



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 17, 2017 – 04:33 PM EDT

PDB ID : 4BIJ
EMDB ID: : EMD-2355
Title : Threading model of T7 large terminase
Authors : Dauden, M.I.; Martin-Benito, J.; Sanchez-Ferrero, J.C.; Pulido-Cid, M.;
Valpuesta, J.M.; Carrascosa, J.L.
Deposited on : unknown
Resolution : 16.00 Å(reported)
Based on PDB ID : 3CPE

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

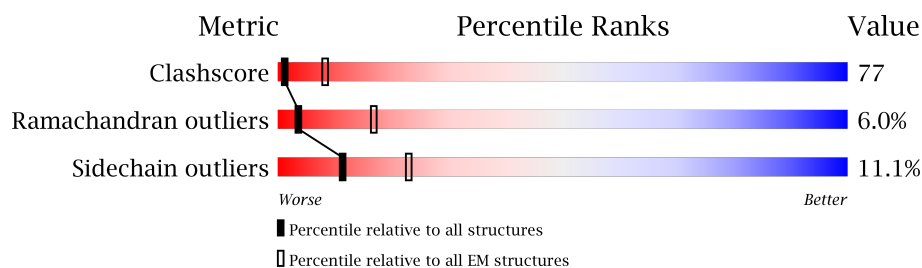
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 16.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	476	
1	B	476	
1	C	476	
1	D	476	
1	E	476	

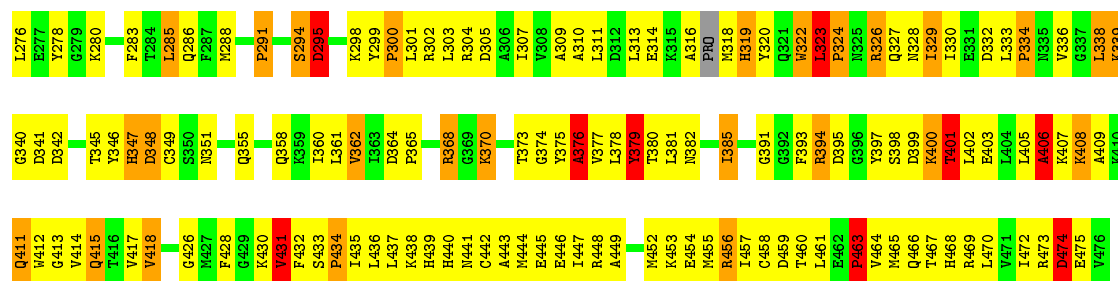
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18855 atoms, of which 0 are hydrogens and 0 are deuteriums.

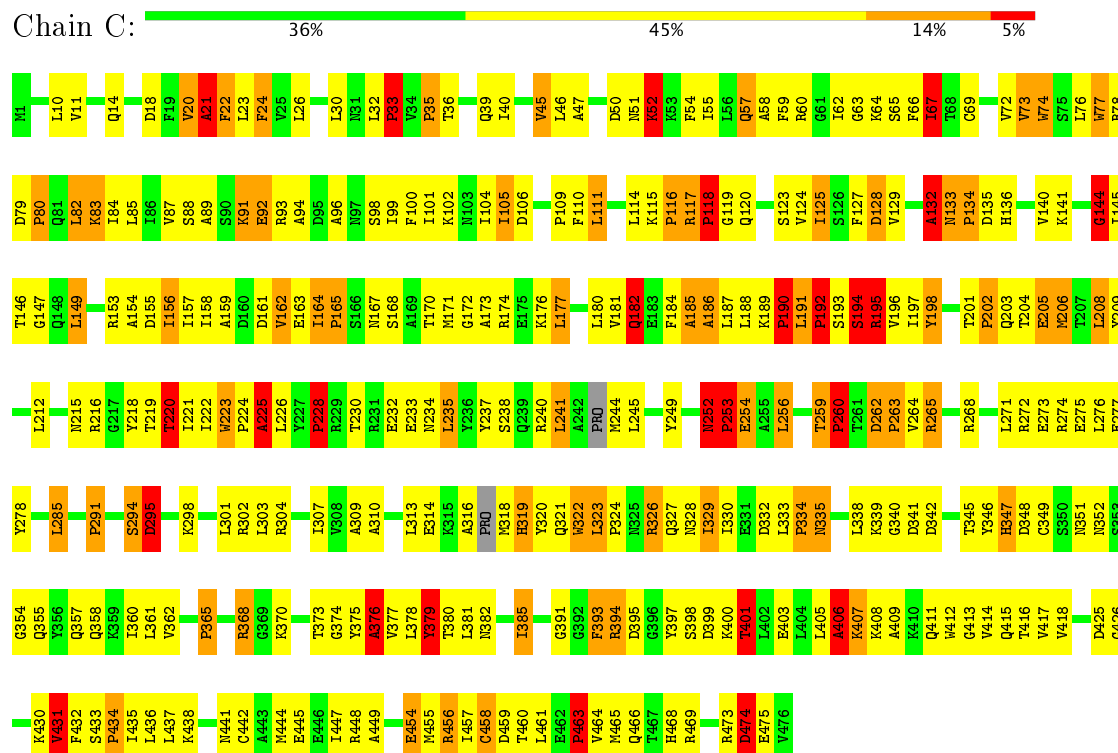
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA MATURASE B.

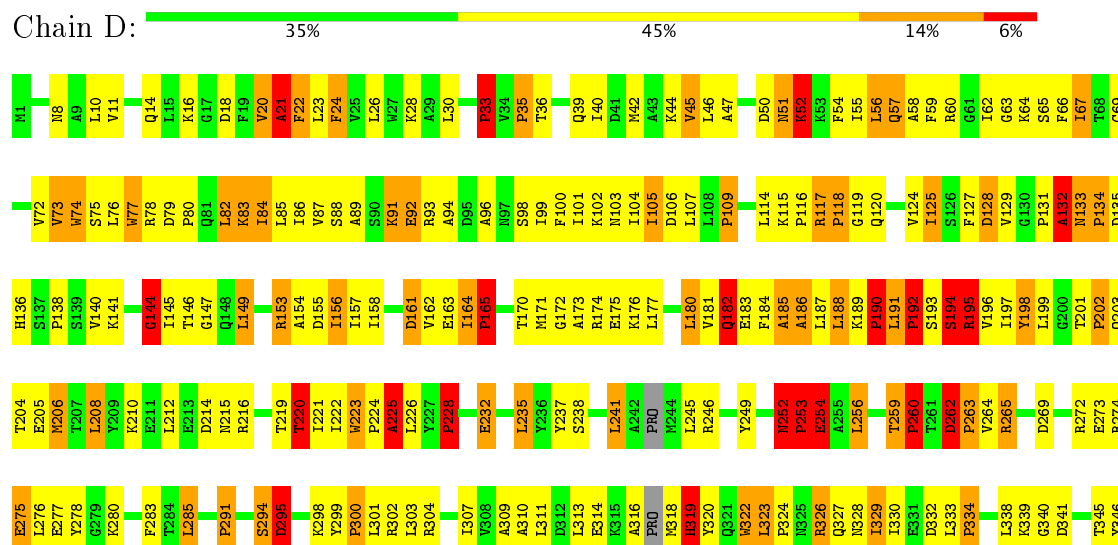
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	474	Total	C	N	O	S	0	0
			3771	2402	648	703	18		
1	B	474	Total	C	N	O	S	0	0
			3771	2402	648	703	18		
1	C	474	Total	C	N	O	S	0	0
			3771	2402	648	703	18		
1	D	474	Total	C	N	O	S	0	0
			3771	2402	648	703	18		
1	E	474	Total	C	N	O	S	0	0
			3771	2402	648	703	18		

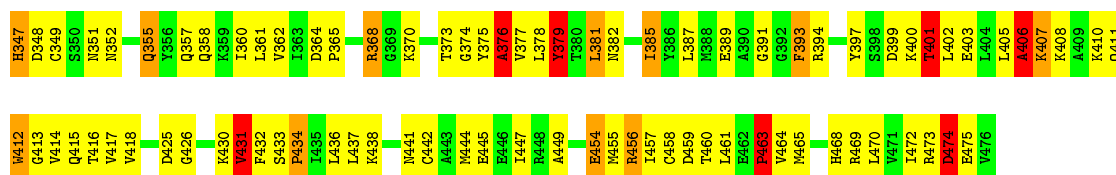


• Molecule 1: DNA MATURASE B



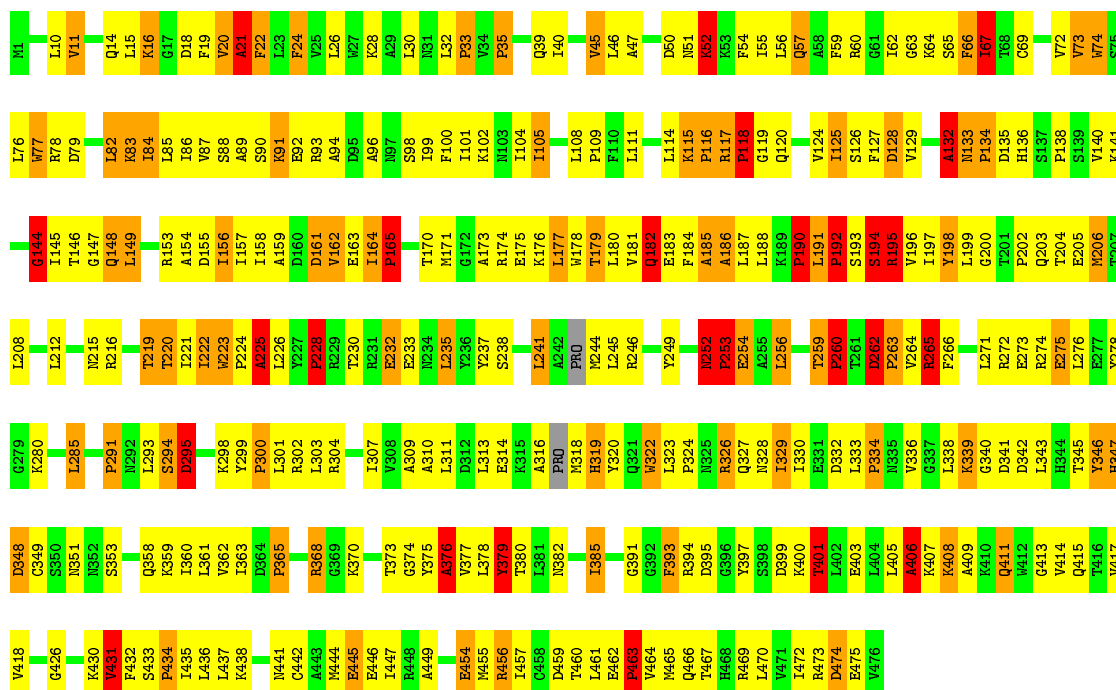
• Molecule 1: DNA MATURASE B





• Molecule 1: DNA MATURASE B

Chain E: 35% 43% 16% 5%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	3650	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PLATE	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	100	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	67000	Depositor
Image detector	FEI EAGLE (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	1.07	22/3850 (0.6%)	1.57	92/5212 (1.8%)
1	B	1.08	22/3850 (0.6%)	1.57	96/5212 (1.8%)
1	C	1.06	23/3850 (0.6%)	1.56	92/5212 (1.8%)
1	D	1.03	22/3850 (0.6%)	1.56	96/5212 (1.8%)
1	E	1.11	22/3850 (0.6%)	1.57	95/5212 (1.8%)
All	All	1.07	111/19250 (0.6%)	1.57	471/26060 (1.8%)

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	13
1	B	0	14
1	C	0	14
1	D	0	14
1	E	0	13
All	All	0	68

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	291	PRO	N-CD	-23.77	1.14	1.47
1	B	134	PRO	N-CD	20.15	1.76	1.47
1	E	300	PRO	N-CD	19.45	1.75	1.47
1	C	291	PRO	N-CD	-19.44	1.20	1.47
1	B	291	PRO	N-CD	-19.19	1.21	1.47
1	E	134	PRO	N-CD	19.02	1.74	1.47
1	A	291	PRO	N-CD	-17.56	1.23	1.47
1	A	134	PRO	N-CD	17.18	1.72	1.47
1	D	291	PRO	N-CD	-16.88	1.24	1.47
1	C	134	PRO	N-CD	16.13	1.70	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	434	PRO	N-CD	15.65	1.69	1.47
1	D	300	PRO	N-CD	15.54	1.69	1.47
1	B	434	PRO	N-CD	15.18	1.69	1.47
1	D	434	PRO	N-CD	14.48	1.68	1.47
1	A	434	PRO	N-CD	14.41	1.68	1.47
1	E	116	PRO	N-CD	14.01	1.67	1.47
1	E	434	PRO	N-CD	13.64	1.67	1.47
1	B	116	PRO	N-CD	12.91	1.66	1.47
1	A	300	PRO	N-CD	12.89	1.65	1.47
1	D	202	PRO	N-CD	12.76	1.65	1.47
1	C	116	PRO	N-CD	12.33	1.65	1.47
1	D	134	PRO	N-CD	12.02	1.64	1.47
1	C	202	PRO	N-CD	11.85	1.64	1.47
1	E	365	PRO	N-CD	11.79	1.64	1.47
1	A	190	PRO	N-CD	11.50	1.64	1.47
1	B	260	PRO	N-CD	11.43	1.63	1.47
1	B	300	PRO	N-CD	11.38	1.63	1.47
1	B	202	PRO	N-CD	11.36	1.63	1.47
1	A	202	PRO	N-CD	11.35	1.63	1.47
1	C	190	PRO	N-CD	11.32	1.63	1.47
1	E	33	PRO	N-CD	-10.99	1.32	1.47
1	A	260	PRO	N-CD	10.66	1.62	1.47
1	D	260	PRO	N-CD	10.16	1.62	1.47
1	A	365	PRO	N-CD	10.16	1.62	1.47
1	D	253	PRO	N-CD	10.12	1.62	1.47
1	D	80	PRO	N-CD	-9.98	1.33	1.47
1	E	253	PRO	N-CD	9.84	1.61	1.47
1	C	253	PRO	N-CD	9.75	1.61	1.47
1	A	33	PRO	N-CD	-9.70	1.34	1.47
1	C	365	PRO	N-CD	9.65	1.61	1.47
1	B	118	PRO	N-CD	9.35	1.60	1.47
1	A	253	PRO	N-CD	9.32	1.60	1.47
1	B	253	PRO	N-CD	9.27	1.60	1.47
1	B	190	PRO	N-CD	8.81	1.60	1.47
1	D	190	PRO	N-CD	8.03	1.59	1.47
1	C	165	PRO	N-CD	-7.50	1.37	1.47
1	A	35	PRO	N-CD	7.43	1.58	1.47
1	C	223	TRP	NE1-CE2	-7.23	1.28	1.37
1	B	223	TRP	NE1-CE2	-7.14	1.28	1.37
1	D	223	TRP	NE1-CE2	-7.08	1.28	1.37
1	E	223	TRP	NE1-CE2	-7.08	1.28	1.37
1	A	223	TRP	NE1-CE2	-7.04	1.28	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	77	TRP	CD2-CE2	-6.96	1.32	1.41
1	B	77	TRP	CD2-CE2	-6.94	1.33	1.41
1	A	77	TRP	CD2-CE2	-6.91	1.33	1.41
1	C	77	TRP	CD2-CE2	-6.90	1.33	1.41
1	D	77	TRP	CD2-CE2	-6.88	1.33	1.41
1	B	463	PRO	N-CD	-6.67	1.38	1.47
1	C	260	PRO	N-CD	6.44	1.56	1.47
1	E	463	PRO	N-CD	-6.35	1.39	1.47
1	D	463	PRO	N-CD	-6.14	1.39	1.47
1	E	77	TRP	NE1-CE2	-6.10	1.29	1.37
1	C	77	TRP	NE1-CE2	-6.08	1.29	1.37
1	A	77	TRP	NE1-CE2	-6.05	1.29	1.37
1	D	77	TRP	NE1-CE2	-6.03	1.29	1.37
1	B	77	TRP	NE1-CE2	-6.00	1.29	1.37
1	C	194	SER	CA-CB	-5.95	1.44	1.52
1	E	194	SER	CA-CB	-5.91	1.44	1.52
1	A	194	SER	CA-CB	-5.91	1.44	1.52
1	B	194	SER	CA-CB	-5.90	1.44	1.52
1	D	194	SER	CA-CB	-5.88	1.44	1.52
1	E	379	TYR	CE2-CZ	-5.88	1.30	1.38
1	A	379	TYR	CE2-CZ	-5.80	1.31	1.38
1	C	379	TYR	CE2-CZ	-5.79	1.31	1.38
1	D	379	TYR	CE2-CZ	-5.79	1.31	1.38
1	B	379	TYR	CE2-CZ	-5.78	1.31	1.38
1	C	35	PRO	N-CD	5.65	1.55	1.47
1	E	77	TRP	CZ3-CH2	-5.64	1.31	1.40
1	C	77	TRP	CZ3-CH2	-5.60	1.31	1.40
1	D	77	TRP	CZ3-CH2	-5.58	1.31	1.40
1	D	35	PRO	N-CD	5.55	1.55	1.47
1	B	77	TRP	CZ3-CH2	-5.52	1.31	1.40
1	C	463	PRO	N-CD	-5.52	1.40	1.47
1	A	77	TRP	CZ3-CH2	-5.46	1.31	1.40
1	B	223	TRP	CD1-NE1	-5.43	1.28	1.38
1	D	223	TRP	CD1-NE1	-5.43	1.28	1.38
1	A	223	TRP	CD1-NE1	-5.41	1.28	1.38
1	E	138	PRO	N-CD	5.41	1.55	1.47
1	E	223	TRP	CD1-NE1	-5.39	1.28	1.38
1	C	223	TRP	CD1-NE1	-5.38	1.28	1.38
1	C	109	PRO	N-CD	-5.37	1.40	1.47
1	E	260	PRO	N-CD	5.37	1.55	1.47
1	D	131	PRO	N-CD	-5.29	1.40	1.47
1	E	35	PRO	N-CD	5.29	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	322	TRP	NE1-CE2	-5.26	1.30	1.37
1	D	322	TRP	NE1-CE2	-5.25	1.30	1.37
1	B	322	TRP	NE1-CE2	-5.24	1.30	1.37
1	C	192	PRO	N-CA	-5.20	1.38	1.47
1	C	322	TRP	NE1-CE2	-5.20	1.30	1.37
1	B	324	PRO	N-CD	5.20	1.55	1.47
1	A	322	TRP	NE1-CE2	-5.18	1.30	1.37
1	D	192	PRO	N-CA	-5.15	1.38	1.47
1	E	192	PRO	N-CA	-5.14	1.38	1.47
1	A	77	TRP	CD1-NE1	-5.14	1.29	1.38
1	C	77	TRP	CD1-NE1	-5.13	1.29	1.38
1	A	192	PRO	N-CA	-5.13	1.38	1.47
1	B	192	PRO	N-CA	-5.12	1.38	1.47
1	B	77	TRP	CD1-NE1	-5.11	1.29	1.38
1	E	77	TRP	CD1-NE1	-5.10	1.29	1.38
1	D	77	TRP	CD1-NE1	-5.10	1.29	1.38
1	A	463	PRO	N-CD	-5.06	1.40	1.47

All (471) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	PRO	N-CD-CG	15.74	126.81	103.20
1	A	291	PRO	N-CD-CG	15.70	126.75	103.20
1	E	77	TRP	CH2-CZ2-CE2	14.73	132.13	117.40
1	A	77	TRP	CH2-CZ2-CE2	14.71	132.12	117.40
1	B	77	TRP	CH2-CZ2-CE2	14.71	132.10	117.40
1	D	77	TRP	CH2-CZ2-CE2	14.69	132.09	117.40
1	C	77	TRP	CH2-CZ2-CE2	14.64	132.04	117.40
1	C	291	PRO	N-CD-CG	14.42	124.83	103.20
1	E	192	PRO	N-CD-CG	13.94	124.12	103.20
1	A	192	PRO	N-CD-CG	13.92	124.09	103.20
1	A	379	TYR	CZ-CE2-CD2	13.90	132.31	119.80
1	B	379	TYR	CZ-CE2-CD2	13.83	132.25	119.80
1	E	379	TYR	CZ-CE2-CD2	13.81	132.23	119.80
1	C	379	TYR	CZ-CE2-CD2	13.75	132.18	119.80
1	D	379	TYR	CZ-CE2-CD2	13.74	132.16	119.80
1	B	192	PRO	N-CD-CG	13.34	123.21	103.20
1	E	291	PRO	N-CD-CG	13.25	123.07	103.20
1	B	77	TRP	CZ3-CH2-CZ2	-12.67	106.39	121.60
1	A	77	TRP	CZ3-CH2-CZ2	-12.67	106.40	121.60
1	D	77	TRP	CZ3-CH2-CZ2	-12.67	106.40	121.60
1	E	77	TRP	CZ3-CH2-CZ2	-12.63	106.44	121.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	77	TRP	CZ3-CH2-CZ2	-12.61	106.47	121.60
1	C	192	PRO	N-CD-CG	12.53	121.99	103.20
1	D	291	PRO	N-CD-CG	12.13	121.39	103.20
1	D	192	PRO	N-CD-CG	12.12	121.39	103.20
1	D	463	PRO	N-CD-CG	12.02	121.22	103.20
1	B	463	PRO	N-CD-CG	11.94	121.11	103.20
1	E	463	PRO	N-CD-CG	11.93	121.09	103.20
1	C	463	PRO	N-CD-CG	11.82	120.93	103.20
1	A	463	PRO	N-CD-CG	11.60	120.60	103.20
1	E	192	PRO	CA-N-CD	-11.37	95.59	111.50
1	A	192	PRO	CA-N-CD	-11.31	95.67	111.50
1	B	192	PRO	CA-N-CD	-10.91	96.22	111.50
1	A	379	TYR	CG-CD2-CE2	-10.68	112.76	121.30
1	D	192	PRO	CA-N-CD	-10.63	96.61	111.50
1	E	379	TYR	CG-CD2-CE2	-10.61	112.81	121.30
1	C	379	TYR	CG-CD2-CE2	-10.55	112.86	121.30
1	B	379	TYR	CG-CD2-CE2	-10.54	112.87	121.30
1	D	379	TYR	CG-CD2-CE2	-10.51	112.89	121.30
1	C	192	PRO	CA-N-CD	-10.49	96.82	111.50
1	E	73	VAL	CG1-CB-CG2	-10.07	94.79	110.90
1	A	73	VAL	CG1-CB-CG2	-10.05	94.83	110.90
1	D	73	VAL	CG1-CB-CG2	-10.04	94.84	110.90
1	B	73	VAL	CG1-CB-CG2	-10.02	94.86	110.90
1	C	73	VAL	CG1-CB-CG2	-10.01	94.89	110.90
1	E	190	PRO	N-CD-CG	9.90	118.05	103.20
1	C	195	ARG	NE-CZ-NH2	-9.75	115.42	120.30
1	A	165	PRO	N-CD-CG	9.72	117.78	103.20
1	A	188	LEU	CB-CG-CD1	-9.67	94.56	111.00
1	B	188	LEU	CB-CG-CD1	-9.67	94.57	111.00
1	D	188	LEU	CB-CG-CD1	-9.66	94.57	111.00
1	C	188	LEU	CB-CG-CD1	-9.64	94.61	111.00
1	E	188	LEU	CB-CG-CD1	-9.64	94.61	111.00
1	D	195	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	B	195	ARG	NE-CZ-NH2	-9.59	115.50	120.30
1	D	463	PRO	CA-N-CD	-9.58	98.08	111.50
1	C	463	PRO	CA-N-CD	-9.54	98.14	111.50
1	A	195	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	A	463	PRO	CA-N-CD	-9.45	98.27	111.50
1	E	195	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	B	431	VAL	CG1-CB-CG2	-9.39	95.88	110.90
1	C	225	ALA	N-CA-CB	9.37	123.22	110.10
1	B	225	ALA	N-CA-CB	9.37	123.22	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ALA	N-CA-CB	9.36	123.21	110.10
1	A	431	VAL	CG1-CB-CG2	-9.36	95.92	110.90
1	C	431	VAL	CG1-CB-CG2	-9.36	95.92	110.90
1	E	431	VAL	CG1-CB-CG2	-9.35	95.93	110.90
1	E	463	PRO	CA-N-CD	-9.35	98.41	111.50
1	E	225	ALA	N-CA-CB	9.35	123.18	110.10
1	D	225	ALA	N-CA-CB	9.34	123.18	110.10
1	D	431	VAL	CG1-CB-CG2	-9.32	95.98	110.90
1	D	165	PRO	N-CD-CG	9.10	116.86	103.20
1	B	165	PRO	N-CD-CG	9.10	116.84	103.20
1	B	463	PRO	CA-N-CD	-9.09	98.78	111.50
1	E	368	ARG	NE-CZ-NH2	9.05	124.83	120.30
1	A	368	ARG	NE-CZ-NH2	9.05	124.82	120.30
1	E	190	PRO	CA-N-CD	-9.04	98.84	111.50
1	A	118	PRO	N-CD-CG	-8.97	89.74	103.20
1	C	368	ARG	NE-CZ-NH2	8.95	124.77	120.30
1	A	291	PRO	CA-N-CD	-8.92	99.01	111.50
1	B	368	ARG	NE-CZ-NH2	8.92	124.76	120.30
1	D	368	ARG	NE-CZ-NH2	8.91	124.75	120.30
1	B	165	PRO	CA-N-CD	-8.87	99.09	111.50
1	E	165	PRO	N-CD-CG	8.81	116.41	103.20
1	D	165	PRO	CA-N-CD	-8.72	99.30	111.50
1	E	165	PRO	CA-N-CD	-8.71	99.31	111.50
1	C	237	TYR	CB-CG-CD1	-8.59	115.85	121.00
1	A	237	TYR	CB-CG-CD1	-8.58	115.85	121.00
1	E	237	TYR	CB-CG-CD1	-8.58	115.85	121.00
1	D	237	TYR	CB-CG-CD1	-8.57	115.86	121.00
1	E	376	ALA	CB-CA-C	8.52	122.88	110.10
1	A	319	HIS	N-CA-CB	-8.49	95.31	110.60
1	D	319	HIS	N-CA-CB	-8.49	95.31	110.60
1	C	319	HIS	N-CA-CB	-8.48	95.33	110.60
1	D	376	ALA	CB-CA-C	8.48	122.83	110.10
1	E	319	HIS	N-CA-CB	-8.48	95.33	110.60
1	B	376	ALA	CB-CA-C	8.48	122.82	110.10
1	C	376	ALA	CB-CA-C	8.48	122.82	110.10
1	A	376	ALA	CB-CA-C	8.46	122.79	110.10
1	B	319	HIS	N-CA-CB	-8.46	95.37	110.60
1	B	237	TYR	CB-CG-CD1	-8.45	115.93	121.00
1	C	165	PRO	N-CD-CG	8.30	115.66	103.20
1	B	291	PRO	CA-N-CD	-8.22	99.99	111.50
1	C	190	PRO	CA-N-CD	-8.12	100.14	111.50
1	A	190	PRO	CA-N-CD	-8.09	100.18	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	132	ALA	CB-CA-C	-8.09	97.97	110.10
1	A	132	ALA	CB-CA-C	-8.08	97.98	110.10
1	E	132	ALA	CB-CA-C	-8.07	97.99	110.10
1	C	132	ALA	CB-CA-C	-8.03	98.06	110.10
1	B	132	ALA	CB-CA-C	-8.02	98.06	110.10
1	C	118	PRO	N-CD-CG	-8.02	91.17	103.20
1	D	228	PRO	CA-N-CD	-7.97	100.34	111.50
1	C	228	PRO	CA-N-CD	-7.97	100.34	111.50
1	E	228	PRO	CA-N-CD	-7.96	100.35	111.50
1	E	300	PRO	N-CD-CG	-7.96	91.26	103.20
1	A	228	PRO	CA-N-CD	-7.95	100.37	111.50
1	E	118	PRO	N-CD-CG	-7.94	91.29	103.20
1	B	182	GLN	N-CA-CB	7.93	124.88	110.60
1	B	228	PRO	CA-N-CD	-7.93	100.39	111.50
1	C	182	GLN	N-CA-CB	7.93	124.87	110.60
1	D	182	GLN	N-CA-CB	7.91	124.84	110.60
1	E	182	GLN	N-CA-CB	7.91	124.83	110.60
1	A	182	GLN	N-CA-CB	7.90	124.83	110.60
1	D	190	PRO	CA-N-CD	-7.85	100.50	111.50
1	A	165	PRO	CA-N-CD	-7.83	100.54	111.50
1	D	128	ASP	CB-CG-OD2	-7.82	111.27	118.30
1	E	365	PRO	N-CD-CG	-7.82	91.48	103.20
1	B	33	PRO	CA-N-CD	-7.81	100.56	111.50
1	A	128	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	B	190	PRO	CA-N-CD	-7.79	100.59	111.50
1	E	128	ASP	CB-CG-OD2	-7.79	111.29	118.30
1	C	128	ASP	CB-CG-OD2	-7.77	111.31	118.30
1	B	128	ASP	CB-CG-OD2	-7.77	111.31	118.30
1	A	194	SER	CB-CA-C	7.70	124.72	110.10
1	E	194	SER	CB-CA-C	7.69	124.72	110.10
1	C	194	SER	CB-CA-C	7.68	124.70	110.10
1	B	194	SER	CB-CA-C	7.67	124.67	110.10
1	A	259	THR	O-C-N	-7.67	106.53	121.10
1	D	259	THR	O-C-N	-7.66	106.54	121.10
1	E	259	THR	O-C-N	-7.65	106.56	121.10
1	D	194	SER	CB-CA-C	7.63	124.61	110.10
1	B	259	THR	O-C-N	-7.63	106.60	121.10
1	C	259	THR	O-C-N	-7.63	106.60	121.10
1	C	252	ASN	C-N-CD	-7.59	103.90	120.60
1	E	252	ASN	C-N-CD	-7.54	104.02	120.60
1	A	105	ILE	CG1-CB-CG2	7.51	127.92	111.40
1	E	33	PRO	N-CD-CG	7.51	114.47	103.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	ASN	C-N-CD	-7.50	104.09	120.60
1	E	105	ILE	CG1-CB-CG2	7.48	127.86	111.40
1	C	105	ILE	CG1-CB-CG2	7.47	127.84	111.40
1	B	105	ILE	CG1-CB-CG2	7.47	127.83	111.40
1	D	105	ILE	CG1-CB-CG2	7.47	127.83	111.40
1	A	252	ASN	C-N-CD	-7.46	104.19	120.60
1	A	33	PRO	N-CD-CG	7.42	114.33	103.20
1	B	117	ARG	C-N-CD	-7.39	104.35	120.60
1	A	365	PRO	N-CD-CG	-7.35	92.18	103.20
1	A	322	TRP	CG-CD1-NE1	7.32	117.42	110.10
1	D	322	TRP	CG-CD1-NE1	7.31	117.41	110.10
1	C	322	TRP	CG-CD1-NE1	7.30	117.40	110.10
1	B	322	TRP	CG-CD1-NE1	7.27	117.37	110.10
1	E	322	TRP	CG-CD1-NE1	7.25	117.35	110.10
1	E	186	ALA	CA-C-O	-7.22	104.93	120.10
1	A	186	ALA	CA-C-O	-7.22	104.94	120.10
1	C	186	ALA	CA-C-O	-7.20	104.97	120.10
1	B	186	ALA	CA-C-O	-7.17	105.04	120.10
1	D	186	ALA	CA-C-O	-7.15	105.08	120.10
1	C	456	ARG	NE-CZ-NH1	-7.13	116.74	120.30
1	B	456	ARG	NE-CZ-NH1	-7.09	116.76	120.30
1	D	456	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	B	294	SER	N-CA-CB	-7.07	99.90	110.50
1	D	294	SER	N-CA-CB	-7.07	99.90	110.50
1	A	456	ARG	NE-CZ-NH1	-7.07	116.77	120.30
1	E	294	SER	N-CA-CB	-7.06	99.90	110.50
1	C	291	PRO	CA-N-CD	-7.05	101.63	111.50
1	C	294	SER	N-CA-CB	-7.05	99.93	110.50
1	A	294	SER	N-CA-CB	-7.04	99.94	110.50
1	C	365	PRO	N-CD-CG	-7.04	92.64	103.20
1	E	456	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	C	469	ARG	CB-CA-C	-6.97	96.46	110.40
1	D	469	ARG	CB-CA-C	-6.96	96.47	110.40
1	E	469	ARG	CB-CA-C	-6.96	96.47	110.40
1	A	469	ARG	CB-CA-C	-6.96	96.49	110.40
1	B	469	ARG	CB-CA-C	-6.95	96.49	110.40
1	C	33	PRO	N-CD-CG	6.93	113.59	103.20
1	D	33	PRO	N-CD-CG	6.92	113.58	103.20
1	E	262	ASP	C-N-CD	-6.90	105.42	120.60
1	D	77	TRP	CE3-CZ3-CH2	6.87	128.76	121.20
1	C	77	TRP	CE3-CZ3-CH2	6.83	128.72	121.20
1	A	206	MET	CG-SD-CE	-6.82	89.28	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	TRP	CE3-CZ3-CH2	6.82	128.71	121.20
1	B	262	ASP	C-N-CD	-6.82	105.60	120.60
1	E	77	TRP	CE3-CZ3-CH2	6.81	128.70	121.20
1	D	206	MET	CG-SD-CE	-6.81	89.30	100.20
1	B	206	MET	CG-SD-CE	-6.81	89.30	100.20
1	C	206	MET	CG-SD-CE	-6.81	89.31	100.20
1	E	206	MET	CG-SD-CE	-6.81	89.31	100.20
1	A	262	ASP	C-N-CD	-6.80	105.65	120.60
1	A	77	TRP	CE3-CZ3-CH2	6.78	128.65	121.20
1	B	324	PRO	CA-N-CD	-6.78	102.01	111.50
1	C	401	THR	CA-CB-CG2	-6.74	102.97	112.40
1	C	262	ASP	C-N-CD	-6.71	105.85	120.60
1	E	401	THR	CA-CB-CG2	-6.70	103.02	112.40
1	A	182	GLN	CB-CA-C	-6.69	97.02	110.40
1	B	182	GLN	CB-CA-C	-6.69	97.02	110.40
1	D	182	GLN	CB-CA-C	-6.69	97.02	110.40
1	D	252	ASN	C-N-CD	-6.68	105.90	120.60
1	E	182	GLN	CB-CA-C	-6.68	97.03	110.40
1	E	225	ALA	O-C-N	-6.68	112.01	122.70
1	D	401	THR	CA-CB-CG2	-6.68	103.05	112.40
1	B	401	THR	CA-CB-CG2	-6.67	103.06	112.40
1	A	401	THR	CA-CB-CG2	-6.66	103.07	112.40
1	C	182	GLN	CB-CA-C	-6.66	97.08	110.40
1	B	118	PRO	N-CD-CG	-6.64	93.24	103.20
1	A	225	ALA	O-C-N	-6.63	112.08	122.70
1	B	225	ALA	O-C-N	-6.62	112.10	122.70
1	C	225	ALA	O-C-N	-6.62	112.11	122.70
1	D	225	ALA	O-C-N	-6.62	112.11	122.70
1	B	295	ASP	O-C-N	-6.62	112.12	122.70
1	E	295	ASP	O-C-N	-6.61	112.12	122.70
1	D	295	ASP	O-C-N	-6.60	112.14	122.70
1	E	117	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	A	295	ASP	O-C-N	-6.60	112.14	122.70
1	D	291	PRO	CA-N-CD	-6.60	102.27	111.50
1	D	300	PRO	N-CD-CG	-6.60	93.31	103.20
1	C	295	ASP	O-C-N	-6.57	112.20	122.70
1	C	33	PRO	CA-N-CD	-6.55	102.33	111.50
1	A	117	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	C	117	ARG	NE-CZ-NH1	-6.51	117.05	120.30
1	C	324	PRO	CA-N-CD	-6.51	102.39	111.50
1	B	241	LEU	CB-CG-CD2	6.50	122.06	111.00
1	C	241	LEU	CB-CG-CD2	6.48	122.02	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	324	PRO	CA-N-CD	-6.48	102.43	111.50
1	A	241	LEU	CB-CG-CD2	6.46	121.99	111.00
1	D	241	LEU	CB-CG-CD2	6.46	121.98	111.00
1	C	319	HIS	CA-CB-CG	6.44	124.56	113.60
1	D	319	HIS	CA-CB-CG	6.44	124.55	113.60
1	E	241	LEU	CB-CG-CD2	6.44	121.94	111.00
1	B	319	HIS	CA-CB-CG	6.42	124.52	113.60
1	A	319	HIS	CA-CB-CG	6.41	124.50	113.60
1	B	33	PRO	N-CD-CG	6.39	112.79	103.20
1	C	368	ARG	NE-CZ-NH1	-6.35	117.12	120.30
1	D	368	ARG	NE-CZ-NH1	-6.35	117.12	120.30
1	A	368	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	D	33	PRO	CA-N-CD	-6.30	102.69	111.50
1	A	67	ILE	CA-CB-CG2	-6.29	98.32	110.90
1	D	117	ARG	NE-CZ-NH1	-6.29	117.16	120.30
1	E	368	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	D	67	ILE	CA-CB-CG2	-6.28	98.35	110.90
1	E	67	ILE	CA-CB-CG2	-6.27	98.35	110.90
1	B	117	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	B	67	ILE	CA-CB-CG2	-6.26	98.38	110.90
1	A	232	GLU	OE1-CD-OE2	6.26	130.81	123.30
1	C	67	ILE	CA-CB-CG2	-6.26	98.39	110.90
1	B	368	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	B	232	GLU	OE1-CD-OE2	6.20	130.74	123.30
1	B	134	PRO	N-CD-CG	-6.19	93.91	103.20
1	C	109	PRO	N-CD-CG	6.19	112.48	103.20
1	C	232	GLU	OE1-CD-OE2	6.19	130.73	123.30
1	A	397	TYR	CD1-CE1-CZ	6.15	125.33	119.80
1	B	397	TYR	CD1-CE1-CZ	6.14	125.33	119.80
1	D	397	TYR	CD1-CE1-CZ	6.14	125.33	119.80
1	E	220	THR	CA-CB-CG2	-6.14	103.81	112.40
1	D	232	GLU	OE1-CD-OE2	6.13	130.66	123.30
1	D	262	ASP	C-N-CD	-6.13	107.11	120.60
1	E	397	TYR	CD1-CE1-CZ	6.13	125.32	119.80
1	A	220	THR	CA-CB-CG2	-6.13	103.82	112.40
1	E	232	GLU	OE1-CD-OE2	6.12	130.65	123.30
1	E	324	PRO	N-CD-CG	6.12	112.38	103.20
1	C	397	TYR	CD1-CE1-CZ	6.12	125.31	119.80
1	D	220	THR	CA-CB-CG2	-6.11	103.84	112.40
1	B	220	THR	CA-CB-CG2	-6.11	103.85	112.40
1	C	220	THR	CA-CB-CG2	-6.10	103.86	112.40
1	E	376	ALA	O-C-N	-6.07	113.00	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	ALA	O-C-N	-6.06	113.00	122.70
1	B	376	ALA	O-C-N	-6.06	113.01	122.70
1	C	376	ALA	O-C-N	-6.05	113.02	122.70
1	D	376	ALA	O-C-N	-6.04	113.04	122.70
1	A	401	THR	OG1-CB-CG2	6.04	123.88	110.00
1	E	401	THR	OG1-CB-CG2	6.02	123.85	110.00
1	B	22	PHE	CG-CD1-CE1	6.02	127.42	120.80
1	B	401	THR	OG1-CB-CG2	6.01	123.82	110.00
1	D	401	THR	OG1-CB-CG2	6.01	123.82	110.00
1	E	22	PHE	CG-CD2-CE2	6.00	127.40	120.80
1	C	401	THR	OG1-CB-CG2	6.00	123.81	110.00
1	A	22	PHE	CG-CD2-CE2	6.00	127.40	120.80
1	D	22	PHE	CG-CD1-CE1	5.99	127.39	120.80
1	C	22	PHE	CG-CD1-CE1	5.97	127.36	120.80
1	E	52	LYS	N-CA-CB	-5.96	99.86	110.60
1	A	52	LYS	N-CA-CB	-5.96	99.87	110.60
1	C	52	LYS	N-CA-CB	-5.95	99.89	110.60
1	E	291	PRO	CA-N-CD	-5.95	103.17	111.50
1	B	52	LYS	N-CA-CB	-5.95	99.90	110.60
1	D	52	LYS	N-CA-CB	-5.94	99.90	110.60
1	A	195	ARG	N-CA-CB	5.88	121.18	110.60
1	D	190	PRO	N-CD-CG	5.88	112.02	103.20
1	D	195	ARG	N-CA-CB	5.87	121.16	110.60
1	B	195	ARG	N-CA-CB	5.86	121.14	110.60
1	D	195	ARG	CD-NE-CZ	-5.86	115.40	123.60
1	D	144	GLY	CA-C-O	-5.85	110.06	120.60
1	E	195	ARG	N-CA-CB	5.85	121.14	110.60
1	C	195	ARG	N-CA-CB	5.85	121.13	110.60
1	A	195	ARG	CD-NE-CZ	-5.84	115.42	123.60
1	C	195	ARG	CD-NE-CZ	-5.84	115.42	123.60
1	E	109	PRO	N-CD-CG	5.84	111.96	103.20
1	E	144	GLY	CA-C-O	-5.83	110.10	120.60
1	A	144	GLY	CA-C-O	-5.83	110.10	120.60
1	E	195	ARG	CD-NE-CZ	-5.82	115.46	123.60
1	C	144	GLY	CA-C-O	-5.81	110.14	120.60
1	B	195	ARG	CD-NE-CZ	-5.81	115.46	123.60
1	B	144	GLY	CA-C-O	-5.81	110.15	120.60
1	B	456	ARG	CD-NE-CZ	5.79	131.71	123.60
1	D	265	ARG	CD-NE-CZ	5.77	131.67	123.60
1	C	265	ARG	CD-NE-CZ	5.76	131.66	123.60
1	C	456	ARG	CD-NE-CZ	5.75	131.65	123.60
1	B	265	ARG	CD-NE-CZ	5.75	131.64	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	324	PRO	N-CD-CG	5.74	111.82	103.20
1	A	265	ARG	CD-NE-CZ	5.74	131.63	123.60
1	D	326	ARG	NE-CZ-NH2	5.73	123.17	120.30
1	E	265	ARG	CD-NE-CZ	5.73	131.62	123.60
1	D	456	ARG	CD-NE-CZ	5.72	131.61	123.60
1	E	456	ARG	CD-NE-CZ	5.72	131.60	123.60
1	A	109	PRO	N-CD-CG	5.71	111.77	103.20
1	A	456	ARG	CD-NE-CZ	5.71	131.59	123.60
1	E	454	GLU	CG-CD-OE1	-5.71	106.89	118.30
1	B	198	TYR	CB-CG-CD2	5.71	124.42	121.00
1	B	454	GLU	CG-CD-OE1	-5.70	106.91	118.30
1	D	379	TYR	CB-CG-CD1	5.70	124.42	121.00
1	E	198	TYR	CB-CG-CD2	5.70	124.42	121.00
1	E	326	ARG	NE-CZ-NH2	5.69	123.15	120.30
1	A	454	GLU	CG-CD-OE1	-5.69	106.92	118.30
1	D	20	VAL	CG1-CB-CG2	-5.69	101.80	110.90
1	B	20	VAL	CG1-CB-CG2	-5.68	101.81	110.90
1	C	322	TRP	CD1-NE1-CE2	-5.68	103.89	109.00
1	C	454	GLU	CG-CD-OE1	-5.67	106.96	118.30
1	E	134	PRO	N-CD-CG	-5.67	94.69	103.20
1	C	20	VAL	CG1-CB-CG2	-5.67	101.83	110.90
1	E	20	VAL	CG1-CB-CG2	-5.67	101.83	110.90
1	A	20	VAL	CG1-CB-CG2	-5.67	101.84	110.90
1	A	74	TRP	CH2-CZ2-CE2	5.66	123.06	117.40
1	D	235	LEU	CD1-CG-CD2	5.66	127.48	110.50
1	D	322	TRP	CD1-NE1-CE2	-5.65	103.91	109.00
1	D	454	GLU	CG-CD-OE1	-5.65	107.00	118.30
1	C	74	TRP	CH2-CZ2-CE2	5.65	123.05	117.40
1	C	326	ARG	NE-CZ-NH2	5.65	123.12	120.30
1	A	235	LEU	CD1-CG-CD2	5.65	127.44	110.50
1	A	324	PRO	CA-N-CD	-5.64	103.60	111.50
1	C	235	LEU	CD1-CG-CD2	5.64	127.43	110.50
1	E	235	LEU	CD1-CG-CD2	5.64	127.43	110.50
1	A	322	TRP	CD1-NE1-CE2	-5.64	103.92	109.00
1	A	198	TYR	CB-CG-CD2	5.63	124.38	121.00
1	E	379	TYR	CB-CG-CD1	5.63	124.38	121.00
1	B	235	LEU	CD1-CG-CD2	5.63	127.39	110.50
1	A	326	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	B	182	GLN	CG-CD-OE1	5.61	132.82	121.60
1	E	324	PRO	CA-N-CD	-5.61	103.64	111.50
1	D	182	GLN	CG-CD-OE1	5.61	132.81	121.60
1	D	198	TYR	CB-CG-CD2	5.61	124.36	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	322	TRP	CD1-NE1-CE2	-5.60	103.96	109.00
1	C	182	GLN	CG-CD-OE1	5.59	132.79	121.60
1	B	322	TRP	CD1-NE1-CE2	-5.59	103.97	109.00
1	E	74	TRP	CH2-CZ2-CE2	5.59	122.99	117.40
1	A	182	GLN	CG-CD-OE1	5.58	132.77	121.60
1	A	300	PRO	N-CD-CG	-5.58	94.82	103.20
1	D	74	TRP	CH2-CZ2-CE2	5.58	122.98	117.40
1	B	74	TRP	CH2-CZ2-CE2	5.57	122.97	117.40
1	B	324	PRO	N-CD-CG	5.56	111.54	103.20
1	C	379	TYR	CB-CG-CD1	5.55	124.33	121.00
1	B	326	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	E	182	GLN	CG-CD-OE1	5.54	132.69	121.60
1	C	324	PRO	N-CD-CG	5.53	111.49	103.20
1	A	379	TYR	CB-CG-CD1	5.51	124.30	121.00
1	B	456	ARG	NE-CZ-NH2	5.51	123.05	120.30
1	C	198	TYR	CB-CG-CD2	5.51	124.30	121.00
1	E	52	LYS	CA-CB-CG	5.51	125.51	113.40
1	B	109	PRO	N-CD-CG	5.50	111.45	103.20
1	B	52	LYS	CA-CB-CG	5.50	125.49	113.40
1	A	52	LYS	CA-CB-CG	5.49	125.47	113.40
1	C	185	ALA	CB-CA-C	-5.49	101.87	110.10
1	A	185	ALA	CB-CA-C	-5.48	101.87	110.10
1	B	185	ALA	CB-CA-C	-5.48	101.89	110.10
1	C	52	LYS	CA-CB-CG	5.48	125.45	113.40
1	D	52	LYS	CA-CB-CG	5.47	125.43	113.40
1	D	185	ALA	CB-CA-C	-5.47	101.90	110.10
1	D	198	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	C	434	PRO	CA-N-CD	-5.44	103.88	111.50
1	E	185	ALA	CB-CA-C	-5.44	101.94	110.10
1	E	198	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	B	190	PRO	N-CD-CG	5.42	111.33	103.20
1	E	57	GLN	CG-CD-OE1	-5.42	110.76	121.60
1	E	376	ALA	CA-C-O	5.41	131.46	120.10
1	C	198	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	B	379	TYR	CB-CG-CD1	5.39	124.24	121.00
1	D	376	ALA	CA-C-O	5.39	131.43	120.10
1	A	376	ALA	CA-C-O	5.39	131.42	120.10
1	B	376	ALA	CA-C-O	5.38	131.41	120.10
1	B	57	GLN	CG-CD-OE1	-5.38	110.84	121.60
1	C	376	ALA	CA-C-O	5.38	131.39	120.10
1	B	434	PRO	CA-N-CD	-5.37	103.98	111.50
1	B	198	TYR	CB-CG-CD1	-5.37	117.78	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	D	456	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	A	456	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	C	456	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	A	115	LYS	C-N-CD	-5.34	108.85	120.60
1	C	57	GLN	CG-CD-OE1	-5.33	110.94	121.60
1	E	456	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	A	57	GLN	CG-CD-OE1	-5.33	110.95	121.60
1	A	434	PRO	CA-N-CD	-5.30	104.08	111.50
1	D	57	GLN	CG-CD-OE1	-5.30	111.00	121.60
1	D	434	PRO	CA-N-CD	-5.30	104.08	111.50
1	D	109	PRO	N-CD-CG	5.30	111.15	103.20
1	D	109	PRO	CA-N-CD	-5.29	104.09	111.50
1	B	80	PRO	CA-N-CD	-5.29	104.10	111.50
1	C	156	ILE	CG1-CB-CG2	5.28	123.02	111.40
1	A	156	ILE	CG1-CB-CG2	5.26	122.97	111.40
1	B	156	ILE	CG1-CB-CG2	5.26	122.97	111.40
1	E	156	ILE	CG1-CB-CG2	5.25	122.95	111.40
1	D	156	ILE	CG1-CB-CG2	5.24	122.92	111.40
1	A	186	ALA	O-C-N	5.23	131.07	122.70
1	E	434	PRO	CA-N-CD	-5.21	104.20	111.50
1	E	186	ALA	O-C-N	5.21	131.03	122.70
1	E	22	PHE	CB-CG-CD1	5.20	124.44	120.80
1	C	186	ALA	O-C-N	5.18	130.99	122.70
1	A	275	GLU	OE1-CD-OE2	5.17	129.50	123.30
1	D	186	ALA	O-C-N	5.17	130.97	122.70
1	B	21	ALA	CA-C-O	-5.16	109.26	120.10
1	B	186	ALA	O-C-N	5.16	130.96	122.70
1	D	275	GLU	OE1-CD-OE2	5.16	129.49	123.30
1	B	322	TRP	CD1-CG-CD2	-5.15	102.18	106.30
1	A	322	TRP	CD1-CG-CD2	-5.15	102.18	106.30
1	A	21	ALA	CA-C-O	-5.14	109.30	120.10
1	A	22	PHE	CB-CG-CD1	5.14	124.40	120.80
1	B	323	LEU	C-N-CD	-5.14	109.29	120.60
1	E	21	ALA	CA-C-O	-5.14	109.30	120.10
1	C	21	ALA	CA-C-O	-5.14	109.31	120.10
1	D	21	ALA	CA-C-O	-5.13	109.32	120.10
1	A	379	TYR	CE1-CZ-CE2	-5.13	111.59	119.80
1	D	322	TRP	CD1-CG-CD2	-5.13	102.20	106.30
1	D	323	LEU	C-N-CD	-5.13	109.32	120.60
1	B	379	TYR	CE1-CZ-CE2	-5.12	111.60	119.80
1	D	115	LYS	C-N-CD	-5.12	109.33	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	GLU	OE1-CD-OE2	5.12	129.45	123.30
1	B	22	PHE	CB-CG-CD2	5.11	124.38	120.80
1	B	92	GLU	OE1-CD-OE2	5.11	129.43	123.30
1	C	322	TRP	CD1-CG-CD2	-5.10	102.22	106.30
1	B	260	PRO	CA-N-CD	-5.10	104.36	111.50
1	C	379	TYR	CE1-CZ-CE2	-5.09	111.65	119.80
1	C	275	GLU	OE1-CD-OE2	5.09	129.41	123.30
1	A	368	ARG	CD-NE-CZ	5.09	130.72	123.60
1	E	275	GLU	OE1-CD-OE2	5.06	129.37	123.30
1	C	92	GLU	OE1-CD-OE2	5.06	129.37	123.30
1	C	323	LEU	C-N-CD	-5.06	109.48	120.60
1	C	22	PHE	CB-CG-CD2	5.05	124.34	120.80
1	E	368	ARG	CD-NE-CZ	5.05	130.67	123.60
1	D	379	TYR	CE1-CZ-CE2	-5.05	111.72	119.80
1	B	368	ARG	CD-NE-CZ	5.04	130.66	123.60
1	C	256	LEU	CA-C-O	-5.04	109.51	120.10
1	E	256	LEU	CA-C-O	-5.04	109.52	120.10
1	D	260	PRO	CA-N-CD	-5.03	104.46	111.50
1	E	379	TYR	CE1-CZ-CE2	-5.03	111.75	119.80
1	D	368	ARG	CD-NE-CZ	5.03	130.64	123.60
1	E	322	TRP	CD1-CG-CD2	-5.03	102.28	106.30
1	C	368	ARG	CD-NE-CZ	5.03	130.64	123.60
1	D	256	LEU	CA-C-O	-5.02	109.55	120.10
1	A	256	LEU	CA-C-O	-5.02	109.56	120.10
1	E	116	PRO	N-CD-CG	-5.02	95.67	103.20
1	E	179	THR	CA-CB-CG2	-5.01	105.39	112.40
1	E	235	LEU	CB-CG-CD2	-5.01	102.49	111.00
1	A	235	LEU	CB-CG-CD2	-5.01	102.49	111.00
1	D	92	GLU	OE1-CD-OE2	5.01	129.31	123.30
1	D	22	PHE	CB-CG-CD2	5.00	124.30	120.80

