2.54	0.43
1:E:185:THR:CG2	1:E:187:GLN:CG	2.80	0.43
1:E:206:TRP:CD1	1:E:207:SER:N	2.87	0.43
1:E:433:ILE:HG21	1:E:571:TYR:OH	2.19	0.43
1:E:571:TYR:CE2	1:E:590:MET:SD	3.11	0.43
1:F:206:TRP:CD1	1:F:207:SER:N	2.87	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:225:ASN:OD1	1:G:229:VAL:HG12	2.17	0.43
1:G:268:ILE:HD12	1:G:268:ILE:HA	1.92	0.43
1:H:102:GLY:HA3	1:H:152:VAL:HG13	2.00	0.43
1:H:449:GLN:O	1:H:450:GLY:C	2.57	0.43
1:A:50:LEU:H	1:A:55:ARG:CD	2.30	0.43
1:A:272:LYS:CG	1:A:273:LEU:N	2.68	0.43
1:A:455:MET:HE3	1:A:455:MET:HB2	1.87	0.43
1:B:190:ALA:HB2	1:B:206:TRP:CD1	2.54	0.43
1:B:222:PHE:HB3	1:B:255:PHE:HB3	2.00	0.43
1:B:588:ASN:CG	1:B:589:ASP:N	2.65	0.43
1:B:594:LEU:O	1:B:598:ILE:HG13	2.19	0.43
1:C:102:GLY:CA	1:C:152:VAL:HG13	2.49	0.43
1:C:485:PHE:CG	1:D:485:PHE:CD2	3.06	0.43
1:D:102:GLY:CA	1:D:152:VAL:HG13	2.49	0.43
1:D:219:PHE:CE1	1:D:428:ARG:NE	2.87	0.43
1:D:567:ALA:O	1:D:571:TYR:HD1	2.02	0.43
1:D:636:MET:HE2	1:D:637:ARG:N	2.33	0.43
1:E:254:LYS:O	1:E:255:PHE:CG	2.70	0.43
1:E:339:TRP:HA	1:E:342:GLN:CB	2.36	0.43
1:E:387:ILE:HD12	1:E:450:GLY:HA2	2.01	0.43
1:E:390:PHE:N	1:E:390:PHE:CD1	2.87	0.43
1:E:435:GLN:O	1:E:439:ALA:N	2.51	0.43
1:E:484:ASP:C	1:E:486:PHE:H	2.22	0.43
1:E:524:CYS:SG	1:E:643:VAL:HG11	2.59	0.43
1:F:272:LYS:CG	1:F:273:LEU:N	2.63	0.43
1:F:361:LEU:HA	1:F:361:LEU:HD23	1.85	0.43
1:F:528:ARG:HA	1:F:530:VAL:HG22	2.01	0.43
1:F:579:ARG:HA	1:F:582:ARG:NH2	2.33	0.43
1:G:195:GLU:O	1:G:196:GLN:HB2	2.19	0.43
1:G:361:LEU:HD23	1:G:361:LEU:HA	1.85	0.43
1:H:307:LEU:HD23	1:H:307:LEU:O	2.18	0.43
1:H:416:ASP:OD1	1:H:416:ASP:N	2.39	0.43
1:A:120:GLY:CA	1:A:123:ARG:HB2	2.47	0.43
1:A:387:ILE:HD12	1:A:450:GLY:N	2.34	0.43
1:B:346:ILE:HG23	1:B:346:ILE:O	2.18	0.43
1:B:449:GLN:NE2	1:B:453:THR:CG2	2.82	0.43
1:C:68:LEU:HB3	1:C:135:TYR:HE2	1.83	0.43
1:C:171:LYS:O	1:C:171:LYS:CG	2.62	0.43
1:C:665:VAL:CG2	1:D:665:VAL:CG2	2.96	0.43
1:D:68:LEU:HB3	1:D:135:TYR:CE2	2.52	0.43
1:D:105:ARG:HG3	1:D:105:ARG:NH1	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:ALA:O	1:D:215:CYS:N	2.52	0.43
1:D:272:LYS:O	1:D:273:LEU:C	2.57	0.43
1:D:501:MET:C	1:D:505:ILE:HD11	2.38	0.43
1:E:296:ASN:CG	1:E:297:VAL:N	2.72	0.43
1:E:296:ASN:ND2	1:E:302:ALA:HB2	2.33	0.43
1:E:563:LEU:CD2	1:E:596:LEU:HB2	2.36	0.43
1:F:312:LEU:HA	1:F:312:LEU:HD23	1.50	0.43
1:F:408:GLU:HA	1:F:408:GLU:OE2	2.19	0.43
1:G:140:ARG:NH2	1:G:174:ASP:OD2	2.51	0.43
1:G:153:LEU:HD22	1:G:162:HIS:HD1	1.81	0.43
1:G:430:TRP:O	1:G:431:GLY:C	2.57	0.43
1:G:433:ILE:HG21	1:G:571:TYR:OH	2.19	0.43
1:G:533:LEU:HD22	1:G:629:VAL:HG13	2.00	0.43
1:H:125:LEU:CA	1:H:162:HIS:NE2	2.70	0.43
1:H:272:LYS:HG2	1:H:273:LEU:HA	2.01	0.43
1:A:68:LEU:HB3	1:A:135:TYR:CE2	2.53	0.42
1:A:297:VAL:HG23	1:A:301:GLN:HE21	1.83	0.42
1:A:373:ASP:O	1:A:374:CYS:CB	2.67	0.42
1:A:387:ILE:CD1	1:A:449:GLN:HG3	2.44	0.42
1:A:441:LYS:HB2	1:A:560:LEU:HD21	1.97	0.42
1:B:103:ASP:O	1:B:105:ARG:N	2.52	0.42
1:B:336:LEU:O	1:B:340:LEU:N	2.52	0.42
1:B:430:TRP:HZ2	1:B:586:ASP:O	2.00	0.42
1:B:579:ARG:HA	1:B:582:ARG:NH2	2.34	0.42
1:C:209:GLY:O	1:C:212:ALA:HB3	2.19	0.42
1:C:246:TYR:CE1	1:C:258:VAL:HB	2.44	0.42
1:C:529:GLU:HG3	1:C:633:MET:HE3	1.99	0.42
1:D:144:ARG:HD2	1:D:171:LYS:HB2	2.00	0.42
1:D:521:VAL:CG1	1:D:643:VAL:HG12	2.49	0.42
1:D:632:VAL:O	1:D:633:MET:SD	2.77	0.42
1:E:18:LYS:HD2	1:E:33:ILE:HB	1.99	0.42
1:E:121:PRO:HA	1:E:124:THR:OG1	2.19	0.42
1:E:260:PRO:HB3	1:E:273:LEU:HD22	2.00	0.42
1:E:469:LYS:HZ2	1:E:630:LYS:CE	2.32	0.42
1:F:233:GLY:O	1:F:235:VAL:N	2.52	0.42
1:G:281:LEU:C	1:G:282:MET:HG2	2.40	0.42
1:H:119:GLU:CB	1:H:121:PRO:HB2	2.49	0.42
1:A:139:ASN:O	1:A:141:ILE:HG13	2.19	0.42
1:A:225:ASN:OD1	1:A:229:VAL:HG12	2.19	0.42
1:A:276:TRP:CE2	1:A:280:MET:HG3	2.54	0.42
1:A:449:GLN:NE2	1:A:453:THR:CG2	2.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:GLU:O	1:A:564:GLU:HG2	2.19	0.42
1:B:50:LEU:H	1:B:55:ARG:CD	2.29	0.42
1:B:222:PHE:HE2	1:B:225:ASN:HB2	1.71	0.42
1:B:281:LEU:O	1:B:282:MET:HG2	2.19	0.42
1:B:540:LEU:HD22	1:B:621:LYS:HE3	2.00	0.42
1:C:146:LEU:HB3	1:C:207:SER:HB2	2.00	0.42
1:C:316:ASN:O	1:C:317:MET:HG2	2.19	0.42
1:C:362:ASN:C	1:C:364:ALA:N	2.71	0.42
1:C:416:ASP:HB3	1:C:591:VAL:HG13	2.01	0.42
1:C:430:TRP:CB	1:C:571:TYR:CD2	3.02	0.42
1:C:436:THR:O	1:C:440:LEU:HG	2.19	0.42
1:C:452:ARG:HE	1:C:550:ASN:HD22	1.67	0.42
1:D:103:ASP:O	1:D:105:ARG:N	2.52	0.42
1:D:319:SER:OG	1:D:403:LEU:HB3	2.17	0.42
1:E:16:GLU:HB3	1:E:17:MET:H	1.68	0.42
1:E:124:THR:OG1	1:E:162:HIS:HE1	2.03	0.42
1:E:362:ASN:C	1:E:364:ALA:N	2.72	0.42
1:F:55:ARG:HE	1:F:55:ARG:HB2	1.52	0.42
1:F:105:ARG:CZ	1:F:149:GLU:OE2	2.67	0.42
1:F:451:GLN:CD	1:F:611:GLN:NE2	2.72	0.42
1:G:408:GLU:OE2	1:G:408:GLU:HA	2.19	0.42
1:H:26:PHE:CE2	1:H:181:GLU:OE2	2.70	0.42
1:H:206:TRP:CD1	1:H:207:SER:N	2.88	0.42
1:A:119:GLU:CB	1:A:121:PRO:HB2	2.50	0.42
1:B:148:PRO:HD2	1:B:149:GLU:OE2	2.19	0.42
1:B:210:THR:O	1:B:211:LEU:C	2.58	0.42
1:B:316:ASN:O	1:B:317:MET:HG2	2.18	0.42
1:B:438:ARG:HH12	1:B:568:ARG:HH21	1.66	0.42
1:B:545:VAL:HG13	1:B:548:GLN:NE2	2.35	0.42
1:C:213:PHE:CE2	1:C:217:THR:OG1	2.69	0.42
1:C:233:GLY:O	1:C:235:VAL:N	2.52	0.42
1:C:410:VAL:O	1:C:411:SER:C	2.57	0.42
1:D:118:LYS:CG	1:D:118:LYS:O	2.65	0.42
1:D:125:LEU:HD12	1:D:129:ILE:HG12	2.01	0.42
1:D:583:THR:O	1:D:584:PRO:C	2.57	0.42
1:E:455:MET:CE	1:E:455:MET:O	2.68	0.42
1:E:494:LEU:CD1	1:E:514:TRP:HB3	2.50	0.42
1:F:346:ILE:HG23	1:F:346:ILE:O	2.19	0.42
1:G:19:GLU:HB3	1:G:20:ARG:H	1.66	0.42
1:G:70:HIS:HB3	1:G:73:VAL:CG1	2.49	0.42
1:G:110:GLN:HB3	1:G:113:ASN:ND2	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:LYS:NZ	1:G:123:ARG:HH12	2.17	0.42
1:G:198:LYS:O	1:G:200:THR:N	2.42	0.42
1:H:190:ALA:O	1:H:191:PRO:C	2.58	0.42
1:H:338:SER:OG	1:H:339:TRP:N	2.52	0.42
1:H:350:GLU:CG	1:H:391:ASP:HB2	2.47	0.42
1:A:124:THR:OG1	1:A:162:HIS:HE1	2.02	0.42
1:A:219:PHE:HB2	1:A:220:ARG:H	1.55	0.42
1:A:312:LEU:HA	1:A:312:LEU:HD23	1.50	0.42
1:A:358:GLY:O	1:A:359:LEU:CB	2.59	0.42
1:B:406:HIS:HA	1:B:407:PRO:HD2	1.83	0.42
1:B:410:VAL:O	1:B:411:SER:C	2.58	0.42
1:B:438:ARG:CG	1:B:564:GLU:CG	2.95	0.42
1:C:50:LEU:H	1:C:55:ARG:CD	2.30	0.42
1:C:222:PHE:HE2	1:C:225:ASN:HB2	1.76	0.42
1:C:315:MET:SD	1:C:321:ARG:HA	2.59	0.42
1:C:412:ILE:HG12	1:C:433:ILE:HD13	2.01	0.42
1:C:449:GLN:NE2	1:C:453:THR:CG2	2.82	0.42
1:C:470:ASN:N	1:C:470:ASN:HD22	2.18	0.42
