



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 19, 2018 – 05:18 pm GMT

PDB ID : 3J2T
EMDB ID: : EMD-5186
Title : An improved model of the human apoptosome
Authors : Yuan, S.; Topf, M.; Akey, C.W.
Deposited on : 2012-12-23
Resolution : 9.50 Å(reported)
Based on PDB ID : 2B4Z, 3SFZ, 1Z6T

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

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

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

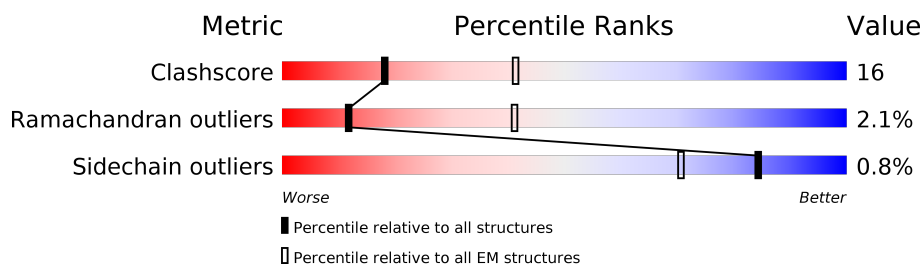
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.50 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	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

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	1263	81% 9% • 9%
1	B	1263	80% 9% • 9%
1	C	1263	81% 9% • 9%
1	D	1263	80% 9% • 9%
1	E	1263	80% 9% • 9%
1	F	1263	81% 8% • 9%
1	G	1263	81% 8% • 9%
2	H	104	81% 17% ••
2	I	104	81% 17% ••

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	104	<div><div></div><div>81%</div><div>17%</div><div>..</div></div>
2	K	104	<div><div></div><div>81%</div><div>17%</div><div>..</div></div>
2	L	104	<div><div></div><div>81%</div><div>17%</div><div>..</div></div>
2	M	104	<div><div></div><div>81%</div><div>17%</div><div>..</div></div>
2	N	104	<div><div></div><div>81%</div><div>17%</div><div>..</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 70189 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 Apoptotic protease-activating factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	B	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	C	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	D	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	E	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	F	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		
1	G	1144	Total	C	N	O	S	0	0
			9139	5789	1569	1720	61		

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP O14727
A	-4	HIS	-	EXPRESSION TAG	UNP O14727
A	-3	HIS	-	EXPRESSION TAG	UNP O14727
A	-2	HIS	-	EXPRESSION TAG	UNP O14727
A	-1	HIS	-	EXPRESSION TAG	UNP O14727
A	0	HIS	-	EXPRESSION TAG	UNP O14727
A	1249	HIS	-	EXPRESSION TAG	UNP O14727
A	1250	HIS	-	EXPRESSION TAG	UNP O14727
A	1251	HIS	-	EXPRESSION TAG	UNP O14727
A	1252	HIS	-	EXPRESSION TAG	UNP O14727
A	1253	HIS	-	EXPRESSION TAG	UNP O14727
A	1254	HIS	-	EXPRESSION TAG	UNP O14727
A	1255	HIS	-	EXPRESSION TAG	UNP O14727
A	1256	HIS	-	EXPRESSION TAG	UNP O14727
A	1257	HIS	-	EXPRESSION TAG	UNP O14727
B	-5	HIS	-	EXPRESSION TAG	UNP O14727