There are no chirality outliers.

All (68) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	GLY	Peptide
1	A	194	SER	Mainchain
1	A	21	ALA	Mainchain
1	A	225	ALA	Mainchain
1	A	295	ASP	Mainchain
1	A	319	HIS	Sidechain
1	A	347	HIS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	379	TYR	Sidechain
1	A	406	ALA	Mainchain,Peptide
1	A	474	ASP	Peptide
1	A	82	LEU	Peptide
1	A	91	LYS	Peptide
1	B	144	GLY	Peptide
1	B	194	SER	Mainchain
1	B	21	ALA	Mainchain
1	B	225	ALA	Mainchain
1	B	295	ASP	Mainchain
1	B	319	HIS	Sidechain
1	B	347	HIS	Peptide
1	B	379	TYR	Sidechain
1	B	406	ALA	Mainchain,Peptide
1	B	474	ASP	Mainchain,Peptide
1	B	82	LEU	Peptide
1	B	91	LYS	Peptide
1	C	144	GLY	Peptide
1	C	194	SER	Mainchain
1	C	21	ALA	Mainchain
1	C	225	ALA	Mainchain
1	C	295	ASP	Mainchain
1	C	319	HIS	Sidechain
1	C	347	HIS	Peptide
1	C	379	TYR	Sidechain
1	C	406	ALA	Mainchain,Peptide
1	C	474	ASP	Mainchain,Peptide
1	C	82	LEU	Peptide
1	C	91	LYS	Peptide
1	D	144	GLY	Peptide
1	D	194	SER	Mainchain
1	D	21	ALA	Mainchain
1	D	225	ALA	Mainchain
1	D	295	ASP	Mainchain
1	D	319	HIS	Sidechain
1	D	347	HIS	Peptide
1	D	379	TYR	Sidechain
1	D	406	ALA	Mainchain,Peptide
1	D	474	ASP	Mainchain,Peptide
1	D	82	LEU	Peptide
1	D	91	LYS	Peptide
1	E	144	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	E	194	SER	Mainchain
1	E	21	ALA	Mainchain
1	E	225	ALA	Mainchain
1	E	295	ASP	Mainchain
1	E	347	HIS	Peptide
1	E	379	TYR	Sidechain
1	E	406	ALA	Mainchain,Peptide
1	E	474	ASP	Mainchain,Peptide
1	E	82	LEU	Peptide
1	E	91	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3771	0	3778	650	0
1	B	3771	0	3776	649	0
1	C	3771	0	3778	670	0
1	D	3771	0	3778	685	0
1	E	3771	0	3778	661	0
All	All	18855	0	18888	2904	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 77.

All (2904) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:TYR:N	1:E:173:ALA:CB	1.69	1.56
1:D:173:ALA:CB	1:E:346:TYR:N	1.69	1.54
1:D:346:TYR:CE1	1:D:349:CYS:HB3	1.41	1.52
1:B:173:ALA:CB	1:C:346:TYR:N	1.69	1.52
1:C:173:ALA:CB	1:D:346:TYR:N	1.69	1.51
1:A:177:LEU:HA	1:B:347:HIS:CD2	1.46	1.51
1:A:173:ALA:CB	1:B:346:TYR:N	1.69	1.50
1:C:346:TYR:CE2	1:C:349:CYS:HB3	1.47	1.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:LEU:HB3	1:D:347:HIS:CD2	1.46	1.48
1:A:401:THR:CG2	1:A:402:LEU:H	1.18	1.44
1:D:173:ALA:HA	1:E:346:TYR:CB	1.50	1.42
1:A:347:HIS:ND1	1:E:177:LEU:CB	1.82	1.41
1:C:173:ALA:HB1	1:D:345:THR:C	1.41	1.40
1:C:173:ALA:CA	1:D:346:TYR:HA	1.51	1.39
1:B:173:ALA:HA	1:C:346:TYR:CB	1.50	1.39
1:E:116:PRO:CD	1:E:116:PRO:N	1.67	1.39
1:A:346:TYR:CB	1:E:173:ALA:HA	1.50	1.39
1:B:173:ALA:HB1	1:C:345:THR:C	1.41	1.39
1:D:173:ALA:CA	1:E:346:TYR:HA	1.51	1.39
1:A:173:ALA:HA	1:B:346:TYR:CB	1.50	1.38
1:E:300:PRO:N	1:E:300:PRO:CD	1.75	1.38
1:B:173:ALA:CA	1:C:346:TYR:HA	1.51	1.38
1:A:173:ALA:CA	1:B:346:TYR:HA	1.51	1.38
1:C:173:ALA:CA	1:D:346:TYR:CA	2.02	1.38
1:B:173:ALA:CA	1:C:346:TYR:CA	2.02	1.38
1:C:173:ALA:HA	1:D:346:TYR:CB	1.50	1.38
1:D:173:ALA:HB1	1:E:345:THR:C	1.41	1.38
1:A:173:ALA:HB1	1:B:345:THR:C	1.41	1.37
1:A:346:TYR:HA	1:E:173:ALA:CA	1.50	1.37
1:A:173:ALA:CA	1:B:346:TYR:CA	2.02	1.37
1:A:345:THR:C	1:E:173:ALA:HB1	1.41	1.36
1:B:134:PRO:N	1:B:134:PRO:CD	1.76	1.36
1:D:173:ALA:CA	1:E:346:TYR:CA	2.02	1.35
1:A:134:PRO:CD	1:A:134:PRO:N	1.71	1.35
1:E:134:PRO:N	1:E:134:PRO:CD	1.74	1.35
1:A:346:TYR:CA	1:E:173:ALA:CA	2.02	1.35
1:B:434:PRO:CD	1:B:434:PRO:N	1.69	1.35
1:C:434:PRO:N	1:C:434:PRO:CD	1.69	1.34
1:D:434:PRO:N	1:D:434:PRO:CD	1.68	1.33
1:D:300:PRO:N	1:D:300:PRO:CD	1.69	1.32
1:A:434:PRO:CD	1:A:434:PRO:N	1.68	1.32
1:A:346:TYR:CA	1:E:173:ALA:HA	1.60	1.32
1:D:176:LYS:HB3	1:E:347:HIS:CB	1.60	1.31
1:B:436:LEU:HA	1:B:439:HIS:CE1	1.65	1.30
1:A:401:THR:CG2	1:A:402:LEU:N	1.77	1.30
1:C:177:LEU:CB	1:D:347:HIS:CD2	2.13	1.30
1:E:182:GLN:NE2	1:E:185:ALA:HB2	1.44	1.29
1:A:173:ALA:HA	1:B:346:TYR:CA	1.61	1.29
1:A:235:LEU:CD2	1:A:245:LEU:HB3	1.61	1.29

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:LEU:HD22	1:C:400:LYS:O	1.28	1.29
1:E:378:LEU:HD22	1:E:400:LYS:O	1.29	1.29
1:C:134:PRO:N	1:C:134:PRO:CD	1.70	1.28
1:C:173:ALA:HA	1:D:346:TYR:CA	1.61	1.28
1:B:235:LEU:CD2	1:B:245:LEU:HB3	1.64	1.27
1:D:401:THR:CG2	1:D:402:LEU:H	1.10	1.27
1:D:378:LEU:HD22	1:D:400:LYS:O	1.25	1.27
1:C:346:TYR:CE2	1:C:349:CYS:CB	2.18	1.26
1:E:235:LEU:CD2	1:E:245:LEU:HB3	1.64	1.26
1:E:163:GLU:OE1	1:E:208:LEU:HB3	1.34	1.26
1:A:235:LEU:CD1	1:A:241:LEU:HD22	1.66	1.26
1:D:173:ALA:HA	1:E:346:TYR:CA	1.60	1.25
1:D:98:SER:HB3	1:D:136:HIS:CE1	1.71	1.25
1:D:177:LEU:HA	1:E:347:HIS:ND1	1.50	1.25
1:B:378:LEU:HD22	1:B:400:LYS:O	1.37	1.25
1:B:173:ALA:HA	1:C:346:TYR:CA	1.60	1.25
1:D:173:ALA:C	1:E:346:TYR:HA	1.57	1.24
1:A:173:ALA:C	1:B:346:TYR:HA	1.57	1.24
1:C:235:LEU:CD2	1:C:245:LEU:HB3	1.69	1.23
1:B:173:ALA:C	1:C:346:TYR:HA	1.57	1.23
1:D:182:GLN:NE2	1:D:185:ALA:HB2	1.51	1.22
1:D:346:TYR:CE1	1:D:349:CYS:CB	2.20	1.22
1:A:346:TYR:HA	1:E:173:ALA:C	1.57	1.22
1:A:274:ARG:HD3	1:A:414:VAL:CG1	1.68	1.21
1:A:182:GLN:NE2	1:A:185:ALA:HB2	1.55	1.21
1:B:182:GLN:NE2	1:B:185:ALA:HB2	1.51	1.21
1:C:173:ALA:C	1:D:346:TYR:HA	1.57	1.21
1:A:437:LEU:HD23	1:A:458:CYS:SG	1.80	1.21
1:B:173:ALA:HA	1:C:346:TYR:HB3	1.22	1.21
1:C:182:GLN:NE2	1:C:185:ALA:HB2	1.55	1.20
1:A:376:ALA:HB2	1:E:181:VAL:O	1.40	1.20
1:A:347:HIS:ND1	1:E:177:LEU:CA	2.04	1.20
1:D:256:LEU:O	1:D:260:PRO:HD2	1.42	1.20
1:A:417:VAL:HB	1:A:465:MET:HG3	1.24	1.19
1:A:220:THR:HG22	1:A:445:GLU:O	1.41	1.19
1:B:163:GLU:OE1	1:B:208:LEU:HB2	1.42	1.19
1:A:181:VAL:O	1:B:376:ALA:HB2	1.40	1.19
1:B:256:LEU:O	1:B:260:PRO:HD2	1.42	1.19
1:C:235:LEU:HD21	1:C:245:LEU:HB3	1.24	1.19
1:D:346:TYR:CZ	1:D:349:CYS:HB3	1.76	1.19
1:D:401:THR:CG2	1:D:402:LEU:N	1.75	1.19