1:D:17:MET:CB	1:D:32:TRP:HB3	2.36	0.42
1:D:186:LEU:CD2	1:D:227:GLN:HG2	2.47	0.42
1:D:195:GLU:O	1:D:196:GLN:HB2	2.19	0.42
1:E:309:LEU:C	1:E:310:LYS:HG3	2.39	0.42
1:E:402:SER:O	1:E:403:LEU:CB	2.66	0.42
1:E:481:ALA:O	1:E:484:ASP:HB2	2.20	0.42
1:E:496:LYS:CB	1:F:655:TRP:NE1	2.39	0.42
1:F:25:GLY:O	1:F:181:GLU:HG3	2.19	0.42
1:F:110:GLN:HB3	1:F:113:ASN:ND2	2.34	0.42
1:F:118:LYS:CB	1:F:264:HIS:O	2.67	0.42
1:F:189:LEU:HD12	1:F:189:LEU:HA	1.69	0.42
1:F:247:ASP:HB3	1:F:248:ASP:H	1.51	0.42
1:F:323:HIS:HB3	1:F:325:TYR:CE1	2.55	0.42
1:F:433:ILE:HB	1:F:571:TYR:OH	2.19	0.42
1:F:437:ILE:HG22	1:F:564:GLU:HB2	2.00	0.42
1:F:484:ASP:C	1:F:486:PHE:H	2.20	0.42
1:G:125:LEU:HD12	1:G:129:ILE:HG12	2.01	0.42
1:G:186:LEU:C	1:G:188:TYR:H	2.22	0.42
1:G:271:GLY:HA2	1:G:275:ARG:NH2	2.34	0.42
1:G:350:GLU:CG	1:G:391:ASP:HB2	2.48	0.42
1:G:583:THR:O	1:G:584:PRO:C	2.58	0.42
1:H:246:TYR:HB2	1:H:256:SER:HB3	2.00	0.42
1:H:528:ARG:HA	1:H:530:VAL:HG22	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:GLU:OE2	1:A:408:GLU:HA	2.18	0.42
1:A:436:THR:O	1:A:440:LEU:HG	2.20	0.42
1:A:583:THR:O	1:A:584:PRO:C	2.58	0.42
1:B:244:VAL:HG22	1:B:282:MET:SD	2.60	0.42
1:B:447:LEU:HD12	1:B:605:VAL:CG2	2.49	0.42
1:B:479:LEU:HD11	1:B:641:LYS:HG3	2.00	0.42
1:C:60:LEU:HD21	1:C:175:GLN:HB3	2.01	0.42
1:C:300:PHE:O	1:C:301:GLN:C	2.55	0.42
1:C:412:ILE:O	1:C:416:ASP:OD1	2.38	0.42
1:C:452:ARG:HD2	1:C:550:ASN:ND2	2.35	0.42
1:C:455:MET:HB2	1:C:455:MET:HE3	1.80	0.42
1:C:528:ARG:HA	1:C:530:VAL:HG22	2.00	0.42
1:C:564:GLU:HG2	1:C:564:GLU:O	2.19	0.42
1:D:484:ASP:O	1:D:485:PHE:C	2.58	0.42
1:E:307:LEU:HD23	1:E:307:LEU:O	2.20	0.42
1:F:387:ILE:HD13	1:F:450:GLY:CA	2.46	0.42
1:F:402:SER:HB2	1:F:403:LEU:H	1.65	0.42
1:F:525:GLY:HA2	1:F:640:GLU:CG	2.49	0.42
1:F:583:THR:O	1:F:584:PRO:C	2.58	0.42
1:F:629:VAL:O	1:F:629:VAL:HG12	2.19	0.42
1:G:50:LEU:H	1:G:55:ARG:CD	2.32	0.42
1:G:115:CYS:HB2	1:G:435:GLN:HG3	2.00	0.42
1:G:269:LEU:C	1:G:271:GLY:N	2.71	0.42
1:A:361:LEU:HD23	1:A:361:LEU:HA	1.86	0.42
1:A:661:ALA:HB1	1:B:662:CYS:SG	2.60	0.42
1:B:33:ILE:HD11	1:B:40:GLN:OE1	2.20	0.42
1:B:402:SER:HB2	1:B:403:LEU:H	1.65	0.42
1:B:533:LEU:O	1:B:537:MET:HG2	2.20	0.42
1:B:581:GLN:H	1:B:582:ARG:HD2	1.84	0.42
1:B:614:LYS:HD3	1:B:614:LYS:HA	1.80	0.42
1:C:486:PHE:O	1:C:486:PHE:CG	2.72	0.42
1:C:502:GLU:N	1:C:502:GLU:OE1	2.53	0.42
1:D:104:LEU:N	1:D:151:ILE:O	2.33	0.42
1:D:118:LYS:HG2	1:D:265:LEU:HA	2.02	0.42
1:D:153:LEU:CA	1:D:162:HIS:HB3	2.39	0.42
1:D:312:LEU:O	1:D:324:THR:HG23	2.20	0.42
1:D:571:TYR:CZ	1:D:590:MET:SD	3.12	0.42
1:D:632:VAL:CG1	1:D:633:MET:HE1	2.48	0.42
1:E:333:LEU:O	1:E:336:LEU:N	2.53	0.42
1:F:144:ARG:HD2	1:F:171:LYS:HB2	2.00	0.42
1:F:186:LEU:C	1:F:188:TYR:H	2.22	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:475:GLU:HG2	1:F:636:MET:HE1	2.02	0.42
1:F:488:SER:O	1:F:492:ILE:HG22	2.20	0.42
1:G:210:THR:O	1:G:211:LEU:C	2.58	0.42
1:G:316:ASN:O	1:G:317:MET:HG2	2.19	0.42
1:G:455:MET:HE2	1:G:455:MET:O	2.20	0.42
1:H:222:PHE:CE2	1:H:225:ASN:CB	2.90	0.42
1:H:315:MET:SD	1:H:321:ARG:HA	2.59	0.42
1:H:336:LEU:O	1:H:340:LEU:N	2.52	0.42
1:H:438:ARG:HG2	1:H:564:GLU:CG	2.49	0.42
1:B:125:LEU:HD21	1:B:215:CYS:SG	2.60	0.42
1:B:140:ARG:NH2	1:B:174:ASP:OD2	2.50	0.42
1:C:103:ASP:O	1:C:105:ARG:N	2.53	0.42
1:C:418:LYS:HB3	1:C:419:ARG:H	1.67	0.42
1:C:430:TRP:O	1:C:431:GLY:C	2.58	0.42
1:D:33:ILE:HG22	1:D:35:GLN:HA	2.02	0.42
1:D:148:PRO:HD2	1:D:149:GLU:OE2	2.20	0.42
1:E:140:ARG:NH2	1:E:174:ASP:OD2	2.51	0.42
1:E:373:ASP:O	1:E:374:CYS:CB	2.67	0.42
1:E:502:GLU:OE1	1:E:502:GLU:N	2.53	0.42
1:E:629:VAL:O	1:E:629:VAL:HG12	2.20	0.42
1:F:119:GLU:CB	1:F:121:PRO:HB2	2.49	0.42
1:F:125:LEU:CA	1:F:162:HIS:NE2	2.71	0.42
1:F:139:ASN:O	1:F:141:ILE:HG13	2.19	0.42
1:F:190:ALA:HB2	1:F:206:TRP:CG	2.55	0.42
1:F:261:THR:HB	1:F:262:PRO:HD2	2.01	0.42
1:G:434:TRP:CZ3	1:G:568:ARG:CG	2.95	0.42
1:G:579:ARG:HA	1:G:582:ARG:NH2	2.34	0.42
1:G:632:VAL:CG1	1:G:633:MET:HE1	2.50	0.42
1:H:225:ASN:OD1	1:H:229:VAL:HG12	2.20	0.42
1:H:361:LEU:HD23	1:H:361:LEU:HA	1.87	0.42
1:A:33:ILE:HD11	1:A:40:GLN:OE1	2.20	0.42
1:A:33:ILE:HG22	1:A:35:GLN:HA	2.02	0.42
1:A:144:ARG:HD2	1:A:171:LYS:HB2	2.02	0.42
1:A:478:GLN:HA	1:B:478:GLN:OE1	2.20	0.42
1:B:455:MET:CE	1:B:455:MET:O	2.68	0.42
1:B:478:GLN:O	1:B:482:LYS:HB3	2.20	0.42
1:C:18:LYS:HG3	1:C:35:GLN:HG2	2.02	0.42
1:C:190:ALA:O	1:C:191:PRO:C	2.58	0.42
1:C:213:PHE:O	1:C:214:GLU:C	2.58	0.42
1:C:416:ASP:OD1	1:C:416:ASP:N	2.39	0.42
1:C:466:SER:HB3	1:C:537:MET:HE1	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:646:ARG:C	1:C:647:GLN:OE1	2.57	0.42
1:D:102:GLY:HA3	1:D:152:VAL:HG13	2.02	0.42
1:D:515:ARG:HA	1:D:518:GLU:OE2	2.19	0.42
1:D:651:GLN:O	1:D:652:GLN:C	2.57	0.42
1:E:120:GLY:O	1:E:123:ARG:CA	2.68	0.42
1:E:134:ARG:CB	1:E:300:PHE:CE1	2.97	0.42
1:F:225:ASN:HB3	1:F:226:TRP:H	1.69	0.42
1:F:272:LYS:HG2	1:F:273:LEU:HA	2.02	0.42
1:F:312:LEU:O	1:F:324:THR:HG23	2.20	0.42
1:F:350:GLU:CG	1:F:391:ASP:HB2	2.46	0.42
1:F:430:TRP:O	1:F:431:GLY:C	2.58	0.42
1:G:139:ASN:O	1:G:141:ILE:HG13	2.19	0.42
1:G:189:LEU:CG	1:G:190:ALA:N	2.68	0.42
1:G:316:ASN:N	1:G:321:ARG:O	2.52	0.42
1:H:198:LYS:C	1:H:200:THR:H	2.23	0.42
1:H:273:LEU:O	1:H:276:TRP:N	2.53	0.42
1:H:581:GLN:H	1:H:582:ARG:HD2	1.85	0.42
1:A:651:GLN:O	1:A:652:GLN:C	2.57	0.42
1:B:312:LEU:O	1:B:324:THR:HG23	2.19	0.42
1:B:358:GLY:O	1:B:359:LEU:CB	2.63	0.42
1:B:583:THR:O	1:B:584:PRO:C	2.58	0.42
1:C:33:ILE:HD11	1:C:40:GLN:OE1	2.20	0.42
1:C:125:LEU:CA	1:C:162:HIS:NE2	2.74	0.42
1:C:517:MET:CE	1:C:647:GLN:OE1	2.68	0.42
1:D:222:PHE:HB2	1:D:255:PHE:HD2	1.85	0.42
1:D:433:ILE:HG23	1:D:594:LEU:HD22	2.01	0.42
1:D:569:ASP:HA	1:D:572:ARG:HB3	2.02	0.42
1:D:646:ARG:HG3	1:D:647:GLN:CD	2.33	0.42
1:D:650:ARG:HA	1:D:650:ARG:HD3	1.67	0.42
1:E:17:MET:CB	1:E:32:TRP:HB3	2.37	0.42
1:E:18:LYS:HZ2	1:E:33:ILE:CD1	2.29	0.42
1:E:70:HIS:HB2	1:E:135:TYR:CD2	2.54	0.42
1:E:102:GLY:CA	1:E:152:VAL:HG13	2.49	0.42
1:E:235:VAL:CG1	1:E:243:ILE:N	2.74	0.42
1:E:272:LYS:HG2	1:E:273:LEU:HA	2.02	0.42
1:E:505:ILE:O	1:E:505:ILE:HG22	2.19	0.42
1:F:105:ARG:HG3	1:F:105:ARG:NH1	2.35	0.42
1:F:272:LYS:O	1:F:273:LEU:C	2.58	0.42
1:G:33:ILE:HD11	1:G:40:GLN:OE1	2.20	0.42
1:G:213:PHE:O	1:G:214:GLU:C	2.58	0.42
1:G:406:HIS:HA	1:G:407:PRO:HD2	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:530:VAL:CA	1:G:533:LEU:HD12	2.32	0.42
1:G:614:LYS:HA	1:G:614:LYS:HD3	1.79	0.42