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	EXPRESSION TAG	UNP O14727
B	-3	HIS	-	EXPRESSION TAG	UNP O14727
B	-2	HIS	-	EXPRESSION TAG	UNP O14727
B	-1	HIS	-	EXPRESSION TAG	UNP O14727
B	0	HIS	-	EXPRESSION TAG	UNP O14727
B	1249	HIS	-	EXPRESSION TAG	UNP O14727
B	1250	HIS	-	EXPRESSION TAG	UNP O14727
B	1251	HIS	-	EXPRESSION TAG	UNP O14727
B	1252	HIS	-	EXPRESSION TAG	UNP O14727
B	1253	HIS	-	EXPRESSION TAG	UNP O14727
B	1254	HIS	-	EXPRESSION TAG	UNP O14727
B	1255	HIS	-	EXPRESSION TAG	UNP O14727
B	1256	HIS	-	EXPRESSION TAG	UNP O14727
B	1257	HIS	-	EXPRESSION TAG	UNP O14727
C	-5	HIS	-	EXPRESSION TAG	UNP O14727
C	-4	HIS	-	EXPRESSION TAG	UNP O14727
C	-3	HIS	-	EXPRESSION TAG	UNP O14727
C	-2	HIS	-	EXPRESSION TAG	UNP O14727
C	-1	HIS	-	EXPRESSION TAG	UNP O14727
C	0	HIS	-	EXPRESSION TAG	UNP O14727
C	1249	HIS	-	EXPRESSION TAG	UNP O14727
C	1250	HIS	-	EXPRESSION TAG	UNP O14727
C	1251	HIS	-	EXPRESSION TAG	UNP O14727
C	1252	HIS	-	EXPRESSION TAG	UNP O14727
C	1253	HIS	-	EXPRESSION TAG	UNP O14727
C	1254	HIS	-	EXPRESSION TAG	UNP O14727
C	1255	HIS	-	EXPRESSION TAG	UNP O14727
C	1256	HIS	-	EXPRESSION TAG	UNP O14727
C	1257	HIS	-	EXPRESSION TAG	UNP O14727
D	-5	HIS	-	EXPRESSION TAG	UNP O14727
D	-4	HIS	-	EXPRESSION TAG	UNP O14727
D	-3	HIS	-	EXPRESSION TAG	UNP O14727
D	-2	HIS	-	EXPRESSION TAG	UNP O14727
D	-1	HIS	-	EXPRESSION TAG	UNP O14727
D	0	HIS	-	EXPRESSION TAG	UNP O14727
D	1249	HIS	-	EXPRESSION TAG	UNP O14727
D	1250	HIS	-	EXPRESSION TAG	UNP O14727
D	1251	HIS	-	EXPRESSION TAG	UNP O14727
D	1252	HIS	-	EXPRESSION TAG	UNP O14727
D	1253	HIS	-	EXPRESSION TAG	UNP O14727
D	1254	HIS	-	EXPRESSION TAG	UNP O14727
D	1255	HIS	-	EXPRESSION TAG	UNP O14727

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1256	HIS	-	EXPRESSION TAG	UNP O14727
D	1257	HIS	-	EXPRESSION TAG	UNP O14727
E	-5	HIS	-	EXPRESSION TAG	UNP O14727
E	-4	HIS	-	EXPRESSION TAG	UNP O14727
E	-3	HIS	-	EXPRESSION TAG	UNP O14727
E	-2	HIS	-	EXPRESSION TAG	UNP O14727
E	-1	HIS	-	EXPRESSION TAG	UNP O14727
E	0	HIS	-	EXPRESSION TAG	UNP O14727
E	1249	HIS	-	EXPRESSION TAG	UNP O14727
E	1250	HIS	-	EXPRESSION TAG	UNP O14727
E	1251	HIS	-	EXPRESSION TAG	UNP O14727
E	1252	HIS	-	EXPRESSION TAG	UNP O14727
E	1253	HIS	-	EXPRESSION TAG	UNP O14727
E	1254	HIS	-	EXPRESSION TAG	UNP O14727
E	1255	HIS	-	EXPRESSION TAG	UNP O14727
E	1256	HIS	-	EXPRESSION TAG	UNP O14727
E	1257	HIS	-	EXPRESSION TAG	UNP O14727
F	-5	HIS	-	EXPRESSION TAG	UNP O14727
F	-4	HIS	-	EXPRESSION TAG	UNP O14727
F	-3	HIS	-	EXPRESSION TAG	UNP O14727
F	-2	HIS	-	EXPRESSION TAG	UNP O14727
F	-1	HIS	-	EXPRESSION TAG	UNP O14727
F	0	HIS	-	EXPRESSION TAG	UNP O14727
F	1249	HIS	-	EXPRESSION TAG	UNP O14727
F	1250	HIS	-	EXPRESSION TAG	UNP O14727
F	1251	HIS	-	EXPRESSION TAG	UNP O14727
F	1252	HIS	-	EXPRESSION TAG	UNP O14727
F	1253	HIS	-	EXPRESSION TAG	UNP O14727
F	1254	HIS	-	EXPRESSION TAG	UNP O14727
F	1255	HIS	-	EXPRESSION TAG	UNP O14727
F	1256	HIS	-	EXPRESSION TAG	UNP O14727
F	1257	HIS	-	EXPRESSION TAG	UNP O14727
G	-5	HIS	-	EXPRESSION TAG	UNP O14727
G	-4	HIS	-	EXPRESSION TAG	UNP O14727
G	-3	HIS	-	EXPRESSION TAG	UNP O14727
G	-2	HIS	-	EXPRESSION TAG	UNP O14727
G	-1	HIS	-	EXPRESSION TAG	UNP O14727
G	0	HIS	-	EXPRESSION TAG	UNP O14727
G	1249	HIS	-	EXPRESSION TAG	UNP O14727
G	1250	HIS	-	EXPRESSION TAG	UNP O14727
G	1251	HIS	-	EXPRESSION TAG	UNP O14727
G	1252	HIS	-	EXPRESSION TAG	UNP O14727