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:VAL:O	1:E:376:ALA:HB2	1.40	1.19
1:B:181:VAL:O	1:C:376:ALA:HB2	1.40	1.18
1:D:235:LEU:HD11	1:D:241:LEU:CD2	1.73	1.18
1:D:173:ALA:CB	1:E:346:TYR:CA	2.21	1.18
1:A:430:LYS:O	1:A:434:PRO:HD3	1.43	1.18
1:C:181:VAL:O	1:D:376:ALA:HB2	1.40	1.18
1:A:346:TYR:CA	1:E:173:ALA:CB	2.21	1.17
1:C:430:LYS:O	1:C:434:PRO:HD3	1.44	1.17
1:A:220:THR:HG21	1:A:446:GLU:CG	1.74	1.17
1:B:430:LYS:O	1:B:434:PRO:HD3	1.43	1.17
1:D:417:VAL:HB	1:D:465:MET:HG3	1.20	1.17
1:C:117:ARG:HB3	1:C:118:PRO:HD3	1.26	1.17
1:C:417:VAL:HB	1:C:465:MET:HG3	1.26	1.17
1:A:345:THR:OG1	1:E:173:ALA:HB3	1.42	1.17
1:A:52:LYS:HB2	1:A:184:PHE:HZ	1.00	1.17
1:A:56:LEU:HG	1:A:222:ILE:CG2	1.74	1.16
1:A:256:LEU:O	1:A:260:PRO:HD2	1.44	1.16
1:B:272:ARG:HB2	1:B:441:ASN:HB2	1.27	1.16
1:D:52:LYS:HB2	1:D:184:PHE:CZ	1.80	1.16
1:D:437:LEU:HD23	1:D:458:CYS:SG	1.85	1.16
1:A:235:LEU:HD21	1:A:245:LEU:HB3	1.17	1.16
1:C:176:LYS:CE	1:D:348:ASP:OD2	1.93	1.16
1:B:52:LYS:HB2	1:B:184:PHE:CZ	1.80	1.16
1:E:52:LYS:HB2	1:E:184:PHE:CZ	1.80	1.16
1:C:173:ALA:CB	1:D:346:TYR:CA	2.21	1.16
1:E:52:LYS:HB2	1:E:184:PHE:HZ	1.02	1.16
1:C:52:LYS:HB2	1:C:184:PHE:CZ	1.80	1.16
1:A:274:ARG:CD	1:A:414:VAL:HG13	1.75	1.15
1:D:313:LEU:HD12	1:D:374:GLY:HA2	1.28	1.15
1:C:174:ARG:NH1	1:D:345:THR:OG1	1.78	1.15
1:D:430:LYS:O	1:D:434:PRO:HD3	1.45	1.15
1:A:52:LYS:HB2	1:A:184:PHE:CZ	1.80	1.15
1:C:159:ALA:HB3	1:C:198:TYR:CD1	1.82	1.15
1:D:370:LYS:HE2	1:D:399:ASP:HB3	1.27	1.15
1:E:313:LEU:HD12	1:E:374:GLY:HA2	1.29	1.14
1:A:124:VAL:HB	1:A:125:ILE:HB	1.23	1.14
1:A:173:ALA:CB	1:B:346:TYR:CA	2.21	1.14
1:C:176:LYS:HE3	1:D:348:ASP:CG	1.67	1.14
1:E:417:VAL:HB	1:E:465:MET:HG3	1.18	1.14
1:B:417:VAL:HB	1:B:465:MET:HG3	1.15	1.14
1:A:313:LEU:HD12	1:A:374:GLY:HA2	1.29	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:430:LYS:O	1:E:434:PRO:HD3	1.44	1.14
1:B:173:ALA:CB	1:C:346:TYR:CA	2.21	1.13
1:B:176:LYS:HB3	1:C:347:HIS:CB	1.78	1.13
1:A:83:LYS:HG3	1:A:155:ASP:CB	1.77	1.13
1:E:256:LEU:O	1:E:260:PRO:HD2	1.47	1.13
1:C:176:LYS:HB2	1:D:347:HIS:H	1.14	1.13
1:A:347:HIS:N	1:E:176:LYS:HB2	1.64	1.13
1:A:173:ALA:HB1	1:B:346:TYR:CA	1.78	1.13
1:D:56:LEU:HG	1:D:222:ILE:HG23	1.22	1.13
1:A:322:TRP:HD1	1:A:456:ARG:HB3	0.98	1.12
1:A:176:LYS:HB2	1:B:347:HIS:N	1.64	1.12
1:D:56:LEU:HG	1:D:222:ILE:CG2	1.79	1.12
1:E:124:VAL:HB	1:E:125:ILE:HB	1.22	1.12
1:A:346:TYR:CA	1:E:173:ALA:HB1	1.78	1.12
1:C:173:ALA:HB3	1:D:345:THR:HG23	1.26	1.12
1:B:173:ALA:HB1	1:C:346:TYR:CA	1.78	1.12
1:C:77:TRP:HE1	1:C:105:ILE:HG12	0.98	1.12
1:A:235:LEU:HD11	1:A:241:LEU:CD2	1.79	1.12
1:A:177:LEU:CA	1:B:347:HIS:CD2	2.32	1.11
1:C:52:LYS:HB2	1:C:184:PHE:HZ	1.03	1.11
1:C:124:VAL:HB	1:C:125:ILE:HB	1.21	1.11
1:C:83:LYS:HE2	1:C:192:PRO:HA	1.17	1.11
1:C:173:ALA:CB	1:D:345:THR:HG23	1.80	1.11
1:C:173:ALA:HB1	1:D:346:TYR:CA	1.78	1.11
1:D:173:ALA:HB1	1:E:346:TYR:CA	1.78	1.11
1:A:117:ARG:HB3	1:A:118:PRO:HD3	1.27	1.11
1:C:181:VAL:HA	1:C:182:GLN:HG2	1.32	1.11
1:B:176:LYS:HB3	1:C:347:HIS:HB3	1.16	1.11
1:D:173:ALA:O	1:E:346:TYR:HA	1.50	1.11
1:A:83:LYS:HG3	1:A:155:ASP:HB2	1.23	1.10
1:B:235:LEU:HD21	1:B:245:LEU:HB3	1.18	1.10
1:B:77:TRP:HE1	1:B:105:ILE:HG12	0.97	1.10
1:A:163:GLU:OE1	1:A:208:LEU:HB2	1.49	1.10
1:A:235:LEU:HD11	1:A:241:LEU:HD22	1.22	1.10
1:E:322:TRP:HD1	1:E:456:ARG:HB3	1.03	1.10
1:C:176:LYS:HB3	1:D:347:HIS:HB3	1.24	1.10
1:C:173:ALA:HA	1:D:346:TYR:HB3	1.21	1.10
1:B:313:LEU:HD12	1:B:374:GLY:HA2	1.29	1.10
1:A:173:ALA:CA	1:B:346:TYR:HB3	1.81	1.10
1:A:401:THR:HG22	1:A:402:LEU:N	1.63	1.10
1:E:117:ARG:HB3	1:E:118:PRO:HD3	1.13	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ALA:O	1:C:346:TYR:HA	1.50	1.10
1:B:18:ASP:OD1	1:B:35:PRO:HG3	1.47	1.09
1:B:173:ALA:CA	1:C:346:TYR:HB3	1.82	1.09
1:D:201:THR:CG2	1:D:202:PRO:HD2	1.83	1.09
1:D:124:VAL:HB	1:D:125:ILE:HB	1.23	1.09
1:B:322:TRP:HD1	1:B:456:ARG:HB3	0.99	1.09
1:A:173:ALA:HA	1:B:346:TYR:HB3	1.17	1.09
1:A:173:ALA:O	1:B:346:TYR:HA	1.50	1.09
1:B:52:LYS:HB2	1:B:184:PHE:HZ	1.01	1.09
1:A:285:LEU:HD11	1:A:434:PRO:HG2	1.23	1.09
1:A:347:HIS:H	1:E:176:LYS:HB2	1.13	1.09
1:B:181:VAL:HA	1:B:182:GLN:HG2	1.34	1.09
1:D:181:VAL:HA	1:D:182:GLN:HG2	1.34	1.09
1:D:322:TRP:HD1	1:D:456:ARG:HB3	1.04	1.09
1:C:173:ALA:CA	1:D:346:TYR:HB3	1.82	1.09
1:C:322:TRP:HD1	1:C:456:ARG:HB3	0.94	1.09
1:C:173:ALA:CA	1:D:346:TYR:CB	2.29	1.09
1:B:124:VAL:HB	1:B:125:ILE:HB	1.23	1.08
1:B:173:ALA:HB1	1:C:346:TYR:N	0.76	1.08
1:E:235:LEU:HD21	1:E:245:LEU:HB3	1.18	1.08
1:A:173:ALA:HB1	1:B:346:TYR:N	0.76	1.08
1:C:322:TRP:CD1	1:C:456:ARG:HB3	1.86	1.08
1:D:52:LYS:HB2	1:D:184:PHE:HZ	1.03	1.08
1:A:181:VAL:HA	1:A:182:GLN:HG2	1.32	1.08
1:A:401:THR:HG23	1:A:402:LEU:N	1.31	1.08
1:C:173:ALA:O	1:D:346:TYR:HA	1.50	1.08
1:C:256:LEU:O	1:C:260:PRO:HD2	1.51	1.08
1:C:176:LYS:HB2	1:D:347:HIS:N	1.69	1.08
1:E:262:ASP:CB	1:E:263:PRO:HD3	1.82	1.08
1:C:173:ALA:HB1	1:D:346:TYR:N	0.75	1.08
1:E:368:ARG:O	1:E:401:THR:HB	1.54	1.07
1:C:368:ARG:O	1:C:401:THR:HB	1.54	1.07
1:A:346:TYR:N	1:E:173:ALA:HB1	0.76	1.07
1:A:347:HIS:HB3	1:E:176:LYS:CB	1.84	1.07
1:A:176:LYS:HB2	1:B:347:HIS:H	1.13	1.07
1:A:89:ALA:O	1:A:140:VAL:HA	1.55	1.07
1:A:220:THR:CG2	1:A:446:GLU:HG2	1.85	1.07
1:D:280:LYS:HZ2	1:D:438:LYS:HA	1.19	1.07
1:E:148:GLN:HE21	1:E:175:GLU:HG3	1.19	1.07
1:D:272:ARG:HB2	1:D:441:ASN:HB2	1.36	1.07
1:A:376:ALA:HA	1:E:181:VAL:HB	1.35	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:ALA:CA	1:E:346:TYR:HB3	1.85	1.07
1:D:235:LEU:CD1	1:D:241:LEU:HD22	1.83	1.07
1:D:291:PRO:HG2	1:D:295:ASP:HB3	1.33	1.07
1:A:346:TYR:HA	1:E:173:ALA:O	1.50	1.07
1:D:173:ALA:HB1	1:E:346:TYR:N	0.75	1.06
1:E:77:TRP:HE1	1:E:105:ILE:HG12	0.96	1.06
1:A:347:HIS:ND1	1:E:177:LEU:HA	1.67	1.06
1:A:347:HIS:ND1	1:E:177:LEU:HB2	1.64	1.06
1:A:182:GLN:HE21	1:A:185:ALA:CB	1.68	1.06
1:A:322:TRP:CD1	1:A:456:ARG:HB3	1.90	1.06
1:C:202:PRO:HD3	1:C:265:ARG:HD2	1.09	1.06
1:D:89:ALA:O	1:D:140:VAL:HA	1.55	1.06
1:E:182:GLN:HE21	1:E:185:ALA:CB	1.69	1.06
1:E:181:VAL:HA	1:E:182:GLN:HG2	1.36	1.06
1:E:273:GLU:HG2	1:E:280:LYS:HZ1	1.19	1.06
1:B:59:PHE:CE2	1:B:60:ARG:O	2.09	1.06
1:D:182:GLN:HE21	1:D:185:ALA:CB	1.68	1.06
1:A:346:TYR:HB3	1:E:173:ALA:HA	1.07	1.06
1:C:176:LYS:HE3	1:D:348:ASP:OD2	1.53	1.06
1:D:173:ALA:HB3	1:E:345:THR:HG23	1.39	1.05
1:C:262:ASP:CB	1:C:263:PRO:HD3	1.84	1.05
1:A:346:TYR:HB3	1:E:173:ALA:CA	1.86	1.05
1:C:182:GLN:HE21	1:C:185:ALA:CB	1.68	1.05
1:B:254:GLU:HG3	1:B:255:ALA:N	1.71	1.05
1:B:368:ARG:HH21	1:B:381:LEU:HD12	1.16	1.05
1:D:173:ALA:HB2	1:E:346:TYR:CD2	1.91	1.05
1:D:176:LYS:HB3	1:E:347:HIS:HB3	1.32	1.05
1:D:401:THR:HG22	1:D:402:LEU:N	1.39	1.05
1:B:368:ARG:O	1:B:401:THR:HB	1.54	1.05
1:B:89:ALA:O	1:B:140:VAL:HA	1.55	1.05
1:C:272:ARG:HB2	1:C:441:ASN:HB2	1.36	1.05
1:D:18:ASP:OD1	1:D:35:PRO:HG3	1.57	1.05
1:C:89:ALA:O	1:C:140:VAL:HA	1.55	1.04
1:B:182:GLN:HE21	1:B:185:ALA:CB	1.68	1.04
1:D:173:ALA:CA	1:E:346:TYR:CB	2.29	1.04
1:D:262:ASP:HB3	1:D:263:PRO:HD3	1.39	1.04
1:E:89:ALA:O	1:E:140:VAL:HA	1.55	1.04
1:A:58:ALA:O	1:A:265:ARG:HD3	1.57	1.04
1:C:73:VAL:CG2	1:C:105:ILE:HG13	1.86	1.04
1:B:202:PRO:CD	1:B:265:ARG:HD2	1.87	1.04
1:E:220:THR:HG21	1:E:446:GLU:HG3	1.09	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ALA:CB	1:B:345:THR:C	2.13	1.04
1:B:322:TRP:CD1	1:B:456:ARG:HB3	1.92	1.04
1:B:176:LYS:HB2	1:C:347:HIS:H	1.20	1.04
1:D:56:LEU:CG	1:D:222:ILE:HG23	1.87	1.04
1:C:83:LYS:NZ	1:C:193:SER:H	1.54	1.04
1:D:176:LYS:HB3	1:E:347:HIS:CA	1.87	1.04
1:B:220:THR:CG2	1:B:446:GLU:HG3	1.88	1.03
1:E:73:VAL:CG2	1:E:105:ILE:HG13	1.87	1.03
1:B:280:LYS:HE2	1:B:438:LYS:HA	1.36	1.03
1:B:77:TRP:NE1	1:B:105:ILE:HG12	1.72	1.03
1:C:346:TYR:CD2	1:C:349:CYS:N	2.26	1.03
1:C:51:ASN:HB2	1:C:54:PHE:CZ	1.94	1.03
1:E:83:LYS:HG2	1:E:155:ASP:HB2	1.33	1.03
1:A:173:ALA:CA	1:B:346:TYR:CB	2.29	1.03
1:E:77:TRP:NE1	1:E:105:ILE:HG12	1.71	1.03
1:B:262:ASP:CB	1:B:263:PRO:HD3	1.84	1.03
1:D:235:LEU:HD11	1:D:241:LEU:HD22	1.09	1.03
1:B:73:VAL:CG2	1:B:105:ILE:HG13	1.87	1.03
1:B:173:ALA:CB	1:C:345:THR:HG23	1.89	1.03
1:B:202:PRO:HD3	1:B:265:ARG:CD	1.88	1.03
1:E:18:ASP:OD1	1:E:35:PRO:HG3	1.57	1.03
1:C:346:TYR:HD2	1:C:349:CYS:N	1.57	1.03
1:A:346:TYR:N	1:A:346:TYR:HD1	1.54	1.03
1:E:235:LEU:HD11	1:E:241:LEU:CD2	1.89	1.03
1:E:51:ASN:HB2	1:E:54:PHE:CZ	1.93	1.03
1:C:176:LYS:CB	1:D:347:HIS:HB3	1.88	1.03
1:C:77:TRP:NE1	1:C:105:ILE:HG12	1.72	1.02
1:A:173:ALA:HB3	1:B:345:THR:HG23	1.39	1.02
1:B:220:THR:HG21	1:B:446:GLU:HG3	1.07	1.02
1:B:378:LEU:HD11	1:B:401:THR:OG1	1.58	1.02
1:A:56:LEU:HG	1:A:222:ILE:HG23	1.40	1.02
1:C:170:THR:HA	1:D:345:THR:HG21	1.37	1.02
1:D:202:PRO:HD3	1:D:265:ARG:HD2	1.03	1.02
1:A:202:PRO:HD3	1:A:265:ARG:CD	1.88	1.02
1:A:280:LYS:HE2	1:A:438:LYS:HA	1.37	1.02
1:B:177:LEU:HA	1:C:347:HIS:CD2	1.95	1.02
1:D:262:ASP:CB	1:D:263:PRO:HD3	1.87	1.02
1:A:345:THR:HB	1:E:174:ARG:NH1	1.73	1.02
1:D:173:ALA:CB	1:E:345:THR:HG23	1.89	1.02
1:A:256:LEU:O	1:A:260:PRO:CD	2.08	1.02
1:C:18:ASP:OD1	1:C:35:PRO:HG3	1.58	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LYS:HE2	1:A:399:ASP:HB3	1.42	1.02
1:B:176:LYS:HE2	1:C:348:ASP:CG	1.80	1.02
1:A:322:TRP:HD1	1:A:456:ARG:CB	1.72	1.02
1:A:173:ALA:CB	1:B:345:THR:HG23	1.89	1.02
1:B:55:ILE:HG22	1:B:57:GLN:OE1	1.58	1.02
1:B:173:ALA:HB3	1:C:345:THR:HG23	1.39	1.02
1:C:173:ALA:CB	1:D:345:THR:C	2.13	1.01
1:E:194:SER:HA	1:E:195:ARG:HB2	1.41	1.01
1:D:133:ASN:H	1:D:134:PRO:HD2	1.25	1.01
1:A:347:HIS:ND1	1:E:177:LEU:HB3	1.76	1.01
1:C:60:ARG:CG	1:C:201:THR:HG21	1.88	1.01
1:D:273:GLU:HG2	1:D:280:LYS:HZ1	1.23	1.01
1:D:173:ALA:HA	1:E:346:TYR:HB3	1.07	1.01
1:A:345:THR:C	1:E:173:ALA:CB	2.14	1.01
1:A:194:SER:HA	1:A:195:ARG:HB2	1.41	1.01
1:B:177:LEU:N	1:C:347:HIS:CB	2.24	1.01
1:D:322:TRP:HD1	1:D:456:ARG:CB	1.72	1.01
1:B:67:ILE:HD12	1:B:67:ILE:N	1.75	1.01
1:E:322:TRP:HD1	1:E:456:ARG:CB	1.73	1.01
1:B:254:GLU:HG3	1:B:255:ALA:H	0.89	1.01
1:C:177:LEU:N	1:D:347:HIS:CB	2.24	1.01
1:E:220:THR:CG2	1:E:446:GLU:HG3	1.90	1.01
1:C:262:ASP:HB3	1:C:263:PRO:HD3	1.40	1.01
1:A:262:ASP:CB	1:A:263:PRO:HD3	1.84	1.00
1:C:322:TRP:HD1	1:C:456:ARG:CB	1.72	1.00
1:B:173:ALA:CA	1:C:346:TYR:CB	2.29	1.00
1:D:177:LEU:N	1:E:347:HIS:CB	2.24	1.00
1:D:58:ALA:O	1:D:265:ARG:HD3	1.60	1.00
1:A:202:PRO:CD	1:A:265:ARG:HD2	1.90	1.00
1:E:265:ARG:HD3	1:E:265:ARG:O	1.61	1.00
1:D:73:VAL:HG22	1:D:105:ILE:HG12	1.43	1.00
1:C:163:GLU:OE1	1:C:208:LEU:HB2	1.61	1.00
1:B:176:LYS:HB2	1:C:347:HIS:N	1.75	1.00
1:A:347:HIS:CB	1:E:177:LEU:N	2.24	1.00
1:B:58:ALA:O	1:B:265:ARG:HD3	1.61	1.00
1:D:176:LYS:CB	1:E:347:HIS:HB3	1.91	1.00
1:D:201:THR:HG22	1:D:202:PRO:HD2	1.44	1.00
1:D:83:LYS:HE3	1:D:156:ILE:HG22	1.42	1.00
1:D:204:THR:HG22	1:D:205:GLU:H	1.24	1.00
1:E:322:TRP:CD1	1:E:456:ARG:HB3	1.96	1.00
1:E:223:TRP:HE1	1:E:265:ARG:HB3	1.23	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:VAL:HG22	1:A:105:ILE:HG12	1.42	1.00
1:B:170:THR:HA	1:C:345:THR:HG21	1.44	1.00
1:B:21:ALA:O	1:B:33:PRO:HD3	1.60	1.00
1:B:322:TRP:HD1	1:B:456:ARG:CB	1.74	1.00
1:C:370:LYS:HE2	1:C:399:ASP:CB	1.91	1.00
1:A:177:LEU:N	1:B:347:HIS:CB	2.24	0.99
1:C:346:TYR:CZ	1:C:349:CYS:HB3	1.96	0.99
1:E:64:LYS:O	1:E:67:ILE:HG13	1.61	0.99
1:D:194:SER:HA	1:D:195:ARG:HB2	1.41	0.99
1:B:254:GLU:CG	1:B:255:ALA:H	1.75	0.99
1:B:256:LEU:O	1:B:260:PRO:CD	2.08	0.99
1:D:313:LEU:CD1	1:D:374:GLY:HA2	1.92	0.99
1:B:59:PHE:CD2	1:B:60:ARG:O	2.15	0.99
1:C:256:LEU:O	1:C:260:PRO:CD	2.10	0.99
1:D:322:TRP:CD1	1:D:456:ARG:HB3	1.97	0.99
1:E:291:PRO:HG2	1:E:295:ASP:HB3	1.45	0.99
1:C:194:SER:HA	1:C:195:ARG:HB2	1.41	0.99
1:B:176:LYS:CB	1:C:347:HIS:HB3	1.92	0.99
1:D:85:LEU:HD22	1:D:136:HIS:CD2	1.98	0.99
1:E:313:LEU:CD1	1:E:374:GLY:HA2	1.92	0.99
1:C:176:LYS:HB3	1:D:347:HIS:CB	1.92	0.99
1:B:194:SER:HA	1:B:195:ARG:HB2	1.41	0.99
1:D:170:THR:HA	1:E:345:THR:HG21	1.44	0.99
1:C:176:LYS:HE2	1:D:348:ASP:OD2	1.59	0.99
1:A:291:PRO:HG2	1:A:295:ASP:HB3	1.44	0.99
1:B:291:PRO:HG2	1:B:295:ASP:HB3	1.44	0.99
1:D:256:LEU:O	1:D:260:PRO:CD	2.10	0.99
1:B:85:LEU:HB3	1:B:136:HIS:HD2	1.27	0.98
1:B:173:ALA:CB	1:C:345:THR:C	2.14	0.98
1:C:370:LYS:HE2	1:C:399:ASP:HB3	1.00	0.98
1:D:378:LEU:CD2	1:D:400:LYS:O	2.11	0.98
1:A:176:LYS:CB	1:B:347:HIS:HB3	1.93	0.98
1:C:235:LEU:HD11	1:C:241:LEU:CD2	1.94	0.98
1:A:18:ASP:OD1	1:A:35:PRO:HG3	1.61	0.98
1:B:194:SER:HA	1:B:195:ARG:CB	1.93	0.98
1:B:159:ALA:HB3	1:B:198:TYR:CD1	1.99	0.98
1:C:83:LYS:HZ3	1:C:193:SER:H	1.11	0.98
1:D:194:SER:HA	1:D:195:ARG:CB	1.93	0.98
1:A:313:LEU:CD1	1:A:374:GLY:HA2	1.93	0.98
1:D:173:ALA:CB	1:E:345:THR:C	2.13	0.98
1:A:170:THR:HA	1:B:345:THR:HG21	1.44	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:401:THR:HG23	1:D:402:LEU:N	1.52	0.97
1:E:370:LYS:HE2	1:E:375:TYR:CE1	1.99	0.97
1:E:417:VAL:CB	1:E:465:MET:HG3	1.93	0.97
1:B:205:GLU:HG2	1:B:209:TYR:CD2	1.99	0.97
1:D:436:LEU:HD22	1:D:457:ILE:HG22	1.46	0.97
1:B:59:PHE:CE1	1:B:62:ILE:HB	1.98	0.97
1:D:202:PRO:HD3	1:D:265:ARG:CD	1.94	0.97
1:C:156:ILE:HB	1:C:194:SER:OG	1.65	0.96
1:C:133:ASN:H	1:C:134:PRO:HD2	1.30	0.96
1:D:98:SER:HB3	1:D:136:HIS:HE1	1.18	0.96
1:A:436:LEU:HD22	1:A:457:ILE:HG22	1.47	0.96
1:D:83:LYS:HE3	1:D:156:ILE:CG2	1.94	0.96
1:A:235:LEU:HD22	1:A:245:LEU:HB3	1.48	0.96
1:D:98:SER:CB	1:D:136:HIS:CE1	2.47	0.96
1:A:374:GLY:O	1:A:378:LEU:HG	1.65	0.96
1:B:220:THR:HG21	1:B:446:GLU:CG	1.94	0.96
1:C:313:LEU:HD12	1:C:374:GLY:HA2	1.47	0.96
1:D:176:LYS:HB3	1:E:347:HIS:N	1.79	0.96
1:A:332:ASP:O	1:A:334:PRO:HD3	1.65	0.96
1:A:194:SER:HA	1:A:195:ARG:CB	1.93	0.96
1:D:57:GLN:OE1	1:D:265:ARG:NH2	1.98	0.95
1:E:256:LEU:O	1:E:260:PRO:CD	2.14	0.95
1:C:202:PRO:HB3	1:C:265:ARG:NH1	1.80	0.95
1:D:401:THR:HG23	1:D:402:LEU:H	0.83	0.95
1:C:291:PRO:HG2	1:C:295:ASP:HB3	1.46	0.95
1:B:177:LEU:HB3	1:C:347:HIS:ND1	1.81	0.95
1:C:163:GLU:HG3	1:C:203:GLN:HB2	1.47	0.95
1:E:329:ILE:HG23	1:E:330:ILE:H	1.31	0.95
1:A:346:TYR:CB	1:E:173:ALA:CA	2.29	0.95
1:B:436:LEU:HD22	1:B:457:ILE:HG22	1.45	0.95
1:D:156:ILE:HB	1:D:194:SER:OG	1.67	0.95
1:E:220:THR:HG21	1:E:446:GLU:CG	1.96	0.95
1:A:156:ILE:HB	1:A:194:SER:OG	1.66	0.95
1:E:332:ASP:O	1:E:334:PRO:HD3	1.66	0.95
1:A:329:ILE:HG23	1:A:330:ILE:H	1.31	0.95
1:A:83:LYS:HD2	1:A:193:SER:O	1.66	0.95
1:D:124:VAL:CB	1:D:125:ILE:HB	1.97	0.95
1:B:163:GLU:HG3	1:B:203:GLN:HB2	1.48	0.95
1:E:194:SER:HA	1:E:195:ARG:CB	1.93	0.95
1:E:370:LYS:HE3	1:E:399:ASP:HB3	1.46	0.95
1:B:368:ARG:NH2	1:B:381:LEU:HD12	1.81	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLU:HG3	1:A:203:GLN:HB2	1.48	0.94
1:A:274:ARG:HD3	1:A:414:VAL:HG13	0.96	0.94
1:B:262:ASP:HB3	1:B:263:PRO:HD3	1.48	0.94
1:B:117:ARG:HB3	1:B:118:PRO:HD3	1.49	0.94
1:B:313:LEU:CD1	1:B:374:GLY:HA2	1.96	0.94
1:C:159:ALA:HB3	1:C:198:TYR:HD1	1.20	0.94
1:C:124:VAL:CB	1:C:125:ILE:HB	1.97	0.94
1:A:202:PRO:HD3	1:A:265:ARG:HD2	0.95	0.94
1:B:177:LEU:N	1:C:347:HIS:HB2	1.82	0.94
1:D:177:LEU:N	1:E:347:HIS:HB2	1.82	0.94
1:A:163:GLU:OE1	1:A:208:LEU:CB	2.14	0.94
1:A:177:LEU:HA	1:B:347:HIS:HD2	1.28	0.94
1:A:77:TRP:HZ2	1:A:105:ILE:HG23	1.33	0.94
1:C:220:THR:O	1:C:445:GLU:OE1	1.86	0.94
1:C:436:LEU:HD22	1:C:457:ILE:HG22	1.50	0.94
1:B:156:ILE:HB	1:B:194:SER:OG	1.67	0.94
1:D:273:GLU:HG2	1:D:280:LYS:NZ	1.81	0.94
1:E:163:GLU:OE1	1:E:208:LEU:CB	2.16	0.94
1:B:332:ASP:O	1:B:334:PRO:HD3	1.66	0.94
1:C:378:LEU:CD2	1:C:400:LYS:O	2.14	0.94
1:E:55:ILE:HG22	1:E:57:GLN:HE21	1.30	0.94
1:A:124:VAL:CB	1:A:125:ILE:HB	1.97	0.94
1:C:332:ASP:O	1:C:334:PRO:HD3	1.66	0.94
1:E:124:VAL:CB	1:E:125:ILE:HB	1.97	0.94
1:E:156:ILE:HB	1:E:194:SER:OG	1.68	0.94
1:E:208:LEU:HD21	1:E:265:ARG:NH2	1.83	0.94
1:E:59:PHE:CE1	1:E:62:ILE:HB	2.03	0.94
1:E:235:LEU:HD11	1:E:241:LEU:HD22	1.49	0.94
1:E:77:TRP:CZ3	1:E:114:LEU:N	2.36	0.94
1:A:101:ILE:O	1:A:105:ILE:HG13	1.66	0.93
1:A:417:VAL:CB	1:A:465:MET:HG3	1.97	0.93
1:A:91:LYS:HB2	1:A:93:ARG:HB2	1.47	0.93
1:B:124:VAL:CB	1:B:125:ILE:HB	1.97	0.93
1:C:59:PHE:CE1	1:C:62:ILE:HB	2.03	0.93
1:D:77:TRP:HZ2	1:D:105:ILE:HG23	1.33	0.93
1:A:177:LEU:N	1:B:347:HIS:HB2	1.82	0.93
1:A:347:HIS:HB3	1:E:176:LYS:HB3	1.47	0.93
1:B:173:ALA:HB1	1:C:346:TYR:H	1.14	0.93
1:C:173:ALA:HB1	1:D:346:TYR:H	1.14	0.93
1:D:163:GLU:OE1	1:D:208:LEU:HB2	1.67	0.93
1:B:77:TRP:CZ3	1:B:114:LEU:N	2.37	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:LEU:HD22	1:D:245:LEU:HB3	1.49	0.93
1:E:378:LEU:CD2	1:E:400:LYS:O	2.15	0.93
1:D:332:ASP:O	1:D:334:PRO:HD3	1.67	0.93
1:D:202:PRO:CD	1:D:265:ARG:HD2	1.97	0.93
1:B:329:ILE:HG23	1:B:330:ILE:H	1.31	0.93
1:D:101:ILE:O	1:D:105:ILE:HG13	1.69	0.93
1:E:83:LYS:CG	1:E:155:ASP:HB2	1.97	0.93
1:C:177:LEU:N	1:D:347:HIS:HB2	1.84	0.92
1:E:436:LEU:HD22	1:E:457:ILE:HG22	1.49	0.92
1:D:176:LYS:CB	1:E:347:HIS:CB	2.48	0.92
1:D:346:TYR:CD1	1:D:349:CYS:N	2.37	0.92
1:A:181:VAL:HB	1:B:376:ALA:HA	1.51	0.92
1:D:235:LEU:CD2	1:D:245:LEU:HB3	1.98	0.92
1:A:176:LYS:CB	1:B:347:HIS:CB	2.48	0.92
1:B:176:LYS:CB	1:C:347:HIS:CB	2.48	0.92
1:A:173:ALA:HA	1:B:346:TYR:HA	1.25	0.92
1:C:430:LYS:O	1:C:434:PRO:CD	2.17	0.92
1:D:329:ILE:HG23	1:D:330:ILE:H	1.32	0.92
1:E:273:GLU:HG2	1:E:280:LYS:NZ	1.83	0.92
1:A:430:LYS:O	1:A:434:PRO:CD	2.18	0.92
1:A:59:PHE:CE1	1:A:62:ILE:HB	2.04	0.92
1:C:417:VAL:CB	1:C:465:MET:HG3	1.98	0.92
1:B:67:ILE:HD12	1:B:67:ILE:H	1.32	0.92
1:C:117:ARG:CB	1:C:118:PRO:HD3	2.00	0.92
1:A:347:HIS:CB	1:E:176:LYS:CB	2.48	0.91
1:C:181:VAL:HB	1:D:376:ALA:HA	1.52	0.91
1:E:235:LEU:CD1	1:E:241:LEU:HD22	2.00	0.91
1:C:329:ILE:HG23	1:C:330:ILE:H	1.32	0.91
1:D:430:LYS:O	1:D:434:PRO:CD	2.18	0.91
1:B:132:ALA:N	1:B:133:ASN:HA	1.86	0.91
1:C:194:SER:HA	1:C:195:ARG:CB	1.94	0.91
1:C:370:LYS:CE	1:C:399:ASP:HB3	1.96	0.91
1:B:430:LYS:O	1:B:434:PRO:CD	2.17	0.91
1:D:173:ALA:HB1	1:E:346:TYR:H	1.14	0.91
1:E:133:ASN:H	1:E:134:PRO:HD2	1.34	0.91
1:A:39:GLN:HB3	1:A:67:ILE:HG12	1.53	0.91
1:B:181:VAL:HB	1:C:376:ALA:HA	1.53	0.91
1:E:117:ARG:CB	1:E:118:PRO:HD3	1.99	0.91
1:E:163:GLU:HG3	1:E:203:GLN:HB2	1.53	0.91
1:B:177:LEU:CA	1:C:347:HIS:CG	2.53	0.91
1:D:329:ILE:HG23	1:D:330:ILE:N	1.83	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:ILE:HG23	1:C:330:ILE:N	1.85	0.91
1:D:163:GLU:HG3	1:D:203:GLN:HB2	1.50	0.91
1:D:379:TYR:O	1:D:385:ILE:HB	1.70	0.91
1:D:322:TRP:CD1	1:D:456:ARG:CB	2.53	0.91
1:E:262:ASP:HB3	1:E:263:PRO:HD3	1.52	0.91
1:A:220:THR:HG21	1:A:446:GLU:HG2	0.94	0.91
1:A:468:HIS:HA	1:A:473:ARG:HD3	1.53	0.91
1:C:235:LEU:HD11	1:C:241:LEU:HD22	1.49	0.91
1:B:177:LEU:HA	1:C:347:HIS:CG	2.05	0.91
1:C:379:TYR:O	1:C:385:ILE:HB	1.70	0.91
1:D:461:LEU:O	1:D:465:MET:HG2	1.71	0.91
1:C:132:ALA:N	1:C:133:ASN:HA	1.86	0.91
1:C:22:PHE:HA	1:C:33:PRO:HD3	1.53	0.91
1:D:132:ALA:N	1:D:133:ASN:HA	1.86	0.90
1:D:176:LYS:CG	1:E:347:HIS:C	2.39	0.90
1:C:77:TRP:CZ3	1:C:114:LEU:N	2.38	0.90
1:D:118:PRO:HD2	1:D:128:ASP:HA	1.54	0.90
1:E:379:TYR:O	1:E:385:ILE:HB	1.70	0.90
1:B:133:ASN:H	1:B:134:PRO:HD2	1.36	0.90
1:C:60:ARG:HG2	1:C:201:THR:HG21	1.51	0.90
1:C:57:GLN:HE21	1:C:265:ARG:NH2	1.68	0.90
1:A:345:THR:OG1	1:E:173:ALA:CB	2.19	0.90
1:B:120:GLN:O	1:B:120:GLN:HG2	1.69	0.90
1:D:163:GLU:OE1	1:D:208:LEU:CB	2.19	0.90
1:E:382:ASN:HB3	1:E:385:ILE:HG12	1.54	0.90
1:A:347:HIS:HB2	1:E:177:LEU:N	1.86	0.90
1:D:468:HIS:HA	1:D:473:ARG:HD3	1.53	0.90
1:A:132:ALA:N	1:A:133:ASN:HA	1.86	0.90
1:A:379:TYR:O	1:A:385:ILE:HB	1.70	0.90
1:B:378:LEU:CD2	1:B:400:LYS:O	2.20	0.90
1:B:117:ARG:CB	1:B:118:PRO:HD3	2.02	0.90
1:C:382:ASN:HB3	1:C:385:ILE:HG12	1.54	0.90
1:D:39:GLN:HB3	1:D:67:ILE:HG12	1.54	0.90
1:A:347:HIS:CG	1:E:177:LEU:HA	2.06	0.90
1:A:329:ILE:HG23	1:A:330:ILE:N	1.85	0.90
1:B:202:PRO:HD3	1:B:265:ARG:HD2	0.95	0.90
1:C:58:ALA:O	1:C:265:ARG:HD3	1.70	0.90
1:E:329:ILE:HG23	1:E:330:ILE:N	1.84	0.90
1:E:322:TRP:CD1	1:E:456:ARG:CB	2.53	0.90
1:A:346:TYR:H	1:E:173:ALA:HB1	1.14	0.89
1:A:173:ALA:HB1	1:B:346:TYR:H	1.14	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LEU:HD12	1:A:241:LEU:HD22	1.49	0.89
1:A:91:LYS:HB3	1:A:93:ARG:H	1.37	0.89
1:C:57:GLN:NE2	1:C:265:ARG:NH2	2.20	0.89
1:C:76:LEU:HB2	1:C:136:HIS:CE1	2.06	0.89
1:D:177:LEU:CA	1:E:347:HIS:CG	2.56	0.89
1:A:177:LEU:CA	1:B:347:HIS:CG	2.55	0.89
1:B:379:TYR:O	1:B:385:ILE:HB	1.71	0.89
1:E:430:LYS:O	1:E:434:PRO:CD	2.19	0.89
1:B:176:LYS:HE2	1:C:348:ASP:OD2	1.71	0.89
1:C:235:LEU:CD1	1:C:241:LEU:HD22	2.02	0.89
1:D:56:LEU:CD2	1:D:222:ILE:HG23	2.03	0.89
1:B:220:THR:HG22	1:B:445:GLU:O	1.72	0.89
1:E:117:ARG:HB3	1:E:118:PRO:CD	2.00	0.89
1:C:174:ARG:NH1	1:D:345:THR:CB	2.36	0.89
1:D:22:PHE:HA	1:D:33:PRO:HD3	1.51	0.89
1:C:176:LYS:CB	1:D:347:HIS:CB	2.48	0.89
1:A:144:GLY:HA2	1:A:146:THR:N	1.88	0.88
1:C:144:GLY:HA2	1:C:146:THR:N	1.88	0.88
1:D:370:LYS:CE	1:D:399:ASP:HB3	2.02	0.88
1:E:132:ALA:N	1:E:133:ASN:HA	1.86	0.88
1:A:345:THR:HA	1:E:174:ARG:HH12	1.38	0.88
1:A:176:LYS:HB3	1:B:347:HIS:HB3	1.52	0.88
1:C:177:LEU:HA	1:D:347:HIS:CG	2.07	0.88
1:C:202:PRO:HD3	1:C:265:ARG:CD	2.02	0.88
1:B:144:GLY:HA2	1:B:146:THR:N	1.88	0.88
1:B:368:ARG:NH2	1:B:381:LEU:CD1	2.37	0.88
1:A:280:LYS:NZ	1:A:437:LEU:HB2	1.89	0.88
1:D:177:LEU:HA	1:E:347:HIS:CG	2.07	0.88
1:E:144:GLY:HA2	1:E:146:THR:N	1.88	0.88
1:E:235:LEU:HD22	1:E:245:LEU:HB3	1.55	0.88
1:A:176:LYS:HB2	1:B:347:HIS:CB	2.03	0.88
1:E:280:LYS:HZ2	1:E:438:LYS:HA	1.33	0.88
1:D:173:ALA:HA	1:E:346:TYR:HA	1.25	0.88
1:A:73:VAL:CG2	1:A:105:ILE:HG12	2.03	0.88
1:B:98:SER:HA	1:B:101:ILE:HD12	1.56	0.88
1:C:301:LEU:HD21	1:C:362:VAL:HG23	1.55	0.88
1:D:202:PRO:HB3	1:D:265:ARG:NH1	1.87	0.88
1:B:329:ILE:HG23	1:B:330:ILE:N	1.87	0.88
1:A:347:HIS:CB	1:E:176:LYS:HB2	2.04	0.88
1:E:83:LYS:CG	1:E:155:ASP:CB	2.53	0.87
1:E:368:ARG:HB2	1:E:401:THR:HG21	1.56	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:VAL:HG11	1:A:447:ILE:HD13	1.55	0.87
1:C:322:TRP:CD1	1:C:456:ARG:CB	2.53	0.87
1:D:144:GLY:HA2	1:D:146:THR:N	1.88	0.87
1:A:347:HIS:HB3	1:E:176:LYS:C	1.94	0.87
1:B:235:LEU:HD22	1:B:245:LEU:HB3	1.54	0.87
1:C:378:LEU:HD21	1:C:401:THR:CG2	2.05	0.87
1:C:468:HIS:HA	1:C:473:ARG:HD3	1.54	0.87
1:A:417:VAL:HB	1:A:465:MET:CG	2.02	0.87
1:C:60:ARG:HG3	1:C:201:THR:HG21	1.53	0.87
1:C:177:LEU:CA	1:D:347:HIS:CD2	2.57	0.87
1:D:181:VAL:HB	1:E:376:ALA:HA	1.57	0.87
1:C:177:LEU:CA	1:D:347:HIS:CG	2.56	0.87
1:E:148:GLN:NE2	1:E:175:GLU:HG3	1.89	0.87
1:B:176:LYS:CE	1:C:348:ASP:OD2	2.22	0.87
1:A:117:ARG:CB	1:A:118:PRO:HD3	2.04	0.87
1:B:461:LEU:O	1:B:465:MET:HG2	1.75	0.87
1:E:370:LYS:HE3	1:E:399:ASP:CB	2.03	0.87
1:A:177:LEU:HA	1:B:347:HIS:CG	2.08	0.86
1:C:437:LEU:CD2	1:C:458:CYS:SG	2.63	0.86
1:C:417:VAL:HB	1:C:465:MET:CG	2.04	0.86
1:A:301:LEU:HD21	1:A:362:VAL:HG23	1.57	0.86
1:D:120:GLN:O	1:D:120:GLN:HG2	1.72	0.86
1:E:182:GLN:HE21	1:E:185:ALA:HB2	0.76	0.86
1:B:351:ASN:HD21	1:B:377:VAL:HA	1.38	0.86
1:C:176:LYS:C	1:D:347:HIS:HB3	1.96	0.86
1:A:98:SER:HA	1:A:101:ILE:HD12	1.58	0.86
1:D:21:ALA:O	1:D:33:PRO:HD2	1.75	0.86
1:D:370:LYS:HB3	1:D:375:TYR:CZ	2.11	0.86
1:B:378:LEU:HD21	1:B:401:THR:CG2	2.06	0.86
1:C:177:LEU:HB3	1:D:347:HIS:HD2	0.86	0.86
1:D:301:LEU:HD21	1:D:362:VAL:HG23	1.58	0.86
1:E:370:LYS:HB3	1:E:375:TYR:CZ	2.10	0.86
1:B:417:VAL:CB	1:B:465:MET:HG3	2.03	0.86
1:E:39:GLN:HB3	1:E:67:ILE:HG21	1.57	0.86
1:C:98:SER:HA	1:C:101:ILE:HD12	1.57	0.86
1:D:201:THR:HG23	1:D:202:PRO:HD2	1.55	0.86
1:D:346:TYR:HD1	1:D:349:CYS:H	0.96	0.86
1:D:351:ASN:HD21	1:D:377:VAL:HA	1.40	0.86
1:C:173:ALA:HB3	1:D:345:THR:CG2	2.04	0.85
1:C:235:LEU:HD22	1:C:245:LEU:HB3	1.57	0.85
1:B:322:TRP:CD1	1:B:456:ARG:CB	2.56	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:LEU:HD21	1:D:401:THR:OG1	1.76	0.85
1:A:132:ALA:N	1:A:133:ASN:OD1	2.10	0.85
1:B:173:ALA:HA	1:C:346:TYR:HA	1.25	0.85
1:C:21:ALA:O	1:C:33:PRO:HD2	1.76	0.85
1:D:436:LEU:CD2	1:D:457:ILE:HG22	2.06	0.85
1:A:347:HIS:CE1	1:E:177:LEU:HB2	2.11	0.85
1:E:83:LYS:HG3	1:E:155:ASP:CB	2.06	0.85
1:D:156:ILE:HB	1:D:194:SER:CB	2.06	0.85
1:C:132:ALA:N	1:C:133:ASN:OD1	2.09	0.85
1:B:132:ALA:N	1:B:133:ASN:OD1	2.09	0.85
1:C:351:ASN:HD21	1:C:377:VAL:HA	1.39	0.85
1:A:347:HIS:CG	1:E:177:LEU:CA	2.59	0.85
1:C:120:GLN:O	1:C:120:GLN:HG2	1.75	0.85
1:C:274:ARG:HD3	1:C:414:VAL:CG1	2.05	0.85
1:C:414:VAL:HG11	1:C:447:ILE:HD13	1.58	0.85
1:E:156:ILE:HB	1:E:194:SER:CB	2.06	0.85
1:B:176:LYS:HB3	1:C:347:HIS:CA	2.07	0.85
1:E:91:LYS:HB3	1:E:93:ARG:H	1.42	0.85
1:A:156:ILE:HB	1:A:194:SER:CB	2.07	0.84
1:E:59:PHE:CD2	1:E:60:ARG:O	2.30	0.84
1:A:351:ASN:HD21	1:A:377:VAL:HA	1.42	0.84
1:A:322:TRP:CD1	1:A:456:ARG:CB	2.53	0.84
1:E:148:GLN:NE2	1:E:175:GLU:CG	2.39	0.84
1:B:368:ARG:HB2	1:B:401:THR:HG21	1.59	0.84
1:B:378:LEU:HD21	1:B:401:THR:HG21	1.60	0.84
1:B:156:ILE:HB	1:B:194:SER:CB	2.07	0.84
1:A:59:PHE:CD2	1:A:60:ARG:O	2.30	0.84
1:C:346:TYR:CD2	1:C:349:CYS:CB	2.60	0.84
1:D:280:LYS:NZ	1:D:438:LYS:HA	1.91	0.84
1:D:98:SER:HA	1:D:101:ILE:HD12	1.57	0.84
1:E:280:LYS:NZ	1:E:438:LYS:HA	1.93	0.84
1:A:370:LYS:HB3	1:A:375:TYR:CZ	2.12	0.84
1:A:417:VAL:CA	1:A:465:MET:HG3	2.07	0.84
1:D:176:LYS:C	1:E:347:HIS:HB3	1.98	0.84
1:E:73:VAL:HG22	1:E:105:ILE:HG13	1.58	0.84
1:C:378:LEU:HD11	1:C:401:THR:OG1	1.78	0.84
1:E:378:LEU:HD21	1:E:401:THR:CG2	2.06	0.84
1:E:220:THR:HG22	1:E:445:GLU:O	1.77	0.84
1:C:39:GLN:HB3	1:C:67:ILE:HG12	1.59	0.84
1:D:177:LEU:HB3	1:E:347:HIS:CD2	2.13	0.84
1:B:73:VAL:HG22	1:B:105:ILE:HG13	1.58	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:PHE:CD1	1:D:225:ALA:HA	2.12	0.83
1:C:174:ARG:HH12	1:D:345:THR:HA	1.42	0.83
1:E:132:ALA:N	1:E:133:ASN:OD1	2.11	0.83
1:C:173:ALA:HA	1:D:346:TYR:HA	1.25	0.83
1:A:176:LYS:C	1:B:347:HIS:HB3	1.99	0.83
1:B:235:LEU:HD21	1:B:245:LEU:CB	2.06	0.83
1:C:202:PRO:CD	1:C:265:ARG:HD2	2.03	0.83
1:C:274:ARG:HD3	1:C:414:VAL:HG12	1.59	0.83
1:D:132:ALA:N	1:D:133:ASN:OD1	2.10	0.83
1:E:436:LEU:CD2	1:E:457:ILE:HG22	2.08	0.83
1:B:176:LYS:C	1:C:347:HIS:HB3	1.99	0.83
1:C:378:LEU:HD21	1:C:401:THR:HG21	1.60	0.83
1:E:98:SER:HA	1:E:101:ILE:HD12	1.60	0.83
1:C:156:ILE:HB	1:C:194:SER:CB	2.07	0.83
1:C:59:PHE:CD2	1:C:60:ARG:O	2.31	0.83
1:A:346:TYR:CD1	1:E:173:ALA:HB2	2.14	0.83
1:A:235:LEU:HD21	1:A:245:LEU:CB	2.04	0.83
1:B:280:LYS:NZ	1:B:437:LEU:HB2	1.92	0.83
1:C:313:LEU:CD1	1:C:374:GLY:HA2	2.09	0.83
1:E:221:ILE:HB	1:E:222:ILE:HG12	1.59	0.83
1:E:382:ASN:CB	1:E:385:ILE:HG12	2.09	0.83
1:C:173:ALA:CB	1:D:346:TYR:CB	2.57	0.83
1:E:378:LEU:HD11	1:E:401:THR:OG1	1.78	0.83
1:A:56:LEU:CG	1:A:222:ILE:HG23	2.07	0.83
1:A:75:SER:HB3	1:A:83:LYS:NZ	1.94	0.83
1:C:181:VAL:HA	1:C:182:GLN:CG	2.08	0.83
1:D:436:LEU:HD22	1:D:457:ILE:CG2	2.09	0.83
1:E:301:LEU:HD21	1:E:362:VAL:HG23	1.60	0.83
1:A:120:GLN:HG2	1:A:120:GLN:O	1.78	0.83
1:C:382:ASN:CB	1:C:385:ILE:HG12	2.08	0.83
1:C:417:VAL:CA	1:C:465:MET:HG3	2.08	0.83
1:E:414:VAL:HG11	1:E:447:ILE:HD13	1.58	0.83
1:D:118:PRO:CG	1:D:129:VAL:H	1.91	0.82
1:D:73:VAL:CG2	1:D:105:ILE:HG12	2.08	0.82
1:D:173:ALA:CB	1:E:346:TYR:CB	2.57	0.82
1:C:22:PHE:HA	1:C:33:PRO:CD	2.10	0.82
1:B:176:LYS:CB	1:C:347:HIS:N	2.42	0.82
1:D:375:TYR:HA	1:D:378:LEU:HD12	1.61	0.82
1:B:177:LEU:HB3	1:C:347:HIS:CG	2.14	0.82
1:E:252:ASN:HB3	1:E:253:PRO:HD3	1.61	0.82
1:B:83:LYS:HZ2	1:B:193:SER:H	1.23	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:HA	1:A:182:GLN:CG	2.08	0.82
1:A:56:LEU:CG	1:A:222:ILE:CG2	2.57	0.82
1:C:176:LYS:CB	1:D:347:HIS:N	2.42	0.82
1:E:77:TRP:HZ3	1:E:114:LEU:N	1.77	0.82
1:E:362:VAL:HG12	1:E:362:VAL:O	1.79	0.82
1:D:176:LYS:CB	1:E:347:HIS:N	2.42	0.82
1:A:346:TYR:CG	1:E:173:ALA:HB2	2.15	0.82
1:E:235:LEU:HD11	1:E:241:LEU:HD23	1.61	0.82
1:A:133:ASN:H	1:A:134:PRO:HD3	1.44	0.82
1:A:87:VAL:HB	1:A:158:ILE:HG13	1.62	0.82
1:A:176:LYS:CB	1:B:347:HIS:N	2.42	0.82
1:E:52:LYS:CB	1:E:184:PHE:HZ	1.91	0.82
1:B:173:ALA:CB	1:C:346:TYR:CB	2.57	0.82
1:C:370:LYS:HB3	1:C:375:TYR:CZ	2.15	0.82
1:A:346:TYR:CB	1:E:173:ALA:CB	2.57	0.82
1:B:87:VAL:HB	1:B:158:ILE:HG13	1.62	0.81
1:E:57:GLN:HB3	1:E:265:ARG:NE	1.94	0.81
1:A:10:LEU:HD23	1:A:11:VAL:HG13	1.62	0.81
1:A:223:TRP:CE3	1:A:444:MET:HB2	2.14	0.81
1:E:85:LEU:HB3	1:E:136:HIS:ND1	1.94	0.81
1:A:347:HIS:N	1:E:176:LYS:CB	2.42	0.81
1:E:378:LEU:HD21	1:E:401:THR:HG21	1.60	0.81
1:E:417:VAL:HB	1:E:465:MET:CG	2.06	0.81
1:B:252:ASN:HB3	1:B:253:PRO:HD3	1.63	0.81
1:A:370:LYS:CE	1:A:399:ASP:HB3	2.10	0.81
1:B:181:VAL:HA	1:B:182:GLN:CG	2.10	0.81
1:C:285:LEU:HD22	1:C:431:VAL:HG13	1.62	0.81
1:E:400:LYS:O	1:E:401:THR:HG23	1.80	0.81
1:A:73:VAL:CG2	1:A:105:ILE:CG1	2.58	0.81
1:A:77:TRP:CZ2	1:A:105:ILE:HG23	2.16	0.81
1:A:77:TRP:HZ3	1:A:114:LEU:HB2	1.46	0.81
1:C:73:VAL:HG22	1:C:105:ILE:HG13	1.61	0.81
1:E:351:ASN:HD21	1:E:377:VAL:HA	1.45	0.81
1:B:177:LEU:H	1:C:347:HIS:HB2	1.44	0.81
1:D:73:VAL:CG2	1:D:105:ILE:CG1	2.58	0.81
1:A:163:GLU:HB2	1:A:208:LEU:HD12	1.62	0.81
1:A:362:VAL:HG12	1:A:362:VAL:O	1.80	0.81
1:A:173:ALA:CB	1:B:346:TYR:CB	2.57	0.81
1:C:252:ASN:HB3	1:C:253:PRO:HD3	1.62	0.81
1:B:223:TRP:CE3	1:B:444:MET:HB2	2.16	0.81
1:C:400:LYS:O	1:C:401:THR:HG23	1.80	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:TRP:HZ3	1:D:114:LEU:HB2	1.45	0.81
1:C:362:VAL:O	1:C:362:VAL:HG12	1.80	0.81
1:E:375:TYR:HA	1:E:378:LEU:HD12	1.62	0.81
1:C:83:LYS:CE	1:C:192:PRO:HA	2.05	0.81
1:E:87:VAL:HB	1:E:158:ILE:HG13	1.62	0.81
1:A:167:ASN:O	1:A:171:MET:SD	2.38	0.80
1:D:177:LEU:CA	1:E:347:HIS:ND1	2.39	0.80
1:E:445:GLU:OE1	1:E:445:GLU:N	2.15	0.80
1:E:73:VAL:HG22	1:E:105:ILE:CG1	2.10	0.80
1:A:117:ARG:HB3	1:A:118:PRO:CD	2.10	0.80
1:A:414:VAL:HA	1:A:417:VAL:HG12	1.61	0.80
1:B:77:TRP:HZ3	1:B:114:LEU:N	1.80	0.80
1:C:173:ALA:O	1:D:346:TYR:CA	2.29	0.80
1:C:163:GLU:HG2	1:C:203:GLN:N	1.97	0.80
1:D:52:LYS:CB	1:D:184:PHE:HZ	1.91	0.80
1:E:235:LEU:HD21	1:E:245:LEU:CB	2.06	0.80
1:B:436:LEU:CD2	1:B:457:ILE:HG22	2.11	0.80
1:C:346:TYR:CE2	1:C:349:CYS:CA	2.65	0.80
1:C:170:THR:HA	1:D:345:THR:CG2	2.10	0.80
1:E:83:LYS:HG3	1:E:155:ASP:HB3	1.61	0.80
1:C:52:LYS:CB	1:C:184:PHE:HZ	1.90	0.80
1:C:436:LEU:CD2	1:C:457:ILE:HG22	2.10	0.80
1:A:346:TYR:CD1	1:E:173:ALA:CB	2.65	0.80
1:A:85:LEU:HB3	1:A:136:HIS:ND1	1.97	0.80
1:D:22:PHE:HA	1:D:33:PRO:CD	2.10	0.80
1:D:362:VAL:O	1:D:362:VAL:HG12	1.79	0.80
1:A:346:TYR:CA	1:E:173:ALA:O	2.30	0.80
1:A:91:LYS:HB3	1:A:93:ARG:N	1.96	0.80
1:B:378:LEU:HD11	1:B:401:THR:HG1	1.42	0.80
1:C:87:VAL:HB	1:C:158:ILE:HG13	1.63	0.80
1:C:375:TYR:HA	1:C:378:LEU:HD12	1.62	0.80
1:E:10:LEU:HD23	1:E:11:VAL:HG13	1.63	0.80
1:A:345:THR:CB	1:E:174:ARG:NH1	2.44	0.80
1:E:186:ALA:O	1:E:190:PRO:HD2	1.82	0.80
1:A:345:THR:HA	1:E:174:ARG:NH1	1.97	0.80
1:A:379:TYR:HA	1:A:385:ILE:HG13	1.64	0.80
1:C:156:ILE:CA	1:C:194:SER:HB3	2.12	0.80
1:D:118:PRO:HG3	1:D:129:VAL:H	1.46	0.80
1:D:87:VAL:HB	1:D:158:ILE:HG13	1.62	0.80
1:E:148:GLN:HE21	1:E:175:GLU:CG	1.93	0.80
1:E:436:LEU:HD22	1:E:457:ILE:CG2	2.11	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ASN:HB3	1:A:253:PRO:HD3	1.63	0.80
1:C:117:ARG:HB3	1:C:118:PRO:CD	2.09	0.80
1:C:73:VAL:HG23	1:C:105:ILE:HG13	1.64	0.80