1:G:629:VAL:O	1:G:629:VAL:HG12	2.20	0.42
1:H:260:PRO:HB3	1:H:273:LEU:HD22	2.01	0.42
1:H:412:ILE:O	1:H:416:ASP:OD1	2.38	0.42
1:A:84:GLN:HB3	1:A:85:LYS:H	1.51	0.42
1:A:143:HIS:NE2	1:A:167:LEU:HB2	2.35	0.42
1:A:235:VAL:CG1	1:A:243:ILE:N	2.74	0.42
1:A:426:LEU:O	1:A:430:TRP:N	2.46	0.42
1:A:484:ASP:O	1:A:485:PHE:C	2.57	0.42
1:A:570:LEU:HD23	1:A:590:MET:CE	2.50	0.42
1:B:269:LEU:HD22	1:B:272:LYS:HB3	2.02	0.42
1:B:500:GLN:HB3	1:B:505:ILE:HG13	2.00	0.42
1:B:503:PHE:N	1:B:505:ILE:HD11	2.32	0.42
1:B:517:MET:SD	1:B:650:ARG:HG3	2.60	0.42
1:C:74:VAL:HG21	1:C:165:ILE:HA	2.01	0.42
1:C:190:ALA:HB2	1:C:206:TRP:CG	2.55	0.42
1:C:307:LEU:HD23	1:C:307:LEU:O	2.20	0.42
1:C:438:ARG:HG2	1:C:564:GLU:CG	2.50	0.42
1:D:402:SER:HB2	1:D:403:LEU:H	1.65	0.42
1:D:570:LEU:CD2	1:D:590:MET:CE	2.98	0.42
1:E:110:GLN:HB3	1:E:113:ASN:ND2	2.34	0.42
1:F:124:THR:OG1	1:F:162:HIS:HE1	2.02	0.42
1:G:21:LEU:HD12	1:G:29:VAL:HG12	2.00	0.42
1:G:110:GLN:O	1:G:111:PHE:CB	2.37	0.42
1:G:253:VAL:HB	1:G:255:PHE:CE1	2.54	0.42
1:G:422:THR:HG22	1:G:426:LEU:CD2	2.49	0.42
1:G:528:ARG:HA	1:G:530:VAL:HG22	2.02	0.42
1:A:198:LYS:C	1:A:200:THR:N	2.73	0.41
1:A:272:LYS:O	1:A:273:LEU:C	2.58	0.41
1:A:503:PHE:HB3	1:B:662:CYS:SG	2.60	0.41
1:B:33:ILE:HG23	1:B:39:GLU:H	1.85	0.41
1:B:430:TRP:O	1:B:431:GLY:C	2.58	0.41
1:B:434:TRP:O	1:B:435:GLN:C	2.55	0.41
1:C:16:GLU:HB3	1:C:17:MET:H	1.68	0.41
1:C:109:ASN:O	1:C:110:GLN:C	2.58	0.41
1:C:273:LEU:O	1:C:276:TRP:N	2.53	0.41
1:C:484:ASP:OD1	1:C:487:ARG:NH1	2.53	0.41
1:C:527:GLU:HG2	1:C:530:VAL:HG13	2.02	0.41
1:C:545:VAL:HG13	1:C:548:GLN:NE2	2.35	0.41
1:D:139:ASN:O	1:D:141:ILE:HG13	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:PHE:HD2	1:D:214:GLU:N	2.18	0.41
1:D:467:LYS:HD3	1:D:467:LYS:HA	1.75	0.41
1:E:190:ALA:O	1:E:191:PRO:C	2.58	0.41
1:E:346:ILE:HG23	1:E:346:ILE:O	2.20	0.41
1:F:133:LEU:O	1:F:134:ARG:C	2.57	0.41
1:G:18:LYS:HZ2	1:G:33:ILE:CD1	2.30	0.41
1:G:276:TRP:HE3	1:G:277:LEU:HD23	1.84	0.41
1:A:210:THR:O	1:A:213:PHE:N	2.53	0.41
1:A:222:PHE:CE2	1:A:225:ASN:CB	2.89	0.41
1:A:250:THR:C	1:A:251:GLY:O	2.58	0.41
1:A:297:VAL:HG23	1:A:301:GLN:NE2	2.35	0.41
1:A:478:GLN:O	1:A:482:LYS:HB3	2.20	0.41
1:A:533:LEU:O	1:A:537:MET:HG2	2.20	0.41
1:A:566:GLN:HG2	1:A:593:LEU:CD1	2.51	0.41
1:A:665:VAL:CG2	1:B:665:VAL:HG21	2.49	0.41
1:B:114:CYS:O	1:B:115:CYS:CB	2.64	0.41
1:C:114:CYS:O	1:C:115:CYS:CB	2.64	0.41
1:C:118:LYS:HZ1	1:C:123:ARG:HH12	1.67	0.41
1:C:144:ARG:HD2	1:C:171:LYS:HB2	2.01	0.41
1:C:533:LEU:O	1:C:537:MET:HG2	2.20	0.41
1:C:569:ASP:HA	1:C:572:ARG:HB3	2.02	0.41
1:D:262:PRO:HG2	1:D:432:GLN:HG2	2.03	0.41
1:E:102:GLY:HA3	1:E:152:VAL:HG13	2.02	0.41
1:E:272:LYS:O	1:E:273:LEU:C	2.57	0.41
1:E:409:SER:CB	1:E:412:ILE:CD1	2.93	0.41
1:E:485:PHE:CD2	1:F:485:PHE:CD2	3.08	0.41
1:E:565:GLU:O	1:E:568:ARG:HB3	2.20	0.41
1:E:583:THR:O	1:E:584:PRO:C	2.58	0.41
1:E:665:VAL:HG11	1:F:664:LYS:O	2.20	0.41
1:F:18:LYS:HG3	1:F:35:GLN:HG2	2.03	0.41
1:F:26:PHE:CE2	1:F:181:GLU:OE1	2.68	0.41
1:F:165:ILE:O	1:F:167:LEU:N	2.48	0.41
1:F:222:PHE:HB2	1:F:255:PHE:HD2	1.85	0.41
1:F:254:LYS:N	1:F:255:PHE:CE1	2.87	0.41
1:F:352:GLU:OE1	1:F:619:LYS:NZ	2.32	0.41
1:F:455:MET:HB2	1:F:455:MET:HE3	1.81	0.41
1:G:185:THR:CG2	1:G:187:GLN:CG	2.80	0.41
1:G:213:PHE:HD2	1:G:214:GLU:N	2.18	0.41
1:H:124:THR:O	1:H:127:SER:N	2.52	0.41
1:H:148:PRO:HD2	1:H:149:GLU:OE2	2.20	0.41
1:H:222:PHE:HB2	1:H:255:PHE:HD2	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:N	1:A:151:ILE:O	2.33	0.41
1:A:124:THR:O	1:A:127:SER:N	2.53	0.41
1:A:268:ILE:HD12	1:A:268:ILE:HA	1.91	0.41
1:A:410:VAL:O	1:A:411:SER:C	2.59	0.41
1:A:430:TRP:CB	1:A:571:TYR:HD2	2.27	0.41
1:A:567:ALA:HA	1:A:590:MET:HE1	2.02	0.41
1:B:195:GLU:O	1:B:196:GLN:HB2	2.20	0.41
1:D:316:ASN:O	1:D:317:MET:HG2	2.21	0.41
1:D:494:LEU:CD1	1:D:514:TRP:HB3	2.50	0.41
1:D:563:LEU:HD21	1:D:596:LEU:HB2	2.02	0.41
1:E:33:ILE:HG22	1:E:35:GLN:HA	2.03	0.41
1:E:103:ASP:O	1:E:106:LYS:N	2.53	0.41
1:E:120:GLY:CA	1:E:123:ARG:HB2	2.48	0.41
1:E:222:PHE:CB	1:E:255:PHE:HB3	2.50	0.41
1:E:434:TRP:HZ3	1:E:568:ARG:HA	1.75	0.41
1:E:527:GLU:C	1:E:529:GLU:H	2.23	0.41
1:F:118:LYS:HG2	1:F:264:HIS:C	2.32	0.41
1:F:118:LYS:HG2	1:F:265:LEU:CA	2.46	0.41
1:F:502:GLU:N	1:F:502:GLU:OE1	2.53	0.41
1:F:517:MET:CG	1:F:646:ARG:HH11	2.18	0.41
1:G:475:GLU:CD	1:G:636:MET:HE1	2.40	0.41
1:H:186:LEU:C	1:H:188:TYR:H	2.22	0.41
1:H:291:ASP:HA	1:H:292:PRO:HD3	1.82	0.41
1:H:443:ASP:O	1:H:446:ARG:CB	2.62	0.41
1:A:315:MET:SD	1:A:321:ARG:HA	2.61	0.41
1:B:70:HIS:HB3	1:B:73:VAL:CG1	2.50	0.41
1:B:455:MET:O	1:B:455:MET:HE3	2.20	0.41
1:B:501:MET:C	1:B:505:ILE:CD1	2.87	0.41
1:C:222:PHE:HB2	1:C:255:PHE:HD2	1.85	0.41
1:C:277:LEU:C	1:C:279:CYS:N	2.74	0.41
1:D:118:LYS:NZ	1:D:123:ARG:HH12	2.18	0.41
1:D:198:LYS:C	1:D:200:THR:N	2.74	0.41
1:D:234:LYS:O	1:D:235:VAL:O	2.38	0.41
1:D:246:TYR:CE1	1:D:258:VAL:HB	2.46	0.41
1:D:414:LEU:O	1:D:418:LYS:HB2	2.20	0.41
1:D:430:TRP:O	1:D:431:GLY:C	2.59	0.41
1:D:434:TRP:O	1:D:435:GLN:C	2.56	0.41
1:E:336:LEU:O	1:E:337:LYS:C	2.57	0.41
1:E:470:ASN:HD22	1:E:470:ASN:N	2.18	0.41
1:E:581:GLN:H	1:E:582:ARG:HD2	1.86	0.41
1:F:102:GLY:CA	1:F:152:VAL:HG13	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:213:PHE:O	1:F:214:GLU:C	2.58	0.41
1:F:268:ILE:HD12	1:F:268:ILE:HA	1.90	0.41
1:F:357:SER:CB	1:F:453:THR:HB	2.51	0.41
1:F:479:LEU:HB3	1:F:640:GLU:OE2	2.21	0.41
1:G:18:LYS:HG3	1:G:35:GLN:HG2	2.03	0.41
1:G:102:GLY:CA	1:G:152:VAL:HG13	2.51	0.41
1:H:189:LEU:CG	1:H:190:ALA:N	2.70	0.41
1:H:222:PHE:HE2	1:H:225:ASN:HB2	1.72	0.41
1:H:451:GLN:NE2	1:H:611:GLN:NE2	2.68	0.41
1:A:110:GLN:HB3	1:A:113:ASN:ND2	2.35	0.41
1:A:422:THR:HG22	1:A:426:LEU:CD2	2.47	0.41
1:A:430:TRP:O	1:A:431:GLY:C	2.59	0.41
1:A:529:GLU:HG3	1:A:633:MET:HE3	1.97	0.41
1:A:547:LEU:HD22	1:A:611:GLN:HG2	2.01	0.41
1:B:16:GLU:C	1:B:17:MET:HG3	2.41	0.41
1:B:198:LYS:C	1:B:200:THR:N	2.73	0.41
1:B:428:ARG:HB2	1:B:429:VAL:H	1.69	0.41
1:B:606:ILE:O	1:B:607:LEU:C	2.58	0.41
1:C:536:LYS:CB	1:C:625:LEU:HD13	2.16	0.41
1:D:70:HIS:HB3	1:D:73:VAL:CG1	2.50	0.41
1:D:614:LYS:HD3	1:D:614:LYS:HA	1.79	0.41
1:E:424:THR:HG1	1:E:425:HIS:HD1	1.54	0.41
1:E:497:TYR:CD2	1:E:497:TYR:C	2.94	0.41
1:F:244:VAL:HG22	1:F:282:MET:SD	2.61	0.41
1:F:260:PRO:HB2	1:F:273:LEU:CD1	2.47	0.41
1:G:55:ARG:HE	1:G:55:ARG:HB2	1.54	0.41
1:G:226:TRP:HD1	1:G:227:GLN:N	2.10	0.41
1:H:32:TRP:HD1	1:H:43:ILE:HD13	1.85	0.41