Continued on next page...

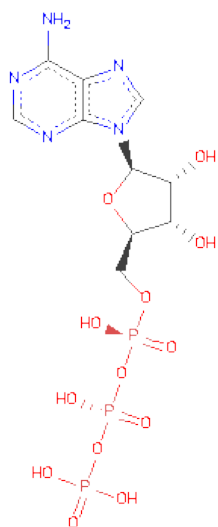
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	1253	HIS	-	EXPRESSION TAG	UNP O14727
G	1254	HIS	-	EXPRESSION TAG	UNP O14727
G	1255	HIS	-	EXPRESSION TAG	UNP O14727
G	1256	HIS	-	EXPRESSION TAG	UNP O14727
G	1257	HIS	-	EXPRESSION TAG	UNP O14727

- Molecule 2 is a protein called Cytochrome c.

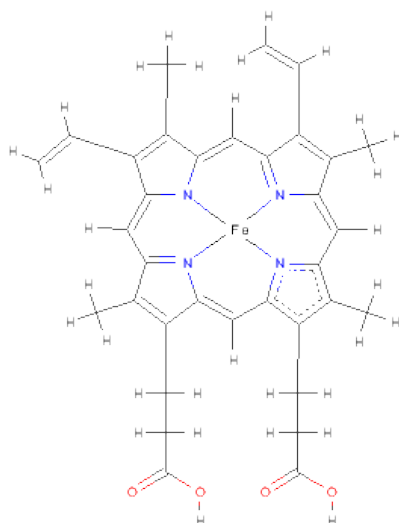
Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	I	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	J	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	K	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	L	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	M	104	Total	C	N	O	S	0	0
			814	517	143	150	4		
2	N	104	Total	C	N	O	S	0	0
			814	517	143	150	4		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
4	H	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
4	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
4	J	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
4	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

Continued on next page...

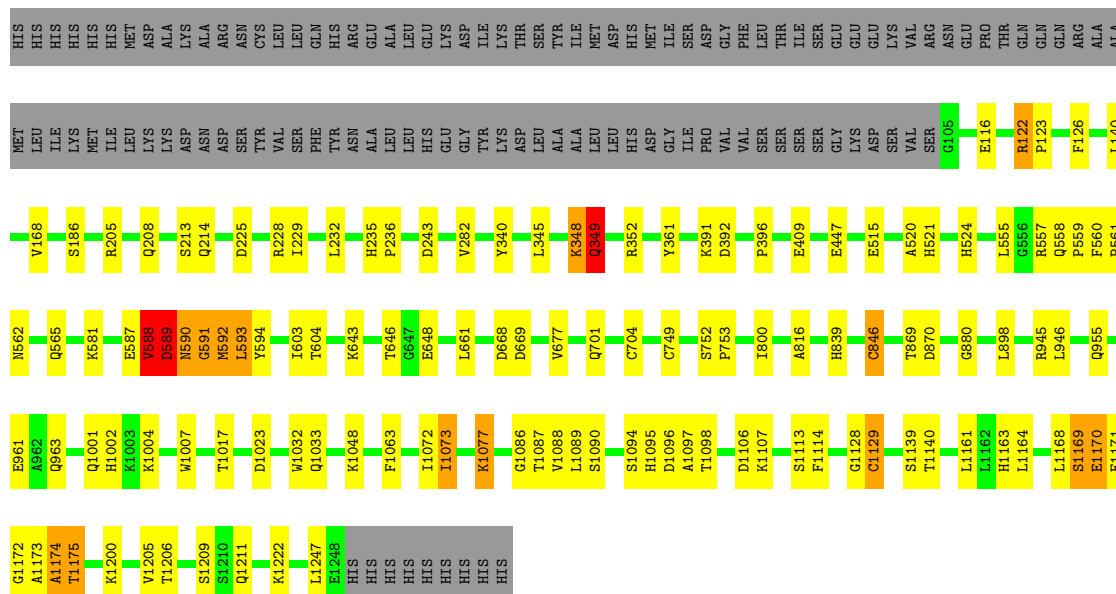
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
4	L	1	Total 43	C 34	Fe 1	N 4	O 4	0
4	M	1	Total 43	C 34	Fe 1	N 4	O 4	0
4	N	1	Total 43	C 34	Fe 1	N 4	O 4	0