1:A:262:ASP:HB3	1:A:263:PRO:HD3	1.62	0.79
1:B:163:GLU:HG2	1:B:203:GLN:N	1.97	0.79
1:D:181:VAL:HA	1:D:182:GLN:CG	2.10	0.79
1:D:163:GLU:HG2	1:D:203:GLN:N	1.97	0.79
1:E:120:GLN:HG2	1:E:120:GLN:O	1.82	0.79
1:C:163:GLU:HB2	1:C:208:LEU:HD12	1.63	0.79
1:D:156:ILE:CA	1:D:194:SER:HB3	2.12	0.79
1:D:379:TYR:HA	1:D:385:ILE:HG13	1.64	0.79
1:D:77:TRP:CZ2	1:D:105:ILE:HG23	2.16	0.79
1:A:83:LYS:CG	1:A:155:ASP:HB2	2.10	0.79
1:A:177:LEU:H	1:B:347:HIS:HB2	1.44	0.79
1:C:436:LEU:HD22	1:C:457:ILE:CG2	2.12	0.79
1:B:436:LEU:HD22	1:B:457:ILE:CG2	2.12	0.79
1:B:73:VAL:HG22	1:B:105:ILE:CG1	2.11	0.79
1:C:177:LEU:H	1:D:347:HIS:HB2	1.46	0.79
1:D:468:HIS:HA	1:D:473:ARG:CD	2.12	0.79
1:E:291:PRO:HG2	1:E:295:ASP:CB	2.12	0.79
1:A:163:GLU:HG2	1:A:203:GLN:N	1.97	0.79
1:A:272:ARG:HB2	1:A:441:ASN:HB2	1.65	0.79
1:B:173:ALA:HB3	1:C:345:THR:CG2	2.13	0.79
1:C:57:GLN:HG3	1:C:212:LEU:HD13	1.65	0.79
1:D:85:LEU:CD2	1:D:136:HIS:CD2	2.65	0.79
1:B:362:VAL:O	1:B:362:VAL:HG13	1.81	0.79
1:C:159:ALA:CB	1:C:198:TYR:CD1	2.65	0.79
1:E:156:ILE:CA	1:E:194:SER:HB3	2.12	0.79
1:E:274:ARG:HD3	1:E:414:VAL:HG12	1.64	0.79
1:A:186:ALA:O	1:A:190:PRO:CD	2.31	0.79
1:A:379:TYR:HB2	1:E:181:VAL:HG21	1.65	0.79
1:A:468:HIS:HA	1:A:473:ARG:CD	2.12	0.79
1:C:174:ARG:HH12	1:D:345:THR:CB	1.96	0.79
1:C:73:VAL:HG22	1:C:105:ILE:CG1	2.13	0.79
1:E:294:SER:HB2	1:E:340:GLY:O	1.83	0.79
1:A:173:ALA:O	1:B:346:TYR:CA	2.29	0.78
1:D:177:LEU:H	1:E:347:HIS:HB2	1.45	0.78
1:A:156:ILE:CA	1:A:194:SER:HB3	2.12	0.78
1:A:173:ALA:HB3	1:B:345:THR:CG2	2.13	0.78
1:C:414:VAL:HA	1:C:417:VAL:HG12	1.63	0.78
1:D:190:PRO:HB2	1:D:192:PRO:HD2	1.64	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:346:TYR:CE1	1:D:349:CYS:CA	2.66	0.78
1:D:294:SER:HB2	1:D:340:GLY:O	1.83	0.78
1:D:77:TRP:CZ3	1:D:114:LEU:HB2	2.17	0.78
1:D:85:LEU:HD22	1:D:136:HIS:HD2	1.45	0.78
1:A:57:GLN:HG3	1:A:212:LEU:HD13	1.65	0.78
1:A:21:ALA:O	1:A:33:PRO:HD3	1.83	0.78
1:B:128:ASP:HB3	1:B:134:PRO:O	1.84	0.78
1:B:156:ILE:CA	1:B:194:SER:HB3	2.12	0.78
1:B:285:LEU:HD22	1:B:431:VAL:HG13	1.65	0.78
1:D:382:ASN:HB3	1:D:385:ILE:HG12	1.64	0.78
1:A:220:THR:HG22	1:A:445:GLU:C	2.04	0.78
1:B:205:GLU:HG2	1:B:209:TYR:HD2	1.45	0.78
1:C:186:ALA:O	1:C:190:PRO:CD	2.32	0.78
1:D:201:THR:CG2	1:D:202:PRO:CD	2.62	0.78
1:A:436:LEU:CD2	1:A:457:ILE:HG22	2.13	0.78
1:C:84:ILE:HG23	1:C:154:ALA:HA	1.65	0.78
1:D:173:ALA:O	1:E:346:TYR:CA	2.29	0.78
1:D:417:VAL:CB	1:D:465:MET:HG3	2.09	0.78
1:B:162:VAL:HB	1:B:208:LEU:HD21	1.66	0.78
1:A:294:SER:HB2	1:A:340:GLY:O	1.83	0.78
1:A:437:LEU:CD2	1:A:458:CYS:SG	2.68	0.78
1:A:57:GLN:OE1	1:A:265:ARG:NH2	2.17	0.78
1:B:167:ASN:O	1:B:171:MET:SD	2.42	0.78
1:B:382:ASN:HB3	1:B:385:ILE:HG12	1.66	0.78
1:D:220:THR:OG1	1:D:445:GLU:HB2	1.83	0.78
1:E:414:VAL:HA	1:E:417:VAL:HG12	1.66	0.78
1:A:144:GLY:HA2	1:A:147:GLY:H	1.48	0.77
1:B:436:LEU:HA	1:B:439:HIS:HE1	1.46	0.77
1:E:417:VAL:CA	1:E:465:MET:HG3	2.14	0.77
1:E:467:THR:HG22	1:E:473:ARG:HG3	1.66	0.77
1:E:85:LEU:HD12	1:E:156:ILE:HG21	1.65	0.77
1:A:177:LEU:HB3	1:B:347:HIS:CG	2.19	0.77
1:A:368:ARG:HB2	1:A:378:LEU:HD21	1.66	0.77
1:C:144:GLY:HA2	1:C:147:GLY:H	1.48	0.77
1:C:346:TYR:HD2	1:C:349:CYS:H	0.81	0.77
1:D:144:GLY:HA2	1:D:147:GLY:H	1.48	0.77
1:E:144:GLY:HA2	1:E:147:GLY:H	1.48	0.77
1:E:163:GLU:HB2	1:E:208:LEU:HD13	1.64	0.77
1:B:173:ALA:O	1:C:346:TYR:CA	2.29	0.77
1:E:163:GLU:HG2	1:E:203:GLN:N	1.99	0.77
1:E:272:ARG:HB2	1:E:441:ASN:HB2	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ILE:HG23	1:B:154:ALA:HA	1.66	0.77
1:E:370:LYS:HE2	1:E:375:TYR:HE1	1.46	0.77
1:A:382:ASN:HB3	1:A:385:ILE:HG12	1.65	0.77
1:A:84:ILE:HG23	1:A:154:ALA:HA	1.65	0.77
1:B:467:THR:HG22	1:B:473:ARG:HG3	1.65	0.77
1:D:173:ALA:HB3	1:E:345:THR:CG2	2.13	0.77
1:A:379:TYR:HB3	1:A:385:ILE:HG21	1.65	0.77
1:B:45:VAL:O	1:B:54:PHE:CE2	2.38	0.77
1:C:10:LEU:HD12	1:C:78:ARG:HD2	1.65	0.77
1:A:262:ASP:HB2	1:A:263:PRO:HD3	1.66	0.77
1:C:235:LEU:HD21	1:C:245:LEU:CB	2.11	0.77
1:E:77:TRP:HE1	1:E:105:ILE:CG1	1.90	0.77
1:C:45:VAL:O	1:C:54:PHE:CE2	2.38	0.77
1:D:182:GLN:HE21	1:D:185:ALA:HB2	0.73	0.77
1:C:174:ARG:NH1	1:D:345:THR:HA	1.99	0.77
1:B:144:GLY:HA2	1:B:147:GLY:H	1.48	0.76
1:A:77:TRP:CZ3	1:A:114:LEU:HB2	2.20	0.76
1:B:73:VAL:HG23	1:B:105:ILE:HG13	1.67	0.76
1:B:294:SER:HB2	1:B:340:GLY:O	1.83	0.76
1:B:400:LYS:O	1:B:401:THR:HG23	1.84	0.76
1:D:56:LEU:CG	1:D:222:ILE:CG2	2.57	0.76
1:D:59:PHE:CZ	1:D:62:ILE:HB	2.20	0.76
1:E:59:PHE:CE2	1:E:60:ARG:O	2.38	0.76
1:B:91:LYS:CB	1:B:93:ARG:H	1.99	0.76
1:B:170:THR:HA	1:C:345:THR:CG2	2.14	0.76
1:C:368:ARG:HB2	1:C:401:THR:HG21	1.67	0.76
1:D:45:VAL:O	1:D:54:PHE:CE2	2.39	0.76
1:A:347:HIS:HB2	1:E:177:LEU:H	1.49	0.76
1:A:170:THR:HA	1:B:345:THR:CG2	2.14	0.76
1:C:173:ALA:C	1:D:345:THR:O	2.24	0.76
1:C:190:PRO:HB2	1:C:192:PRO:HD2	1.67	0.76
1:D:173:ALA:HB2	1:E:346:TYR:CG	2.20	0.76
1:E:91:LYS:HB3	1:E:93:ARG:N	2.00	0.76
1:B:414:VAL:HA	1:B:417:VAL:HG12	1.66	0.76
1:C:182:GLN:HE21	1:C:185:ALA:HB2	0.73	0.76
1:C:294:SER:HB2	1:C:340:GLY:O	1.85	0.76
1:D:128:ASP:HB3	1:D:134:PRO:O	1.84	0.76
1:D:252:ASN:HB3	1:D:253:PRO:HD3	1.67	0.76
1:E:252:ASN:HB3	1:E:253:PRO:CD	2.16	0.76
1:E:470:LEU:HD21	1:E:472:ILE:HD12	1.68	0.76
1:A:77:TRP:HZ2	1:A:105:ILE:CG2	1.99	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LEU:HD22	1:A:457:ILE:CG2	2.15	0.76
1:E:181:VAL:HA	1:E:182:GLN:CG	2.13	0.76
1:A:56:LEU:HG	1:A:222:ILE:HG22	1.67	0.76
1:B:280:LYS:CE	1:B:438:LYS:HA	2.16	0.76
1:C:77:TRP:HZ3	1:C:114:LEU:N	1.82	0.76
1:E:57:GLN:O	1:E:223:TRP:CD1	2.39	0.76
1:E:57:GLN:OE1	1:E:265:ARG:NH2	2.18	0.76
1:A:59:PHE:CE2	1:A:60:ARG:O	2.39	0.76
1:C:220:THR:OG1	1:C:220:THR:O	1.97	0.76
1:D:285:LEU:HD22	1:D:431:VAL:HG13	1.68	0.76
1:D:313:LEU:HD12	1:D:374:GLY:CA	2.11	0.76
1:B:173:ALA:C	1:C:345:THR:O	2.24	0.76
1:C:216:ARG:O	1:C:411:GLN:OE1	2.03	0.76
1:D:173:ALA:C	1:E:345:THR:O	2.24	0.76
1:D:56:LEU:HD13	1:D:199:LEU:HD12	1.68	0.76
1:D:414:VAL:HA	1:D:417:VAL:HG12	1.68	0.76
1:D:170:THR:HA	1:E:345:THR:CG2	2.14	0.76
1:A:133:ASN:H	1:A:134:PRO:CD	2.00	0.75
1:D:470:LEU:HD21	1:D:472:ILE:HD12	1.68	0.75
1:D:177:LEU:HB3	1:E:347:HIS:CG	2.19	0.75
1:A:176:LYS:HB2	1:B:347:HIS:CA	2.15	0.75
1:B:368:ARG:H	1:B:401:THR:CG2	1.99	0.75
1:B:67:ILE:H	1:B:67:ILE:CD1	1.98	0.75
1:C:91:LYS:CB	1:C:93:ARG:H	1.99	0.75
1:A:173:ALA:C	1:B:345:THR:O	2.24	0.75
1:E:291:PRO:HD3	1:E:295:ASP:O	1.85	0.75
1:E:45:VAL:O	1:E:54:PHE:CE2	2.39	0.75
1:A:182:GLN:HE21	1:A:185:ALA:HB2	0.73	0.75
1:B:186:ALA:O	1:B:190:PRO:CD	2.34	0.75
1:B:252:ASN:HB3	1:B:253:PRO:CD	2.17	0.75
1:C:220:THR:CA	1:C:445:GLU:HB2	2.17	0.75
1:D:196:VAL:HG13	1:D:198:TYR:CE1	2.21	0.75
1:D:216:ARG:O	1:D:411:GLN:OE1	2.04	0.75
1:D:346:TYR:CD1	1:D:349:CYS:CB	2.69	0.75
1:E:190:PRO:HB2	1:E:192:PRO:HD2	1.68	0.75
1:E:163:GLU:CD	1:E:208:LEU:HB3	2.07	0.75
1:B:91:LYS:HB3	1:B:93:ARG:H	1.52	0.75
1:C:128:ASP:HB3	1:C:134:PRO:O	1.86	0.75
1:E:128:ASP:HB3	1:E:134:PRO:O	1.87	0.75
1:A:345:THR:O	1:E:173:ALA:C	2.24	0.75
1:A:75:SER:HB3	1:A:83:LYS:HZ1	1.51	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:TRP:HZ2	1:D:105:ILE:CG2	2.00	0.75
1:D:144:GLY:O	1:D:171:MET:HG2	1.87	0.75
1:E:221:ILE:CB	1:E:222:ILE:HG12	2.17	0.75
1:A:252:ASN:HB3	1:A:253:PRO:CD	2.17	0.75
1:A:202:PRO:HB3	1:A:265:ARG:NH1	2.02	0.75
1:A:91:LYS:CB	1:A:93:ARG:H	1.99	0.75
1:C:59:PHE:CE2	1:C:60:ARG:O	2.40	0.75
1:A:190:PRO:HB2	1:A:192:PRO:HD2	1.69	0.74
1:A:313:LEU:HD12	1:A:374:GLY:CA	2.13	0.74
1:C:45:VAL:O	1:C:54:PHE:CZ	2.40	0.74
1:D:437:LEU:CD2	1:D:458:CYS:SG	2.71	0.74
1:A:347:HIS:CA	1:E:176:LYS:HB2	2.16	0.74
1:E:59:PHE:CZ	1:E:62:ILE:HB	2.22	0.74
1:D:186:ALA:O	1:D:190:PRO:CD	2.35	0.74
1:A:45:VAL:O	1:A:54:PHE:CE2	2.40	0.74
1:C:162:VAL:O	1:C:165:PRO:HD2	1.88	0.74
1:C:59:PHE:CZ	1:C:62:ILE:HB	2.21	0.74
1:E:202:PRO:HD3	1:E:265:ARG:HG2	1.70	0.74
1:B:190:PRO:HB2	1:B:192:PRO:HD2	1.67	0.74
1:B:45:VAL:O	1:B:54:PHE:CZ	2.40	0.74
1:A:52:LYS:CB	1:A:184:PHE:HZ	1.91	0.74
1:A:59:PHE:CZ	1:A:62:ILE:HB	2.21	0.74
1:B:156:ILE:HA	1:B:194:SER:HB3	1.69	0.74
1:D:45:VAL:O	1:D:54:PHE:CZ	2.40	0.74
1:D:91:LYS:CB	1:D:93:ARG:H	1.99	0.74
1:E:220:THR:CA	1:E:445:GLU:HB2	2.17	0.74
1:E:45:VAL:O	1:E:54:PHE:CZ	2.40	0.74
1:E:91:LYS:CB	1:E:93:ARG:H	1.99	0.74
1:B:182:GLN:HE21	1:B:185:ALA:HB2	0.73	0.74
1:D:133:ASN:H	1:D:134:PRO:CD	1.99	0.74
1:D:176:LYS:HB3	1:E:347:HIS:H	1.48	0.74
1:D:177:LEU:HA	1:E:347:HIS:HD1	1.51	0.74
1:A:346:TYR:CA	1:E:173:ALA:C	2.44	0.74
1:E:55:ILE:CG2	1:E:57:GLN:HE21	1.99	0.74
1:B:85:LEU:HB3	1:B:136:HIS:CD2	2.19	0.74
1:D:252:ASN:HB3	1:D:253:PRO:CD	2.18	0.74
1:E:272:ARG:HB3	1:E:442:CYS:H	1.53	0.74
1:E:379:TYR:HA	1:E:385:ILE:HG13	1.68	0.74
1:C:174:ARG:NH1	1:D:345:THR:CA	2.51	0.74
1:C:177:LEU:CB	1:D:347:HIS:HD2	1.72	0.74
1:B:379:TYR:HA	1:B:385:ILE:HG13	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ASN:HB3	1:C:253:PRO:CD	2.17	0.74
1:B:159:ALA:HB3	1:B:198:TYR:HD1	1.50	0.74
1:A:45:VAL:O	1:A:54:PHE:CZ	2.40	0.73
1:C:174:ARG:HH12	1:D:345:THR:CA	2.00	0.73
1:D:346:TYR:HD1	1:D:349:CYS:N	1.78	0.73
1:E:370:LYS:HG3	1:E:401:THR:OG1	1.88	0.73
1:A:144:GLY:CA	1:A:147:GLY:H	2.01	0.73
1:A:72:VAL:HG13	1:A:85:LEU:HD13	1.70	0.73
1:C:235:LEU:HD11	1:C:241:LEU:HD23	1.69	0.73
1:C:368:ARG:H	1:C:401:THR:CG2	2.01	0.73
1:C:468:HIS:HA	1:C:473:ARG:CD	2.17	0.73
1:E:73:VAL:HG23	1:E:105:ILE:HG13	1.69	0.73
1:D:156:ILE:HA	1:D:194:SER:HB3	1.69	0.73
1:D:412:TRP:CZ3	1:D:416:THR:OG1	2.41	0.73
1:A:345:THR:CA	1:E:174:ARG:HH12	2.01	0.73
1:A:128:ASP:HB3	1:A:134:PRO:O	1.87	0.73
1:B:83:LYS:NZ	1:B:193:SER:H	1.85	0.73
1:D:144:GLY:CA	1:D:147:GLY:H	2.01	0.73
1:C:176:LYS:HB3	1:D:347:HIS:CA	2.17	0.73
1:A:76:LEU:HG	1:A:134:PRO:HB2	1.69	0.73
1:B:85:LEU:CB	1:B:136:HIS:HD2	2.01	0.73
1:D:373:THR:O	1:D:376:ALA:HB3	1.89	0.73
1:A:91:LYS:CB	1:A:93:ARG:HB2	2.19	0.73
1:E:128:ASP:O	1:E:135:ASP:HB3	1.88	0.73
1:B:144:GLY:CA	1:B:147:GLY:H	2.01	0.73
1:D:51:ASN:HB2	1:D:54:PHE:CZ	2.24	0.73
1:E:156:ILE:HA	1:E:194:SER:HB3	1.69	0.73
1:E:21:ALA:O	1:E:33:PRO:HD3	1.88	0.73
1:C:186:ALA:O	1:C:190:PRO:HD2	1.88	0.73
1:C:373:THR:O	1:C:376:ALA:HB3	1.89	0.73
1:E:144:GLY:CA	1:E:147:GLY:H	2.01	0.73
1:E:313:LEU:HD12	1:E:374:GLY:CA	2.13	0.73
1:E:368:ARG:H	1:E:401:THR:CG2	2.01	0.73
1:A:156:ILE:HA	1:A:194:SER:HB3	1.69	0.72
1:B:181:VAL:CB	1:C:376:ALA:HA	2.19	0.72
1:D:132:ALA:H	1:D:133:ASN:HA	1.54	0.72
1:A:346:TYR:N	1:A:346:TYR:CD1	2.31	0.72
1:A:181:VAL:CB	1:B:376:ALA:HA	2.19	0.72
1:A:345:THR:CA	1:E:174:ARG:NH1	2.52	0.72
1:B:442:CYS:HA	1:B:447:ILE:HD13	1.69	0.72
1:C:163:GLU:OE1	1:C:208:LEU:CB	2.35	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ALA:O	1:A:190:PRO:HD2	1.88	0.72
1:A:220:THR:CA	1:A:445:GLU:HB3	2.18	0.72
1:B:373:THR:O	1:B:376:ALA:HB3	1.89	0.72
1:C:144:GLY:CA	1:C:147:GLY:H	2.01	0.72
1:C:149:LEU:HD23	1:C:174:ARG:HD2	1.71	0.72
1:D:10:LEU:HD23	1:D:11:VAL:HG13	1.70	0.72
1:C:10:LEU:HD23	1:C:11:VAL:HG13	1.69	0.72
1:D:186:ALA:O	1:D:190:PRO:HD2	1.89	0.72
1:E:373:THR:O	1:E:376:ALA:HB3	1.89	0.72
1:A:21:ALA:O	1:A:33:PRO:CD	2.38	0.72
1:B:132:ALA:H	1:B:133:ASN:HA	1.55	0.72
1:C:379:TYR:HA	1:C:385:ILE:HG13	1.71	0.72
1:C:72:VAL:HG13	1:C:85:LEU:HD13	1.70	0.72
1:E:21:ALA:O	1:E:33:PRO:CD	2.38	0.72
1:B:177:LEU:CB	1:C:347:HIS:CG	2.72	0.72
1:E:181:VAL:N	1:E:182:GLN:HB3	2.05	0.72
1:E:272:ARG:CB	1:E:441:ASN:HB2	2.20	0.72
1:D:57:GLN:HG3	1:D:212:LEU:HD13	1.71	0.72
1:D:181:VAL:CB	1:E:376:ALA:HA	2.19	0.72
1:A:204:THR:HG22	1:A:268:ARG:HD3	1.71	0.72
1:A:373:THR:O	1:A:376:ALA:HB3	1.89	0.72
1:B:368:ARG:H	1:B:401:THR:HG22	1.55	0.72
1:A:220:THR:HA	1:A:445:GLU:HB3	1.71	0.72
1:D:329:ILE:CG2	1:D:330:ILE:H	2.03	0.72
1:C:161:ASP:O	1:C:165:PRO:HD3	1.90	0.71
1:D:118:PRO:HG3	1:D:129:VAL:N	2.05	0.71
1:C:177:LEU:HA	1:D:347:HIS:CD2	2.24	0.71
1:A:177:LEU:CB	1:B:347:HIS:CG	2.74	0.71
1:B:313:LEU:HD12	1:B:374:GLY:CA	2.14	0.71
1:C:156:ILE:HA	1:C:194:SER:HB3	1.69	0.71
1:D:291:PRO:HD3	1:D:295:ASP:O	1.90	0.71
1:B:117:ARG:CB	1:B:118:PRO:CD	2.68	0.71
1:B:52:LYS:CB	1:B:184:PHE:HZ	1.91	0.71
1:B:55:ILE:CG2	1:B:57:GLN:OE1	2.38	0.71
1:D:173:ALA:C	1:E:346:TYR:CA	2.44	0.71
1:C:181:VAL:CB	1:D:376:ALA:HA	2.19	0.71
1:E:149:LEU:HD23	1:E:174:ARG:HD2	1.71	0.71
1:E:379:TYR:HB3	1:E:385:ILE:HG21	1.71	0.71
1:A:272:ARG:HB3	1:A:442:CYS:H	1.55	0.71
1:D:338:LEU:HD22	1:D:430:LYS:HG3	1.71	0.71
1:D:223:TRP:CE3	1:D:444:MET:HB2	2.26	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:ALA:H	1:E:133:ASN:HA	1.55	0.71
1:E:370:LYS:CE	1:E:399:ASP:HB3	2.20	0.71
1:B:186:ALA:O	1:B:190:PRO:HD2	1.91	0.71
1:E:368:ARG:H	1:E:401:THR:HG22	1.56	0.71
1:C:91:LYS:HB2	1:C:93:ARG:HB2	1.73	0.71
1:D:177:LEU:HA	1:E:347:HIS:CE1	2.26	0.71
1:D:128:ASP:O	1:D:135:ASP:HB3	1.90	0.71
1:A:51:ASN:HB2	1:A:54:PHE:CZ	2.25	0.70
1:B:382:ASN:CB	1:B:385:ILE:HG12	2.21	0.70
1:C:338:LEU:HD22	1:C:430:LYS:HG3	1.71	0.70
1:D:83:LYS:HD2	1:D:193:SER:O	1.90	0.70
1:E:55:ILE:CG2	1:E:57:GLN:NE2	2.54	0.70
1:B:77:TRP:HE1	1:B:105:ILE:CG1	1.91	0.70
1:C:272:ARG:CB	1:C:441:ASN:HB2	2.20	0.70
1:E:285:LEU:HD22	1:E:431:VAL:HG13	1.73	0.70
1:D:379:TYR:HB3	1:D:385:ILE:HG21	1.71	0.70
1:D:442:CYS:HA	1:D:447:ILE:HD13	1.73	0.70
1:A:280:LYS:HZ1	1:A:437:LEU:HB2	1.56	0.70
1:C:159:ALA:CB	1:C:198:TYR:CE1	2.74	0.70
1:A:346:TYR:CG	1:E:173:ALA:CB	2.73	0.70
1:D:181:VAL:N	1:D:182:GLN:HB3	2.07	0.70
1:B:220:THR:HA	1:B:445:GLU:HB3	1.74	0.70
1:C:145:ILE:HB	1:C:174:ARG:HG3	1.73	0.70
1:C:57:GLN:HE21	1:C:265:ARG:HH22	1.36	0.70
1:C:69:CYS:HA	1:C:101:ILE:HG12	1.74	0.70
1:A:379:TYR:CB	1:E:181:VAL:HG21	2.21	0.70
1:B:51:ASN:HB2	1:B:54:PHE:CZ	2.26	0.70
1:A:235:LEU:HD11	1:A:241:LEU:HD23	1.72	0.70
1:A:347:HIS:HB3	1:E:177:LEU:N	2.02	0.70
1:A:301:LEU:HD22	1:A:360:ILE:O	1.92	0.70
1:B:181:VAL:N	1:B:182:GLN:HB3	2.07	0.70
1:E:69:CYS:HA	1:E:101:ILE:HG12	1.72	0.70
1:B:176:LYS:CB	1:C:347:HIS:CA	2.70	0.70
1:D:133:ASN:N	1:D:134:PRO:HD2	2.04	0.70
1:E:115:LYS:C	1:E:116:PRO:CD	2.57	0.70
1:A:176:LYS:CB	1:B:347:HIS:CA	2.70	0.70
1:C:132:ALA:H	1:C:133:ASN:HA	1.55	0.70
1:C:176:LYS:HB3	1:D:347:HIS:C	2.12	0.70
1:C:285:LEU:HB2	1:C:431:VAL:HG22	1.74	0.70
1:D:72:VAL:HG13	1:D:85:LEU:HD13	1.73	0.70
1:E:301:LEU:HD22	1:E:360:ILE:O	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:370:LYS:HB3	1:E:375:TYR:CE1	2.27	0.70
1:D:124:VAL:CA	1:D:125:ILE:HB	2.22	0.69
1:D:201:THR:HG22	1:D:202:PRO:CD	2.20	0.69
1:A:216:ARG:HA	1:A:219:THR:O	1.92	0.69
1:C:176:LYS:CB	1:D:347:HIS:CA	2.70	0.69
1:C:181:VAL:HG21	1:D:379:TYR:CB	2.23	0.69
1:C:55:ILE:HG22	1:C:57:GLN:OE1	1.92	0.69
1:D:382:ASN:CB	1:D:385:ILE:HG12	2.21	0.69
1:A:347:HIS:CA	1:E:176:LYS:CB	2.70	0.69
1:E:208:LEU:HD21	1:E:265:ARG:HH22	1.57	0.69
1:E:216:ARG:HA	1:E:219:THR:O	1.92	0.69
1:E:39:GLN:HB3	1:E:67:ILE:CG2	2.22	0.69
1:A:124:VAL:CA	1:A:125:ILE:HB	2.22	0.69
1:A:401:THR:HG23	1:A:402:LEU:H	0.54	0.69
1:B:72:VAL:HG11	1:B:101:ILE:HD13	1.75	0.69
1:D:216:ARG:HA	1:D:219:THR:O	1.92	0.69
1:D:91:LYS:HB2	1:D:93:ARG:HB2	1.74	0.69
1:A:382:ASN:CB	1:A:385:ILE:HG12	2.22	0.69
1:B:124:VAL:CA	1:B:125:ILE:HB	2.22	0.69
1:B:285:LEU:HB2	1:B:431:VAL:HG22	1.75	0.69
1:B:436:LEU:CA	1:B:439:HIS:CE1	2.61	0.69
1:E:55:ILE:HG22	1:E:57:GLN:NE2	2.05	0.69
1:A:132:ALA:H	1:A:133:ASN:HA	1.55	0.69
1:B:216:ARG:HA	1:B:219:THR:O	1.92	0.69
1:C:133:ASN:H	1:C:134:PRO:CD	2.05	0.69
1:D:91:LYS:HB2	1:D:93:ARG:CB	2.22	0.69
1:E:221:ILE:CA	1:E:445:GLU:HG2	2.22	0.69
1:A:51:ASN:O	1:A:52:LYS:HB3	1.92	0.69
1:B:69:CYS:HA	1:B:101:ILE:HG12	1.74	0.69
1:D:285:LEU:HB2	1:D:431:VAL:HG22	1.75	0.69
1:A:176:LYS:HG3	1:B:346:TYR:HB2	1.73	0.69
1:A:285:LEU:HG	1:A:431:VAL:HA	1.74	0.69
1:C:216:ARG:HA	1:C:219:THR:O	1.92	0.69
1:E:124:VAL:CA	1:E:125:ILE:HB	2.22	0.69
1:E:39:GLN:CB	1:E:67:ILE:HG21	2.23	0.69
1:E:76:LEU:HG	1:E:134:PRO:HB2	1.74	0.69
1:A:181:VAL:HG21	1:B:379:TYR:CB	2.22	0.69
1:C:368:ARG:H	1:C:401:THR:HG22	1.56	0.69
1:C:91:LYS:HB3	1:C:93:ARG:H	1.57	0.69
1:D:163:GLU:OE1	1:D:208:LEU:HB3	1.93	0.69
1:A:329:ILE:CG2	1:A:330:ILE:H	2.04	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LYS:HA	1:B:195:ARG:HG2	1.75	0.68
1:D:69:CYS:HA	1:D:101:ILE:HG12	1.75	0.68
1:E:57:GLN:HG3	1:E:212:LEU:HD13	1.73	0.68
1:C:181:VAL:N	1:C:182:GLN:HB3	2.08	0.68
1:C:301:LEU:HD22	1:C:360:ILE:O	1.92	0.68
1:B:181:VAL:HG21	1:C:379:TYR:CB	2.23	0.68
1:D:301:LEU:HD22	1:D:360:ILE:O	1.92	0.68
1:C:173:ALA:CB	1:D:345:THR:CG2	2.66	0.68
1:A:346:TYR:HA	1:E:173:ALA:HA	1.25	0.68
1:A:345:THR:CB	1:E:174:ARG:HH12	2.05	0.68
1:E:329:ILE:CG2	1:E:330:ILE:H	2.03	0.68
1:C:91:LYS:HB2	1:C:93:ARG:CB	2.23	0.68
1:E:164:ILE:HG22	1:E:203:GLN:HG3	1.74	0.68
1:B:176:LYS:HB3	1:C:347:HIS:C	2.12	0.68
1:C:173:ALA:CB	1:D:346:TYR:HB3	2.23	0.68
1:C:221:ILE:HB	1:C:222:ILE:HG13	1.74	0.68
1:D:322:TRP:CD1	1:D:456:ARG:HB2	2.29	0.68
1:D:72:VAL:HG11	1:D:101:ILE:HD13	1.75	0.68
1:A:52:LYS:HA	1:A:195:ARG:HG2	1.75	0.68
1:B:72:VAL:HG13	1:B:85:LEU:HD13	1.74	0.68
1:D:56:LEU:CD2	1:D:222:ILE:CG2	2.72	0.68
1:E:52:LYS:HA	1:E:195:ARG:HG2	1.76	0.68
1:E:311:LEU:HD23	1:E:368:ARG:HG2	1.76	0.68
1:A:69:CYS:HA	1:A:101:ILE:HG12	1.74	0.68
1:B:301:LEU:HD22	1:B:360:ILE:O	1.92	0.68
1:D:82:LEU:O	1:D:83:LYS:HB3	1.93	0.68
1:E:221:ILE:HB	1:E:222:ILE:CG1	2.22	0.68
1:A:272:ARG:CB	1:A:441:ASN:HB2	2.24	0.68
1:C:370:LYS:HG2	1:C:401:THR:OG1	1.94	0.68
1:D:83:LYS:HE3	1:D:156:ILE:HG21	1.76	0.68
1:D:181:VAL:HG21	1:E:379:TYR:CB	2.24	0.68
1:A:91:LYS:C	1:A:93:ARG:H	1.98	0.68
1:D:204:THR:CG2	1:D:205:GLU:H	2.02	0.68
1:D:415:GLN:O	1:D:418:VAL:HG12	1.93	0.68
1:D:177:LEU:CB	1:E:347:HIS:CG	2.76	0.67
1:E:156:ILE:HB	1:E:194:SER:HB3	1.76	0.67
1:E:91:LYS:C	1:E:93:ARG:H	1.98	0.67
1:A:181:VAL:N	1:A:182:GLN:HB3	2.08	0.67
1:A:368:ARG:HB2	1:A:378:LEU:CD2	2.24	0.67
1:C:84:ILE:CG2	1:C:154:ALA:HA	2.24	0.67
1:B:173:ALA:CB	1:C:346:TYR:HB3	2.21	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:TYR:HB3	1:C:385:ILE:HG21	1.76	0.67
1:C:415:GLN:O	1:C:418:VAL:HG12	1.94	0.67
1:C:221:ILE:CA	1:C:445:GLU:HG2	2.25	0.67
1:E:314:GLU:O	1:E:314:GLU:HG2	1.93	0.67
1:C:173:ALA:C	1:D:346:TYR:CA	2.44	0.67
1:D:39:GLN:CB	1:D:67:ILE:HG12	2.24	0.67
1:E:370:LYS:HZ2	1:E:403:GLU:HA	1.57	0.67
1:A:314:GLU:HG2	1:A:314:GLU:O	1.94	0.67
1:C:437:LEU:HD23	1:C:458:CYS:SG	2.33	0.67
1:A:376:ALA:HA	1:E:181:VAL:CB	2.19	0.67
1:D:73:VAL:CG2	1:D:105:ILE:HG13	2.25	0.67
1:E:285:LEU:HB2	1:E:431:VAL:HG22	1.75	0.67
1:C:124:VAL:CA	1:C:125:ILE:HB	2.24	0.67
1:D:91:LYS:HB3	1:D:93:ARG:H	1.59	0.67
1:D:173:ALA:CB	1:E:346:TYR:CG	2.78	0.67
1:B:314:GLU:O	1:B:314:GLU:HG2	1.94	0.67
1:B:91:LYS:HB3	1:B:93:ARG:N	2.10	0.67
1:C:118:PRO:HD2	1:C:128:ASP:HA	1.77	0.67
1:A:84:ILE:CG2	1:A:154:ALA:HA	2.24	0.67
1:B:329:ILE:CG2	1:B:330:ILE:H	2.06	0.67
1:C:52:LYS:HA	1:C:195:ARG:HG2	1.75	0.67
1:C:77:TRP:HE1	1:C:105:ILE:CG1	1.91	0.67
1:D:314:GLU:HG2	1:D:314:GLU:O	1.93	0.67
1:E:72:VAL:HG11	1:E:101:ILE:HD13	1.75	0.67
1:E:20:VAL:O	1:E:22:PHE:CD2	2.48	0.67
1:A:329:ILE:CG2	1:A:330:ILE:N	2.58	0.66
1:B:254:GLU:CG	1:B:255:ALA:N	2.45	0.66
1:B:370:LYS:HG3	1:B:401:THR:OG1	1.95	0.66
1:B:280:LYS:NZ	1:B:437:LEU:CB	2.58	0.66
1:C:291:PRO:HG2	1:C:295:ASP:CB	2.24	0.66
1:E:415:GLN:O	1:E:418:VAL:HG12	1.94	0.66
1:A:415:GLN:O	1:A:418:VAL:HG12	1.94	0.66
1:D:156:ILE:HB	1:D:194:SER:HB3	1.77	0.66
1:D:91:LYS:C	1:D:93:ARG:H	1.98	0.66
1:A:39:GLN:CB	1:A:67:ILE:HG12	2.24	0.66
1:D:222:ILE:HA	1:D:445:GLU:OE2	1.96	0.66
1:C:91:LYS:C	1:C:93:ARG:H	1.98	0.66
1:D:220:THR:C	1:D:445:GLU:HB2	2.16	0.66
1:B:91:LYS:C	1:B:93:ARG:H	1.98	0.66
1:C:85:LEU:HD12	1:C:156:ILE:HG21	1.77	0.66
1:C:83:LYS:HE2	1:C:192:PRO:CA	2.10	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:VAL:HG21	1:D:379:TYR:HB2	1.78	0.66
1:A:20:VAL:O	1:A:22:PHE:CD2	2.48	0.66
1:A:414:VAL:CA	1:A:417:VAL:HG12	2.25	0.66
1:C:14:GLN:NE2	1:C:40:ILE:HG12	2.11	0.66
1:E:145:ILE:HB	1:E:174:ARG:HG3	1.76	0.66
1:A:14:GLN:NE2	1:A:40:ILE:HG12	2.10	0.66
1:C:329:ILE:CG2	1:C:330:ILE:H	2.05	0.66
1:C:51:ASN:O	1:C:52:LYS:HB3	1.95	0.66
1:E:118:PRO:HD2	1:E:128:ASP:HA	1.78	0.66
1:E:91:LYS:HB2	1:E:93:ARG:HB2	1.78	0.66
1:C:346:TYR:CD2	1:C:349:CYS:HB2	2.31	0.66
1:E:322:TRP:CD1	1:E:456:ARG:HB2	2.30	0.66
1:A:72:VAL:HG11	1:A:101:ILE:HD13	1.78	0.65
1:A:118:PRO:HD2	1:A:128:ASP:HA	1.77	0.65
1:C:351:ASN:ND2	1:C:377:VAL:HA	2.12	0.65
1:C:437:LEU:HD22	1:C:458:CYS:SG	2.35	0.65
1:D:51:ASN:O	1:D:52:LYS:HB3	1.95	0.65
1:A:280:LYS:HZ3	1:A:437:LEU:CB	2.09	0.65
1:E:291:PRO:CG	1:E:295:ASP:HB3	2.23	0.65
1:A:291:PRO:HD2	1:A:295:ASP:O	1.96	0.65
1:B:220:THR:CA	1:B:445:GLU:HB3	2.27	0.65
1:B:51:ASN:O	1:B:52:LYS:HB3	1.93	0.65
1:C:314:GLU:O	1:C:314:GLU:HG2	1.94	0.65
1:D:220:THR:CA	1:D:445:GLU:HB2	2.27	0.65
1:A:280:LYS:NZ	1:A:437:LEU:CB	2.60	0.65
1:D:145:ILE:HB	1:D:174:ARG:HG3	1.77	0.65
1:D:181:VAL:CG1	1:E:376:ALA:HA	2.26	0.65
1:E:51:ASN:O	1:E:52:LYS:HB3	1.95	0.65
1:A:132:ALA:N	1:A:133:ASN:CA	2.59	0.65
1:D:362:VAL:CG1	1:D:362:VAL:O	2.45	0.65
1:E:220:THR:C	1:E:445:GLU:HB2	2.17	0.65
1:E:348:ASP:OD1	1:E:349:CYS:N	2.30	0.65
1:A:235:LEU:CD2	1:A:245:LEU:CB	2.57	0.65
1:A:85:LEU:HD12	1:A:156:ILE:HG21	1.78	0.65
1:E:84:ILE:CG2	1:E:153:ARG:O	2.44	0.65
1:A:73:VAL:HG23	1:A:105:ILE:CG1	2.27	0.65
1:A:56:LEU:CD2	1:A:222:ILE:HG23	2.26	0.65
1:B:159:ALA:CB	1:B:198:TYR:CD1	2.79	0.65
1:B:274:ARG:HE	1:B:414:VAL:CG1	2.10	0.65
1:B:375:TYR:O	1:B:378:LEU:HB2	1.97	0.65
1:C:132:ALA:H	1:C:133:ASN:CA	2.10	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:LYS:CB	1:E:347:HIS:H	2.06	0.65
1:C:76:LEU:HB2	1:C:136:HIS:HE1	1.60	0.65
1:A:351:ASN:ND2	1:A:377:VAL:HA	2.11	0.65
1:B:149:LEU:HD23	1:B:174:ARG:HG3	1.79	0.65
1:B:156:ILE:HB	1:B:194:SER:HB3	1.78	0.65
1:B:84:ILE:CG2	1:B:154:ALA:HA	2.26	0.65
1:B:91:LYS:HB2	1:B:93:ARG:CB	2.26	0.65
1:C:159:ALA:HB3	1:C:198:TYR:CE1	2.32	0.65
1:D:190:PRO:HB2	1:D:192:PRO:CD	2.25	0.65
1:E:57:GLN:O	1:E:223:TRP:HD1	1.78	0.65
1:C:132:ALA:N	1:C:133:ASN:CA	2.59	0.65
1:C:375:TYR:O	1:C:378:LEU:HB2	1.97	0.65
1:A:132:ALA:H	1:A:133:ASN:CG	2.01	0.64
1:B:323:LEU:HB3	1:B:339:LYS:HB2	1.79	0.64
1:B:329:ILE:CG2	1:B:330:ILE:N	2.60	0.64
1:C:172:GLY:O	1:C:176:LYS:HD3	1.97	0.64
1:C:220:THR:C	1:C:445:GLU:HB2	2.17	0.64
1:E:133:ASN:H	1:E:134:PRO:CD	2.07	0.64
1:A:176:LYS:HB3	1:B:347:HIS:C	2.18	0.64
1:B:128:ASP:O	1:B:135:ASP:HB3	1.97	0.64
1:B:181:VAL:HG21	1:C:379:TYR:HB2	1.79	0.64
1:D:117:ARG:HB3	1:D:118:PRO:HD3	1.79	0.64
1:E:132:ALA:N	1:E:133:ASN:CA	2.59	0.64
1:C:132:ALA:H	1:C:133:ASN:CG	2.01	0.64
1:A:347:HIS:C	1:E:176:LYS:HB3	2.17	0.64
1:A:83:LYS:CD	1:A:193:SER:O	2.44	0.64
1:B:132:ALA:H	1:B:133:ASN:CG	2.01	0.64
1:B:378:LEU:CD1	1:B:401:THR:OG1	2.42	0.64
1:D:375:TYR:O	1:D:378:LEU:HB2	1.97	0.64
1:D:272:ARG:CB	1:D:441:ASN:HB2	2.22	0.64
1:E:119:GLY:HA2	1:E:127:PHE:CD2	2.32	0.64
1:A:309:ALA:CB	1:A:358:GLN:HE22	2.11	0.64
1:D:132:ALA:H	1:D:133:ASN:CA	2.10	0.64
1:D:181:VAL:O	1:D:181:VAL:HG12	1.96	0.64
1:D:347:HIS:HE1	1:D:376:ALA:CB	2.09	0.64
1:A:173:ALA:C	1:B:346:TYR:CA	2.44	0.64
1:C:190:PRO:HB2	1:C:192:PRO:CD	2.27	0.64
1:C:362:VAL:O	1:C:362:VAL:CG1	2.45	0.64
1:E:10:LEU:HD12	1:E:78:ARG:HD2	1.80	0.64
1:E:309:ALA:CB	1:E:358:GLN:HE22	2.11	0.64
1:E:362:VAL:CG1	1:E:362:VAL:O	2.45	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:375:TYR:O	1:E:378:LEU:HB2	1.98	0.64
1:A:181:VAL:HG21	1:B:379:TYR:HB2	1.80	0.64
1:C:159:ALA:HB2	1:C:198:TYR:HE1	1.62	0.64
1:C:370:LYS:HB3	1:C:375:TYR:CE1	2.32	0.64
1:C:382:ASN:HB3	1:C:385:ILE:CG1	2.27	0.64
1:B:10:LEU:HD12	1:B:78:ARG:HD2	1.80	0.64
1:D:235:LEU:HD11	1:D:241:LEU:HD23	1.75	0.64
1:E:132:ALA:H	1:E:133:ASN:CA	2.10	0.64
1:E:382:ASN:HB3	1:E:385:ILE:CG1	2.27	0.64
1:A:370:LYS:HG3	1:A:378:LEU:HD11	1.80	0.64
1:B:91:LYS:HB2	1:B:93:ARG:HB2	1.79	0.64
1:C:177:LEU:N	1:D:347:HIS:HB3	2.05	0.64
1:C:414:VAL:CA	1:C:417:VAL:HG12	2.28	0.64
1:E:351:ASN:ND2	1:E:377:VAL:HA	2.12	0.64
1:B:132:ALA:H	1:B:133:ASN:CA	2.10	0.64
1:A:347:HIS:CB	1:E:176:LYS:HB3	2.20	0.63
1:E:223:TRP:NE1	1:E:265:ARG:HB3	2.05	0.63
1:B:303:LEU:HG	1:B:304:ARG:HG3	1.79	0.63
1:D:132:ALA:H	1:D:133:ASN:CG	2.02	0.63
1:E:226:LEU:HD13	1:E:263:PRO:HB3	1.79	0.63
1:B:132:ALA:N	1:B:133:ASN:CA	2.59	0.63
1:A:347:HIS:CE1	1:E:177:LEU:HA	2.34	0.63
1:E:223:TRP:HE1	1:E:265:ARG:CB	2.06	0.63
1:D:176:LYS:CB	1:E:347:HIS:CA	2.70	0.63
1:A:132:ALA:H	1:A:133:ASN:CA	2.10	0.63
1:A:382:ASN:HB3	1:A:385:ILE:CG1	2.27	0.63
1:D:351:ASN:ND2	1:D:377:VAL:HA	2.11	0.63
1:E:182:GLN:NE2	1:E:185:ALA:CB	2.40	0.63
1:A:362:VAL:CG1	1:A:362:VAL:O	2.46	0.63
1:A:10:LEU:HD12	1:A:78:ARG:HD2	1.81	0.63
1:D:382:ASN:HB3	1:D:385:ILE:CG1	2.28	0.63
1:A:280:LYS:HE2	1:A:438:LYS:CA	2.20	0.63
1:B:294:SER:HB3	1:B:341:ASP:HB3	1.81	0.63
1:C:72:VAL:HG11	1:C:101:ILE:HD13	1.80	0.63
1:E:132:ALA:H	1:E:133:ASN:CG	2.02	0.63
1:B:80:PRO:HD2	1:B:83:LYS:HZ1	1.63	0.63
1:E:208:LEU:HD21	1:E:265:ARG:HH21	1.63	0.63
1:A:83:LYS:HG3	1:A:155:ASP:HB3	1.76	0.62
1:B:133:ASN:H	1:B:134:PRO:CD	2.08	0.62
1:D:117:ARG:HB3	1:D:118:PRO:CD	2.29	0.62
1:D:226:LEU:HB2	1:D:263:PRO:HB3	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:VAL:CG1	1:E:198:TYR:CE1	2.82	0.62
1:B:351:ASN:ND2	1:B:377:VAL:HA	2.11	0.62
1:E:262:ASP:HB2	1:E:263:PRO:HD3	1.76	0.62
1:A:348:ASP:OD1	1:A:349:CYS:N	2.33	0.62
1:C:161:ASP:HB3	1:C:164:ILE:HG22	1.82	0.62
1:D:177:LEU:N	1:E:347:HIS:HB3	2.07	0.62
1:D:162:VAL:HG21	1:D:198:TYR:HB3	1.81	0.62
1:A:346:TYR:HB2	1:E:176:LYS:HG3	1.81	0.62
1:A:226:LEU:HB2	1:A:263:PRO:HB3	1.81	0.62
1:B:362:VAL:O	1:B:362:VAL:CG1	2.47	0.62
1:C:173:ALA:O	1:D:345:THR:O	2.17	0.62
1:C:346:TYR:HE2	1:C:349:CYS:HB3	1.51	0.62
1:D:132:ALA:N	1:D:133:ASN:CA	2.59	0.62
1:A:156:ILE:HB	1:A:194:SER:HB3	1.79	0.62
1:B:226:LEU:HB2	1:B:263:PRO:HB3	1.82	0.62
1:B:346:TYR:HD1	1:B:349:CYS:H	1.42	0.62
1:B:379:TYR:HB3	1:B:385:ILE:HG21	1.82	0.62
1:B:73:VAL:CG2	1:B:105:ILE:CG1	2.68	0.62
1:C:252:ASN:CB	1:C:253:PRO:CD	2.78	0.62
1:D:124:VAL:HB	1:D:125:ILE:CB	2.15	0.62
1:E:272:ARG:HB3	1:E:442:CYS:N	2.14	0.62
1:A:285:LEU:HD22	1:A:285:LEU:N	2.14	0.62
1:B:433:SER:HA	1:B:457:ILE:HD13	1.82	0.62
1:D:181:VAL:HG21	1:E:379:TYR:HB2	1.81	0.62
1:D:173:ALA:O	1:E:345:THR:O	2.18	0.62
1:B:163:GLU:CG	1:B:203:GLN:HB2	2.27	0.62
1:A:173:ALA:O	1:B:345:THR:O	2.18	0.62
1:C:77:TRP:CZ3	1:C:114:LEU:HB2	2.35	0.62
1:E:20:VAL:O	1:E:22:PHE:CE2	2.52	0.62
1:E:72:VAL:HG13	1:E:85:LEU:HD13	1.81	0.62
1:C:309:ALA:CB	1:C:358:GLN:HE22	2.13	0.62
1:A:190:PRO:C	1:A:192:PRO:HD2	2.20	0.62
1:B:328:ASN:HA	1:B:333:LEU:HD22	1.81	0.62
1:D:73:VAL:HG23	1:D:105:ILE:CG1	2.30	0.62
1:E:252:ASN:CB	1:E:253:PRO:CD	2.78	0.62
1:E:414:VAL:CA	1:E:417:VAL:HG12	2.30	0.62
1:A:20:VAL:O	1:A:22:PHE:CE2	2.53	0.61
1:C:159:ALA:HB2	1:C:198:TYR:CE1	2.34	0.61
1:C:378:LEU:CD2	1:C:401:THR:CG2	2.78	0.61
1:C:91:LYS:HB3	1:C:93:ARG:N	2.14	0.61
1:A:417:VAL:HA	1:A:465:MET:HG3	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ALA:CB	1:C:345:THR:CG2	2.73	0.61
1:B:190:PRO:HB2	1:B:192:PRO:CD	2.31	0.61
1:B:77:TRP:CZ3	1:B:114:LEU:HB2	2.35	0.61
1:C:163:GLU:CG	1:C:203:GLN:HB2	2.25	0.61
1:B:311:LEU:HB3	1:B:368:ARG:HG2	1.82	0.61
1:B:414:VAL:CA	1:B:417:VAL:HG12	2.30	0.61
1:C:226:LEU:HB2	1:C:263:PRO:HB3	1.83	0.61
1:C:309:ALA:HB3	1:C:358:GLN:HE22	1.66	0.61
1:D:201:THR:HG23	1:D:202:PRO:CD	2.26	0.61
1:D:320:TYR:H	1:D:456:ARG:HG3	1.65	0.61
1:D:75:SER:HB3	1:D:83:LYS:NZ	2.16	0.61
1:B:124:VAL:HB	1:B:125:ILE:CB	2.16	0.61
1:A:345:THR:O	1:E:173:ALA:O	2.18	0.61
1:A:348:ASP:C	1:A:348:ASP:OD1	2.38	0.61
1:B:39:GLN:HB3	1:B:67:ILE:HG13	1.82	0.61
1:D:79:ASP:HB3	1:D:82:LEU:O	2.00	0.61
1:E:164:ILE:HG13	1:E:165:PRO:HD3	1.82	0.61
1:A:285:LEU:HB3	1:A:431:VAL:HG22	1.83	0.61
1:A:173:ALA:CB	1:B:346:TYR:HB3	2.27	0.61
1:D:173:ALA:CB	1:E:345:THR:CG2	2.73	0.61
1:E:259:THR:HB	1:E:260:PRO:HD3	1.82	0.61
1:E:303:LEU:HG	1:E:304:ARG:HG3	1.82	0.61
1:A:79:ASP:HB3	1:A:82:LEU:O	2.01	0.61
1:B:173:ALA:O	1:C:345:THR:O	2.17	0.61
1:B:85:LEU:HD12	1:B:156:ILE:HG21	1.82	0.61
1:B:96:ALA:HA	1:B:99:ILE:HD12	1.82	0.61
1:C:120:GLN:HA	1:C:124:VAL:O	2.01	0.61
1:E:274:ARG:HD3	1:E:414:VAL:CG1	2.30	0.61
1:A:347:HIS:HB3	1:E:176:LYS:CA	2.31	0.61
1:B:460:THR:HA	1:B:463:PRO:HG2	1.83	0.61
1:B:173:ALA:HB2	1:C:345:THR:HG23	1.81	0.61
1:D:173:ALA:HB2	1:E:345:THR:HG23	1.81	0.61
1:E:320:TYR:H	1:E:456:ARG:HG3	1.66	0.61
1:A:73:VAL:HG23	1:A:105:ILE:HG13	1.83	0.61
1:A:252:ASN:CB	1:A:253:PRO:CD	2.78	0.61
1:C:156:ILE:HB	1:C:194:SER:HB3	1.79	0.61
1:E:105:ILE:HA	1:E:108:LEU:HD12	1.81	0.61
1:A:120:GLN:HA	1:A:124:VAL:O	2.01	0.61
1:C:259:THR:HB	1:C:260:PRO:HD3	1.82	0.61
1:C:323:LEU:HB3	1:C:339:LYS:HB2	1.83	0.61
1:D:84:ILE:CG2	1:D:153:ARG:O	2.49	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:PRO:C	1:E:192:PRO:HD2	2.20	0.61
1:E:235:LEU:HD12	1:E:241:LEU:HD22	1.80	0.61
1:E:328:ASN:HA	1:E:333:LEU:HD22	1.82	0.61
1:A:346:TYR:CD1	1:E:173:ALA:HB1	2.34	0.60
1:A:309:ALA:HB3	1:A:358:GLN:HE22	1.66	0.60
1:B:77:TRP:HZ3	1:B:114:LEU:CA	2.14	0.60
1:A:181:VAL:O	1:B:376:ALA:CB	2.33	0.60
1:B:252:ASN:CB	1:B:253:PRO:CD	2.78	0.60
1:B:280:LYS:HZ1	1:B:437:LEU:HB2	1.65	0.60
1:B:434:PRO:HA	1:B:437:LEU:HD12	1.84	0.60
1:D:118:PRO:CG	1:D:129:VAL:N	2.62	0.60
1:E:148:GLN:NE2	1:E:175:GLU:HG2	2.15	0.60
1:E:348:ASP:C	1:E:348:ASP:OD1	2.37	0.60
1:D:459:ASP:O	1:D:463:PRO:HD2	2.01	0.60
1:A:196:VAL:HG13	1:A:198:TYR:CE1	2.35	0.60
1:C:230:THR:HA	1:C:233:GLU:HG3	1.83	0.60
1:D:120:GLN:HA	1:D:124:VAL:O	2.01	0.60
1:D:303:LEU:HG	1:D:304:ARG:HG3	1.84	0.60
1:D:309:ALA:CB	1:D:358:GLN:HE22	2.14	0.60
1:E:14:GLN:NE2	1:E:40:ILE:HG12	2.16	0.60
1:A:459:ASP:O	1:A:463:PRO:CD	2.49	0.60
1:B:368:ARG:NH2	1:B:381:LEU:HD13	2.17	0.60
1:C:96:ALA:HA	1:C:99:ILE:HD12	1.83	0.60
1:E:301:LEU:HB2	1:E:361:LEU:HD23	1.83	0.60
1:A:119:GLY:HA2	1:A:127:PHE:CD1	2.37	0.60
1:A:370:LYS:O	1:A:375:TYR:CE1	2.54	0.60
1:B:172:GLY:O	1:B:176:LYS:HD2	2.02	0.60
1:E:235:LEU:CD1	1:E:241:LEU:CD2	2.65	0.60
1:E:56:LEU:HD23	1:E:222:ILE:HB	1.83	0.60
1:E:79:ASP:HB3	1:E:82:LEU:O	2.00	0.60
1:A:56:LEU:CD2	1:A:222:ILE:CG2	2.80	0.60
1:A:73:VAL:CG2	1:A:105:ILE:HG13	2.30	0.60
1:B:120:GLN:HA	1:B:124:VAL:O	2.01	0.60
1:A:173:ALA:HB2	1:B:345:THR:HG23	1.81	0.60
1:B:272:ARG:HB3	1:B:442:CYS:HB2	1.82	0.60
1:D:156:ILE:CB	1:D:194:SER:HB3	2.32	0.60
1:E:156:ILE:CB	1:E:194:SER:HB3	2.31	0.60
1:C:417:VAL:HA	1:C:465:MET:HG3	1.83	0.60
1:E:329:ILE:CG2	1:E:330:ILE:N	2.57	0.60
1:E:459:ASP:O	1:E:463:PRO:CD	2.50	0.60
1:C:459:ASP:O	1:C:463:PRO:HD2	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:ASN:CB	1:D:253:PRO:CD	2.80	0.60
1:B:84:ILE:HG13	1:B:135:ASP:OD1	2.02	0.59
1:D:118:PRO:HG2	1:D:129:VAL:H	1.67	0.59
1:D:414:VAL:O	1:D:417:VAL:HG12	2.01	0.59
1:E:378:LEU:HD11	1:E:401:THR:HG1	1.68	0.59
1:A:163:GLU:CG	1:A:203:GLN:HB2	2.27	0.59
1:C:346:TYR:CE2	1:C:349:CYS:N	2.70	0.59
1:C:83:LYS:NZ	1:C:193:SER:N	2.39	0.59
1:D:73:VAL:HG23	1:D:105:ILE:HG13	1.82	0.59
1:D:414:VAL:CA	1:D:417:VAL:HG12	2.32	0.59
1:D:221:ILE:CA	1:D:445:GLU:HG2	2.33	0.59
1:E:187:LEU:HB3	1:E:192:PRO:HB2	1.84	0.59