1:H:33:ILE:HG22	1:H:35:GLN:HA	2.02	0.41
1:H:423:TYR:CE1	1:H:425:HIS:O	2.74	0.41
1:A:70:HIS:HB3	1:A:73:VAL:CG1	2.50	0.41
1:A:195:GLU:O	1:A:196:GLN:HB2	2.20	0.41
1:A:510:LEU:HD22	1:A:653:GLU:HB2	2.02	0.41
1:A:517:MET:HG3	1:A:646:ARG:HH11	1.85	0.41
1:A:581:GLN:H	1:A:582:ARG:HD2	1.84	0.41
1:B:120:GLY:O	1:B:123:ARG:CA	2.69	0.41
1:B:186:LEU:C	1:B:188:TYR:H	2.22	0.41
1:B:261:THR:HB	1:B:262:PRO:HD2	2.02	0.41
1:B:488:SER:O	1:B:492:ILE:HG22	2.20	0.41
1:C:210:THR:O	1:C:211:LEU:C	2.59	0.41
1:C:346:ILE:HA	1:C:347:PRO:HD3	1.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:GLN:O	1:C:439:ALA:N	2.51	0.41
1:D:209:GLY:O	1:D:212:ALA:HB3	2.21	0.41
1:D:281:LEU:C	1:D:282:MET:HG2	2.41	0.41
1:E:455:MET:O	1:E:455:MET:HE3	2.21	0.41
1:E:469:LYS:HZ3	1:E:630:LYS:HE2	1.84	0.41
1:E:500:GLN:HE22	1:F:659:LYS:HG2	1.85	0.41
1:E:563:LEU:HD21	1:E:596:LEU:CB	2.35	0.41
1:F:33:ILE:HG22	1:F:35:GLN:HA	2.02	0.41
1:F:234:LYS:O	1:F:235:VAL:O	2.38	0.41
1:F:235:VAL:CG1	1:F:243:ILE:N	2.72	0.41
1:F:459:LEU:O	1:F:459:LEU:HD23	2.21	0.41
1:F:473:THR:HB	1:F:533:LEU:HD13	2.03	0.41
1:F:581:GLN:H	1:F:582:ARG:HD2	1.85	0.41
1:G:455:MET:O	1:G:455:MET:CE	2.68	0.41
1:G:472:MET:CG	1:G:633:MET:CB	2.99	0.41
1:H:18:LYS:HG3	1:H:35:GLN:HG2	2.03	0.41
1:H:144:ARG:HD2	1:H:171:LYS:HB2	2.01	0.41
1:H:195:GLU:O	1:H:196:GLN:HB2	2.20	0.41
1:H:346:ILE:HG23	1:H:346:ILE:O	2.20	0.41
1:A:206:TRP:CD1	1:A:207:SER:N	2.88	0.41
1:A:307:LEU:O	1:A:307:LEU:HD23	2.21	0.41
1:A:437:ILE:CG1	1:A:594:LEU:HD12	2.50	0.41
1:A:642:ILE:C	1:A:644:VAL:H	2.22	0.41
1:A:658:LEU:CD1	1:B:658:LEU:HA	2.51	0.41
1:B:139:ASN:O	1:B:141:ILE:HG13	2.21	0.41
1:B:144:ARG:HD2	1:B:171:LYS:HB2	2.00	0.41
1:B:226:TRP:CG	1:B:227:GLN:N	2.62	0.41
1:B:265:LEU:HG	1:B:266:SER:H	1.86	0.41
1:C:119:GLU:CB	1:C:121:PRO:HB2	2.50	0.41
1:C:119:GLU:HB2	1:C:121:PRO:N	2.36	0.41
1:C:515:ARG:HA	1:C:518:GLU:OE2	2.20	0.41
1:C:527:GLU:C	1:C:529:GLU:N	2.73	0.41
1:C:539:ALA:O	1:C:543:ASP:HB2	2.20	0.41
1:D:18:LYS:HG3	1:D:35:GLN:HG2	2.02	0.41
1:D:222:PHE:HE2	1:D:225:ASN:HB2	1.72	0.41
1:D:449:GLN:NE2	1:D:453:THR:CG2	2.83	0.41
1:D:646:ARG:CG	1:D:647:GLN:NE2	2.54	0.41
1:E:33:ILE:HD11	1:E:40:GLN:OE1	2.20	0.41
1:E:387:ILE:HD12	1:E:450:GLY:CA	2.49	0.41
1:E:533:LEU:O	1:E:537:MET:HG2	2.20	0.41
1:E:569:ASP:HA	1:E:572:ARG:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:LEU:HB3	1:F:250:THR:H	1.38	0.41
1:F:533:LEU:O	1:F:537:MET:HG2	2.20	0.41
1:F:660:ILE:C	1:F:662:CYS:N	2.68	0.41
1:G:33:ILE:HG22	1:G:35:GLN:HA	2.02	0.41
1:A:362:ASN:C	1:A:364:ALA:N	2.72	0.41
1:B:412:ILE:HG12	1:B:433:ILE:HD13	2.03	0.41
1:C:114:CYS:O	1:C:114:CYS:SG	2.79	0.41
1:C:189:LEU:HD12	1:C:207:SER:HB3	2.03	0.41
1:C:451:GLN:OE1	1:C:611:GLN:NE2	2.54	0.41
1:C:480:LYS:O	1:C:483:LEU:HB3	2.20	0.41
1:C:571:TYR:CE1	1:C:590:MET:HE1	2.56	0.41
1:D:119:GLU:HB2	1:D:121:PRO:N	2.36	0.41
1:D:121:PRO:HA	1:D:124:THR:OG1	2.21	0.41
1:D:497:TYR:CD2	1:D:497:TYR:C	2.93	0.41
1:D:540:LEU:HD13	1:D:622:ALA:HB2	2.03	0.41
1:E:105:ARG:HG3	1:E:105:ARG:NH1	2.31	0.41
1:E:139:ASN:O	1:E:141:ILE:HG13	2.21	0.41
1:F:16:GLU:C	1:F:17:MET:HG3	2.41	0.41
1:F:222:PHE:CB	1:F:255:PHE:HB3	2.50	0.41
1:F:281:LEU:C	1:F:282:MET:HG2	2.41	0.41
1:F:540:LEU:CD1	1:F:622:ALA:HB2	2.50	0.41
1:G:16:GLU:C	1:G:17:MET:HG3	2.41	0.41
1:G:142:ILE:HG22	1:G:144:ARG:H	1.86	0.41
1:H:25:GLY:HA2	1:H:169:TYR:OH	2.21	0.41
1:H:533:LEU:O	1:H:537:MET:HG2	2.20	0.41
1:H:564:GLU:HG2	1:H:564:GLU:O	2.20	0.41
1:H:610:ASP:O	1:H:613:SER:HB3	2.20	0.41
1:H:636:MET:HE2	1:H:637:ARG:N	2.35	0.41
1:A:246:TYR:CE1	1:A:258:VAL:HB	2.45	0.41
1:A:281:LEU:C	1:A:282:MET:HG2	2.41	0.41
1:A:336:LEU:O	1:A:337:LYS:C	2.59	0.41
1:B:55:ARG:HE	1:B:55:ARG:HB2	1.53	0.41
1:B:222:PHE:HB2	1:B:255:PHE:HD2	1.86	0.41
1:B:285:GLN:O	1:B:285:GLN:CG	2.69	0.41
1:B:629:VAL:HG12	1:B:629:VAL:O	2.21	0.41
1:B:656:ASN:OD1	1:B:656:ASN:O	2.39	0.41
1:C:148:PRO:HD2	1:C:149:GLU:OE2	2.21	0.41
1:C:387:ILE:HG21	1:C:450:GLY:HA2	2.03	0.41
1:C:437:ILE:HG12	1:C:597:ALA:HB3	2.03	0.41
1:C:654:LEU:HD12	1:D:655:TRP:CZ3	2.56	0.41
1:C:655:TRP:CZ3	1:D:654:LEU:HD12	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ASN:O	1:D:164:ILE:HG22	2.21	0.41
1:D:118:LYS:CB	1:D:264:HIS:O	2.69	0.41
1:D:484:ASP:OD1	1:D:487:ARG:NH1	2.54	0.41
1:D:485:PHE:CD1	1:D:485:PHE:C	2.94	0.41
1:D:564:GLU:O	1:D:564:GLU:HG2	2.20	0.41
1:E:142:ILE:HG12	1:E:201:VAL:HA	2.02	0.41
1:E:260:PRO:HB2	1:E:273:LEU:CD1	2.50	0.41
1:E:268:ILE:HD12	1:E:268:ILE:HA	1.90	0.41
1:E:273:LEU:O	1:E:276:TRP:N	2.54	0.41
1:E:455:MET:HE3	1:E:455:MET:HB2	1.80	0.41
1:E:459:LEU:HD23	1:E:459:LEU:O	2.21	0.41
1:E:486:PHE:O	1:E:486:PHE:CG	2.73	0.41
1:E:503:PHE:N	1:E:505:ILE:HD11	2.29	0.41
1:E:515:ARG:HA	1:E:518:GLU:OE2	2.21	0.41
1:E:527:GLU:HG2	1:E:530:VAL:CG1	2.50	0.41
1:E:528:ARG:HA	1:E:530:VAL:HG22	2.03	0.41
1:F:148:PRO:HG3	1:F:188:TYR:OH	2.21	0.41
1:F:276:TRP:HE3	1:F:277:LEU:HD23	1.85	0.41
1:F:455:MET:O	1:F:455:MET:CE	2.69	0.41
1:F:503:PHE:C	1:F:505:ILE:HG13	2.40	0.41
1:F:579:ARG:NH2	1:G:580:ASP:HB3	2.36	0.41
1:G:119:GLU:HB3	1:G:121:PRO:CD	2.43	0.41
1:G:273:LEU:O	1:G:276:TRP:N	2.54	0.41
1:G:276:TRP:CE2	1:G:280:MET:HG3	2.55	0.41
1:G:346:ILE:HA	1:G:347:PRO:HD3	1.84	0.41
1:G:567:ALA:O	1:G:571:TYR:CD1	2.74	0.41
1:H:107:TYR:CA	1:H:110:GLN:HB2	2.51	0.41
1:H:159:ARG:HD3	1:H:375:THR:HG21	2.03	0.41
1:H:169:TYR:CD2	1:H:169:TYR:N	2.89	0.41
1:A:148:PRO:HG3	1:A:188:TYR:OH	2.20	0.41
1:B:125:LEU:HD12	1:B:129:ILE:HG12	2.02	0.41
1:B:373:ASP:O	1:B:374:CYS:CB	2.69	0.41
1:B:497:TYR:CD2	1:B:497:TYR:C	2.93	0.41
1:B:502:GLU:OE1	1:B:502:GLU:N	2.54	0.41
1:B:603:LYS:O	1:B:606:ILE:HG13	2.21	0.41
1:C:102:GLY:O	1:C:103:ASP:C	2.60	0.41
1:C:250:THR:C	1:C:251:GLY:O	2.58	0.41
1:C:336:LEU:O	1:C:337:LYS:C	2.60	0.41
1:D:120:GLY:C	1:D:123:ARG:H	2.25	0.41
1:D:222:PHE:CB	1:D:255:PHE:HB3	2.51	0.41
1:D:346:ILE:HA	1:D:347:PRO:HD3	1.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:LYS:CG	1:E:118:LYS:O	2.68	0.41
1:E:148:PRO:HD2	1:E:149:GLU:OE2	2.21	0.41
1:E:250:THR:C	1:E:251:GLY:O	2.58	0.41
1:E:476:CYS:HB2	1:E:636:MET:SD	2.61	0.41
1:E:651:GLN:O	1:E:652:GLN:C	2.59	0.41
1:E:654:LEU:HD21	1:F:654:LEU:HD21	1.70	0.41
1:F:210:THR:N	1:F:281:LEU:HD11	2.35	0.41
1:F:438:ARG:HG2	1:F:564:GLU:OE1	2.21	0.41
1:F:539:ALA:O	1:F:543:ASP:HB2	2.21	0.41
1:G:222:PHE:HB2	1:G:255:PHE:HD2	1.85	0.41
1:G:261:THR:HB	1:G:262:PRO:HD2	2.03	0.41