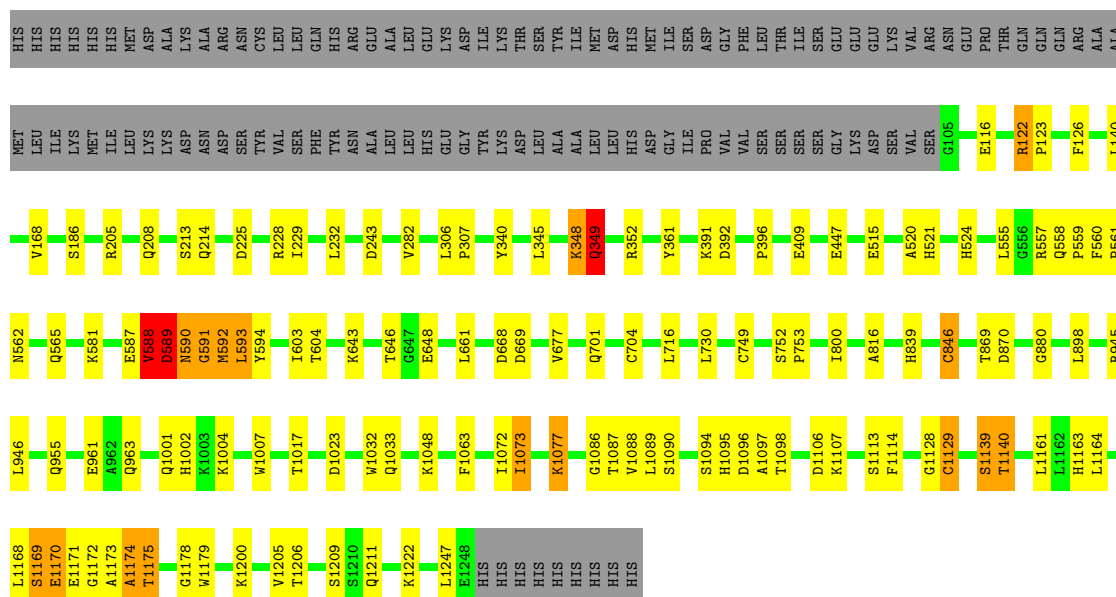
- Molecule 1: Apoptotic protease-activating factor 1

Chain C: 81% 9% 9%



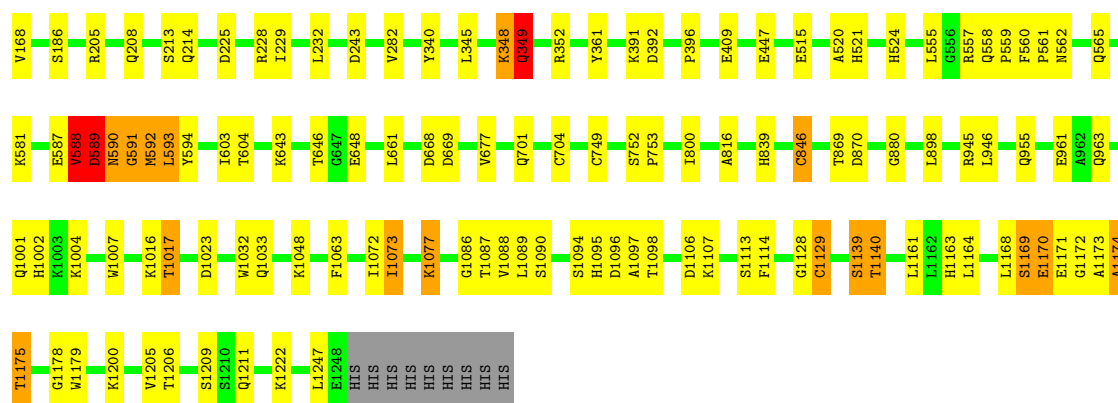
- Molecule 1: Apoptotic protease-activating factor 1

Chain D: 80% 9% 9%



- Molecule 1: Apoptotic protease-activating factor 1

Chain E: 80% 9% 9%



• Molecule 2: Cytochrome c

Chain H: 81% 17% ..