1:A:177:LEU:CB	1:B:347:HIS:CD2	2.85	0.59
1:C:77:TRP:HZ3	1:C:114:LEU:CA	2.15	0.59
1:C:459:ASP:O	1:C:463:PRO:CD	2.49	0.59
1:D:235:LEU:HD21	1:D:245:LEU:HB3	1.84	0.59
1:D:75:SER:HB3	1:D:83:LYS:HZ1	1.66	0.59
1:E:378:LEU:CD2	1:E:401:THR:CG2	2.78	0.59
1:A:56:LEU:HD13	1:A:199:LEU:HD12	1.84	0.59
1:A:272:ARG:HB3	1:A:442:CYS:N	2.16	0.59
1:A:177:LEU:N	1:B:347:HIS:CG	2.70	0.59
1:B:459:ASP:O	1:B:463:PRO:CD	2.50	0.59
1:C:187:LEU:HB3	1:C:192:PRO:HB2	1.83	0.59
1:D:91:LYS:HB3	1:D:93:ARG:N	2.16	0.59
1:E:77:TRP:HZ3	1:E:114:LEU:CA	2.15	0.59
1:B:414:VAL:O	1:B:417:VAL:HG12	2.02	0.59
1:C:84:ILE:HG22	1:C:153:ARG:O	2.03	0.59
1:D:460:THR:HA	1:D:463:PRO:HG2	1.84	0.59
1:B:280:LYS:HZ3	1:B:437:LEU:CB	2.13	0.59
1:E:120:GLN:HA	1:E:124:VAL:O	2.01	0.59
1:B:84:ILE:HG22	1:B:153:ARG:O	2.03	0.59
1:B:181:VAL:O	1:C:376:ALA:CB	2.33	0.59
1:B:187:LEU:HB3	1:B:192:PRO:HB2	1.84	0.59
1:A:176:LYS:CG	1:B:346:TYR:HB2	2.33	0.59
1:C:100:PHE:O	1:C:104:ILE:HG12	2.03	0.59
1:A:376:ALA:CB	1:E:181:VAL:O	2.33	0.59
1:A:322:TRP:CD1	1:A:456:ARG:HB2	2.36	0.59
1:B:51:ASN:CB	1:B:54:PHE:CZ	2.86	0.59
1:C:46:LEU:HD22	1:C:197:ILE:HG12	1.84	0.59
1:C:79:ASP:HB3	1:C:82:LEU:O	2.03	0.59
1:D:163:GLU:CG	1:D:203:GLN:HB2	2.28	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ALA:HB2	1:D:345:THR:HG23	1.77	0.59
1:E:414:VAL:O	1:E:417:VAL:HG12	2.02	0.59
1:A:176:LYS:HB3	1:B:347:HIS:CB	2.21	0.59
1:C:66:PHE:O	1:C:69:CYS:SG	2.61	0.59
1:D:273:GLU:CG	1:D:280:LYS:HZ1	2.05	0.59
1:D:459:ASP:O	1:D:463:PRO:CD	2.50	0.59
1:E:226:LEU:HB2	1:E:263:PRO:HB3	1.85	0.59
1:A:89:ALA:HB3	1:A:94:ALA:HB2	1.84	0.59
1:C:187:LEU:O	1:C:192:PRO:HD2	2.02	0.59
1:D:59:PHE:CD2	1:D:60:ARG:O	2.56	0.59
1:E:326:ARG:HD3	1:E:333:LEU:HB3	1.84	0.59
1:E:89:ALA:HB3	1:E:94:ALA:HB2	1.84	0.59
1:E:96:ALA:HA	1:E:99:ILE:HD12	1.84	0.59
1:A:414:VAL:HA	1:A:417:VAL:CG1	2.31	0.58
1:B:14:GLN:NE2	1:B:40:ILE:HG12	2.18	0.58
1:B:156:ILE:CB	1:B:194:SER:HB3	2.32	0.58
1:B:181:VAL:O	1:B:181:VAL:HG12	2.03	0.58
1:D:196:VAL:CG1	1:D:198:TYR:CZ	2.86	0.58
1:D:346:TYR:CE1	1:D:349:CYS:N	2.71	0.58
1:A:259:THR:HB	1:A:260:PRO:HD3	1.84	0.58
1:A:303:LEU:HG	1:A:304:ARG:HG3	1.85	0.58
1:A:459:ASP:O	1:A:463:PRO:HD2	2.02	0.58
1:C:73:VAL:CG2	1:C:105:ILE:CG1	2.68	0.58
1:C:89:ALA:HB3	1:C:94:ALA:HB2	1.84	0.58
1:D:433:SER:C	1:D:434:PRO:CD	2.65	0.58
1:E:221:ILE:CA	1:E:222:ILE:HG12	2.32	0.58
1:A:84:ILE:HG22	1:A:153:ARG:O	2.03	0.58
1:B:272:ARG:CB	1:B:441:ASN:HB2	2.18	0.58
1:C:172:GLY:O	1:C:176:LYS:CD	2.51	0.58
1:C:177:LEU:HB3	1:D:347:HIS:CG	2.23	0.58
1:D:85:LEU:HD12	1:D:156:ILE:HG21	1.84	0.58
1:B:100:PHE:O	1:B:104:ILE:HG12	2.03	0.58
1:B:291:PRO:HD2	1:B:295:ASP:O	2.03	0.58
1:B:368:ARG:HB2	1:B:378:LEU:HD21	1.85	0.58
1:B:382:ASN:HB3	1:B:385:ILE:CG1	2.33	0.58
1:C:156:ILE:CB	1:C:194:SER:HB3	2.33	0.58
1:B:181:VAL:CG1	1:C:376:ALA:HA	2.33	0.58
1:C:87:VAL:HA	1:C:158:ILE:O	2.04	0.58
1:D:84:ILE:HG12	1:D:154:ALA:HA	1.85	0.58
1:E:459:ASP:O	1:E:463:PRO:HD2	2.03	0.58
1:B:10:LEU:HD23	1:B:11:VAL:HG13	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:LEU:HD13	1:B:400:LYS:O	2.04	0.58
1:D:187:LEU:HB3	1:D:192:PRO:HB2	1.84	0.58
1:D:177:LEU:N	1:E:347:HIS:CG	2.71	0.58
1:A:187:LEU:HB3	1:A:192:PRO:HB2	1.83	0.58
1:A:82:LEU:O	1:A:134:PRO:HG3	2.04	0.58
1:B:232:GLU:HB3	1:B:246:ARG:HG2	1.85	0.58
1:B:368:ARG:CB	1:B:401:THR:HG21	2.33	0.58
1:B:89:ALA:HB3	1:B:94:ALA:HB2	1.84	0.58
1:E:434:PRO:HA	1:E:437:LEU:HD12	1.86	0.58
1:A:256:LEU:O	1:A:260:PRO:HD3	2.03	0.58
1:B:79:ASP:HB3	1:B:82:LEU:O	2.04	0.58
1:D:196:VAL:CG1	1:D:198:TYR:CE1	2.86	0.58
1:E:141:LYS:HZ3	1:E:171:MET:HB2	1.69	0.58
1:E:66:PHE:O	1:E:69:CYS:SG	2.61	0.58
1:A:189:LYS:HB2	1:A:190:PRO:HD3	1.86	0.58
1:A:320:TYR:H	1:A:456:ARG:HG3	1.69	0.58
1:B:259:THR:HB	1:B:260:PRO:HD3	1.86	0.58
1:B:59:PHE:CZ	1:B:62:ILE:HB	2.37	0.58
1:B:87:VAL:HA	1:B:158:ILE:O	2.04	0.58
1:C:285:LEU:CB	1:C:431:VAL:HG22	2.34	0.58
1:D:87:VAL:HA	1:D:158:ILE:O	2.04	0.58
1:D:176:LYS:HB3	1:E:347:HIS:HB2	1.71	0.58
1:D:187:LEU:O	1:D:192:PRO:HD2	2.03	0.58
1:D:323:LEU:HB3	1:D:339:LYS:HB2	1.84	0.58
1:D:223:TRP:N	1:D:445:GLU:OE2	2.37	0.58
1:D:89:ALA:HB3	1:D:94:ALA:HB2	1.84	0.58
1:A:347:HIS:CG	1:E:177:LEU:N	2.72	0.58
1:E:460:THR:HA	1:E:463:PRO:HG2	1.84	0.58
1:A:51:ASN:CB	1:A:54:PHE:CZ	2.87	0.58
1:B:66:PHE:O	1:B:69:CYS:SG	2.61	0.58
1:D:449:ALA:HB2	1:D:455:MET:HB3	1.86	0.58
1:D:10:LEU:HD12	1:D:78:ARG:HD2	1.85	0.58
1:E:265:ARG:HD3	1:E:265:ARG:C	2.23	0.58
1:B:57:GLN:HG2	1:B:212:LEU:HD13	1.85	0.58
1:C:133:ASN:N	1:C:134:PRO:HD2	2.12	0.58
1:C:346:TYR:CD2	1:C:349:CYS:CA	2.87	0.58
1:C:55:ILE:CG2	1:C:57:GLN:OE1	2.52	0.58
1:D:204:THR:HG22	1:D:205:GLU:N	2.08	0.58
1:E:87:VAL:HA	1:E:158:ILE:O	2.04	0.58
1:D:77:TRP:HE1	1:D:105:ILE:HG12	1.69	0.57
1:E:46:LEU:HD22	1:E:197:ILE:HG12	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LEU:N	1:C:347:HIS:CG	2.70	0.57
1:C:368:ARG:CB	1:C:401:THR:HG21	2.34	0.57
1:D:272:ARG:HB3	1:D:442:CYS:HB2	1.85	0.57
1:D:370:LYS:O	1:D:375:TYR:CE1	2.57	0.57
1:D:84:ILE:HG23	1:D:153:ARG:O	2.04	0.57
1:A:87:VAL:HA	1:A:158:ILE:O	2.04	0.57
1:D:346:TYR:HB2	1:D:348:ASP:HB3	1.87	0.57
1:D:66:PHE:O	1:D:69:CYS:SG	2.61	0.57
1:B:230:THR:HA	1:B:233:GLU:HG3	1.85	0.57
1:B:320:TYR:H	1:B:456:ARG:HG3	1.69	0.57
1:C:181:VAL:CG1	1:D:376:ALA:HA	2.34	0.57
1:C:460:THR:HA	1:C:463:PRO:HG2	1.86	0.57
1:D:259:THR:HB	1:D:260:PRO:HD3	1.85	0.57
1:E:220:THR:HB	1:E:445:GLU:HB2	1.86	0.57
1:E:83:LYS:HG2	1:E:155:ASP:CB	2.14	0.57
1:A:181:VAL:HG12	1:A:181:VAL:O	2.05	0.57
1:A:156:ILE:CB	1:A:194:SER:HB3	2.33	0.57
1:B:348:ASP:C	1:B:348:ASP:OD1	2.43	0.57
1:C:119:GLY:HA2	1:C:127:PHE:CD1	2.39	0.57
1:C:177:LEU:N	1:D:347:HIS:CG	2.71	0.57
1:A:468:HIS:CA	1:A:473:ARG:HD3	2.31	0.57
1:A:77:TRP:HE1	1:A:105:ILE:HG12	1.69	0.57
1:B:21:ALA:O	1:B:33:PRO:CD	2.45	0.57
1:B:280:LYS:HE2	1:B:438:LYS:CA	2.25	0.57
1:B:375:TYR:HA	1:B:378:LEU:HD12	1.86	0.57
1:B:285:LEU:CB	1:B:431:VAL:HG22	2.34	0.57
1:B:470:LEU:HD21	1:B:472:ILE:HD12	1.85	0.57
1:D:51:ASN:CB	1:D:54:PHE:CZ	2.88	0.57
1:A:186:ALA:O	1:A:190:PRO:HD3	2.05	0.57
1:B:348:ASP:OD1	1:B:349:CYS:N	2.38	0.57
1:C:220:THR:CB	1:C:445:GLU:HB2	2.35	0.57
1:C:276:LEU:HD23	1:C:278:TYR:HB2	1.87	0.57
1:C:414:VAL:O	1:C:417:VAL:HG12	2.04	0.57
1:D:468:HIS:CA	1:D:473:ARG:HD3	2.32	0.57
1:A:193:SER:O	1:A:194:SER:HB2	2.05	0.57
1:A:66:PHE:O	1:A:69:CYS:SG	2.61	0.57
1:B:176:LYS:CD	1:C:348:ASP:OD2	2.49	0.57
1:B:190:PRO:C	1:B:192:PRO:HD2	2.25	0.57
1:B:262:ASP:HB2	1:B:263:PRO:HD3	1.80	0.57
1:C:64:LYS:HA	1:C:67:ILE:HD12	1.87	0.57
1:D:85:LEU:HD12	1:D:156:ILE:HD13	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:PRO:CD	1:D:295:ASP:O	2.53	0.57
1:D:291:PRO:CG	1:D:295:ASP:HB3	2.20	0.57
1:E:190:PRO:HB2	1:E:192:PRO:CD	2.34	0.57
1:E:368:ARG:HB2	1:E:378:LEU:HD21	1.85	0.57
1:E:449:ALA:HB2	1:E:455:MET:HB3	1.87	0.57
1:A:181:VAL:CG1	1:B:376:ALA:HA	2.35	0.57
1:B:435:ILE:HA	1:B:438:LYS:HG3	1.87	0.57
1:B:449:ALA:HB2	1:B:455:MET:HB3	1.86	0.57
1:C:76:LEU:CB	1:C:136:HIS:CE1	2.85	0.57
1:E:220:THR:CB	1:E:445:GLU:HB2	2.35	0.57
1:E:365:PRO:HA	1:E:391:GLY:O	2.05	0.57
1:A:274:ARG:HD2	1:A:417:VAL:HG13	1.85	0.57
1:A:449:ALA:HB2	1:A:455:MET:HB3	1.87	0.57
1:A:96:ALA:HA	1:A:99:ILE:HD12	1.85	0.57
1:B:83:LYS:HE2	1:B:192:PRO:HA	1.86	0.57
1:D:59:PHE:CE1	1:D:225:ALA:O	2.57	0.57
1:D:311:LEU:HD23	1:D:368:ARG:HD3	1.86	0.57
1:D:319:HIS:CB	1:D:456:ARG:HE	2.18	0.57
1:A:232:GLU:HB3	1:A:246:ARG:HG2	1.86	0.56
1:B:42:MET:HG3	1:B:56:LEU:HD21	1.87	0.56
1:B:84:ILE:CG2	1:B:153:ARG:O	2.52	0.56
1:C:433:SER:C	1:C:434:PRO:CD	2.66	0.56
1:D:285:LEU:CB	1:D:431:VAL:HG22	2.34	0.56
1:A:378:LEU:HD13	1:A:400:LYS:O	2.06	0.56
1:A:42:MET:HG3	1:A:56:LEU:HD21	1.85	0.56
1:B:163:GLU:OE1	1:B:208:LEU:CB	2.35	0.56
1:B:368:ARG:HH22	1:B:381:LEU:HD13	1.68	0.56
1:E:26:LEU:H	1:E:26:LEU:HD23	1.70	0.56
1:A:365:PRO:HA	1:A:391:GLY:O	2.05	0.56
1:B:365:PRO:HA	1:B:391:GLY:O	2.05	0.56
1:C:365:PRO:HA	1:C:391:GLY:O	2.05	0.56
1:A:470:LEU:HD21	1:A:472:ILE:HD12	1.87	0.56
1:C:449:ALA:HB2	1:C:455:MET:HB3	1.87	0.56
1:D:196:VAL:HG11	1:D:198:TYR:CZ	2.40	0.56
1:B:322:TRP:CD1	1:B:456:ARG:HB2	2.40	0.56
1:C:181:VAL:O	1:D:376:ALA:CB	2.33	0.56
1:D:156:ILE:CB	1:D:194:SER:CB	2.83	0.56
1:D:181:VAL:O	1:E:376:ALA:CB	2.33	0.56
1:E:115:LYS:HA	1:E:116:PRO:HD3	1.88	0.56
1:B:156:ILE:CB	1:B:194:SER:CB	2.83	0.56
1:B:173:ALA:HB3	1:C:345:THR:C	2.23	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ALA:C	1:C:346:TYR:CA	2.44	0.56
1:D:365:PRO:HA	1:D:391:GLY:O	2.05	0.56
1:E:85:LEU:HD12	1:E:156:ILE:HD13	1.86	0.56
1:E:196:VAL:HG13	1:E:198:TYR:CE1	2.41	0.56
1:A:460:THR:HA	1:A:463:PRO:HG2	1.87	0.56
1:C:193:SER:O	1:C:194:SER:HB2	2.05	0.56
1:C:322:TRP:CD1	1:C:456:ARG:HB2	2.40	0.56
1:E:91:LYS:HB2	1:E:93:ARG:CB	2.35	0.56
1:A:156:ILE:CB	1:A:194:SER:CB	2.83	0.56
1:C:368:ARG:HB2	1:C:378:LEU:HD21	1.88	0.56
1:C:91:LYS:C	1:C:93:ARG:N	2.59	0.56
1:E:156:ILE:CB	1:E:194:SER:CB	2.83	0.56
1:A:120:GLN:CG	1:A:120:GLN:O	2.52	0.56
1:A:434:PRO:HA	1:A:437:LEU:HD12	1.87	0.56
1:B:193:SER:O	1:B:194:SER:HB2	2.05	0.56
1:C:156:ILE:CB	1:C:194:SER:CB	2.83	0.56
1:C:346:TYR:HE2	1:C:349:CYS:CA	2.17	0.56
1:C:346:TYR:HE2	1:C:349:CYS:C	2.08	0.56
1:C:176:LYS:CA	1:D:347:HIS:HB3	2.36	0.56
1:E:77:TRP:CZ3	1:E:114:LEU:HB2	2.40	0.56
1:A:100:PHE:O	1:A:104:ILE:HG12	2.06	0.56
1:B:163:GLU:HG3	1:B:203:GLN:CB	2.29	0.56
1:C:26:LEU:H	1:C:26:LEU:HD23	1.70	0.56
1:C:370:LYS:CG	1:C:401:THR:OG1	2.54	0.56
1:B:309:ALA:CB	1:B:358:GLN:HE22	2.18	0.55
1:B:298:LYS:NZ	1:B:430:LYS:HA	2.21	0.55
1:D:193:SER:O	1:D:194:SER:HB2	2.06	0.55
1:A:326:ARG:O	1:A:328:ASN:OD1	2.25	0.55
1:A:469:ARG:O	1:A:469:ARG:HG2	2.05	0.55
1:C:181:VAL:HG12	1:C:181:VAL:O	2.04	0.55
1:C:85:LEU:HD12	1:C:156:ILE:HD13	1.88	0.55
1:E:115:LYS:HA	1:E:116:PRO:CD	2.36	0.55
1:E:144:GLY:O	1:E:171:MET:HG2	2.07	0.55
1:E:368:ARG:CB	1:E:401:THR:HG21	2.34	0.55
1:A:370:LYS:C	1:A:375:TYR:CE1	2.79	0.55
1:B:159:ALA:CB	1:B:198:TYR:CE1	2.90	0.55
1:D:118:PRO:HG2	1:D:128:ASP:N	2.21	0.55
1:C:173:ALA:HB3	1:D:345:THR:C	2.22	0.55
1:D:417:VAL:HA	1:D:465:MET:SD	2.46	0.55
1:D:52:LYS:HA	1:D:195:ARG:HG2	1.88	0.55
1:E:64:LYS:HB2	1:E:199:LEU:HD21	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:LEU:HB3	1:C:136:HIS:HD1	1.71	0.55
1:C:141:LYS:HZ3	1:C:171:MET:HB2	1.70	0.55
1:C:202:PRO:HB3	1:C:265:ARG:HH12	1.71	0.55
1:D:26:LEU:HD23	1:D:26:LEU:H	1.70	0.55
1:D:347:HIS:HE1	1:D:376:ALA:HB1	1.69	0.55
1:D:381:LEU:HD23	1:D:387:LEU:HB2	1.89	0.55
1:A:190:PRO:HB2	1:A:192:PRO:CD	2.35	0.55
1:A:322:TRP:CH2	1:A:457:ILE:HD12	2.42	0.55
1:C:83:LYS:HZ3	1:C:193:SER:N	1.92	0.55
1:D:23:LEU:HG	1:D:33:PRO:HG3	1.88	0.55
1:E:322:TRP:CH2	1:E:457:ILE:HD12	2.42	0.55
1:D:181:VAL:HG21	1:E:379:TYR:CG	2.41	0.55
1:B:274:ARG:NE	1:B:414:VAL:CG1	2.69	0.55
1:B:73:VAL:HG22	1:B:105:ILE:HG12	1.87	0.55
1:B:91:LYS:C	1:B:93:ARG:N	2.59	0.55
1:C:117:ARG:CB	1:C:118:PRO:CD	2.79	0.55
1:C:346:TYR:HB2	1:C:348:ASP:HB3	1.89	0.55
1:D:77:TRP:CE3	1:D:77:TRP:HA	2.41	0.55
1:D:91:LYS:C	1:D:93:ARG:N	2.59	0.55
1:A:173:ALA:CB	1:B:345:THR:CG2	2.73	0.55
1:B:346:TYR:CD1	1:B:349:CYS:N	2.72	0.55
1:B:459:ASP:O	1:B:463:PRO:HD2	2.07	0.55
1:D:24:PHE:CD2	1:D:30:LEU:HD13	2.42	0.55
1:D:368:ARG:HB2	1:D:378:LEU:HD21	1.89	0.55
1:E:196:VAL:CG1	1:E:198:TYR:CZ	2.90	0.55
1:E:319:HIS:HB3	1:E:456:ARG:HE	1.71	0.55
1:E:51:ASN:HB2	1:E:54:PHE:HZ	1.64	0.55
1:A:414:VAL:O	1:A:417:VAL:HG12	2.07	0.55
1:D:322:TRP:CZ3	1:D:457:ILE:HD12	2.42	0.55
1:D:417:VAL:HB	1:D:465:MET:CG	2.13	0.55
1:C:186:ALA:O	1:C:190:PRO:HD3	2.06	0.55
1:C:235:LEU:HD12	1:C:241:LEU:HD22	1.84	0.55
1:C:303:LEU:HG	1:C:304:ARG:HG3	1.89	0.55
1:B:176:LYS:CE	1:C:348:ASP:CG	2.48	0.55
1:D:262:ASP:CB	1:D:263:PRO:CD	2.76	0.55
1:A:274:ARG:CD	1:A:414:VAL:CG1	2.57	0.54
1:A:433:SER:C	1:A:434:PRO:CD	2.65	0.54
1:B:189:LYS:HB2	1:B:190:PRO:HD3	1.90	0.54
1:B:221:ILE:C	1:B:445:GLU:HG3	2.28	0.54
1:C:84:ILE:CG2	1:C:153:ARG:O	2.54	0.54
1:C:322:TRP:CH2	1:C:457:ILE:HD12	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:PHE:O	1:D:104:ILE:HG12	2.06	0.54
1:B:256:LEU:O	1:B:260:PRO:HD3	2.05	0.54
1:C:177:LEU:HB2	1:D:347:HIS:CD2	2.31	0.54
1:E:73:VAL:HG22	1:E:105:ILE:HG12	1.87	0.54
1:C:378:LEU:HD11	1:C:401:THR:HG1	1.72	0.54
1:E:91:LYS:C	1:E:93:ARG:N	2.59	0.54
1:A:83:LYS:O	1:A:134:PRO:HA	2.08	0.54
1:A:235:LEU:CD1	1:A:241:LEU:CD2	2.51	0.54
1:A:26:LEU:HD23	1:A:26:LEU:H	1.72	0.54
1:A:328:ASN:HA	1:A:333:LEU:HD22	1.90	0.54
1:B:10:LEU:HG	1:B:78:ARG:HB3	1.90	0.54
1:B:186:ALA:O	1:B:190:PRO:HD3	2.08	0.54
1:B:301:LEU:HD13	1:B:361:LEU:HA	1.90	0.54
1:C:414:VAL:HA	1:C:417:VAL:CG1	2.35	0.54
1:C:320:TYR:H	1:C:456:ARG:HG3	1.71	0.54
1:D:322:TRP:CH2	1:D:457:ILE:HD12	2.42	0.54
1:D:73:VAL:HG13	1:D:77:TRP:HD1	1.72	0.54
1:B:85:LEU:HD12	1:B:156:ILE:HD13	1.88	0.54
1:C:163:GLU:HG3	1:C:203:GLN:CB	2.29	0.54
1:C:328:ASN:HA	1:C:333:LEU:HD22	1.89	0.54
1:D:55:ILE:HG22	1:D:57:GLN:HE21	1.73	0.54
1:A:163:GLU:OE1	1:A:208:LEU:HB3	2.02	0.54
1:B:433:SER:C	1:B:434:PRO:CD	2.66	0.54
1:B:83:LYS:O	1:B:134:PRO:HA	2.08	0.54
1:C:120:GLN:O	1:C:120:GLN:CG	2.54	0.54
1:D:370:LYS:NZ	1:D:375:TYR:CE2	2.75	0.54
1:A:375:TYR:HA	1:A:378:LEU:HD12	1.89	0.54
1:A:368:ARG:CB	1:A:378:LEU:HD21	2.36	0.54
1:A:84:ILE:CG2	1:A:153:ARG:O	2.54	0.54
1:C:301:LEU:HD13	1:C:361:LEU:HA	1.90	0.54
1:D:441:ASN:C	1:D:447:ILE:HG23	2.28	0.54
1:E:298:LYS:NZ	1:E:430:LYS:HA	2.23	0.54
1:A:141:LYS:O	1:A:144:GLY:O	2.26	0.54
1:B:141:LYS:O	1:B:144:GLY:O	2.26	0.54
1:D:301:LEU:HD13	1:D:361:LEU:HA	1.90	0.54
1:E:193:SER:O	1:E:194:SER:HB2	2.08	0.54
1:E:323:LEU:HB3	1:E:339:LYS:HB2	1.89	0.54
1:B:406:ALA:O	1:B:408:LYS:N	2.41	0.54
1:C:124:VAL:HB	1:C:125:ILE:CB	2.16	0.54
1:C:291:PRO:CD	1:C:295:ASP:O	2.56	0.54
1:D:311:LEU:HB3	1:D:368:ARG:HG2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:LYS:O	1:E:134:PRO:HA	2.08	0.54
1:E:406:ALA:O	1:E:408:LYS:N	2.41	0.54
1:A:57:GLN:HB3	1:A:265:ARG:CZ	2.37	0.54
1:B:415:GLN:O	1:B:418:VAL:HG12	2.07	0.54
1:B:10:LEU:O	1:B:74:TRP:CZ2	2.61	0.54
1:C:39:GLN:CB	1:C:67:ILE:HG12	2.35	0.54
1:D:83:LYS:O	1:D:134:PRO:HA	2.08	0.54
1:D:141:LYS:O	1:D:144:GLY:O	2.26	0.54
1:A:73:VAL:HG13	1:A:77:TRP:HD1	1.73	0.53
1:B:46:LEU:HD22	1:B:197:ILE:HG12	1.89	0.53
1:C:141:LYS:O	1:C:144:GLY:O	2.26	0.53
1:C:57:GLN:HB3	1:C:265:ARG:CZ	2.38	0.53
1:C:45:VAL:HG22	1:C:54:PHE:CE1	2.44	0.53
1:D:176:LYS:CA	1:E:347:HIS:HB3	2.38	0.53
1:A:91:LYS:C	1:A:93:ARG:N	2.59	0.53
1:C:378:LEU:CD1	1:C:401:THR:OG1	2.54	0.53
1:D:59:PHE:HD1	1:D:225:ALA:HA	1.69	0.53
1:D:225:ALA:O	1:D:228:PRO:HD2	2.09	0.53
1:D:298:LYS:NZ	1:D:430:LYS:HA	2.23	0.53
1:D:346:TYR:HE1	1:D:349:CYS:C	2.12	0.53
1:B:433:SER:HB2	1:B:457:ILE:CD1	2.38	0.53
1:C:225:ALA:O	1:C:228:PRO:HD2	2.09	0.53
1:C:272:ARG:HB3	1:C:442:CYS:HB2	1.89	0.53
1:D:272:ARG:HB2	1:D:441:ASN:CB	2.26	0.53
1:E:301:LEU:HG	1:E:302:ARG:N	2.24	0.53
1:D:173:ALA:HB3	1:E:345:THR:C	2.22	0.53
1:E:359:LYS:HD2	1:E:363:ILE:HD13	1.90	0.53
1:E:301:LEU:HD13	1:E:361:LEU:HA	1.90	0.53
1:E:285:LEU:CB	1:E:431:VAL:HG22	2.38	0.53
1:A:133:ASN:N	1:A:134:PRO:CD	2.71	0.53
1:A:64:LYS:HA	1:A:67:ILE:HD12	1.91	0.53
1:A:10:LEU:O	1:A:74:TRP:CZ2	2.61	0.53
1:B:45:VAL:HG22	1:B:54:PHE:CE1	2.44	0.53
1:C:83:LYS:O	1:C:134:PRO:HA	2.08	0.53
1:C:164:ILE:N	1:C:165:PRO:CD	2.72	0.53
1:C:73:VAL:HG22	1:C:105:ILE:HG12	1.88	0.53
1:D:136:HIS:ND1	1:D:138:PRO:HD3	2.22	0.53
1:E:141:LYS:O	1:E:144:GLY:O	2.26	0.53
1:A:294:SER:HB2	1:A:340:GLY:C	2.29	0.53
1:A:366:SER:HB3	1:A:368:ARG:HE	1.72	0.53
1:B:235:LEU:HD12	1:B:241:LEU:HG	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:LYS:HZ2	1:C:430:LYS:HA	1.73	0.53
1:E:378:LEU:CD1	1:E:401:THR:OG1	2.54	0.53
1:A:298:LYS:HZ2	1:A:430:LYS:HA	1.74	0.53
1:B:39:GLN:HB3	1:B:67:ILE:CG1	2.38	0.53
1:C:256:LEU:O	1:C:260:PRO:HD3	2.02	0.53
1:B:173:ALA:HB2	1:C:346:TYR:HD1	1.73	0.53
1:D:310:ALA:HB2	1:D:464:VAL:HG23	1.91	0.53
1:E:100:PHE:O	1:E:104:ILE:HG12	2.09	0.53
1:E:124:VAL:HB	1:E:125:ILE:CB	2.16	0.53
1:E:186:ALA:O	1:E:190:PRO:CD	2.54	0.53
1:E:225:ALA:O	1:E:228:PRO:HD2	2.09	0.53
1:E:310:ALA:HB2	1:E:464:VAL:HG23	1.91	0.53
1:A:301:LEU:HD13	1:A:361:LEU:HA	1.90	0.53
1:A:406:ALA:O	1:A:408:LYS:N	2.41	0.53
1:A:77:TRP:CE3	1:A:77:TRP:HA	2.42	0.53
1:B:173:ALA:HB3	1:C:345:THR:CB	2.39	0.53
1:A:173:ALA:HB2	1:B:346:TYR:CD2	2.44	0.53
1:C:406:ALA:O	1:C:408:LYS:N	2.41	0.53
1:C:298:LYS:NZ	1:C:430:LYS:HA	2.24	0.53
1:C:174:ARG:CZ	1:D:345:THR:OG1	2.53	0.53
1:C:176:LYS:HG2	1:D:346:TYR:HB2	1.90	0.53
1:A:128:ASP:O	1:A:135:ASP:HB3	2.09	0.53
1:B:202:PRO:HB3	1:B:265:ARG:NH1	2.23	0.53
1:B:298:LYS:HZ2	1:B:430:LYS:HA	1.74	0.53
1:D:173:ALA:HB3	1:E:345:THR:CB	2.39	0.53
1:E:161:ASP:O	1:E:165:PRO:CD	2.57	0.53
1:E:190:PRO:HB2	1:E:192:PRO:HG2	1.91	0.53
1:A:314:GLU:O	1:A:314:GLU:CG	2.57	0.53
1:A:347:HIS:CA	1:E:176:LYS:HB3	2.39	0.53
1:B:225:ALA:O	1:B:228:PRO:HD2	2.08	0.53
1:C:322:TRP:CZ3	1:C:457:ILE:HD12	2.44	0.53
1:D:189:LYS:HB2	1:D:190:PRO:HD3	1.90	0.53
1:D:274:ARG:HD3	1:D:417:VAL:HG13	1.90	0.53
1:D:314:GLU:CG	1:D:314:GLU:O	2.57	0.53
1:E:230:THR:HA	1:E:233:GLU:HG3	1.90	0.53
1:E:294:SER:HB2	1:E:340:GLY:C	2.29	0.53
1:A:414:VAL:C	1:A:417:VAL:HG12	2.29	0.53
1:C:265:ARG:O	1:C:265:ARG:HG3	2.08	0.53
1:C:313:LEU:HD11	1:C:377:VAL:HB	1.90	0.53
1:C:310:ALA:HB2	1:C:464:VAL:HG23	1.91	0.53
1:D:406:ALA:O	1:D:408:LYS:N	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ARG:CB	1:A:118:PRO:CD	2.81	0.52
1:B:73:VAL:HG21	1:B:104:ILE:HB	1.90	0.52
1:D:301:LEU:HG	1:D:302:ARG:N	2.24	0.52
1:C:173:ALA:HB3	1:D:345:THR:CB	2.39	0.52
1:E:368:ARG:HD2	1:E:378:LEU:HD23	1.90	0.52
1:A:176:LYS:HB2	1:B:347:HIS:HB2	1.90	0.52
1:B:56:LEU:HB2	1:B:199:LEU:HG	1.91	0.52
1:B:307:ILE:HD13	1:B:327:GLN:HA	1.91	0.52
1:C:77:TRP:HZ3	1:C:114:LEU:HB2	1.73	0.52
1:D:161:ASP:HB3	1:D:164:ILE:HG22	1.91	0.52
1:A:280:LYS:CE	1:A:438:LYS:HA	2.24	0.52
1:B:294:SER:HB2	1:B:340:GLY:C	2.29	0.52
1:B:440:HIS:CG	1:B:458:CYS:HG	2.28	0.52
1:B:310:ALA:HB2	1:B:464:VAL:HG23	1.91	0.52
1:C:202:PRO:CB	1:C:265:ARG:NH1	2.66	0.52
1:C:294:SER:HB2	1:C:340:GLY:C	2.29	0.52
1:E:84:ILE:HG23	1:E:153:ARG:O	2.08	0.52
1:E:181:VAL:N	1:E:182:GLN:CB	2.73	0.52
1:E:19:PHE:O	1:E:32:LEU:HD21	2.10	0.52
1:E:266:PHE:CE1	1:E:272:ARG:HG3	2.44	0.52
1:A:190:PRO:HB2	1:A:192:PRO:HG2	1.91	0.52
1:A:196:VAL:HG13	1:A:198:TYR:HE1	1.73	0.52
1:A:14:GLN:OE1	1:A:40:ILE:HG23	2.09	0.52
1:B:376:ALA:O	1:B:377:VAL:C	2.47	0.52
1:C:193:SER:HB2	1:C:195:ARG:NH2	2.25	0.52
1:D:141:LYS:HZ3	1:D:171:MET:HB2	1.74	0.52
1:D:173:ALA:HB1	1:E:345:THR:CA	2.36	0.52
1:C:170:THR:CA	1:D:345:THR:HG21	2.27	0.52
1:B:274:ARG:NE	1:B:414:VAL:HG12	2.24	0.52
1:C:190:PRO:C	1:C:192:PRO:HD2	2.30	0.52
1:E:414:VAL:HA	1:E:417:VAL:CG1	2.38	0.52
1:A:225:ALA:O	1:A:228:PRO:HD2	2.09	0.52
1:A:310:ALA:HB2	1:A:464:VAL:HG23	1.91	0.52
1:C:235:LEU:CD1	1:C:241:LEU:CD2	2.70	0.52
1:C:262:ASP:CB	1:C:263:PRO:CD	2.74	0.52
1:C:272:ARG:HB3	1:C:442:CYS:H	1.74	0.52
1:C:51:ASN:HB2	1:C:54:PHE:HZ	1.66	0.52
1:D:294:SER:HB2	1:D:340:GLY:C	2.29	0.52
1:E:14:GLN:OE1	1:E:40:ILE:HG23	2.10	0.52
1:C:468:HIS:HD2	1:C:468:HIS:O	1.92	0.52
1:C:57:GLN:NE2	1:C:265:ARG:HH21	2.03	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:PRO:HB3	1:E:127:PHE:CZ	2.45	0.52
1:E:119:GLY:HA2	1:E:127:PHE:HD2	1.74	0.52
1:E:221:ILE:HA	1:E:445:GLU:HG2	1.88	0.52
1:A:191:LEU:N	1:A:192:PRO:HD2	2.25	0.52
1:A:298:LYS:NZ	1:A:430:LYS:HA	2.25	0.52
1:A:311:LEU:HB3	1:A:368:ARG:HG3	1.92	0.52
1:B:394:ARG:HB3	1:B:400:LYS:HD3	1.91	0.52
1:B:77:TRP:HZ3	1:B:114:LEU:HB2	1.75	0.52
1:C:181:VAL:N	1:C:182:GLN:CB	2.73	0.52
1:C:291:PRO:HD3	1:C:295:ASP:O	2.10	0.52
1:D:125:ILE:O	1:D:125:ILE:CG2	2.58	0.52
1:D:220:THR:CB	1:D:445:GLU:HB2	2.39	0.52
1:E:196:VAL:HG11	1:E:198:TYR:CZ	2.45	0.52
1:A:144:GLY:O	1:A:171:MET:HG2	2.10	0.52
1:A:176:LYS:HB3	1:B:347:HIS:CA	2.40	0.52
1:B:300:PRO:HB2	1:B:302:ARG:HH12	1.75	0.52
1:C:119:GLY:HA2	1:C:127:PHE:HD1	1.74	0.52
1:C:14:GLN:OE1	1:C:40:ILE:HG23	2.09	0.52
1:E:125:ILE:O	1:E:125:ILE:CG2	2.58	0.52
1:E:208:LEU:CD2	1:E:265:ARG:HH22	2.23	0.52
1:E:314:GLU:O	1:E:314:GLU:CG	2.57	0.52
1:A:173:ALA:HB3	1:B:345:THR:CB	2.39	0.52
1:A:176:LYS:CA	1:B:347:HIS:HB3	2.40	0.52
1:D:319:HIS:HB3	1:D:456:ARG:HE	1.75	0.52
1:B:161:ASP:O	1:B:165:PRO:CD	2.58	0.51
1:B:21:ALA:HB3	1:B:33:PRO:HG3	1.92	0.51
1:C:128:ASP:O	1:C:135:ASP:HB3	2.09	0.51
1:C:294:SER:OG	1:C:341:ASP:HB2	2.10	0.51
1:D:193:SER:HB2	1:D:195:ARG:NH2	2.25	0.51
1:B:291:PRO:HG2	1:B:295:ASP:CB	2.28	0.51
1:B:294:SER:CB	1:B:341:ASP:HB3	2.41	0.51
1:B:414:VAL:HA	1:B:417:VAL:CG1	2.38	0.51
1:C:414:VAL:C	1:C:417:VAL:HG12	2.30	0.51
1:D:161:ASP:O	1:D:165:PRO:CD	2.58	0.51
1:A:345:THR:OG1	1:E:170:THR:HA	2.09	0.51
1:A:181:VAL:N	1:A:182:GLN:CB	2.73	0.51
1:A:322:TRP:CZ3	1:A:457:ILE:HD12	2.45	0.51
1:B:125:ILE:CG2	1:B:125:ILE:O	2.58	0.51
1:C:162:VAL:C	1:C:165:PRO:HD2	2.30	0.51
1:B:176:LYS:CA	1:C:347:HIS:HB3	2.39	0.51
1:C:176:LYS:C	1:D:347:HIS:CB	2.66	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:LYS:C	1:D:375:TYR:CE1	2.84	0.51
1:E:76:LEU:HB2	1:E:136:HIS:CE1	2.46	0.51
1:E:313:LEU:CD1	1:E:374:GLY:CA	2.79	0.51
1:D:59:PHE:CD1	1:D:225:ALA:CA	2.89	0.51
1:C:376:ALA:O	1:C:377:VAL:C	2.47	0.51
1:E:417:VAL:HA	1:E:465:MET:HG3	1.92	0.51
1:A:124:VAL:HB	1:A:125:ILE:CB	2.16	0.51
1:A:24:PHE:CD2	1:A:30:LEU:HD13	2.46	0.51
1:A:53:LYS:HD3	1:A:196:VAL:HB	1.91	0.51
1:B:181:VAL:N	1:B:182:GLN:CB	2.73	0.51
1:B:414:VAL:C	1:B:417:VAL:HG12	2.31	0.51
1:B:441:ASN:C	1:B:447:ILE:HG23	2.31	0.51
1:E:191:LEU:N	1:E:192:PRO:HD2	2.25	0.51
1:E:370:LYS:CG	1:E:401:THR:OG1	2.56	0.51
1:D:355:GLN:HB2	1:D:381:LEU:HD21	1.92	0.51
1:E:117:ARG:HD3	1:E:118:PRO:HD3	1.93	0.51
1:E:24:PHE:CD2	1:E:30:LEU:HD13	2.46	0.51
1:A:85:LEU:CB	1:A:136:HIS:ND1	2.72	0.51
1:A:301:LEU:HG	1:A:302:ARG:N	2.24	0.51
1:A:323:LEU:HB3	1:A:339:LYS:HB2	1.92	0.51
1:B:272:ARG:HB3	1:B:442:CYS:CB	2.41	0.51
1:C:176:LYS:HB2	1:D:347:HIS:CB	2.33	0.51
1:D:83:LYS:HG3	1:D:155:ASP:HB2	1.91	0.51
1:D:468:HIS:HA	1:D:473:ARG:NE	2.26	0.51
1:E:319:HIS:CB	1:E:456:ARG:HE	2.24	0.51
1:B:52:LYS:CB	1:B:184:PHE:CZ	2.74	0.51
1:C:24:PHE:CD2	1:C:30:LEU:HD13	2.46	0.51
1:C:314:GLU:O	1:C:314:GLU:CG	2.57	0.51
1:D:190:PRO:C	1:D:192:PRO:HD2	2.31	0.51
1:D:370:LYS:HE3	1:D:403:GLU:HA	1.93	0.51
1:D:432:PHE:HD1	1:D:432:PHE:N	2.09	0.51
1:E:322:TRP:CZ3	1:E:457:ILE:HD12	2.46	0.51
1:C:73:VAL:HG21	1:C:104:ILE:HB	1.92	0.51
1:C:76:LEU:HG	1:C:134:PRO:HB2	1.92	0.51
1:D:370:LYS:HG3	1:D:378:LEU:HD11	1.91	0.51
1:E:376:ALA:O	1:E:377:VAL:C	2.47	0.51
1:E:435:ILE:HA	1:E:438:LYS:HG3	1.92	0.51
1:E:73:VAL:HG21	1:E:104:ILE:HB	1.93	0.51
1:A:125:ILE:CG2	1:A:125:ILE:O	2.58	0.50
1:B:301:LEU:HG	1:B:302:ARG:N	2.25	0.50
1:B:314:GLU:O	1:B:314:GLU:CG	2.57	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:LEU:O	1:C:74:TRP:CZ2	2.64	0.50
1:D:14:GLN:NE2	1:D:40:ILE:HG12	2.26	0.50
1:A:345:THR:CA	1:E:173:ALA:HB1	2.36	0.50
1:E:45:VAL:HG22	1:E:54:PHE:CE1	2.45	0.50
1:E:85:LEU:HA	1:E:156:ILE:HG23	1.92	0.50
1:E:85:LEU:HD12	1:E:156:ILE:CG2	2.37	0.50
1:A:177:LEU:HB3	1:B:347:HIS:ND1	2.27	0.50
1:A:313:LEU:CD1	1:A:374:GLY:CA	2.80	0.50
1:C:189:LYS:HB2	1:C:190:PRO:HD3	1.93	0.50
1:C:181:VAL:HG21	1:D:379:TYR:CG	2.46	0.50
1:E:111:LEU:HD23	1:E:111:LEU:H	1.76	0.50
1:E:414:VAL:C	1:E:417:VAL:HG12	2.31	0.50
1:B:280:LYS:HZ1	1:B:438:LYS:N	2.09	0.50
1:B:432:PHE:HD1	1:B:432:PHE:N	2.09	0.50
1:A:285:LEU:CB	1:A:431:VAL:HG22	2.40	0.50
1:A:376:ALA:O	1:A:377:VAL:C	2.47	0.50
1:B:117:ARG:HB2	1:B:118:PRO:CD	2.40	0.50
1:C:176:LYS:HD2	1:C:176:LYS:N	2.25	0.50
1:D:85:LEU:HA	1:D:156:ILE:HG23	1.93	0.50
1:D:220:THR:HG23	1:D:220:THR:O	2.09	0.50
1:E:177:LEU:HD12	1:E:177:LEU:C	2.31	0.50
1:E:45:VAL:HG21	1:E:222:ILE:HD11	1.93	0.50
1:A:54:PHE:HD1	1:A:221:ILE:HD13	1.77	0.50
1:B:59:PHE:CD2	1:B:263:PRO:HA	2.47	0.50
1:B:10:LEU:O	1:B:74:TRP:HZ2	1.94	0.50
1:C:190:PRO:C	1:C:192:PRO:CD	2.80	0.50
1:C:378:LEU:CD2	1:C:401:THR:HG23	2.41	0.50
1:C:88:SER:HB3	1:C:141:LYS:CG	2.41	0.50
1:D:163:GLU:HG3	1:D:203:GLN:CB	2.34	0.50
1:D:180:LEU:HD21	1:E:380:THR:OG1	2.11	0.50
1:D:181:VAL:N	1:D:182:GLN:CB	2.73	0.50
1:D:298:LYS:HZ2	1:D:430:LYS:HA	1.77	0.50
1:E:370:LYS:CE	1:E:375:TYR:CE1	2.86	0.50
1:C:125:ILE:CG2	1:C:125:ILE:O	2.59	0.50
1:D:414:VAL:C	1:D:417:VAL:HG12	2.32	0.50
1:D:73:VAL:HG21	1:D:104:ILE:HB	1.93	0.50
1:B:286:GLN:HG2	1:B:288:MET:HE2	1.94	0.50
1:B:313:LEU:HD11	1:B:377:VAL:HB	1.92	0.50
1:C:301:LEU:HG	1:C:302:ARG:N	2.25	0.50
1:C:468:HIS:CA	1:C:473:ARG:HD3	2.35	0.50
1:D:96:ALA:HA	1:D:99:ILE:HD12	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LEU:N	1:B:192:PRO:HD2	2.26	0.50
1:B:291:PRO:CD	1:B:295:ASP:O	2.60	0.50
1:B:433:SER:CA	1:B:457:ILE:HD13	2.42	0.50
1:D:272:ARG:HB3	1:D:442:CYS:CB	2.42	0.50
1:D:59:PHE:HD2	1:D:60:ARG:O	1.95	0.50
1:D:10:LEU:O	1:D:74:TRP:CZ2	2.64	0.50
1:A:116:PRO:HB3	1:A:127:PHE:CZ	2.47	0.50
1:A:311:LEU:HD23	1:A:368:ARG:HG2	1.94	0.50
1:C:85:LEU:HB3	1:C:136:HIS:ND1	2.27	0.50
1:C:435:ILE:HA	1:C:438:LYS:HG3	1.94	0.50
1:D:280:LYS:HZ2	1:D:438:LYS:CA	2.08	0.50
1:E:309:ALA:HB2	1:E:358:GLN:HE22	1.77	0.50
1:E:417:VAL:HA	1:E:465:MET:SD	2.51	0.50
1:A:162:VAL:C	1:A:165:PRO:HD2	2.33	0.49
1:A:311:LEU:HB2	1:A:323:LEU:HD12	1.93	0.49
1:D:21:ALA:O	1:D:22:PHE:CD1	2.65	0.49
1:E:76:LEU:CG	1:E:134:PRO:HB2	2.42	0.49
1:E:73:VAL:HG22	1:E:77:TRP:HE1	1.77	0.49
1:A:163:GLU:HG3	1:A:203:GLN:CB	2.33	0.49
1:B:326:ARG:HD3	1:B:333:LEU:HB3	1.92	0.49
1:C:144:GLY:O	1:C:171:MET:HG2	2.12	0.49
1:C:415:GLN:O	1:C:418:VAL:CG1	2.60	0.49
1:D:136:HIS:CE1	1:D:138:PRO:HD3	2.46	0.49
1:D:190:PRO:C	1:D:192:PRO:CD	2.80	0.49
1:D:58:ALA:C	1:D:265:ARG:HD3	2.30	0.49
1:E:415:GLN:O	1:E:418:VAL:CG1	2.60	0.49
1:A:375:TYR:O	1:A:378:LEU:HB2	2.12	0.49
1:A:415:GLN:O	1:A:418:VAL:CG1	2.60	0.49
1:D:125:ILE:O	1:D:138:PRO:HD2	2.12	0.49
1:C:173:ALA:HB2	1:D:346:TYR:CD2	2.47	0.49
1:E:190:PRO:CB	1:E:192:PRO:HD2	2.41	0.49
1:A:10:LEU:O	1:A:74:TRP:HZ2	1.94	0.49
1:A:161:ASP:O	1:A:165:PRO:CD	2.60	0.49
1:A:52:LYS:CB	1:A:184:PHE:CZ	2.73	0.49
1:B:76:LEU:HB3	1:B:136:HIS:CE1	2.47	0.49
1:B:187:LEU:O	1:B:192:PRO:HD2	2.12	0.49
1:C:173:ALA:HB1	1:D:345:THR:CA	2.36	0.49
1:B:173:ALA:HB2	1:C:346:TYR:CD1	2.47	0.49
1:D:256:LEU:O	1:D:260:PRO:HD3	2.09	0.49
1:D:55:ILE:CG2	1:D:57:GLN:HE21	2.25	0.49
1:E:144:GLY:HA2	1:E:147:GLY:N	2.23	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:309:ALA:HB3	1:E:358:GLN:HE22	1.77	0.49
1:A:58:ALA:C	1:A:265:ARG:HD3	2.31	0.49
1:A:345:THR:C	1:E:173:ALA:HB3	2.22	0.49
1:A:468:HIS:HA	1:A:473:ARG:NE	2.26	0.49
1:B:190:PRO:HB2	1:B:192:PRO:HG2	1.94	0.49
1:C:157:ILE:HB	1:C:196:VAL:HG22	1.94	0.49
1:D:98:SER:HB2	1:D:136:HIS:CE1	2.44	0.49
1:D:172:GLY:HA2	1:D:175:GLU:OE1	2.12	0.49
1:E:378:LEU:CD2	1:E:401:THR:HG23	2.42	0.49
1:E:221:ILE:N	1:E:445:GLU:HG2	2.27	0.49
1:A:313:LEU:HD11	1:A:377:VAL:HB	1.94	0.49
1:B:177:LEU:CB	1:C:347:HIS:ND1	2.66	0.49
1:C:73:VAL:HG22	1:C:77:TRP:HE1	1.76	0.49
1:D:299:TYR:HA	1:D:300:PRO:CD	2.42	0.49
1:E:118:PRO:HG2	1:E:129:VAL:HB	1.95	0.49
1:E:293:LEU:HD13	1:E:353:SER:HB2	1.94	0.49
1:E:54:PHE:HD1	1:E:221:ILE:HD13	1.78	0.49
1:A:114:LEU:O	1:A:116:PRO:HD3	2.12	0.49
1:A:119:GLY:HA2	1:A:127:PHE:HD1	1.73	0.49
1:C:249:TYR:O	1:C:253:PRO:HD2	2.13	0.49
1:C:23:LEU:HG	1:C:33:PRO:HG3	1.95	0.49
1:D:173:ALA:HB2	1:E:346:TYR:HD2	1.68	0.49
1:D:149:LEU:HG	1:D:174:ARG:HH11	1.78	0.49
1:D:157:ILE:HB	1:D:196:VAL:HG22	1.94	0.49
1:E:202:PRO:HB3	1:E:265:ARG:CZ	2.43	0.49
1:E:57:GLN:C	1:E:265:ARG:HG3	2.33	0.49
1:B:159:ALA:HB2	1:B:198:TYR:CE1	2.47	0.49
1:B:307:ILE:C	1:B:364:ASP:OD1	2.51	0.49
1:E:161:ASP:HB3	1:E:164:ILE:HG12	1.93	0.49
1:E:16:LYS:HD2	1:E:16:LYS:C	2.33	0.49
1:A:226:LEU:HD13	1:A:263:PRO:HB3	1.94	0.49
1:B:262:ASP:CB	1:B:263:PRO:CD	2.73	0.49
1:E:190:PRO:HB2	1:E:192:PRO:CG	2.43	0.49
1:E:163:GLU:CG	1:E:203:GLN:HB2	2.35	0.49
1:E:57:GLN:CG	1:E:212:LEU:HD13	2.40	0.49
1:A:144:GLY:HA2	1:A:147:GLY:N	2.23	0.49
1:A:266:PHE:CE1	1:A:272:ARG:HG3	2.48	0.49
1:B:190:PRO:HB2	1:B:192:PRO:CG	2.43	0.49
1:B:57:GLN:CD	1:B:57:GLN:N	2.66	0.49
1:C:111:LEU:HD23	1:C:111:LEU:H	1.77	0.49
1:C:368:ARG:H	1:C:401:THR:HG21	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:VAL:HA	1:D:417:VAL:CG1	2.41	0.49
1:D:54:PHE:HD1	1:D:221:ILE:HD13	1.78	0.49
1:E:294:SER:OG	1:E:341:ASP:HB2	2.13	0.49
1:A:141:LYS:HZ3	1:A:171:MET:HB2	1.78	0.48
1:A:157:ILE:HB	1:A:196:VAL:HG22	1.94	0.48
1:A:307:ILE:HD13	1:A:327:GLN:HA	1.95	0.48
1:B:190:PRO:CB	1:B:192:PRO:HD2	2.41	0.48
1:B:21:ALA:O	1:B:22:PHE:CD1	2.66	0.48
1:B:443:ALA:HB1	1:B:448:ARG:NH2	2.27	0.48
1:C:273:GLU:HA	1:C:441:ASN:HA	1.95	0.48
1:C:221:ILE:HA	1:C:445:GLU:HG2	1.95	0.48
1:D:376:ALA:O	1:D:377:VAL:C	2.47	0.48
1:E:162:VAL:C	1:E:165:PRO:HD2	2.34	0.48
1:B:119:GLY:HA2	1:B:127:PHE:CD2	2.48	0.48
1:B:159:ALA:HB3	1:B:198:TYR:CE1	2.47	0.48
1:B:378:LEU:CD2	1:B:401:THR:CG2	2.84	0.48
1:C:155:ASP:O	1:C:194:SER:C	2.52	0.48
1:C:191:LEU:N	1:C:192:PRO:HD2	2.28	0.48
1:C:21:ALA:O	1:C:22:PHE:CD1	2.66	0.48
1:C:54:PHE:HD1	1:C:221:ILE:HD13	1.78	0.48
1:D:299:TYR:C	1:D:300:PRO:CD	2.68	0.48
1:E:313:LEU:HD11	1:E:377:VAL:HB	1.95	0.48
1:A:190:PRO:HB2	1:A:192:PRO:CG	2.44	0.48
1:A:291:PRO:CD	1:A:295:ASP:O	2.61	0.48
1:B:111:LEU:HD23	1:B:111:LEU:H	1.77	0.48
1:B:155:ASP:O	1:B:194:SER:C	2.52	0.48
1:C:181:VAL:CA	1:C:182:GLN:CG	2.88	0.48
1:D:88:SER:HB3	1:D:141:LYS:CG	2.42	0.48
1:D:155:ASP:O	1:D:194:SER:C	2.52	0.48
1:D:322:TRP:HB3	1:D:460:THR:HG21	1.96	0.48
1:D:273:GLU:HA	1:D:441:ASN:HA	1.95	0.48
1:B:73:VAL:HG22	1:B:77:TRP:HE1	1.79	0.48
1:C:164:ILE:N	1:C:165:PRO:HD3	2.28	0.48
1:C:417:VAL:HG23	1:C:465:MET:HE2	1.94	0.48
1:D:144:GLY:HA2	1:D:147:GLY:N	2.23	0.48
1:E:155:ASP:O	1:E:194:SER:C	2.52	0.48
1:A:155:ASP:O	1:A:194:SER:C	2.52	0.48
1:A:57:GLN:CG	1:A:212:LEU:HD13	2.41	0.48
1:B:157:ILE:HB	1:B:196:VAL:HG22	1.94	0.48
1:B:368:ARG:H	1:B:401:THR:HG21	1.74	0.48
1:C:10:LEU:O	1:C:74:TRP:HZ2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:LYS:O	1:C:401:THR:CG2	2.58	0.48
1:C:322:TRP:HB3	1:C:460:THR:HG21	1.96	0.48
1:D:10:LEU:O	1:D:74:TRP:HZ2	1.96	0.48
1:D:21:ALA:C	1:D:33:PRO:HD2	2.34	0.48
1:D:313:LEU:HD11	1:D:377:VAL:HB	1.95	0.48
1:D:415:GLN:O	1:D:418:VAL:CG1	2.60	0.48
1:D:434:PRO:HA	1:D:437:LEU:HD12	1.94	0.48
1:D:45:VAL:HG22	1:D:54:PHE:CE1	2.48	0.48
1:A:190:PRO:CB	1:A:192:PRO:HD2	2.41	0.48
1:A:322:TRP:HB3	1:A:460:THR:HG21	1.96	0.48
1:A:382:ASN:CB	1:A:385:ILE:CG1	2.90	0.48
1:B:465:MET:O	1:B:468:HIS:HB3	2.14	0.48
1:C:403:GLU:HG2	1:C:405:LEU:H	1.78	0.48
1:C:82:LEU:C	1:C:83:LYS:HG3	2.34	0.48
1:C:85:LEU:HA	1:C:156:ILE:HG23	1.95	0.48
1:D:338:LEU:HD23	1:D:457:ILE:HD11	1.95	0.48
1:D:73:VAL:HG13	1:D:77:TRP:CD1	2.47	0.48
1:E:307:ILE:HD13	1:E:327:GLN:HA	1.95	0.48
1:A:46:LEU:CD2	1:A:54:PHE:HB2	2.43	0.48
1:B:141:LYS:HZ3	1:B:171:MET:HB2	1.78	0.48
1:B:439:HIS:CD2	1:B:453:LYS:HB3	2.49	0.48
1:C:190:PRO:CB	1:C:192:PRO:HD2	2.42	0.48
1:E:161:ASP:O	1:E:165:PRO:HD3	2.14	0.48