1:G:436:THR:O	1:G:440:LEU:HG	2.20	0.41
1:G:533:LEU:HD21	1:G:633:MET:HE3	2.03	0.41
1:H:58:TRP:CZ3	1:H:62:ILE:HG13	2.57	0.41
1:H:140:ARG:NH2	1:H:174:ASP:OD2	2.52	0.41
1:H:210:THR:O	1:H:211:LEU:C	2.60	0.41
1:H:276:TRP:CE2	1:H:280:MET:HG3	2.56	0.41
1:H:583:THR:O	1:H:585:GLY:N	2.54	0.41
1:A:150:ASN:ND2	1:A:167:LEU:CD1	2.82	0.40
1:A:497:TYR:CD2	1:A:497:TYR:C	2.94	0.40
1:B:102:GLY:O	1:B:103:ASP:C	2.60	0.40
1:B:260:PRO:HB2	1:B:273:LEU:CD1	2.49	0.40
1:B:505:ILE:O	1:B:505:ILE:HG22	2.22	0.40
1:C:186:LEU:HD23	1:C:227:GLN:HG2	2.03	0.40
1:C:208:PHE:O	1:C:211:LEU:HB3	2.22	0.40
1:C:357:SER:HB3	1:C:453:THR:CB	2.41	0.40
1:D:169:TYR:N	1:D:169:TYR:CD2	2.89	0.40
1:D:206:TRP:CD1	1:D:207:SER:N	2.89	0.40
1:D:250:THR:C	1:D:251:GLY:O	2.59	0.40
1:E:50:LEU:N	1:E:55:ARG:HD3	2.35	0.40
1:E:467:LYS:HD3	1:E:467:LYS:HA	1.75	0.40
1:E:482:LYS:C	1:E:484:ASP:H	2.23	0.40
1:F:143:HIS:NE2	1:F:167:LEU:HB2	2.35	0.40
1:F:195:GLU:O	1:F:196:GLN:HB2	2.20	0.40
1:F:296:ASN:CG	1:F:297:VAL:N	2.75	0.40
1:F:441:LYS:HB2	1:F:560:LEU:HD22	2.03	0.40
1:F:515:ARG:HA	1:F:518:GLU:OE2	2.21	0.40
1:F:570:LEU:CB	1:F:590:MET:HE2	2.51	0.40
1:G:373:ASP:O	1:G:374:CYS:CB	2.68	0.40
1:H:68:LEU:HD11	1:H:141:ILE:CD1	2.51	0.40
1:H:437:ILE:HG12	1:H:597:ALA:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:449:GLN:O	1:H:453:THR:HG23	2.21	0.40
1:A:190:ALA:O	1:A:191:PRO:C	2.60	0.40
1:A:213:PHE:O	1:A:214:GLU:C	2.59	0.40
1:A:480:LYS:HZ2	1:A:527:GLU:HB2	1.86	0.40
1:A:629:VAL:HG12	1:A:629:VAL:O	2.21	0.40
1:B:208:PHE:O	1:B:211:LEU:HB3	2.21	0.40
1:C:614:LYS:HD3	1:C:614:LYS:HA	1.80	0.40
1:D:269:LEU:HD23	1:D:269:LEU:HA	1.89	0.40
1:D:361:LEU:HD23	1:D:361:LEU:HA	1.85	0.40
1:D:567:ALA:O	1:D:571:TYR:CD1	2.74	0.40
1:D:580:ASP:O	1:D:580:ASP:CG	2.60	0.40
1:E:102:GLY:O	1:E:103:ASP:C	2.59	0.40
1:E:336:LEU:O	1:E:340:LEU:N	2.54	0.40
1:E:428:ARG:HB2	1:E:429:VAL:H	1.69	0.40
1:E:545:VAL:HG13	1:E:548:GLN:NE2	2.36	0.40
1:F:33:ILE:HD11	1:F:40:GLN:OE1	2.21	0.40
1:F:497:TYR:CD2	1:F:511:LEU:HD22	2.50	0.40
1:F:517:MET:HE1	1:F:647:GLN:OE1	2.18	0.40
1:F:606:ILE:O	1:F:607:LEU:C	2.58	0.40
1:F:651:GLN:O	1:F:652:GLN:C	2.59	0.40
1:G:190:ALA:O	1:G:191:PRO:C	2.59	0.40
1:G:212:ALA:O	1:G:215:CYS:N	2.55	0.40
1:G:423:TYR:CE1	1:G:425:HIS:O	2.74	0.40
1:G:571:TYR:OH	1:G:590:MET:SD	2.79	0.40
1:A:208:PHE:O	1:A:211:LEU:HB3	2.21	0.40
1:A:285:GLN:O	1:A:285:GLN:CG	2.69	0.40
1:A:438:ARG:HH11	1:A:568:ARG:HH21	1.67	0.40
1:A:449:GLN:O	1:A:453:THR:HG23	2.20	0.40
1:A:482:LYS:C	1:A:484:ASP:N	2.74	0.40
1:A:488:SER:O	1:A:492:ILE:HG22	2.21	0.40
1:B:276:TRP:CE2	1:B:280:MET:HG3	2.56	0.40
1:B:485:PHE:CD1	1:B:485:PHE:C	2.95	0.40
1:C:120:GLY:O	1:C:123:ARG:CA	2.69	0.40
1:C:135:TYR:O	1:C:139:ASN:ND2	2.52	0.40
1:C:434:TRP:HZ3	1:C:568:ARG:CB	2.35	0.40
1:C:441:LYS:HB2	1:C:560:LEU:HD21	2.02	0.40
1:C:481:ALA:O	1:C:484:ASP:HB2	2.22	0.40
1:C:485:PHE:CB	1:D:485:PHE:CE2	3.05	0.40
1:C:497:TYR:CD2	1:C:497:TYR:C	2.93	0.40
1:D:50:LEU:N	1:D:55:ARG:HD3	2.36	0.40
1:D:60:LEU:HD21	1:D:175:GLN:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:ASN:O	1:D:110:GLN:C	2.60	0.40
1:D:142:ILE:HG22	1:D:144:ARG:H	1.86	0.40
1:D:484:ASP:C	1:D:486:PHE:H	2.22	0.40
1:E:209:GLY:O	1:E:212:ALA:HB3	2.21	0.40
1:E:246:TYR:CE1	1:E:258:VAL:HB	2.44	0.40
1:E:316:ASN:O	1:E:317:MET:HG2	2.21	0.40
1:E:410:VAL:O	1:E:411:SER:C	2.59	0.40
1:E:414:LEU:O	1:E:418:LYS:HB2	2.22	0.40
1:E:654:LEU:HD22	1:F:654:LEU:CD2	2.45	0.40
1:F:32:TRP:HD1	1:F:43:ILE:HD13	1.86	0.40
1:F:260:PRO:HB3	1:F:273:LEU:CD2	2.51	0.40
1:F:486:PHE:O	1:F:486:PHE:CG	2.75	0.40
1:G:105:ARG:NE	1:G:149:GLU:OE2	2.55	0.40
1:G:118:LYS:HZ1	1:G:123:ARG:HH22	1.68	0.40
1:G:247:ASP:HB3	1:G:248:ASP:H	1.47	0.40
1:G:402:SER:HB2	1:G:403:LEU:H	1.66	0.40
1:G:409:SER:CB	1:G:412:ILE:CD1	2.92	0.40
1:H:118:LYS:HZ1	1:H:123:ARG:HH12	1.68	0.40
1:B:110:GLN:HB3	1:B:113:ASN:ND2	2.35	0.40
1:B:247:ASP:HB3	1:B:248:ASP:H	1.50	0.40
1:B:260:PRO:O	1:B:261:THR:OG1	2.37	0.40
1:B:316:ASN:N	1:B:321:ARG:O	2.54	0.40
1:B:484:ASP:OD1	1:B:487:ARG:NH1	2.54	0.40
1:C:28:TYR:HD2	1:C:45:GLN:NE2	2.19	0.40
1:C:32:TRP:HD1	1:C:43:ILE:HD13	1.86	0.40
1:C:273:LEU:HB3	1:C:274:GLU:H	1.73	0.40
1:C:312:LEU:O	1:C:324:THR:HG23	2.21	0.40
1:C:462:ASN:ND2	1:C:540:LEU:HB3	2.37	0.40
1:C:485:PHE:CG	1:D:485:PHE:CE2	3.09	0.40
1:C:632:VAL:O	1:C:633:MET:SD	2.79	0.40
1:D:143:HIS:NE2	1:D:167:LEU:HB2	2.36	0.40
1:D:307:LEU:O	1:D:307:LEU:HD23	2.20	0.40
1:D:434:TRP:NE1	1:D:435:GLN:OE1	2.55	0.40
1:D:476:CYS:CB	1:D:636:MET:SD	3.09	0.40
1:E:321:ARG:NE	1:E:443:ASP:OD1	2.54	0.40
1:E:406:HIS:HA	1:E:407:PRO:HD2	1.84	0.40
1:E:426:LEU:O	1:E:430:TRP:N	2.45	0.40
1:E:449:GLN:O	1:E:453:THR:HG23	2.21	0.40
1:F:276:TRP:CE2	1:F:280:MET:HG3	2.56	0.40
1:F:481:ALA:O	1:F:484:ASP:HB2	2.22	0.40
1:F:490:ILE:O	1:F:490:ILE:CG2	2.68	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:569:ASP:HA	1:F:572:ARG:HB3	2.03	0.40
1:G:58:TRP:CZ3	1:G:62:ILE:HG13	2.57	0.40
1:G:565:GLU:O	1:G:568:ARG:HB3	2.22	0.40
1:G:567:ALA:O	1:G:571:TYR:HD1	2.03	0.40
1:G:569:ASP:HA	1:G:572:ARG:HB3	2.03	0.40
1:H:33:ILE:HD11	1:H:40:GLN:OE1	2.21	0.40
1:H:185:THR:CG2	1:H:187:GLN:CG	2.83	0.40
1:H:629:VAL:O	1:H:629:VAL:HG12	2.21	0.40
1:A:222:PHE:CZ	1:A:225:ASN:CB	3.04	0.40
1:A:346:ILE:HA	1:A:347:PRO:HD3	1.84	0.40
1:A:530:VAL:CA	1:A:533:LEU:HD12	2.32	0.40
1:A:565:GLU:O	1:A:568:ARG:HB3	2.20	0.40
1:B:28:TYR:HD2	1:B:45:GLN:NE2	2.19	0.40
1:B:104:LEU:N	1:B:151:ILE:O	2.33	0.40
1:B:135:TYR:O	1:B:139:ASN:ND2	2.51	0.40
1:B:272:LYS:HG2	1:B:273:LEU:HA	2.02	0.40
1:B:277:LEU:C	1:B:279:CYS:N	2.74	0.40
1:B:333:LEU:O	1:B:336:LEU:N	2.54	0.40
1:C:291:ASP:HA	1:C:292:PRO:HD3	1.82	0.40
1:C:296:ASN:CG	1:C:297:VAL:N	2.75	0.40
1:D:16:GLU:C	1:D:17:MET:HG3	2.42	0.40
1:D:33:ILE:HD11	1:D:40:GLN:OE1	2.21	0.40
1:D:70:HIS:NE2	1:D:131:SER:O	2.54	0.40
1:D:272:LYS:HG2	1:D:273:LEU:HA	2.03	0.40
1:F:114:CYS:O	1:F:114:CYS:SG	2.80	0.40
1:F:186:LEU:HD23	1:F:227:GLN:HG2	2.03	0.40
1:F:410:VAL:O	1:F:413:VAL:HG12	2.22	0.40
1:G:122:ILE:O	1:G:126:LEU:HB2	2.22	0.40
1:G:269:LEU:HD22	1:G:272:LYS:HB3	2.03	0.40
1:G:473:THR:HB	1:G:533:LEU:HD13	2.04	0.40
1:H:333:LEU:O	1:H:336:LEU:N	2.55	0.40
1:H:569:ASP:HA	1:H:572:ARG:HB3	2.03	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:MET:SD	1:E:364:ALA:O[1_565]	1.61	0.59
1:E:515:ARG:NH1	1:H:394:LYS:NZ[1_465]	1.76	0.44
1:B:617:VAL:CG2	1:C:519:GLN:OE1[1_465]	1.96	0.24