1:E:249:TYR:O	1:E:253:PRO:HD2	2.13	0.48
1:E:400:LYS:O	1:E:401:THR:CG2	2.58	0.48
1:A:91:LYS:CA	1:A:93:ARG:H	2.27	0.48
1:B:181:VAL:HG21	1:C:379:TYR:CG	2.48	0.48
1:C:91:LYS:CA	1:C:93:ARG:H	2.27	0.48
1:D:91:LYS:CA	1:D:93:ARG:H	2.27	0.48
1:D:176:LYS:CG	1:E:347:HIS:HB3	2.42	0.48
1:B:432:PHE:CD1	1:B:432:PHE:N	2.81	0.48
1:C:226:LEU:HD13	1:C:263:PRO:HB3	1.95	0.48
1:C:432:PHE:N	1:C:432:PHE:HD1	2.11	0.48
1:C:77:TRP:HZ3	1:C:114:LEU:CB	2.26	0.48
1:A:380:THR:OG1	1:E:180:LEU:HD21	2.14	0.48
1:C:291:PRO:CG	1:C:295:ASP:HB3	2.32	0.48
1:D:294:SER:OG	1:D:341:ASP:HB2	2.13	0.48
1:E:77:TRP:CE2	1:E:105:ILE:HG12	2.45	0.48
1:A:294:SER:OG	1:A:341:ASP:HB2	2.14	0.47
1:B:161:ASP:O	1:B:165:PRO:HD2	2.14	0.47
1:B:76:LEU:HD11	1:B:128:ASP:OD2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:PRO:HD2	1:C:128:ASP:CA	2.43	0.47
1:C:21:ALA:C	1:C:33:PRO:HD2	2.34	0.47
1:C:382:ASN:CG	1:C:385:ILE:HG12	2.34	0.47
1:D:309:ALA:HB2	1:D:358:GLN:HE22	1.78	0.47
1:E:115:LYS:CA	1:E:116:PRO:CD	2.91	0.47
1:E:275:GLU:OE2	1:E:437:LEU:HD22	2.14	0.47
1:E:326:ARG:O	1:E:328:ASN:OD1	2.32	0.47
1:A:433:SER:CA	1:A:434:PRO:CD	2.92	0.47
1:B:259:THR:O	1:B:264:VAL:HG23	2.14	0.47
1:B:322:TRP:HB3	1:B:460:THR:HG21	1.97	0.47
1:C:307:ILE:HD13	1:C:327:GLN:HA	1.95	0.47
1:D:117:ARG:CB	1:D:118:PRO:HD3	2.43	0.47
1:D:55:ILE:CG2	1:D:57:GLN:NE2	2.77	0.47
1:E:322:TRP:HB3	1:E:460:THR:HG21	1.96	0.47
1:E:88:SER:HB3	1:E:141:LYS:CG	2.44	0.47
1:B:190:PRO:C	1:B:192:PRO:CD	2.82	0.47
1:B:91:LYS:CA	1:B:93:ARG:H	2.27	0.47
1:C:190:PRO:HB2	1:C:192:PRO:HG2	1.96	0.47
1:C:338:LEU:HD23	1:C:457:ILE:HD11	1.97	0.47
1:E:91:LYS:CA	1:E:93:ARG:H	2.27	0.47
1:A:249:TYR:O	1:A:253:PRO:HD2	2.14	0.47
1:A:45:VAL:HG22	1:A:54:PHE:CE1	2.49	0.47
1:B:88:SER:HB3	1:B:141:LYS:CG	2.45	0.47
1:A:56:LEU:HB2	1:A:199:LEU:HG	1.96	0.47
1:C:190:PRO:HB2	1:C:192:PRO:CG	2.44	0.47
1:C:223:TRP:O	1:C:223:TRP:CE3	2.67	0.47
1:C:234:ASN:OD1	1:C:240:ARG:HD3	2.14	0.47
1:D:265:ARG:O	1:D:265:ARG:HG3	2.15	0.47
1:E:232:GLU:HB3	1:E:246:ARG:HG2	1.97	0.47
1:E:338:LEU:HD23	1:E:457:ILE:HD11	1.96	0.47
1:A:262:ASP:CB	1:A:263:PRO:CD	2.74	0.47
1:A:73:VAL:HG21	1:A:104:ILE:HB	1.95	0.47
1:B:173:ALA:HB1	1:C:345:THR:CA	2.36	0.47
1:B:316:ALA:O	1:B:318:MET:HB2	2.13	0.47
1:C:83:LYS:CE	1:C:193:SER:H	2.23	0.47
1:E:444:MET:HA	1:E:445:GLU:HA	1.56	0.47
1:E:46:LEU:HD22	1:E:197:ILE:CG1	2.45	0.47
1:B:77:TRP:CE2	1:B:105:ILE:HG12	2.47	0.47
1:B:161:ASP:HB3	1:B:164:ILE:HG22	1.96	0.47
1:B:57:GLN:O	1:B:223:TRP:HD1	1.98	0.47
1:B:433:SER:CA	1:B:434:PRO:CD	2.93	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LYS:CB	1:C:184:PHE:CZ	2.73	0.47
1:D:20:VAL:HA	1:D:22:PHE:CZ	2.49	0.47
1:C:173:ALA:HB2	1:D:346:TYR:HD2	1.79	0.47
1:D:368:ARG:NH2	1:D:381:LEU:HB3	2.29	0.47
1:D:433:SER:CA	1:D:434:PRO:CD	2.92	0.47
1:A:417:VAL:N	1:A:465:MET:HG3	2.28	0.47
1:B:77:TRP:HZ3	1:B:114:LEU:CB	2.27	0.47
1:D:76:LEU:HD11	1:D:128:ASP:OD2	2.14	0.47
1:D:432:PHE:N	1:D:432:PHE:CD1	2.81	0.47
1:D:441:ASN:O	1:D:447:ILE:HG23	2.15	0.47
1:A:326:ARG:HD3	1:A:333:LEU:HB3	1.96	0.47
1:A:465:MET:O	1:A:468:HIS:HB3	2.14	0.47
1:B:182:GLN:NE2	1:B:185:ALA:CB	2.46	0.47
1:B:273:GLU:HA	1:B:441:ASN:HA	1.95	0.47
1:C:241:LEU:HG	1:C:244:MET:HB2	1.97	0.47
1:E:208:LEU:CD2	1:E:265:ARG:NH2	2.67	0.47
1:E:273:GLU:HA	1:E:441:ASN:HA	1.95	0.47
1:A:161:ASP:O	1:A:165:PRO:HD3	2.14	0.47
1:A:235:LEU:HD23	1:A:235:LEU:HA	1.52	0.47
1:A:347:HIS:HE2	1:A:376:ALA:CB	2.28	0.47
1:A:273:GLU:HA	1:A:441:ASN:HA	1.95	0.47
1:B:235:LEU:HA	1:B:235:LEU:HD23	1.50	0.47
1:B:249:TYR:O	1:B:253:PRO:HD2	2.14	0.47
1:B:265:ARG:HG3	1:B:265:ARG:HH11	1.80	0.47
1:B:280:LYS:NZ	1:B:437:LEU:C	2.69	0.47
1:B:76:LEU:CB	1:B:136:HIS:CE1	2.98	0.47
1:C:272:ARG:HB3	1:C:442:CYS:CB	2.44	0.47
1:C:316:ALA:O	1:C:318:MET:HB2	2.14	0.47
1:C:370:LYS:O	1:C:375:TYR:CE2	2.68	0.47
1:C:313:LEU:CD2	1:C:377:VAL:HG21	2.45	0.47
1:D:119:GLY:HA2	1:D:127:PHE:CD2	2.49	0.47
1:D:59:PHE:HB2	1:D:263:PRO:HA	1.96	0.47
1:D:202:PRO:CB	1:D:265:ARG:NH1	2.71	0.47
1:A:54:PHE:O	1:A:55:ILE:HD13	2.15	0.47
1:C:346:TYR:HE2	1:C:349:CYS:CB	2.12	0.47
1:D:272:ARG:HB3	1:D:442:CYS:H	1.78	0.47
1:A:73:VAL:HG13	1:A:77:TRP:CD1	2.49	0.46
1:B:309:ALA:HB3	1:B:358:GLN:HE22	1.78	0.46
1:A:173:ALA:HB3	1:B:345:THR:C	2.22	0.46
1:B:417:VAL:HG23	1:B:465:MET:CE	2.45	0.46
1:C:417:VAL:N	1:C:465:MET:HG3	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:PHE:CE1	1:D:225:ALA:C	2.89	0.46
1:D:232:GLU:HB3	1:D:246:ARG:HG2	1.96	0.46
1:E:19:PHE:C	1:E:32:LEU:HD21	2.36	0.46
1:E:57:GLN:HB3	1:E:265:ARG:CZ	2.44	0.46
1:A:85:LEU:HA	1:A:156:ILE:HG23	1.97	0.46
1:A:57:GLN:O	1:A:223:TRP:HD1	1.99	0.46
1:B:220:THR:HG23	1:B:411:GLN:CD	2.35	0.46
1:C:176:LYS:HB2	1:D:347:HIS:CA	2.37	0.46
1:C:433:SER:CA	1:C:434:PRO:CD	2.93	0.46
1:D:114:LEU:O	1:D:116:PRO:HD3	2.15	0.46
1:D:307:ILE:HD13	1:D:327:GLN:HA	1.97	0.46
1:A:118:PRO:HD2	1:A:128:ASP:CA	2.42	0.46
1:B:428:PHE:HE1	1:B:461:LEU:HD22	1.79	0.46
1:B:432:PHE:O	1:B:436:LEU:HD13	2.16	0.46
1:B:280:LYS:HZ3	1:B:437:LEU:HB3	1.81	0.46
1:B:45:VAL:HG12	1:B:46:LEU:HG	1.98	0.46
1:C:46:LEU:HD22	1:C:197:ILE:CG1	2.45	0.46
1:D:190:PRO:CB	1:D:192:PRO:HD2	2.40	0.46
1:E:221:ILE:HA	1:E:222:ILE:HG12	1.96	0.46
1:E:346:TYR:CE1	1:E:349:CYS:HB3	2.51	0.46
1:A:141:LYS:HG2	1:A:171:MET:HE2	1.97	0.46
1:A:293:LEU:HD13	1:A:353:SER:HB2	1.97	0.46
1:A:85:LEU:HD12	1:A:156:ILE:HD13	1.96	0.46
1:B:144:GLY:HA2	1:B:147:GLY:N	2.23	0.46
1:B:235:LEU:CD1	1:B:241:LEU:HG	2.44	0.46
1:C:259:THR:O	1:C:264:VAL:HG23	2.15	0.46
1:D:117:ARG:CB	1:D:118:PRO:CD	2.93	0.46
1:D:412:TRP:CE3	1:D:416:THR:OG1	2.66	0.46
1:E:241:LEU:HG	1:E:244:MET:HB2	1.96	0.46
1:E:45:VAL:HG12	1:E:46:LEU:HG	1.98	0.46
1:A:181:VAL:CA	1:A:182:GLN:CG	2.88	0.46
1:C:116:PRO:HB3	1:C:127:PHE:CZ	2.50	0.46
1:C:118:PRO:HG2	1:C:129:VAL:HB	1.97	0.46
1:D:193:SER:HB2	1:D:195:ARG:HH22	1.80	0.46
1:D:57:GLN:HB3	1:D:265:ARG:CZ	2.44	0.46
1:D:91:LYS:CB	1:D:93:ARG:N	2.74	0.46
1:E:22:PHE:HA	1:E:33:PRO:HD3	1.97	0.46
1:A:280:LYS:HZ3	1:A:437:LEU:HB3	1.79	0.46
1:B:85:LEU:HA	1:B:156:ILE:HG23	1.96	0.46
1:C:144:GLY:HA2	1:C:147:GLY:N	2.23	0.46
1:C:168:SER:HA	1:C:171:MET:SD	2.55	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ALA:HB2	1:C:346:TYR:HB3	1.96	0.46
1:C:274:ARG:CD	1:C:414:VAL:CG1	2.86	0.46
1:C:444:MET:HA	1:C:445:GLU:HA	1.56	0.46
1:D:56:LEU:HD21	1:D:222:ILE:CG2	2.45	0.46
1:E:73:VAL:HG13	1:E:77:TRP:CD1	2.51	0.46
1:B:20:VAL:HA	1:B:22:PHE:CZ	2.51	0.46
1:C:355:GLN:HB2	1:C:381:LEU:HD21	1.97	0.46
1:C:432:PHE:N	1:C:432:PHE:CD1	2.83	0.46
1:D:191:LEU:N	1:D:192:PRO:HD2	2.31	0.46
1:E:162:VAL:HG23	1:E:208:LEU:HD12	1.98	0.46
1:E:222:ILE:HA	1:E:445:GLU:OE2	2.16	0.46
1:A:55:ILE:HG22	1:A:57:GLN:NE2	2.31	0.46
1:D:57:GLN:CG	1:D:212:LEU:HD13	2.41	0.46
1:D:259:THR:O	1:D:264:VAL:HG23	2.16	0.46
1:D:378:LEU:CD2	1:D:401:THR:OG1	2.55	0.46
1:A:323:LEU:O	1:A:338:LEU:HA	2.16	0.46
1:A:76:LEU:HB2	1:A:136:HIS:CE1	2.51	0.46
1:B:378:LEU:CD2	1:B:401:THR:HG23	2.46	0.46
1:B:76:LEU:HG	1:B:134:PRO:HB2	1.96	0.46
1:D:181:VAL:CA	1:D:182:GLN:CG	2.90	0.46
1:D:190:PRO:HB2	1:D:192:PRO:CG	2.45	0.46
1:D:193:SER:O	1:D:194:SER:CB	2.64	0.46
1:D:444:MET:HA	1:D:445:GLU:HA	1.56	0.46
1:E:118:PRO:HD2	1:E:128:ASP:CA	2.44	0.46
1:A:291:PRO:HG2	1:A:295:ASP:CB	2.32	0.46
1:E:85:LEU:CB	1:E:136:HIS:ND1	2.73	0.46
1:A:345:THR:CB	1:E:173:ALA:HB3	2.39	0.46
1:B:274:ARG:HE	1:B:414:VAL:HG11	1.81	0.45
1:B:327:GLN:HG2	1:B:329:ILE:HG22	1.97	0.45
1:C:145:ILE:CB	1:C:174:ARG:HG3	2.46	0.45
1:C:45:VAL:HG12	1:C:46:LEU:HG	1.98	0.45
1:D:46:LEU:CD2	1:D:54:PHE:HB2	2.46	0.45
1:A:193:SER:O	1:A:194:SER:CB	2.64	0.45
1:B:351:ASN:HB3	1:B:381:LEU:HG	1.98	0.45
1:B:441:ASN:O	1:B:447:ILE:HG23	2.15	0.45
1:B:82:LEU:O	1:B:83:LYS:HB2	2.17	0.45
1:C:158:ILE:HG22	1:C:197:ILE:HB	1.99	0.45
1:C:57:GLN:CG	1:C:212:LEU:HD13	2.41	0.45
1:B:173:ALA:HB2	1:C:346:TYR:CB	2.45	0.45
1:D:161:ASP:O	1:D:165:PRO:HD2	2.16	0.45
1:D:162:VAL:C	1:D:165:PRO:HD2	2.36	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:PRO:C	1:E:192:PRO:CD	2.84	0.45
1:E:156:ILE:HD11	1:E:197:ILE:HD13	1.98	0.45
1:E:259:THR:O	1:E:264:VAL:HG23	2.15	0.45
1:A:259:THR:O	1:A:264:VAL:HG23	2.16	0.45
1:A:46:LEU:HD22	1:A:197:ILE:CG1	2.47	0.45
1:B:159:ALA:HB1	1:B:162:VAL:CG1	2.47	0.45
1:B:355:GLN:HB2	1:B:381:LEU:HD21	1.99	0.45
1:B:370:LYS:NZ	1:B:399:ASP:HA	2.32	0.45
1:C:76:LEU:HD11	1:C:128:ASP:OD2	2.17	0.45
1:D:403:GLU:HG2	1:D:405:LEU:H	1.81	0.45
1:A:276:LEU:HD23	1:A:278:TYR:HB2	1.97	0.45
1:B:144:GLY:O	1:B:171:MET:HG2	2.16	0.45
1:B:57:GLN:CG	1:B:212:LEU:HD13	2.47	0.45
1:B:221:ILE:HB	1:B:222:ILE:HG13	1.98	0.45
1:B:323:LEU:O	1:B:338:LEU:HA	2.16	0.45
1:C:159:ALA:HB1	1:C:162:VAL:CG1	2.46	0.45
1:C:323:LEU:O	1:C:338:LEU:HA	2.16	0.45
1:C:72:VAL:HG13	1:C:85:LEU:CD1	2.42	0.45
1:D:158:ILE:HG22	1:D:197:ILE:HB	1.99	0.45
1:D:161:ASP:O	1:D:164:ILE:HG22	2.16	0.45
1:D:174:ARG:HD3	1:D:174:ARG:HA	1.77	0.45
1:D:309:ALA:HB3	1:D:358:GLN:HE22	1.80	0.45
1:D:75:SER:CB	1:D:83:LYS:HZ1	2.29	0.45
1:E:84:ILE:HG12	1:E:154:ALA:HA	1.99	0.45
1:A:161:ASP:O	1:A:164:ILE:HG22	2.17	0.45
1:D:202:PRO:HD3	1:D:265:ARG:HA	1.98	0.45
1:D:323:LEU:O	1:D:338:LEU:HA	2.16	0.45
1:D:36:THR:HB	1:D:39:GLN:HG3	1.97	0.45
1:D:221:ILE:C	1:D:445:GLU:HG2	2.36	0.45
1:D:79:ASP:CB	1:D:82:LEU:O	2.65	0.45
1:E:368:ARG:H	1:E:401:THR:HG21	1.77	0.45
1:E:379:TYR:O	1:E:385:ILE:CB	2.55	0.45
1:C:156:ILE:HD11	1:C:197:ILE:HD13	1.98	0.45
1:E:159:ALA:HB1	1:E:162:VAL:CG1	2.46	0.45
1:E:190:PRO:O	1:E:191:LEU:HB2	2.17	0.45
1:E:193:SER:O	1:E:194:SER:CB	2.64	0.45
1:E:158:ILE:HG22	1:E:197:ILE:HB	1.99	0.45
1:E:323:LEU:O	1:E:338:LEU:HA	2.16	0.45
1:A:190:PRO:O	1:A:191:LEU:HB2	2.17	0.45
1:B:299:TYR:HD2	1:B:336:VAL:HG12	1.81	0.45
1:B:456:ARG:HD3	1:B:456:ARG:HA	1.78	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:VAL:HG13	1:B:77:TRP:CD1	2.52	0.45
1:B:77:TRP:CH2	1:B:113:GLU:HG3	2.52	0.45
1:D:186:ALA:O	1:D:190:PRO:HD3	2.13	0.45
1:D:465:MET:O	1:D:468:HIS:HB3	2.16	0.45
1:E:382:ASN:CG	1:E:385:ILE:HG12	2.36	0.45
1:A:118:PRO:HG2	1:A:129:VAL:HB	1.98	0.45
1:A:190:PRO:C	1:A:192:PRO:CD	2.84	0.45
1:A:235:LEU:HD22	1:A:245:LEU:CB	2.32	0.45
1:A:85:LEU:HD13	1:A:136:HIS:CE1	2.51	0.45
1:B:226:LEU:HD13	1:B:263:PRO:HB3	1.99	0.45
1:B:394:ARG:O	1:B:394:ARG:HG2	2.17	0.45
1:C:313:LEU:HD21	1:C:377:VAL:HG21	1.98	0.45
1:C:79:ASP:CB	1:C:82:LEU:O	2.65	0.45
1:E:163:GLU:HG3	1:E:203:GLN:CB	2.37	0.45
1:A:110:PHE:CG	1:A:111:LEU:N	2.85	0.45
1:A:347:HIS:C	1:E:176:LYS:CB	2.86	0.45
1:A:39:GLN:HG2	1:A:67:ILE:HD11	1.97	0.45
1:A:173:ALA:HB2	1:B:346:TYR:CB	2.45	0.45
1:C:191:LEU:N	1:C:192:PRO:CD	2.80	0.45
1:C:221:ILE:N	1:C:445:GLU:HG2	2.32	0.45
1:E:299:TYR:HA	1:E:300:PRO:CD	2.47	0.45
1:E:394:ARG:HB3	1:E:400:LYS:HA	1.98	0.45
1:E:77:TRP:HZ3	1:E:114:LEU:HB2	1.81	0.45
1:A:181:VAL:HG21	1:B:379:TYR:CD2	2.51	0.45
1:B:158:ILE:HG22	1:B:197:ILE:HB	1.99	0.45
1:B:378:LEU:HD21	1:B:401:THR:HG23	1.97	0.45
1:B:79:ASP:CB	1:B:82:LEU:O	2.65	0.45
1:C:468:HIS:HA	1:C:473:ARG:NE	2.31	0.45
1:D:177:LEU:CB	1:E:347:HIS:CD2	2.91	0.45
1:D:202:PRO:HB3	1:D:265:ARG:HH12	1.79	0.45
1:A:265:ARG:O	1:A:265:ARG:HG3	2.17	0.44
1:B:145:ILE:N	1:B:171:MET:HG3	2.32	0.44
1:B:57:GLN:HG3	1:B:265:ARG:NH2	2.32	0.44
1:C:144:GLY:HA2	1:C:146:THR:H	1.79	0.44
1:D:182:GLN:NE2	1:D:185:ALA:CB	2.46	0.44
1:C:173:ALA:HB2	1:D:346:TYR:CB	2.45	0.44
1:A:294:SER:CB	1:A:341:ASP:HB2	2.48	0.44
1:A:370:LYS:HE3	1:A:403:GLU:HA	1.98	0.44
1:A:370:LYS:HG2	1:A:375:TYR:CD2	2.53	0.44
1:A:79:ASP:CB	1:A:82:LEU:O	2.65	0.44
1:B:180:LEU:HD13	1:B:180:LEU:HA	1.77	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:VAL:HG13	1:B:77:TRP:HD1	1.82	0.44
1:D:316:ALA:O	1:D:318:MET:HB2	2.17	0.44
1:E:411:GLN:HA	1:E:411:GLN:OE1	2.12	0.44
1:E:461:LEU:O	1:E:465:MET:HG2	2.17	0.44
1:C:193:SER:O	1:C:194:SER:CB	2.64	0.44
1:C:83:LYS:HD3	1:C:193:SER:O	2.17	0.44
1:C:272:ARG:HB3	1:C:442:CYS:N	2.32	0.44
1:D:161:ASP:O	1:D:165:PRO:HD3	2.18	0.44
1:E:16:LYS:HE2	1:E:74:TRP:HB2	1.99	0.44
1:A:316:ALA:O	1:A:318:MET:HB2	2.17	0.44
1:A:394:ARG:N	1:A:394:ARG:HD3	2.31	0.44
1:A:55:ILE:HG22	1:A:57:GLN:HE21	1.81	0.44
1:B:193:SER:O	1:B:194:SER:CB	2.64	0.44
1:B:266:PHE:CZ	1:B:272:ARG:HG2	2.52	0.44
1:C:221:ILE:CB	1:C:222:ILE:HG13	2.46	0.44
1:C:448:ARG:HG2	1:C:455:MET:SD	2.57	0.44
1:E:10:LEU:HB2	1:E:78:ARG:HD2	2.00	0.44
1:A:435:ILE:HA	1:A:438:LYS:HG3	1.99	0.44
1:B:162:VAL:C	1:B:165:PRO:HD2	2.37	0.44
1:B:190:PRO:O	1:B:191:LEU:HB2	2.17	0.44
1:B:57:GLN:CD	1:B:212:LEU:HD13	2.38	0.44
1:B:30:LEU:HD12	1:B:30:LEU:HA	1.84	0.44
1:B:403:GLU:HG2	1:B:405:LEU:H	1.82	0.44
1:C:161:ASP:O	1:C:164:ILE:HG22	2.18	0.44
1:D:226:LEU:HD13	1:D:263:PRO:HB3	1.98	0.44
1:D:346:TYR:CD1	1:D:349:CYS:CA	2.97	0.44
1:E:276:LEU:HD23	1:E:278:TYR:HB2	1.98	0.44
1:E:320:TYR:CD2	1:E:342:ASP:HB3	2.53	0.44
1:E:403:GLU:HG2	1:E:405:LEU:H	1.83	0.44
1:A:37:LYS:HG2	1:A:38:CYS:N	2.33	0.44
1:A:73:VAL:HG22	1:A:77:TRP:HE1	1.83	0.44
1:B:124:VAL:HA	1:B:125:ILE:HB	1.98	0.44
1:B:173:ALA:CB	1:C:345:THR:CA	2.95	0.44
1:A:181:VAL:HG21	1:B:379:TYR:CG	2.52	0.44
1:E:161:ASP:O	1:E:165:PRO:HD2	2.18	0.44
1:D:176:LYS:CB	1:E:347:HIS:C	2.86	0.44
1:D:176:LYS:HB2	1:E:347:HIS:N	2.28	0.44
1:A:173:ALA:HB1	1:B:345:THR:CA	2.36	0.44
1:A:346:TYR:CD2	1:A:349:CYS:HB2	2.53	0.44
1:C:190:PRO:O	1:C:191:LEU:HB2	2.17	0.44
1:C:370:LYS:HG2	1:C:378:LEU:HD11	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:409:ALA:HB1	1:E:466:GLN:OE1	2.17	0.44
1:E:73:VAL:HG13	1:E:77:TRP:HD1	1.83	0.44
1:A:456:ARG:HA	1:A:456:ARG:HD3	1.80	0.44
1:B:311:LEU:HD13	1:B:323:LEU:HD12	2.00	0.44
1:A:170:THR:CA	1:B:345:THR:HG21	2.33	0.44
1:D:173:ALA:C	1:E:345:THR:C	2.77	0.44
1:D:285:LEU:HG	1:D:285:LEU:H	1.49	0.44
1:D:379:TYR:O	1:D:385:ILE:CB	2.55	0.44
1:E:413:GLY:O	1:E:465:MET:CB	2.66	0.44
1:E:441:ASN:O	1:E:447:ILE:HG23	2.18	0.44
1:A:235:LEU:HD22	1:A:245:LEU:HD23	1.99	0.44
1:A:72:VAL:HG13	1:A:85:LEU:CD1	2.44	0.44
1:B:202:PRO:HD3	1:B:265:ARG:HA	2.00	0.44
1:C:125:ILE:HG22	1:C:125:ILE:O	2.17	0.44
1:D:190:PRO:O	1:D:191:LEU:HB2	2.18	0.44
1:E:370:LYS:CE	1:E:375:TYR:HE1	2.25	0.44
1:E:456:ARG:HA	1:E:456:ARG:HD3	1.79	0.44
1:A:370:LYS:HB3	1:A:375:TYR:CE1	2.51	0.43
1:A:275:GLU:OE1	1:A:437:LEU:HD13	2.18	0.43
1:B:173:ALA:C	1:C:345:THR:C	2.77	0.43
1:B:79:ASP:OD1	1:B:83:LYS:HD2	2.18	0.43
1:C:215:ASN:O	1:C:219:THR:HG22	2.18	0.43
1:C:294:SER:CB	1:C:341:ASP:HB2	2.48	0.43
1:C:394:ARG:O	1:C:394:ARG:HG2	2.16	0.43
1:C:413:GLY:O	1:C:465:MET:CB	2.66	0.43
1:D:176:LYS:CE	1:D:180:LEU:HD22	2.48	0.43
1:D:413:GLY:O	1:D:465:MET:CB	2.66	0.43
1:E:446:GLU:HB3	1:E:447:ILE:H	1.66	0.43
1:A:158:ILE:HG22	1:A:197:ILE:HB	1.99	0.43
1:A:371:ASP:O	1:A:375:TYR:HD1	2.01	0.43
1:A:441:ASN:O	1:A:447:ILE:HG23	2.17	0.43
1:B:235:LEU:CD2	1:B:245:LEU:CB	2.61	0.43
1:C:202:PRO:HD3	1:C:265:ARG:HA	1.99	0.43
1:D:191:LEU:N	1:D:192:PRO:CD	2.81	0.43
1:D:215:ASN:O	1:D:219:THR:HG22	2.19	0.43
1:D:407:LYS:O	1:D:411:GLN:HG2	2.18	0.43
1:A:284:THR:C	1:A:285:LEU:HD22	2.38	0.43
1:A:403:GLU:HG2	1:A:405:LEU:H	1.83	0.43
1:A:441:ASN:C	1:A:447:ILE:HG23	2.38	0.43
1:B:176:LYS:CB	1:C:347:HIS:C	2.86	0.43
1:E:177:LEU:HG	1:E:178:TRP:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:ASP:CB	1:E:82:LEU:O	2.65	0.43
1:A:125:ILE:HG22	1:A:125:ILE:O	2.19	0.43
1:A:88:SER:HB3	1:A:141:LYS:CG	2.49	0.43
1:B:119:GLY:HA2	1:B:127:PHE:HD2	1.83	0.43
1:B:156:ILE:HD11	1:B:197:ILE:HD13	1.99	0.43
1:B:46:LEU:HD22	1:B:197:ILE:CG1	2.48	0.43
1:C:329:ILE:HG23	1:C:330:ILE:HG12	2.00	0.43
1:C:379:TYR:O	1:C:385:ILE:CB	2.55	0.43
1:C:47:ALA:O	1:C:50:ASP:O	2.37	0.43
1:D:101:ILE:HG22	1:D:105:ILE:HD11	2.00	0.43
1:E:18:ASP:O	1:E:32:LEU:HD13	2.18	0.43
1:A:413:GLY:O	1:A:465:MET:CB	2.66	0.43
1:A:47:ALA:O	1:A:50:ASP:O	2.37	0.43
1:B:32:LEU:HD12	1:B:32:LEU:H	1.84	0.43
1:C:58:ALA:C	1:C:265:ARG:HD3	2.37	0.43
1:D:194:SER:H	1:D:195:ARG:HG3	1.83	0.43
1:E:125:ILE:HG22	1:E:125:ILE:O	2.18	0.43
1:A:345:THR:C	1:E:173:ALA:C	2.77	0.43
1:A:215:ASN:O	1:A:219:THR:HG22	2.18	0.43
1:B:33:PRO:O	1:B:33:PRO:CD	2.66	0.43
1:D:10:LEU:HG	1:D:78:ARG:HB3	2.01	0.43
1:D:76:LEU:HD12	1:D:134:PRO:HB2	2.00	0.43
1:D:176:LYS:HE3	1:D:180:LEU:HD13	1.99	0.43
1:D:410:LYS:O	1:D:414:VAL:HG23	2.18	0.43
1:D:76:LEU:HG	1:D:134:PRO:HB2	2.00	0.43
1:A:202:PRO:HD3	1:A:265:ARG:HA	2.01	0.43
1:B:417:VAL:HA	1:B:465:MET:SD	2.59	0.43
1:B:413:GLY:O	1:B:465:MET:CB	2.66	0.43
1:C:88:SER:HB3	1:C:141:LYS:HD2	2.01	0.43
1:C:162:VAL:HA	1:C:165:PRO:HG2	2.00	0.43
1:C:32:LEU:HD12	1:C:32:LEU:H	1.84	0.43
1:D:347:HIS:CE1	1:D:376:ALA:HB1	2.52	0.43
1:D:432:PHE:O	1:D:436:LEU:HD13	2.19	0.43
1:D:47:ALA:O	1:D:50:ASP:O	2.37	0.43
1:E:294:SER:CB	1:E:341:ASP:HB2	2.48	0.43
1:E:220:THR:HA	1:E:445:GLU:HB2	1.99	0.43
1:A:265:ARG:HH11	1:A:265:ARG:HG3	1.84	0.43
1:A:299:TYR:HD2	1:A:336:VAL:HG12	1.84	0.43
1:A:82:LEU:O	1:A:83:LYS:HB3	2.18	0.43
1:B:159:ALA:CB	1:B:162:VAL:CG1	2.97	0.43
1:B:428:PHE:CE1	1:B:461:LEU:HD22	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:GLN:HB3	1:B:265:ARG:CZ	2.49	0.43
1:C:220:THR:HA	1:C:445:GLU:HB2	1.98	0.43
1:D:273:GLU:OE2	1:D:441:ASN:HB3	2.19	0.43
1:E:432:PHE:O	1:E:436:LEU:HD13	2.19	0.43
1:A:161:ASP:HB3	1:A:164:ILE:HG22	2.00	0.43
1:A:173:ALA:C	1:B:345:THR:C	2.77	0.43
1:B:307:ILE:O	1:B:364:ASP:OD1	2.36	0.43
1:B:446:GLU:HB3	1:B:447:ILE:H	1.66	0.43
1:B:459:ASP:O	1:B:463:PRO:HD3	2.19	0.43
1:B:91:LYS:CB	1:B:93:ARG:N	2.74	0.43
1:C:326:ARG:HD2	1:C:335:ASN:HA	2.01	0.43
1:C:285:LEU:CD2	1:C:431:VAL:HG13	2.40	0.43
1:C:436:LEU:HG	1:C:454:GLU:O	2.19	0.43
1:C:456:ARG:HA	1:C:456:ARG:HD3	1.80	0.43
1:D:190:PRO:HB2	1:D:192:PRO:HG2	1.99	0.43
1:D:381:LEU:HD22	1:D:389:GLU:HB2	2.01	0.43
1:D:436:LEU:HG	1:D:454:GLU:O	2.19	0.43
1:E:199:LEU:HD12	1:E:200:GLY:N	2.34	0.43
1:E:346:TYR:HB2	1:E:348:ASP:OD1	2.19	0.43
1:E:77:TRP:HZ3	1:E:114:LEU:CB	2.32	0.43
1:A:144:GLY:HA2	1:A:146:THR:H	1.79	0.43
1:A:162:VAL:HG21	1:A:198:TYR:HD2	1.84	0.43
1:B:161:ASP:O	1:B:165:PRO:HD3	2.19	0.43
1:B:47:ALA:O	1:B:50:ASP:O	2.37	0.43
1:B:77:TRP:CZ3	1:B:114:LEU:CB	3.02	0.43
1:C:173:ALA:C	1:D:345:THR:C	2.77	0.43
1:C:338:LEU:HD22	1:C:430:LYS:CG	2.47	0.43
1:C:354:GLY:O	1:C:358:GLN:HG2	2.18	0.43
1:C:368:ARG:HD3	1:C:377:VAL:HG12	1.99	0.43
1:C:368:ARG:N	1:C:401:THR:CG2	2.79	0.43
1:D:346:TYR:CD1	1:D:349:CYS:HB2	2.54	0.43
1:D:381:LEU:HD23	1:D:381:LEU:HA	1.79	0.43
1:E:159:ALA:HB3	1:E:198:TYR:CD1	2.53	0.43
1:E:159:ALA:CB	1:E:162:VAL:CG1	2.97	0.43
1:E:274:ARG:CD	1:E:414:VAL:CG1	2.97	0.43
1:A:145:ILE:HB	1:A:174:ARG:HD2	2.00	0.42
1:B:199:LEU:HD23	1:B:200:GLY:N	2.34	0.42
1:B:305:ASP:O	1:B:362:VAL:HG11	2.19	0.42
1:B:274:ARG:HD2	1:B:418:VAL:HB	2.00	0.42
1:B:76:LEU:HA	1:B:79:ASP:OD2	2.19	0.42
1:C:36:THR:HB	1:C:39:GLN:HG3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:PRO:HB3	1:D:127:PHE:CZ	2.54	0.42
1:D:285:LEU:CD2	1:D:431:VAL:HG13	2.45	0.42
1:D:64:LYS:HA	1:D:67:ILE:HD12	2.00	0.42
1:E:133:ASN:N	1:E:134:PRO:CD	2.80	0.42
1:A:309:ALA:HB2	1:A:364:ASP:OD2	2.19	0.42
1:A:51:ASN:HB3	1:A:52:LYS:H	1.73	0.42
1:B:125:ILE:HG22	1:B:125:ILE:O	2.19	0.42
1:B:145:ILE:H	1:B:171:MET:HG3	1.84	0.42
1:C:77:TRP:CE2	1:C:105:ILE:HG12	2.46	0.42
1:C:73:VAL:HG13	1:C:77:TRP:HD1	1.84	0.42
1:D:155:ASP:C	1:D:194:SER:CB	2.87	0.42
1:C:176:LYS:CB	1:D:347:HIS:C	2.86	0.42
1:D:370:LYS:NZ	1:D:375:TYR:HE2	2.15	0.42
1:D:378:LEU:HD11	1:D:401:THR:HB	2.02	0.42
1:A:344:HIS:HA	1:A:346:TYR:CE1	2.55	0.42
1:A:413:GLY:O	1:A:465:MET:HB3	2.18	0.42
1:B:368:ARG:N	1:B:401:THR:CG2	2.76	0.42
1:C:20:VAL:HA	1:C:22:PHE:CZ	2.54	0.42
1:D:181:VAL:CG1	1:E:376:ALA:CA	2.95	0.42
1:E:291:PRO:CD	1:E:295:ASP:O	2.61	0.42
1:A:36:THR:HB	1:A:39:GLN:HG3	2.01	0.42
1:B:400:LYS:O	1:B:401:THR:CG2	2.60	0.42
1:C:83:LYS:CE	1:C:193:SER:N	2.82	0.42
1:C:173:ALA:HB2	1:D:346:TYR:HB3	1.99	0.42
1:E:155:ASP:C	1:E:194:SER:CB	2.88	0.42
1:E:15:LEU:HG	1:E:19:PHE:CD2	2.54	0.42
1:E:181:VAL:CA	1:E:182:GLN:CG	2.93	0.42
1:E:47:ALA:O	1:E:50:ASP:O	2.37	0.42
1:A:46:LEU:HD23	1:A:54:PHE:CD2	2.55	0.42
1:B:338:LEU:HD13	1:B:430:LYS:CG	2.50	0.42
1:B:444:MET:HA	1:B:445:GLU:HA	1.56	0.42
1:B:220:THR:O	1:B:445:GLU:HB2	2.20	0.42
1:C:413:GLY:O	1:C:465:MET:HB3	2.19	0.42
1:C:79:ASP:OD1	1:C:83:LYS:HD2	2.19	0.42
1:D:382:ASN:CB	1:D:385:ILE:CG1	2.90	0.42
1:D:57:GLN:O	1:D:223:TRP:HD1	2.02	0.42
1:E:436:LEU:HG	1:E:454:GLU:O	2.19	0.42
1:A:155:ASP:C	1:A:194:SER:CB	2.88	0.42
1:A:30:LEU:HA	1:A:30:LEU:HD12	1.87	0.42
1:A:220:THR:C	1:A:445:GLU:CB	2.88	0.42
1:B:76:LEU:HB2	1:B:136:HIS:NE2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:TYR:CD1	1:B:342:ASP:HB3	2.54	0.42
1:B:51:ASN:HB2	1:B:54:PHE:HZ	1.83	0.42
1:C:141:LYS:NZ	1:C:171:MET:HB2	2.34	0.42
1:C:433:SER:HA	1:C:457:ILE:HG21	2.02	0.42
1:C:432:PHE:O	1:C:436:LEU:HD13	2.19	0.42
1:D:313:LEU:HD22	1:D:377:VAL:HG21	2.01	0.42
1:A:329:ILE:HG23	1:A:330:ILE:HG12	2.01	0.42
1:B:10:LEU:HA	1:B:78:ARG:HG3	2.01	0.42
1:B:155:ASP:C	1:B:194:SER:CB	2.88	0.42
1:A:176:LYS:CB	1:B:347:HIS:C	2.86	0.42
1:C:30:LEU:HD12	1:C:30:LEU:HA	1.88	0.42
1:D:52:LYS:CB	1:D:184:PHE:CZ	2.73	0.42
1:E:225:ALA:O	1:E:228:PRO:CD	2.68	0.42
1:E:285:LEU:HG	1:E:285:LEU:H	1.47	0.42
1:E:379:TYR:CA	1:E:385:ILE:HG13	2.45	0.42
1:A:124:VAL:HA	1:A:125:ILE:HB	1.98	0.42
1:A:351:ASN:ND2	1:A:380:THR:HB	2.34	0.42
1:B:88:SER:HB3	1:B:141:LYS:HB2	2.01	0.42
1:B:252:ASN:C	1:B:254:GLU:N	2.73	0.42
1:C:155:ASP:C	1:C:194:SER:CB	2.88	0.42
1:C:441:ASN:O	1:C:447:ILE:HG23	2.19	0.42
1:D:144:GLY:HA2	1:D:146:THR:H	1.80	0.42
1:D:155:ASP:O	1:D:194:SER:CB	2.68	0.42
1:D:313:LEU:CD1	1:D:374:GLY:CA	2.79	0.42
1:D:294:SER:CB	1:D:341:ASP:HB2	2.49	0.42
1:D:346:TYR:CZ	1:D:349:CYS:CB	2.71	0.42
1:E:223:TRP:CZ2	1:E:225:ALA:HB2	2.55	0.42
1:E:235:LEU:CD2	1:E:245:LEU:CB	2.61	0.42
1:E:413:GLY:O	1:E:465:MET:HB3	2.20	0.42
1:A:21:ALA:HB3	1:A:33:PRO:HG3	2.01	0.42
1:A:357:GLN:HE22	1:A:361:LEU:HD11	1.85	0.42
1:B:191:LEU:N	1:B:192:PRO:CD	2.82	0.42
1:B:220:THR:C	1:B:445:GLU:CB	2.88	0.42
1:B:433:SER:HB2	1:B:457:ILE:HD13	2.02	0.42
1:C:252:ASN:C	1:C:254:GLU:N	2.73	0.42
1:C:80:PRO:HD2	1:C:83:LYS:HZ2	1.85	0.42
1:D:85:LEU:CD2	1:D:136:HIS:HD2	2.17	0.42
1:D:193:SER:HB2	1:D:195:ARG:CZ	2.50	0.42
1:E:155:ASP:O	1:E:194:SER:CB	2.68	0.42
1:E:299:TYR:HD2	1:E:336:VAL:HG12	1.85	0.42
1:A:333:LEU:O	1:A:426:GLY:HA2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:SER:HB3	1:A:83:LYS:HZ3	1.79	0.42
1:B:155:ASP:O	1:B:194:SER:CB	2.68	0.42
1:B:468:HIS:HA	1:B:473:ARG:HE	1.85	0.42
1:C:39:GLN:HG2	1:C:67:ILE:HD11	2.02	0.42
1:C:73:VAL:HG13	1:C:77:TRP:CD1	2.55	0.42
1:D:103:ASN:O	1:D:107:LEU:HG	2.20	0.42
1:D:173:ALA:CB	1:E:346:TYR:H	1.92	0.42
1:D:265:ARG:HH11	1:D:265:ARG:HG3	1.84	0.42
1:E:252:ASN:C	1:E:254:GLU:N	2.73	0.42
1:E:307:ILE:HG21	1:E:361:LEU:HD13	2.01	0.42
1:A:225:ALA:O	1:A:228:PRO:CD	2.68	0.41
1:A:354:GLY:O	1:A:358:GLN:HG2	2.20	0.41
1:A:364:ASP:HA	1:A:365:PRO:HD3	1.97	0.41
1:A:84:ILE:HB	1:A:135:ASP:OD2	2.20	0.41
1:B:174:ARG:HD2	1:B:174:ARG:HA	1.87	0.41
1:C:155:ASP:O	1:C:194:SER:CB	2.68	0.41
1:C:393:PHE:O	1:C:401:THR:HA	2.20	0.41
1:C:88:SER:CB	1:C:141:LYS:HD2	2.50	0.41
1:D:145:ILE:HG21	1:D:170:THR:HB	2.02	0.41
1:D:370:LYS:HG2	1:D:375:TYR:CD2	2.55	0.41
1:E:393:PHE:O	1:E:401:THR:HA	2.20	0.41
1:A:393:PHE:O	1:A:401:THR:HA	2.20	0.41
1:A:173:ALA:O	1:B:347:HIS:N	2.53	0.41
1:B:409:ALA:HB1	1:B:466:GLN:OE1	2.20	0.41
1:C:159:ALA:CB	1:C:162:VAL:CG1	2.98	0.41
1:C:225:ALA:O	1:C:228:PRO:CD	2.68	0.41
1:D:225:ALA:O	1:D:228:PRO:CD	2.68	0.41
1:D:370:LYS:HB3	1:D:375:TYR:CE1	2.53	0.41
1:E:16:LYS:HD2	1:E:16:LYS:O	2.20	0.41
1:E:441:ASN:C	1:E:447:ILE:HG23	2.40	0.41
1:E:63:GLY:O	1:E:66:PHE:HB2	2.21	0.41
1:A:145:ILE:HG21	1:A:170:THR:HB	2.02	0.41
1:A:10:LEU:HA	1:A:78:ARG:HG3	2.02	0.41
1:B:159:ALA:HB2	1:B:198:TYR:HE1	1.84	0.41
1:B:173:ALA:O	1:C:347:HIS:N	2.53	0.41
1:C:110:PHE:CG	1:C:111:LEU:N	2.89	0.41
1:C:60:ARG:HG2	1:C:201:THR:CG2	2.35	0.41
1:D:118:PRO:HG3	1:D:129:VAL:HB	2.02	0.41
1:D:125:ILE:O	1:D:125:ILE:HG22	2.19	0.41
1:D:56:LEU:HB2	1:D:199:LEU:HG	2.02	0.41
1:D:56:LEU:HD23	1:D:222:ILE:HG23	1.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:ASN:C	1:D:254:GLU:N	2.73	0.41
1:D:393:PHE:O	1:D:401:THR:HA	2.20	0.41
1:E:316:ALA:O	1:E:318:MET:HB2	2.20	0.41
1:D:173:ALA:O	1:E:347:HIS:N	2.53	0.41
1:A:193:SER:HB2	1:A:195:ARG:NH2	2.35	0.41
1:A:280:LYS:HA	1:A:283:PHE:CD2	2.55	0.41
1:A:432:PHE:O	1:A:436:LEU:HD13	2.20	0.41
1:A:436:LEU:HG	1:A:454:GLU:O	2.21	0.41
1:A:63:GLY:O	1:A:66:PHE:HB2	2.20	0.41
1:B:110:PHE:CG	1:B:111:LEU:N	2.88	0.41
1:B:433:SER:HB2	1:B:457:ILE:HD11	2.03	0.41
1:C:173:ALA:O	1:D:347:HIS:N	2.53	0.41
1:C:84:ILE:HB	1:C:135:ASP:OD2	2.21	0.41
1:D:118:PRO:HG3	1:D:129:VAL:CB	2.51	0.41
1:D:188:LEU:HD23	1:D:188:LEU:HA	1.91	0.41
1:D:333:LEU:O	1:D:426:GLY:HA2	2.21	0.41
1:D:364:ASP:C	1:D:364:ASP:OD1	2.59	0.41
1:E:272:ARG:HB3	1:E:441:ASN:HB2	2.02	0.41
1:A:173:ALA:CB	1:B:346:TYR:H	1.92	0.41
1:A:156:ILE:HD11	1:A:197:ILE:HD13	2.02	0.41
1:A:327:GLN:HG2	1:A:329:ILE:HG22	2.01	0.41
1:A:382:ASN:CG	1:A:385:ILE:HG12	2.40	0.41
1:B:161:ASP:O	1:B:164:ILE:HG22	2.20	0.41
1:B:225:ALA:O	1:B:228:PRO:CD	2.68	0.41
1:B:333:LEU:O	1:B:426:GLY:HA2	2.21	0.41
1:B:402:LEU:HD22	1:B:466:GLN:NE2	2.35	0.41
1:C:205:GLU:HG2	1:C:209:TYR:CD2	2.55	0.41
1:D:272:ARG:HB3	1:D:442:CYS:N	2.35	0.41
1:D:326:ARG:NH2	1:D:333:LEU:HD22	2.35	0.41
1:D:63:GLY:O	1:D:66:PHE:HB2	2.20	0.41
1:E:51:ASN:HB2	1:E:54:PHE:CE2	2.51	0.41
1:B:223:TRP:CE3	1:B:444:MET:CB	2.97	0.41
1:B:63:GLY:O	1:B:66:PHE:HB2	2.21	0.41
1:C:235:LEU:HA	1:C:235:LEU:HD23	1.49	0.41
1:D:149:LEU:HG	1:D:174:ARG:NH1	2.36	0.41
1:A:59:PHE:HB2	1:A:263:PRO:HA	2.03	0.41
1:B:276:LEU:HG	1:B:278:TYR:H	1.85	0.41
1:B:280:LYS:HZ1	1:B:437:LEU:C	2.24	0.41
1:C:357:GLN:NE2	1:C:361:LEU:HD11	2.36	0.41
1:C:333:LEU:O	1:C:426:GLY:HA2	2.20	0.41
1:C:441:ASN:C	1:C:447:ILE:HG23	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:LEU:HD22	1:D:197:ILE:CG1	2.50	0.41
1:D:88:SER:HB3	1:D:141:LYS:HB2	2.02	0.41
1:A:174:ARG:NE	1:A:174:ARG:HA	2.35	0.41
1:A:155:ASP:O	1:A:194:SER:CB	2.68	0.41
1:A:56:LEU:HD23	1:A:222:ILE:HG23	2.01	0.41
1:B:347:HIS:CE1	1:B:373:THR:HA	2.56	0.41
1:B:470:LEU:HG	1:B:472:ILE:H	1.86	0.41
1:C:167:ASN:O	1:C:171:MET:CE	2.68	0.41
1:C:218:TYR:O	1:C:408:LYS:HD3	2.21	0.41
1:D:276:LEU:HD23	1:D:278:TYR:HB2	2.02	0.41
1:D:72:VAL:HG13	1:D:85:LEU:CD1	2.48	0.41
1:E:351:ASN:ND2	1:E:380:THR:HB	2.36	0.41
1:A:252:ASN:C	1:A:254:GLU:N	2.73	0.41
1:A:320:TYR:CD1	1:A:342:ASP:HB3	2.56	0.41
1:A:347:HIS:N	1:E:173:ALA:O	2.53	0.41
1:A:409:ALA:HA	1:A:466:GLN:NE2	2.36	0.41
1:B:265:ARG:HG3	1:B:265:ARG:O	2.21	0.41
1:B:272:ARG:HD3	1:B:442:CYS:HB2	2.02	0.41
1:D:313:LEU:CD2	1:D:377:VAL:HG21	2.51	0.41
1:A:345:THR:CA	1:E:173:ALA:CB	2.95	0.41
1:E:220:THR:C	1:E:445:GLU:CB	2.87	0.41
1:E:271:LEU:HA	1:E:271:LEU:HD13	1.90	0.41
1:E:374:GLY:O	1:E:378:LEU:HG	2.21	0.41
1:E:86:ILE:O	1:E:157:ILE:HA	2.21	0.41
1:A:370:LYS:HG2	1:A:375:TYR:CE2	2.56	0.41
1:A:370:LYS:HE3	1:A:403:GLU:CA	2.50	0.41
1:C:124:VAL:HA	1:C:125:ILE:HB	2.00	0.41
1:C:351:ASN:CG	1:C:380:THR:HB	2.41	0.41
1:D:249:TYR:O	1:D:253:PRO:HD2	2.21	0.41
1:D:382:ASN:CG	1:D:385:ILE:HG12	2.41	0.41
1:E:52:LYS:CB	1:E:184:PHE:CZ	2.74	0.41
1:E:333:LEU:O	1:E:426:GLY:HA2	2.21	0.41
1:E:370:LYS:O	1:E:375:TYR:CE2	2.73	0.41
1:E:59:PHE:HB2	1:E:263:PRO:HA	2.03	0.41
1:A:459:ASP:O	1:A:463:PRO:HD3	2.20	0.41
1:B:182:GLN:HG3	1:B:185:ALA:H	1.86	0.41
1:B:83:LYS:CE	1:B:192:PRO:HA	2.50	0.41
1:C:133:ASN:N	1:C:134:PRO:CD	2.77	0.41
1:C:314:GLU:OE1	1:C:321:GLN:HB2	2.21	0.41
1:C:409:ALA:HA	1:C:466:GLN:OE1	2.21	0.41
1:D:182:GLN:HG3	1:D:185:ALA:H	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:VAL:CG1	1:E:108:LEU:HD23	2.51	0.41
1:E:55:ILE:HD13	1:E:215:ASN:CG	2.41	0.41
1:E:433:SER:HA	1:E:457:ILE:HD13	2.03	0.41
1:A:173:ALA:CB	1:B:345:THR:CA	2.95	0.40
1:A:55:ILE:HD12	1:A:198:TYR:HB2	2.03	0.40
1:A:88:SER:HB3	1:A:141:LYS:HB2	2.02	0.40
1:B:116:PRO:HB3	1:B:127:PHE:CZ	2.56	0.40
1:B:382:ASN:CG	1:B:385:ILE:HG12	2.41	0.40
1:B:379:TYR:CB	1:B:385:ILE:HG21	2.49	0.40
1:B:433:SER:HA	1:B:457:ILE:HG21	2.03	0.40
1:C:99:ILE:O	1:C:102:LYS:HB2	2.21	0.40
1:C:220:THR:C	1:C:445:GLU:CB	2.87	0.40
1:C:407:LYS:O	1:C:411:GLN:HG2	2.20	0.40
1:D:124:VAL:HA	1:D:125:ILE:HB	1.97	0.40
1:E:235:LEU:HD23	1:E:235:LEU:HA	1.49	0.40
1:E:30:LEU:HA	1:E:30:LEU:HD12	1.87	0.40
1:E:330:ILE:HG13	1:E:332:ASP:O	2.21	0.40
1:A:22:PHE:HA	1:A:33:PRO:HD3	2.03	0.40
1:C:416:THR:HB	1:C:465:MET:HB3	2.03	0.40
1:D:86:ILE:O	1:D:157:ILE:HA	2.21	0.40
1:D:280:LYS:HA	1:D:283:PHE:CD2	2.56	0.40
1:D:328:ASN:CG	1:D:328:ASN:O	2.59	0.40
1:D:329:ILE:CG2	1:D:330:ILE:N	2.56	0.40
1:D:91:LYS:HB2	1:D:93:ARG:HB3	2.01	0.40
1:E:182:GLN:HG3	1:E:185:ALA:H	1.85	0.40
1:E:382:ASN:CB	1:E:385:ILE:CG1	2.88	0.40
1:A:174:ARG:HE	1:A:174:ARG:HA	1.86	0.40
1:A:382:ASN:ND2	1:A:400:LYS:HD3	2.37	0.40
1:A:433:SER:HA	1:A:457:ILE:HG21	2.02	0.40
1:C:461:LEU:O	1:C:465:MET:HG2	2.22	0.40
1:C:59:PHE:HB2	1:C:263:PRO:HA	2.03	0.40
1:C:63:GLY:O	1:C:66:PHE:HB2	2.21	0.40
1:D:275:GLU:OE1	1:D:437:LEU:HD13	2.21	0.40
1:E:21:ALA:C	1:E:33:PRO:HG3	2.42	0.40
1:E:415:GLN:C	1:E:418:VAL:HG12	2.41	0.40
1:E:99:ILE:O	1:E:102:LYS:HB2	2.21	0.40
1:A:145:ILE:H	1:A:145:ILE:HG23	1.67	0.40
1:A:180:LEU:HA	1:A:180:LEU:HD13	1.76	0.40
1:A:163:GLU:CG	1:A:203:GLN:N	2.78	0.40
1:A:56:LEU:HD21	1:A:222:ILE:HG21	2.04	0.40
1:A:79:ASP:OD2	1:A:83:LYS:HE2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LYS:HD3	1:A:92:GLU:HB2	2.04	0.40
1:B:133:ASN:N	1:B:134:PRO:CD	2.81	0.40
1:B:20:VAL:CG1	1:B:109:PRO:HD2	2.51	0.40
1:B:54:PHE:HD1	1:B:221:ILE:HD12	1.86	0.40
1:B:272:ARG:HB3	1:B:442:CYS:H	1.86	0.40
1:B:351:ASN:CG	1:B:380:THR:HB	2.42	0.40
1:B:457:ILE:O	1:B:460:THR:HG22	2.22	0.40
1:B:54:PHE:CD1	1:B:221:ILE:HD12	2.57	0.40
1:C:320:TYR:CD1	1:C:342:ASP:HB3	2.56	0.40
1:C:417:VAL:HG23	1:C:465:MET:CE	2.51	0.40
1:D:173:ALA:CB	1:E:345:THR:CA	2.95	0.40
1:D:415:GLN:C	1:D:418:VAL:HG12	2.41	0.40
1:D:99:ILE:O	1:D:102:LYS:HB2	2.21	0.40
1:E:124:VAL:HA	1:E:125:ILE:HB	1.98	0.40
1:E:187:LEU:O	1:E:192:PRO:HD2	2.21	0.40
1:E:252:ASN:C	1:E:254:GLU:H	2.25	0.40
1:E:21:ALA:HB3	1:E:33:PRO:HG3	2.03	0.40
1:E:73:VAL:CG2	1:E:105:ILE:CG1	2.69	0.40
1:A:99:ILE:O	1:A:102:LYS:HB2	2.21	0.40
1:A:84:ILE:HG13	1:A:135:ASP:OD1	2.21	0.40
1:A:379:TYR:CA	1:A:385:ILE:HG13	2.43	0.40
1:A:370:LYS:NZ	1:A:399:ASP:HB3	2.34	0.40
1:B:311:LEU:HB2	1:B:323:LEU:HD12	2.03	0.40
1:B:338:LEU:HD13	1:B:430:LYS:HB2	2.03	0.40
1:E:163:GLU:HG2	1:E:203:GLN:H	1.82	0.40
1:E:191:LEU:N	1:E:192:PRO:CD	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	468/476 (98%)	394 (84%)	46 (10%)	28 (6%)	2	23
1	B	468/476 (98%)	394 (84%)	46 (10%)	28 (6%)	2	23
1	C	468/476 (98%)	394 (84%)	46 (10%)	28 (6%)	2	23
1	D	468/476 (98%)	394 (84%)	46 (10%)	28 (6%)	2	23
1	E	468/476 (98%)	394 (84%)	46 (10%)	28 (6%)	2	23
All	All	2340/2380 (98%)	1970 (84%)	230 (10%)	140 (6%)	3	23