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:GLU:OE1	1:C:295:PRO:CB[1_565]	2.01	0.19
1:A:522:GLU:OE1	1:C:295:PRO:CG[1_565]	2.04	0.16
1:B:394:LYS:NZ	1:C:515:ARG:NH1[1_465]	2.19	0.01

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	610/676 (90%)	360 (59%)	145 (24%)	105 (17%)	0 2
1	B	610/676 (90%)	362 (59%)	143 (23%)	105 (17%)	0 2
1	C	610/676 (90%)	359 (59%)	147 (24%)	104 (17%)	0 2
1	D	610/676 (90%)	363 (60%)	143 (23%)	104 (17%)	0 2
1	E	610/676 (90%)	361 (59%)	147 (24%)	102 (17%)	0 3
1	F	610/676 (90%)	362 (59%)	144 (24%)	104 (17%)	0 2
1	G	527/676 (78%)	310 (59%)	126 (24%)	91 (17%)	0 2
1	H	527/676 (78%)	313 (59%)	121 (23%)	93 (18%)	0 2
All	All	4714/5408 (87%)	2790 (59%)	1116 (24%)	808 (17%)	0 2

All (808) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	GLY
1	A	106	LYS
1	A	110	GLN
1	A	111	PHE
1	A	166	ASP
1	A	171	LYS
1	A	183	VAL
1	A	187	GLN
1	A	191	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	195	GLU
1	A	202	THR
1	A	214	GLU
1	A	231	TRP
1	A	235	VAL
1	A	300	PHE
1	A	319	SER
1	A	330	ASN
1	A	350	GLU
1	A	359	LEU
1	A	372	ILE
1	A	403	LEU
1	A	419	ARG
1	A	420	PRO
1	A	424	THR
1	A	506	THR
1	A	528	ARG
1	A	582	ARG
1	A	584	PRO
1	A	588	ASN
1	B	101	GLY
1	B	106	LYS
1	B	110	GLN
1	B	111	PHE
1	B	166	ASP
1	B	171	LYS
1	B	183	VAL
1	B	187	GLN
1	B	191	PRO
1	B	195	GLU
1	B	201	VAL
1	B	202	THR
1	B	231	TRP
1	B	235	VAL
1	B	300	PHE
1	B	319	SER
1	B	330	ASN
1	B	350	GLU
1	B	359	LEU
1	B	363	SER
1	B	372	ILE
1	B	403	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	419	ARG
1	B	420	PRO
1	B	424	THR
1	B	506	THR
1	B	528	ARG
1	B	582	ARG
1	B	584	PRO
1	B	661	ALA
1	C	101	GLY
1	C	106	LYS
1	C	110	GLN
1	C	111	PHE
1	C	166	ASP
1	C	171	LYS
1	C	183	VAL
1	C	187	GLN
1	C	191	PRO
1	C	195	GLU
1	C	201	VAL
1	C	202	THR
1	C	231	TRP
1	C	235	VAL
1	C	273	LEU
1	C	300	PHE
1	C	319	SER
1	C	330	ASN
1	C	350	GLU
1	C	359	LEU
1	C	363	SER
1	C	372	ILE
1	C	403	LEU
1	C	419	ARG
1	C	420	PRO
1	C	424	THR
1	C	506	THR
1	C	528	ARG
1	C	582	ARG
1	C	584	PRO
1	C	661	ALA
1	D	101	GLY
1	D	106	LYS
1	D	110	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	111	PHE
1	D	166	ASP
1	D	171	LYS
1	D	183	VAL
1	D	187	GLN
1	D	191	PRO
1	D	195	GLU
1	D	201	VAL
1	D	202	THR
1	D	231	TRP
1	D	235	VAL
1	D	300	PHE
1	D	319	SER
1	D	330	ASN
1	D	350	GLU
1	D	359	LEU
1	D	363	SER
1	D	372	ILE
1	D	386	LEU
1	D	403	LEU
1	D	419	ARG
1	D	420	PRO
1	D	424	THR
1	D	506	THR
1	D	582	ARG
1	D	584	PRO
1	D	661	ALA
1	E	101	GLY
1	E	106	LYS
1	E	110	GLN
1	E	111	PHE
1	E	166	ASP
1	E	171	LYS
1	E	183	VAL
1	E	187	GLN
1	E	191	PRO
1	E	195	GLU
1	E	202	THR
1	E	231	TRP
1	E	235	VAL
1	E	273	LEU
1	E	300	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	319	SER
1	E	330	ASN
1	E	350	GLU
1	E	359	LEU
1	E	372	ILE
1	E	403	LEU
1	E	419	ARG
1	E	420	PRO
1	E	424	THR
1	E	506	THR
1	E	582	ARG
1	E	584	PRO
1	E	661	ALA
1	F	101	GLY
1	F	106	LYS
1	F	110	GLN
1	F	111	PHE
1	F	166	ASP
1	F	171	LYS
1	F	183	VAL
1	F	187	GLN
1	F	191	PRO
1	F	195	GLU
1	F	201	VAL
1	F	202	THR
1	F	214	GLU
1	F	231	TRP
1	F	235	VAL
1	F	273	LEU
1	F	300	PHE
1	F	319	SER
1	F	330	ASN
1	F	350	GLU
1	F	359	LEU
1	F	372	ILE
1	F	403	LEU
1	F	419	ARG
1	F	420	PRO
1	F	424	THR
1	F	506	THR
1	F	582	ARG
1	F	584	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	101	GLY
1	G	106	LYS
1	G	110	GLN
1	G	111	PHE
1	G	166	ASP
1	G	171	LYS
1	G	183	VAL
1	G	187	GLN
1	G	191	PRO
1	G	195	GLU
1	G	201	VAL
1	G	202	THR
1	G	231	TRP
1	G	235	VAL
1	G	273	LEU
1	G	300	PHE
1	G	319	SER
1	G	330	ASN
1	G	350	GLU
1	G	359	LEU
1	G	363	SER
1	G	372	ILE
1	G	403	LEU
1	G	419	ARG
1	G	420	PRO
1	G	424	THR
1	G	582	ARG
1	G	584	PRO
1	H	101	GLY
1	H	106	LYS
1	H	110	GLN
1	H	111	PHE
1	H	166	ASP
1	H	171	LYS
1	H	183	VAL
1	H	187	GLN
1	H	191	PRO
1	H	195	GLU
1	H	201	VAL
1	H	202	THR
1	H	231	TRP
1	H	235	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	273	LEU
1	H	300	PHE
1	H	319	SER
1	H	330	ASN
1	H	350	GLU
1	H	359	LEU
1	H	372	ILE
1	H	403	LEU
1	H	419	ARG
1	H	420	PRO
1	H	424	THR
1	H	582	ARG
1	H	584	PRO
1	H	588	ASN
1	A	36	ASP
1	A	74	VAL
1	A	103	ASP
1	A	134	ARG
1	A	179	CYS
1	A	184	GLY
1	A	189	LEU
1	A	201	VAL
1	A	222	PHE
1	A	250	THR
1	A	251	GLY
1	A	273	LEU
1	A	298	GLY
1	A	308	SER
1	A	317	MET
1	A	363	SER
1	A	371	VAL
1	A	374	CYS
1	A	385	ASP
1	A	386	LEU
1	A	503	PHE
1	A	661	ALA
1	B	36	ASP
1	B	74	VAL
1	B	103	ASP
1	B	134	ARG
1	B	160	LEU
1	B	179	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	184	GLY
1	B	189	LEU
1	B	214	GLU
1	B	222	PHE
1	B	250	THR
1	B	251	GLY
1	B	273	LEU
1	B	298	GLY
1	B	317	MET
1	B	320	GLY
1	B	321	ARG
1	B	371	VAL
1	B	374	CYS
1	B	385	ASP
1	B	386	LEU
1	B	476	CYS
1	B	588	ASN
1	C	36	ASP
1	C	74	VAL
1	C	85	LYS
1	C	134	ARG
1	C	160	LEU
1	C	179	CYS
1	C	184	GLY
1	C	214	GLU
1	C	222	PHE
1	C	230	GLN
1	C	250	THR
1	C	251	GLY
1	C	298	GLY
1	C	308	SER
1	C	317	MET
1	C	371	VAL
1	C	374	CYS
1	C	385	ASP
1	C	386	LEU
1	C	427	ARG
1	C	588	ASN
1	C	643	VAL
1	D	36	ASP
1	D	74	VAL
1	D	103	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	134	ARG
1	D	160	LEU
1	D	179	CYS
1	D	184	GLY
1	D	189	LEU
1	D	213	PHE
1	D	214	GLU
1	D	222	PHE
1	D	250	THR
1	D	251	GLY
1	D	273	LEU
1	D	298	GLY
1	D	317	MET
1	D	320	GLY
1	D	321	ARG
1	D	371	VAL
1	D	374	CYS
1	D	385	ASP
1	D	528	ARG
1	D	588	ASN
1	D	643	VAL
1	E	36	ASP
1	E	74	VAL
1	E	103	ASP
1	E	134	ARG
1	E	160	LEU
1	E	179	CYS
1	E	184	GLY
1	E	189	LEU
1	E	201	VAL
1	E	214	GLU
1	E	222	PHE
1	E	250	THR
1	E	251	GLY
1	E	298	GLY
1	E	308	SER
1	E	317	MET
1	E	320	GLY
1	E	363	SER
1	E	371	VAL
1	E	374	CYS
1	E	385	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	386	LEU
1	E	503	PHE
1	E	528	ARG
1	E	588	ASN
1	E	643	VAL
1	F	36	ASP
1	F	74	VAL
1	F	103	ASP
1	F	134	ARG
1	F	160	LEU
1	F	179	CYS
1	F	184	GLY
1	F	189	LEU
1	F	213	PHE
1	F	222	PHE
1	F	250	THR
1	F	251	GLY
1	F	298	GLY
1	F	308	SER
1	F	317	MET
1	F	320	GLY
1	F	363	SER
1	F	371	VAL
1	F	374	CYS
1	F	385	ASP
1	F	386	LEU
1	F	503	PHE
1	F	588	ASN
1	F	643	VAL
1	F	661	ALA
1	G	36	ASP
1	G	74	VAL
1	G	103	ASP
1	G	134	ARG
1	G	160	LEU
1	G	179	CYS
1	G	184	GLY
1	G	189	LEU
1	G	214	GLU
1	G	222	PHE
1	G	230	GLN
1	G	250	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	251	GLY
1	G	298	GLY
1	G	308	SER
1	G	317	MET
1	G	371	VAL
1	G	374	CYS
1	G	385	ASP
1	G	386	LEU
1	G	588	ASN
1	H	36	ASP
1	H	74	VAL
1	H	103	ASP
1	H	134	ARG
1	H	160	LEU
1	H	179	CYS
1	H	184	GLY
1	H	189	LEU
1	H	222	PHE
1	H	230	GLN
1	H	250	THR
1	H	251	GLY
1	H	298	GLY
1	H	308	SER
1	H	317	MET
1	H	363	SER
1	H	371	VAL
1	H	374	CYS
1	H	385	ASP
1	H	386	LEU
1	A	48	GLN
1	A	49	GLU
1	A	85	LYS
1	A	105	ARG
1	A	115	CYS
1	A	160	LEU
1	A	194	LEU
1	A	213	PHE
1	A	218	GLY
1	A	230	GLN
1	A	234	LYS
1	A	320	GLY
1	A	321	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	333	LEU
1	A	348	GLU
1	A	364	ALA
1	A	409	SER
1	A	507	SER
1	A	508	GLU
1	A	530	VAL
1	A	550	ASN
1	A	583	THR
1	A	587	SER
1	A	597	ALA
1	A	643	VAL
1	B	48	GLN
1	B	49	GLU
1	B	85	LYS
1	B	105	ARG
1	B	115	CYS
1	B	194	LEU
1	B	213	PHE
1	B	218	GLY
1	B	230	GLN
1	B	234	LYS
1	B	308	SER
1	B	333	LEU
1	B	348	GLU
1	B	364	ALA
1	B	409	SER
1	B	427	ARG
1	B	450	GLY
1	B	489	SER
1	B	507	SER
1	B	508	GLU
1	B	530	VAL
1	B	550	ASN
1	B	583	THR
1	B	587	SER
1	B	597	ALA
1	B	643	VAL
1	C	48	GLN
1	C	49	GLU
1	C	103	ASP
1	C	105	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	115	CYS
1	C	189	LEU
1	C	194	LEU
1	C	213	PHE
1	C	234	LYS
1	C	320	GLY
1	C	321	ARG
1	C	333	LEU
1	C	348	GLU
1	C	364	ALA
1	C	409	SER
1	C	450	GLY
1	C	483	LEU
1	C	489	SER
1	C	503	PHE
1	C	508	GLU
1	C	530	VAL
1	C	550	ASN
1	C	583	THR
1	C	587	SER
1	C	597	ALA
1	D	48	GLN
1	D	49	GLU
1	D	85	LYS
1	D	105	ARG
1	D	115	CYS
1	D	194	LEU
1	D	230	GLN
1	D	234	LYS
1	D	308	SER
1	D	333	LEU
1	D	348	GLU
1	D	364	ALA
1	D	409	SER
1	D	450	GLY
1	D	483	LEU
1	D	503	PHE
1	D	508	GLU
1	D	530	VAL
1	D	550	ASN
1	D	583	THR
1	D	587	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	597	ALA
1	E	48	GLN
1	E	49	GLU
1	E	85	LYS
1	E	115	CYS
1	E	194	LEU
1	E	213	PHE
1	E	230	GLN
1	E	234	LYS
1	E	321	ARG
1	E	333	LEU
1	E	348	GLU
1	E	364	ALA
1	E	409	SER
1	E	427	ARG
1	E	483	LEU
1	E	507	SER
1	E	508	GLU
1	E	530	VAL
1	E	550	ASN
1	E	583	THR
1	E	587	SER
1	F	49	GLU
1	F	85	LYS
1	F	105	ARG
1	F	115	CYS
1	F	194	LEU
1	F	218	GLY
1	F	230	GLN
1	F	234	LYS
1	F	321	ARG
1	F	333	LEU
1	F	348	GLU
1	F	364	ALA
1	F	409	SER
1	F	489	SER
1	F	507	SER
1	F	508	GLU
1	F	528	ARG
1	F	530	VAL
1	F	550	ASN
1	F	583	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	587	SER
1	G	48	GLN
1	G	49	GLU
1	G	85	LYS
1	G	194	LEU
1	G	213	PHE
1	G	218	GLY
1	G	234	LYS
1	G	320	GLY
1	G	321	ARG
1	G	333	LEU
1	G	348	GLU
1	G	409	SER
1	G	530	VAL
1	G	550	ASN
1	G	583	THR
1	G	587	SER
1	G	597	ALA
1	H	48	GLN
1	H	49	GLU
1	H	85	LYS
1	H	105	ARG
1	H	115	CYS
1	H	194	LEU
1	H	214	GLU
1	H	234	LYS
1	H	320	GLY
1	H	321	ARG
1	H	333	LEU
1	H	348	GLU
1	H	364	ALA
1	H	409	SER
1	H	427	ARG
1	H	450	GLY
1	H	530	VAL
1	H	550	ASN
1	H	583	THR
1	H	587	SER
1	H	597	ALA
1	A	121	PRO
1	A	144	ARG
1	A	199	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	284	HIS
1	A	418	LYS
1	A	427	ARG
1	A	450	GLY
1	A	483	LEU
1	A	489	SER
1	A	549	ARG
1	A	629	VAL
1	B	121	PRO
1	B	144	ARG
1	B	199	TYR
1	B	284	HIS
1	B	309	LEU
1	B	418	LYS
1	B	503	PHE
1	B	549	ARG
1	B	629	VAL
1	C	78	GLU
1	C	121	PRO
1	C	144	ARG
1	C	218	GLY
1	C	284	HIS
1	C	418	LYS
1	C	507	SER
1	C	549	ARG
1	C	629	VAL
1	D	121	PRO
1	D	144	ARG
1	D	218	GLY
1	D	418	LYS
1	D	427	ARG
1	D	489	SER
1	D	507	SER
1	D	549	ARG
1	D	629	VAL
1	D	644	VAL
1	E	105	ARG
1	E	121	PRO
1	E	144	ARG
1	E	218	GLY
1	E	418	LYS
1	E	450	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	489	SER
1	E	549	ARG
1	E	597	ALA
1	E	629	VAL
1	F	48	GLN
1	F	144	ARG
1	F	418	LYS
1	F	427	ARG
1	F	450	GLY
1	F	483	LEU
1	F	549	ARG
1	F	597	ALA
1	F	629	VAL
1	G	105	ARG
1	G	115	CYS
1	G	121	PRO
1	G	144	ARG
1	G	364	ALA
1	G	418	LYS
1	G	427	ARG
1	G	549	ARG
1	G	629	VAL
1	H	121	PRO
1	H	144	ARG
1	H	213	PHE
1	H	218	GLY
1	H	284	HIS
1	H	309	LEU
1	H	418	LYS
1	H	549	ARG
1	H	629	VAL
1	A	72	ASN
1	A	78	GLU
1	A	220	ARG
1	A	227	GLN
1	A	261	THR
1	A	309	LEU
1	A	445	ALA
1	A	644	VAL
1	B	72	ASN
1	B	78	GLU
1	B	220	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	261	THR
1	B	388	PHE
1	B	483	LEU
1	B	644	VAL
1	C	72	ASN
1	C	220	ARG
1	C	261	THR
1	C	445	ALA
1	C	644	VAL
1	D	78	GLU
1	D	220	ARG
1	D	261	THR
1	D	284	HIS
1	D	309	LEU
1	D	388	PHE
1	D	445	ALA
1	E	35	GLN
1	E	78	GLU
1	E	220	ARG
1	E	261	THR
1	E	284	HIS
1	E	644	VAL
1	F	78	GLU
1	F	121	PRO
1	F	199	TYR
1	F	220	ARG
1	F	261	THR
1	F	284	HIS
1	F	388	PHE
1	F	431	GLY
1	F	445	ALA
1	F	644	VAL
1	G	72	ASN
1	G	78	GLU
1	G	193	LEU
1	G	220	ARG
1	G	227	GLN
1	G	261	THR
1	G	284	HIS
1	G	309	LEU
1	G	450	GLY
1	H	78	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	220	ARG
1	H	261	THR
1	H	431	GLY
1	H	445	ALA
1	A	35	GLN
1	A	388	PHE
1	A	431	GLY
1	A	626	SER
1	A	665	VAL
1	B	227	GLN
1	B	431	GLY
1	B	577	ARG
1	B	626	SER
1	B	665	VAL
1	C	193	LEU
1	C	199	TYR
1	C	227	GLN
1	C	388	PHE
1	C	431	GLY
1	C	577	ARG
1	C	626	SER
1	C	665	VAL
1	D	199	TYR
1	D	227	GLN
1	D	626	SER
1	D	665	VAL
1	E	72	ASN
1	E	431	GLY
1	E	445	ALA
1	E	577	ARG
1	E	626	SER
1	E	665	VAL
1	F	72	ASN
1	F	227	GLN
1	F	626	SER
1	F	665	VAL
1	G	388	PHE
1	G	577	ARG
1	H	72	ASN
1	H	199	TYR
1	A	407	PRO
1	A	577	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	407	PRO
1	D	431	GLY
1	F	577	ARG
1	G	407	PRO
1	G	431	GLY
1	G	626	SER
1	H	227	GLN
1	H	407	PRO
1	H	577	ARG
1	H	626	SER
1	B	165	ILE
1	B	407	PRO
1	C	407	PRO
1	D	165	ILE
1	D	577	ARG
1	E	227	GLN
1	E	407	PRO
1	F	165	ILE
1	F	407	PRO
1	A	165	ILE
1	B	387	ILE
1	C	165	ILE
1	E	165	ILE
1	F	387	ILE
1	G	165	ILE
1	H	165	ILE
1	B	260	PRO
1	D	260	PRO
1	D	295	PRO
1	D	387	ILE
1	E	295	PRO
1	E	387	ILE
1	F	260	PRO
1	F	295	PRO
1	G	260	PRO
1	H	260	PRO
1	H	295	PRO
1	A	260	PRO
1	A	295	PRO
1	B	295	PRO
1	C	260	PRO
1	C	295	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	387	ILE