All (140) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	LYS
1	A	92	GLU
1	A	125	ILE
1	A	132	ALA
1	A	182	GLN
1	A	191	LEU
1	A	194	SER
1	A	195	ARG
1	A	252	ASN
1	A	253	PRO
1	A	376	ALA
1	A	401	THR
1	A	407	LYS
1	A	475	GLU
1	B	83	LYS
1	B	92	GLU
1	B	125	ILE
1	B	132	ALA
1	B	182	GLN
1	B	191	LEU
1	B	194	SER
1	B	195	ARG
1	B	252	ASN
1	B	253	PRO
1	B	376	ALA
1	B	401	THR
1	B	407	LYS
1	B	475	GLU
1	C	83	LYS
1	C	92	GLU
1	C	125	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	132	ALA
1	C	182	GLN
1	C	191	LEU
1	C	194	SER
1	C	195	ARG
1	C	252	ASN
1	C	253	PRO
1	C	376	ALA
1	C	401	THR
1	C	407	LYS
1	C	475	GLU
1	D	83	LYS
1	D	92	GLU
1	D	125	ILE
1	D	132	ALA
1	D	182	GLN
1	D	191	LEU
1	D	194	SER
1	D	195	ARG
1	D	252	ASN
1	D	253	PRO
1	D	376	ALA
1	D	401	THR
1	D	407	LYS
1	D	475	GLU
1	E	83	LYS
1	E	92	GLU
1	E	125	ILE
1	E	132	ALA
1	E	182	GLN
1	E	191	LEU
1	E	194	SER
1	E	195	ARG
1	E	252	ASN
1	E	253	PRO
1	E	376	ALA
1	E	401	THR
1	E	407	LYS
1	E	475	GLU
1	A	52	LYS
1	A	474	ASP
1	B	52	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	474	ASP
1	C	52	LYS
1	C	474	ASP
1	D	52	LYS
1	D	474	ASP
1	E	52	LYS
1	E	474	ASP
1	A	192	PRO
1	B	192	PRO
1	C	192	PRO
1	D	192	PRO
1	E	192	PRO
1	A	133	ASN
1	A	206	MET
1	A	224	PRO
1	A	254	GLU
1	B	133	ASN
1	B	206	MET
1	B	224	PRO
1	B	254	GLU
1	C	133	ASN
1	C	206	MET
1	C	224	PRO
1	C	254	GLU
1	D	133	ASN
1	D	206	MET
1	D	224	PRO
1	D	254	GLU
1	E	133	ASN
1	E	206	MET
1	E	224	PRO
1	E	254	GLU
1	A	164	ILE
1	A	385	ILE
1	A	406	ALA
1	B	164	ILE
1	B	385	ILE
1	B	406	ALA
1	C	164	ILE
1	C	385	ILE
1	C	406	ALA
1	D	164	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	385	ILE
1	D	406	ALA
1	E	164	ILE
1	E	385	ILE
1	E	406	ALA
1	A	334	PRO
1	B	334	PRO
1	C	334	PRO
1	D	334	PRO
1	E	334	PRO
1	A	118	PRO
1	A	329	ILE
1	B	118	PRO
1	B	329	ILE
1	C	118	PRO
1	C	329	ILE
1	D	118	PRO
1	D	329	ILE
1	E	118	PRO
1	E	329	ILE
1	A	263	PRO
1	B	263	PRO
1	C	263	PRO
1	D	263	PRO
1	E	263	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	409/411 (100%)	372 (91%)	37 (9%)	11	38
1	B	409/411 (100%)	347 (85%)	62 (15%)	3	19
1	C	409/411 (100%)	370 (90%)	39 (10%)	10	36
1	D	409/411 (100%)	363 (89%)	46 (11%)	7	29
1	E	409/411 (100%)	365 (89%)	44 (11%)	7	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2045/2055 (100%)	1817 (89%)	228 (11%)	11	29