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	563/609 (92%)	520 (92%)	43 (8%)	13 45
1	B	563/609 (92%)	521 (92%)	42 (8%)	13 45
1	C	563/609 (92%)	520 (92%)	43 (8%)	13 45
1	D	563/609 (92%)	519 (92%)	44 (8%)	12 44
1	E	563/609 (92%)	520 (92%)	43 (8%)	13 45
1	F	563/609 (92%)	521 (92%)	42 (8%)	13 45
1	G	488/609 (80%)	456 (93%)	32 (7%)	16 51
1	H	488/609 (80%)	455 (93%)	33 (7%)	16 50
All	All	4354/4872 (89%)	4032 (93%)	322 (7%)	13 46

All (322) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	51	SER
1	A	114	CYS
1	A	123	ARG
1	A	134	ARG
1	A	145	ASP
1	A	150	ASN
1	A	210	THR
1	A	234	LYS
1	A	248	ASP
1	A	263	ASN
1	A	266	SER
1	A	278	GLN
1	A	301	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	313	SER
1	A	314	VAL
1	A	330	ASN
1	A	357	SER
1	A	390	PHE
1	A	408	GLU
1	A	422	THR
1	A	424	THR
1	A	429	VAL
1	A	434	TRP
1	A	436	THR
1	A	444	CYS
1	A	448	LEU
1	A	453	THR
1	A	455	MET
1	A	479	LEU
1	A	490	ILE
1	A	494	LEU
1	A	497	TYR
1	A	505	ILE
1	A	517	MET
1	A	535	ASP
1	A	564	GLU
1	A	590	MET
1	A	610	ASP
1	A	616	VAL
1	A	654	LEU
1	A	659	LYS
1	A	662	CYS
1	B	16	GLU
1	B	51	SER
1	B	114	CYS
1	B	123	ARG
1	B	134	ARG
1	B	145	ASP
1	B	150	ASN
1	B	210	THR
1	B	234	LYS
1	B	248	ASP
1	B	263	ASN
1	B	266	SER
1	B	278	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	301	GLN
1	B	313	SER
1	B	330	ASN
1	B	339	TRP
1	B	357	SER
1	B	390	PHE
1	B	408	GLU
1	B	422	THR
1	B	424	THR
1	B	429	VAL
1	B	434	TRP
1	B	436	THR
1	B	444	CYS
1	B	448	LEU
1	B	453	THR
1	B	455	MET
1	B	479	LEU
1	B	490	ILE
1	B	494	LEU
1	B	497	TYR
1	B	505	ILE
1	B	517	MET
1	B	535	ASP
1	B	564	GLU
1	B	590	MET
1	B	616	VAL
1	B	654	LEU
1	B	659	LYS
1	B	662	CYS
1	C	16	GLU
1	C	51	SER
1	C	114	CYS
1	C	123	ARG
1	C	134	ARG
1	C	145	ASP
1	C	150	ASN
1	C	210	THR
1	C	234	LYS
1	C	248	ASP
1	C	263	ASN
1	C	266	SER
1	C	278	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	301	GLN
1	C	313	SER
1	C	314	VAL
1	C	330	ASN
1	C	357	SER
1	C	390	PHE
1	C	408	GLU
1	C	422	THR
1	C	424	THR
1	C	429	VAL
1	C	434	TRP
1	C	436	THR
1	C	444	CYS
1	C	448	LEU
1	C	453	THR
1	C	455	MET
1	C	479	LEU
1	C	490	ILE
1	C	497	TYR
1	C	505	ILE
1	C	517	MET
1	C	564	GLU
1	C	590	MET
1	C	602	GLU
1	C	606	ILE
1	C	610	ASP
1	C	616	VAL
1	C	654	LEU
1	C	659	LYS
1	C	662	CYS
1	D	16	GLU
1	D	51	SER
1	D	114	CYS
1	D	123	ARG
1	D	134	ARG
1	D	145	ASP
1	D	150	ASN
1	D	210	THR
1	D	219	PHE
1	D	234	LYS
1	D	248	ASP
1	D	263	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	266	SER
1	D	278	GLN
1	D	301	GLN
1	D	313	SER
1	D	330	ASN
1	D	339	TRP
1	D	357	SER
1	D	390	PHE
1	D	408	GLU
1	D	422	THR
1	D	424	THR
1	D	429	VAL
1	D	434	TRP
1	D	436	THR
1	D	444	CYS
1	D	448	LEU
1	D	453	THR
1	D	455	MET
1	D	479	LEU
1	D	490	ILE
1	D	494	LEU
1	D	497	TYR
1	D	505	ILE
1	D	517	MET
1	D	564	GLU
1	D	590	MET
1	D	602	GLU
1	D	610	ASP
1	D	616	VAL
1	D	654	LEU
1	D	659	LYS
1	D	662	CYS
1	E	16	GLU
1	E	51	SER
1	E	114	CYS
1	E	123	ARG
1	E	134	ARG
1	E	145	ASP
1	E	150	ASN
1	E	210	THR
1	E	219	PHE
1	E	234	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	248	ASP
1	E	263	ASN
1	E	266	SER
1	E	278	GLN
1	E	301	GLN
1	E	313	SER
1	E	314	VAL
1	E	330	ASN
1	E	357	SER
1	E	390	PHE
1	E	408	GLU
1	E	422	THR
1	E	424	THR
1	E	429	VAL
1	E	434	TRP
1	E	436	THR
1	E	444	CYS
1	E	448	LEU
1	E	453	THR
1	E	455	MET
1	E	479	LEU
1	E	490	ILE
1	E	497	TYR
1	E	505	ILE
1	E	517	MET
1	E	564	GLU
1	E	590	MET
1	E	606	ILE
1	E	610	ASP
1	E	616	VAL
1	E	654	LEU
1	E	659	LYS
1	E	662	CYS
1	F	16	GLU
1	F	51	SER
1	F	114	CYS
1	F	123	ARG
1	F	134	ARG
1	F	145	ASP
1	F	150	ASN
1	F	210	THR
1	F	219	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	234	LYS
1	F	248	ASP
1	F	263	ASN
1	F	266	SER
1	F	278	GLN
1	F	301	GLN
1	F	313	SER
1	F	330	ASN
1	F	339	TRP
1	F	357	SER
1	F	390	PHE
1	F	408	GLU
1	F	422	THR
1	F	424	THR
1	F	429	VAL
1	F	434	TRP
1	F	444	CYS
1	F	448	LEU
1	F	453	THR
1	F	455	MET
1	F	479	LEU
1	F	490	ILE
1	F	497	TYR
1	F	505	ILE
1	F	517	MET
1	F	564	GLU
1	F	590	MET
1	F	602	GLU
1	F	610	ASP
1	F	616	VAL
1	F	654	LEU
1	F	659	LYS
1	F	662	CYS
1	G	16	GLU
1	G	51	SER
1	G	114	CYS
1	G	123	ARG
1	G	134	ARG
1	G	145	ASP
1	G	150	ASN
1	G	210	THR
1	G	234	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	248	ASP
1	G	263	ASN
1	G	266	SER
1	G	278	GLN
1	G	301	GLN
1	G	313	SER
1	G	330	ASN
1	G	357	SER
1	G	390	PHE
1	G	408	GLU
1	G	422	THR
1	G	424	THR
1	G	429	VAL
1	G	434	TRP
1	G	444	CYS
1	G	448	LEU
1	G	453	THR
1	G	455	MET
1	G	564	GLU
1	G	590	MET
1	G	602	GLU
1	G	610	ASP
1	G	616	VAL
1	H	16	GLU
1	H	51	SER
1	H	114	CYS
1	H	123	ARG
1	H	134	ARG
1	H	145	ASP
1	H	150	ASN
1	H	210	THR
1	H	234	LYS
1	H	248	ASP
1	H	263	ASN
1	H	266	SER
1	H	278	GLN
1	H	301	GLN
1	H	313	SER
1	H	330	ASN
1	H	339	TRP
1	H	357	SER
1	H	390	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	408	GLU
1	H	422	THR
1	H	424	THR
1	H	429	VAL
1	H	434	TRP
1	H	436	THR
1	H	444	CYS
1	H	448	LEU
1	H	453	THR
1	H	455	MET
1	H	535	ASP
1	H	564	GLU
1	H	590	MET
1	H	616	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	143	HIS
1	A	196	GLN
1	A	263	ASN
1	A	264	HIS
1	A	294	ASN
1	A	301	GLN
1	A	332	ASN
1	A	449	GLN
1	A	462	ASN
1	A	470	ASN
1	A	478	GLN
1	A	491	GLN
1	A	500	GLN
1	A	541	GLN
1	A	550	ASN
1	A	651	GLN
1	B	70	HIS
1	B	109	ASN
1	B	143	HIS
1	B	196	GLN
1	B	263	ASN
1	B	264	HIS
1	B	294	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	301	GLN
1	B	332	ASN
1	B	449	GLN
1	B	451	GLN
1	B	470	ASN
1	B	491	GLN
1	B	500	GLN
1	B	550	ASN
1	B	651	GLN
1	C	70	HIS
1	C	143	HIS
1	C	196	GLN
1	C	263	ASN
1	C	294	ASN
1	C	301	GLN
1	C	332	ASN
1	C	342	GLN
1	C	449	GLN
1	C	462	ASN
1	C	491	GLN
1	C	500	GLN
1	C	541	GLN
1	C	550	ASN
1	C	651	GLN
1	D	109	ASN
1	D	143	HIS
1	D	196	GLN
1	D	263	ASN
1	D	264	HIS
1	D	294	ASN
1	D	301	GLN
1	D	332	ASN
1	D	449	GLN
1	D	478	GLN
1	D	491	GLN
1	D	500	GLN
1	D	550	ASN
1	D	647	GLN
1	D	651	GLN
1	E	70	HIS
1	E	109	ASN
1	E	143	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	196	GLN
1	E	263	ASN
1	E	264	HIS
1	E	294	ASN
1	E	301	GLN
1	E	332	ASN
1	E	342	GLN
1	E	449	GLN
1	E	462	ASN
1	E	478	GLN
1	E	491	GLN
1	E	500	GLN
1	E	541	GLN
1	E	550	ASN
1	E	651	GLN
1	F	70	HIS
1	F	109	ASN
1	F	143	HIS
1	F	196	GLN
1	F	263	ASN
1	F	264	HIS
1	F	294	ASN
1	F	301	GLN
1	F	332	ASN
1	F	449	GLN
1	F	457	ASN
1	F	470	ASN
1	F	478	GLN
1	F	491	GLN
1	F	500	GLN
1	F	550	ASN
1	F	599	GLN
1	F	651	GLN
1	G	84	GLN
1	G	109	ASN
1	G	143	HIS
1	G	196	GLN
1	G	263	ASN
1	G	294	ASN
1	G	301	GLN
1	G	332	ASN
1	G	449	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	550	ASN
1	G	611	GLN
1	H	70	HIS
1	H	84	GLN
1	H	109	ASN
1	H	143	HIS
1	H	196	GLN
1	H	263	ASN
1	H	264	HIS
1	H	294	ASN
1	H	301	GLN
1	H	332	ASN
1	H	449	GLN
1	H	470	ASN
1	H	611	GLN