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	24	PHE
1	A	37	LYS
1	A	44	LYS
1	A	45	VAL
1	A	51	ASN
1	A	65	SER
1	A	90	SER
1	A	93	ARG
1	A	106	ASP
1	A	111	LEU
1	A	152	SER
1	A	161	ASP
1	A	174	ARG
1	A	190	PRO
1	A	192	PRO
1	A	208	LEU
1	A	220	THR
1	A	228	PRO
1	A	238	SER
1	A	250	ASP
1	A	260	PRO
1	A	271	LEU
1	A	346	TYR
1	A	348	ASP
1	A	357	GLN
1	A	368	ARG
1	A	393	PHE
1	A	394	ARG
1	A	395	ASP
1	A	401	THR
1	A	411	GLN
1	A	420	GLU
1	A	425	ASP
1	A	431	VAL
1	A	463	PRO
1	A	474	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	16	LYS
1	B	24	PHE
1	B	33	PRO
1	B	45	VAL
1	B	51	ASN
1	B	65	SER
1	B	66	PHE
1	B	67	ILE
1	B	80	PRO
1	B	90	SER
1	B	106	ASP
1	B	126	SER
1	B	149	LEU
1	B	153	ARG
1	B	161	ASP
1	B	165	PRO
1	B	174	ARG
1	B	176	LYS
1	B	177	LEU
1	B	190	PRO
1	B	192	PRO
1	B	204	THR
1	B	205	GLU
1	B	206	MET
1	B	208	LEU
1	B	213	GLU
1	B	214	ASP
1	B	219	THR
1	B	222	ILE
1	B	228	PRO
1	B	238	SER
1	B	240	ARG
1	B	241	LEU
1	B	250	ASP
1	B	260	PRO
1	B	268	ARG
1	B	271	LEU
1	B	272	ARG
1	B	283	PHE
1	B	285	LEU
1	B	323	LEU
1	B	324	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	338	LEU
1	B	339	LYS
1	B	348	ASP
1	B	362	VAL
1	B	370	LYS
1	B	379	TYR
1	B	393	PHE
1	B	394	ARG
1	B	395	ASP
1	B	398	SER
1	B	400	LYS
1	B	408	LYS
1	B	411	GLN
1	B	412	TRP
1	B	415	GLN
1	B	418	VAL
1	B	431	VAL
1	B	452	MET
1	B	463	PRO
1	B	474	ASP
1	C	24	PHE
1	C	33	PRO
1	C	45	VAL
1	C	65	SER
1	C	67	ILE
1	C	80	PRO
1	C	106	ASP
1	C	111	LEU
1	C	115	LYS
1	C	123	SER
1	C	149	LEU
1	C	162	VAL
1	C	177	LEU
1	C	180	LEU
1	C	190	PRO
1	C	192	PRO
1	C	204	THR
1	C	205	GLU
1	C	208	LEU
1	C	220	THR
1	C	228	PRO
1	C	238	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	260	PRO
1	C	268	ARG
1	C	271	LEU
1	C	277	GLU
1	C	285	LEU
1	C	335	ASN
1	C	352	ASN
1	C	393	PHE
1	C	394	ARG
1	C	395	ASP
1	C	398	SER
1	C	412	TRP
1	C	425	ASP
1	C	431	VAL
1	C	458	CYS
1	C	463	PRO
1	C	474	ASP
1	D	8	ASN
1	D	16	LYS
1	D	24	PHE
1	D	28	LYS
1	D	33	PRO
1	D	42	MET
1	D	44	LYS
1	D	45	VAL
1	D	51	ASN
1	D	52	LYS
1	D	56	LEU
1	D	65	SER
1	D	84	ILE
1	D	106	ASP
1	D	109	PRO
1	D	149	LEU
1	D	153	ARG
1	D	161	ASP
1	D	165	PRO
1	D	180	LEU
1	D	183	GLU
1	D	190	PRO
1	D	192	PRO
1	D	208	LEU
1	D	210	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	214	ASP
1	D	220	THR
1	D	228	PRO
1	D	238	SER
1	D	254	GLU
1	D	260	PRO
1	D	262	ASP
1	D	269	ASP
1	D	277	GLU
1	D	285	LEU
1	D	352	ASN
1	D	355	GLN
1	D	357	GLN
1	D	381	LEU
1	D	393	PHE
1	D	394	ARG
1	D	412	TRP
1	D	425	ASP
1	D	431	VAL
1	D	463	PRO
1	D	474	ASP
1	E	11	VAL
1	E	16	LYS
1	E	24	PHE
1	E	28	LYS
1	E	45	VAL
1	E	65	SER
1	E	66	PHE
1	E	67	ILE
1	E	84	ILE
1	E	90	SER
1	E	115	LYS
1	E	126	SER
1	E	148	GLN
1	E	149	LEU
1	E	161	ASP
1	E	162	VAL
1	E	165	PRO
1	E	177	LEU
1	E	179	THR
1	E	183	GLU
1	E	190	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	192	PRO
1	E	204	THR
1	E	205	GLU
1	E	219	THR
1	E	222	ILE
1	E	228	PRO
1	E	238	SER
1	E	260	PRO
1	E	262	ASP
1	E	265	ARG
1	E	285	LEU
1	E	339	LYS
1	E	343	LEU
1	E	346	TYR
1	E	348	ASP
1	E	393	PHE
1	E	395	ASP
1	E	408	LYS
1	E	411	GLN
1	E	431	VAL
1	E	445	GLU
1	E	462	GLU
1	E	463	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	ASN
1	A	351	ASN
1	A	357	GLN
1	A	358	GLN
1	B	136	HIS
1	B	182	GLN
1	B	325	ASN
1	B	347	HIS
1	B	351	ASN
1	B	358	GLN
1	C	57	GLN
1	C	325	ASN
1	C	335	ASN
1	C	351	ASN
1	C	352	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	357	GLN
1	C	358	GLN
1	C	411	GLN
1	C	415	GLN
1	D	136	HIS
1	D	182	GLN
1	D	325	ASN
1	D	347	HIS
1	D	351	ASN
1	D	352	ASN
1	D	358	GLN
1	D	411	GLN
1	E	148	GLN
1	E	182	GLN
1	E	325	ASN
1	E	351	ASN
1	E	357	GLN
1	E	358	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.