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

There are no RNA molecules in this entry.

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

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

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

There are no monosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	622/676 (92%)	0.26	42 (6%) 17 10	76, 189, 275, 337	0
1	B	622/676 (92%)	0.30	42 (6%) 17 10	71, 191, 274, 336	0
1	C	622/676 (92%)	0.34	30 (4%) 30 19	58, 188, 275, 327	0
1	D	622/676 (92%)	0.25	50 (8%) 12 7	85, 194, 278, 327	0
1	E	622/676 (92%)	0.37	36 (5%) 23 13	74, 190, 274, 330	0
1	F	622/676 (92%)	0.30	49 (7%) 12 7	93, 200, 283, 331	0
1	G	541/676 (80%)	0.42	62 (11%) 4 3	96, 214, 302, 387	0
1	H	541/676 (80%)	0.32	44 (8%) 12 7	79, 194, 293, 423	0
All	All	4814/5408 (89%)	0.32	355 (7%) 14 9	58, 195, 283, 423	0

All (355) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	93	LEU	11.5
1	G	571	TYR	9.8
1	F	40	GLN	8.2
1	H	47	ARG	8.0
1	E	199	TYR	7.9
1	F	155	PRO	7.8
1	A	65	MET	7.3
1	A	41	VAL	7.1
1	E	17	MET	6.8
1	G	454	SER	6.6
1	H	537	MET	6.6
1	D	87	ALA	6.2
1	B	47	ARG	6.1
1	D	65	MET	6.0
1	H	388	PHE	5.8
1	G	389	LEU	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	510	LEU	5.7
1	G	390	PHE	5.7
1	D	93	LEU	5.6
1	F	54	ASN	5.6
1	F	298	GLY	5.5
1	B	39	GLU	5.4
1	F	571	TYR	5.3
1	B	41	VAL	5.3
1	G	93	LEU	5.2
1	C	93	LEU	5.2
1	C	89	ASN	5.1
1	G	327	VAL	5.0
1	F	497	TYR	5.0
1	D	437	ILE	4.9
1	F	65	MET	4.9
1	G	41	VAL	4.9
1	F	41	VAL	4.9
1	F	199	TYR	4.9
1	A	172	GLU	4.9
1	G	65	MET	4.8
1	B	42	ALA	4.8
1	D	625	LEU	4.7
1	E	571	TYR	4.7
1	G	469	LYS	4.7
1	G	351	GLN	4.7
1	H	571	TYR	4.7
1	A	40	GLN	4.6
1	D	654	LEU	4.6
1	H	528	ARG	4.6
1	E	41	VAL	4.6
1	D	40	GLN	4.5
1	D	17	MET	4.5
1	H	41	VAL	4.5
1	H	31	ARG	4.4
1	G	236	ARG	4.4
1	B	666	ARG	4.4
1	F	32	TRP	4.4
1	D	571	TYR	4.3
1	H	40	GLN	4.3
1	H	42	ALA	4.2
1	G	388	PHE	4.2
1	C	92	PRO	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	640	GLU	4.0
1	E	47	ARG	4.0
1	E	32	TRP	4.0
1	H	39	GLU	4.0
1	D	94	LEU	4.0
1	A	472	MET	4.0
1	H	93	LEU	3.9
1	D	166	ASP	3.9
1	B	17	MET	3.9
1	H	533	LEU	3.9
1	H	159	ARG	3.9
1	D	608	ILE	3.8
1	E	244	VAL	3.8
1	B	87	ALA	3.8
1	E	40	GLN	3.7
1	G	360	ALA	3.7
1	E	39	GLU	3.7
1	A	506	THR	3.7
1	H	544	SER	3.7
1	C	17	MET	3.7
1	G	437	ILE	3.7
1	D	578	PRO	3.7
1	A	236	ARG	3.7
1	A	367	LEU	3.6
1	G	40	GLN	3.6
1	D	80	PRO	3.6
1	G	402	SER	3.6
1	F	481	ALA	3.6
1	F	88	PRO	3.6
1	D	141	ILE	3.6
1	G	636	MET	3.6
1	B	93	LEU	3.6
1	B	353	LEU	3.5
1	F	365	GLN	3.5
1	C	244	VAL	3.5
1	A	77	ARG	3.5
1	F	73	VAL	3.5
1	F	93	LEU	3.5
1	B	40	GLN	3.5
1	B	497	TYR	3.5
1	F	61	GLU	3.5
1	H	96	MET	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	157	PRO	3.4
1	C	41	VAL	3.4
1	H	30	LEU	3.4
1	H	95	ALA	3.4
1	A	503	PHE	3.4
1	B	394	LYS	3.4
1	F	39	GLU	3.4
1	H	367	LEU	3.4
1	H	29	VAL	3.4
1	C	32	TRP	3.4
1	G	47	ARG	3.4
1	F	615	THR	3.4
1	A	141	ILE	3.4
1	A	176	GLY	3.4
1	B	43	ILE	3.4
1	G	370	TYR	3.4
1	C	629	VAL	3.3
1	H	37	THR	3.3
1	B	485	PHE	3.3
1	E	198	LYS	3.3
1	B	354	LEU	3.3
1	C	96	MET	3.3
1	G	470	ASN	3.3
1	F	514	TRP	3.3
1	A	39	GLU	3.3
1	G	404	PRO	3.2
1	H	38	GLY	3.2
1	F	176	GLY	3.2
1	H	32	TRP	3.2
1	B	327	VAL	3.2
1	B	388	PHE	3.2
1	F	666	ARG	3.1
1	A	62	ILE	3.1
1	E	384	GLY	3.1
1	F	299	CYS	3.1
1	D	164	ILE	3.1
1	H	88	PRO	3.1
1	E	160	LEU	3.1
1	G	353	LEU	3.1
1	G	401	ILE	3.1
1	G	603	LYS	3.1
1	C	94	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	41	VAL	3.1
1	D	197	LYS	3.1
1	A	384	GLY	3.1
1	D	514	TRP	3.1
1	G	45	GLN	3.0
1	B	32	TRP	3.0
1	D	85	LYS	3.0
1	E	629	VAL	3.0
1	F	37	THR	3.0
1	B	571	TYR	3.0
1	F	38	GLY	3.0
1	H	65	MET	3.0
1	F	200	THR	3.0
1	G	46	CYS	3.0
1	B	367	LEU	2.9
1	D	21	LEU	2.9
1	E	61	GLU	2.9
1	H	635	LEU	2.9
1	G	365	GLN	2.9
1	D	510	LEU	2.9
1	G	473	THR	2.9
1	F	197	LYS	2.9
1	B	95	ALA	2.9
1	C	77	ARG	2.9
1	F	51	SER	2.9
1	A	175	GLN	2.9
1	G	39	GLU	2.9
1	B	37	THR	2.9
1	E	563	LEU	2.9
1	E	175	GLN	2.9
1	H	61	GLU	2.8
1	C	571	TYR	2.8
1	H	634	ASN	2.8
1	B	21	LEU	2.8
1	F	87	ALA	2.8
1	A	388	PHE	2.8
1	B	30	LEU	2.8
1	G	455	MET	2.8
1	D	354	LEU	2.8
1	A	87	ALA	2.8
1	C	153	LEU	2.8
1	D	525	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	45	GLN	2.8
1	H	541	GLN	2.8
1	D	236	ARG	2.8
1	A	507	SER	2.8
1	G	141	ILE	2.8
1	D	46	CYS	2.8
1	H	370	TYR	2.8
1	D	447	LEU	2.8
1	G	468	LYS	2.7
1	D	198	LYS	2.7
1	A	170	ALA	2.7
1	E	295	PRO	2.7
1	H	454	SER	2.7
1	G	30	LEU	2.7
1	A	171	LYS	2.7
1	F	366	PRO	2.7
1	G	625	LEU	2.7
1	C	278	GLN	2.7
1	D	172	GLU	2.7
1	A	447	LEU	2.7
1	H	475	GLU	2.7
1	A	58	TRP	2.6
1	E	294	ASN	2.6
1	F	158	GLN	2.6
1	C	508	GLU	2.6
1	A	536	LYS	2.6
1	G	38	GLY	2.6
1	G	80	PRO	2.6
1	E	57	ARG	2.6
1	F	233	GLY	2.6
1	A	199	TYR	2.6
1	H	43	ILE	2.6
1	G	535	ASP	2.6
1	G	367	LEU	2.6
1	D	600	SER	2.6
1	G	366	PRO	2.6
1	H	551	PRO	2.6
1	H	56	GLU	2.6
1	D	388	PHE	2.6
1	C	415	GLN	2.5
1	D	58	TRP	2.5
1	F	513	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	533	LEU	2.5
1	E	284	HIS	2.5
1	F	205	TYR	2.5
1	F	590	MET	2.5
1	G	433	ILE	2.5
1	F	394	LYS	2.5
1	B	68	LEU	2.5
1	C	279	CYS	2.5
1	A	69	ASN	2.5
1	F	367	LEU	2.5
1	B	640	GLU	2.5
1	E	567	ALA	2.5
1	B	447	LEU	2.4
1	A	61	GLU	2.4
1	C	515	ARG	2.4
1	F	175	GLN	2.4
1	F	156	GLY	2.4
1	A	21	LEU	2.4
1	D	77	ARG	2.4
1	H	94	LEU	2.4
1	B	38	GLY	2.4
1	B	551	PRO	2.4
1	A	370	TYR	2.4
1	C	518	GLU	2.4
1	D	62	ILE	2.4
1	D	208	PHE	2.4
1	G	94	LEU	2.4
1	F	654	LEU	2.4
1	G	55	ARG	2.4
1	G	73	VAL	2.4
1	C	292	PRO	2.4
1	A	80	PRO	2.4
1	D	170	ALA	2.4
1	F	567	ALA	2.4
1	D	81	ASP	2.4
1	G	32	TRP	2.3
1	D	593	LEU	2.3
1	E	507	SER	2.3
1	B	94	LEU	2.3
1	G	540	LEU	2.3
1	A	44	LYS	2.3
1	F	46	CYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	290	THR	2.3
1	C	293	GLN	2.3
1	D	42	ALA	2.3
1	G	607	LEU	2.3
1	C	469	LYS	2.3
1	E	469	LYS	2.3
1	A	88	PRO	2.3
1	F	52	PRO	2.3
1	E	550	ASN	2.3
1	E	291	ASP	2.3
1	B	629	VAL	2.3
1	B	386	LEU	2.3
1	C	370	TYR	2.3
1	G	394	LYS	2.3
1	C	305	SER	2.3
1	E	482	LYS	2.3
1	F	42	ALA	2.3
1	C	648	GLU	2.2
1	B	454	SER	2.2
1	H	327	VAL	2.2
1	G	352	GLU	2.2
1	C	88	PRO	2.2
1	D	60	LEU	2.2
1	H	632	VAL	2.2
1	H	453	THR	2.2
1	F	591	VAL	2.2
1	G	205	TYR	2.2
1	A	42	ALA	2.2
1	E	625	LEU	2.2
1	H	34	HIS	2.2
1	D	39	GLU	2.2
1	A	371	VAL	2.2
1	D	415	GLN	2.2
1	D	327	VAL	2.2
1	G	472	MET	2.2
1	D	541	GLN	2.2
1	A	86	LEU	2.2
1	E	53	LYS	2.2
1	G	529	GLU	2.2
1	E	415	GLN	2.2
1	G	451	GLN	2.2
1	B	80	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	327	VAL	2.2
1	A	571	TYR	2.2
1	B	494	LEU	2.2
1	E	155	PRO	2.2
1	C	54	ASN	2.2
1	D	650	ARG	2.2
1	G	303	LEU	2.2
1	E	504	GLY	2.1
1	F	593	LEU	2.1
1	G	604	ARG	2.1
1	H	160	LEU	2.1
1	G	629	VAL	2.1
1	A	327	VAL	2.1
1	H	44	LYS	2.1
1	D	88	PRO	2.1
1	H	153	LEU	2.1
1	A	143	HIS	2.1
1	G	406	HIS	2.1
1	D	479	LEU	2.1
1	A	366	PRO	2.1
1	B	34	HIS	2.1
1	G	166	ASP	2.1
1	B	472	MET	2.1
1	C	294	ASN	2.1
1	A	96	MET	2.1
1	E	541	GLN	2.1
1	G	393	ARG	2.1
1	H	78	GLU	2.1
1	A	92	PRO	2.1
1	B	473	THR	2.1
1	E	393	ARG	2.1
1	B	236	ARG	2.0
1	D	367	LEU	2.0
1	E	159	ARG	2.0
1	G	168	GLY	2.0
1	F	172	GLU	2.0
1	B	326	PRO	2.0
1	E	77	ARG	2.0
1	E	292	PRO	2.0
1	D	96	MET	2.0
1	B	559	THR	2.0
1	G	57	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	615	THR	2.0
1	B	521	VAL	2.0
1	G	452	ARG	2.0

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

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

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

There are no monosaccharides 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.