• Molecule 2: Cytochrome c

Chain I: 81% 17% ..



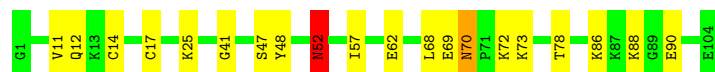
• Molecule 2: Cytochrome c

Chain J: 81% 17% ..



• Molecule 2: Cytochrome c

Chain K: 81% 17% ..



• Molecule 2: Cytochrome c

Chain L: 81% 17% ..

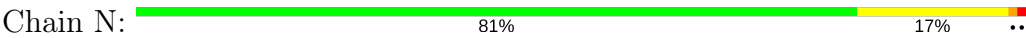


• Molecule 2: Cytochrome c

Chain M: 81% 17% ..



● Molecule 2: Cytochrome c



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	34000	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTF correction was done on each particle image based on summed power spectra from each micrograph.	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	62000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	A	0.85	1/9337 (0.0%)	0.82	8/12636 (0.1%)
1	B	0.85	1/9337 (0.0%)	0.82	8/12636 (0.1%)
1	C	0.85	1/9337 (0.0%)	0.82	8/12636 (0.1%)
1	D	0.85	1/9337 (0.0%)	0.82	8/12636 (0.1%)
1	E	0.85	1/9337 (0.0%)	0.82	8/12636 (0.1%)
1	F	0.85	1/9337 (0.0%)	0.82	8/12636 (0.1%)
1	G	0.85	1/9337 (0.0%)	0.82	8/12636 (0.1%)
2	H	0.86	4/830 (0.5%)	0.96	3/1105 (0.3%)
2	I	0.86	4/830 (0.5%)	0.96	3/1105 (0.3%)
2	J	0.86	4/830 (0.5%)	0.96	3/1105 (0.3%)
2	K	0.86	4/830 (0.5%)	0.96	3/1105 (0.3%)
2	L	0.86	4/830 (0.5%)	0.96	3/1105 (0.3%)
2	M	0.86	4/830 (0.5%)	0.96	3/1105 (0.3%)
2	N	0.86	4/830 (0.5%)	0.96	3/1105 (0.3%)
All	All	0.85	35/71169 (0.0%)	0.83	77/96187 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
2	H	0	1
2	I	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	J	0	1
2	K	0	1
2	L	0	1
2	M	0	1
2	N	0	1
All	All	0	21

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	52	ASN	CG-OD1	15.38	1.57	1.24
2	M	52	ASN	CG-OD1	15.37	1.57	1.24
2	L	52	ASN	CG-OD1	15.37	1.57	1.24
2	H	52	ASN	CG-OD1	15.36	1.57	1.24
2	J	52	ASN	CG-OD1	15.35	1.57	1.24
2	K	52	ASN	CG-OD1	15.35	1.57	1.24
2	I	52	ASN	CG-OD1	15.34	1.57	1.24
2	K	62	GLU	CG-CD	13.59	1.72	1.51
2	M	62	GLU	CG-CD	13.58	1.72	1.51
2	H	62	GLU	CG-CD	13.58	1.72	1.51
2	L	62	GLU	CG-CD	13.58	1.72	1.51
2	I	62	GLU	CG-CD	13.57	1.72	1.51
2	N	62	GLU	CG-CD	13.57	1.72	1.51
2	J	62	GLU	CG-CD	13.57	1.72	1.51
2	J	12	GLN	CB-CG	-6.21	1.35	1.52
2	K	12	GLN	CB-CG	-6.21	1.35	1.52
2	L	12	GLN	CB-CG	-6.21	1.35	1.52
2	H	12	GLN	CB-CG	-6.21	1.35	1.52
2	I	12	GLN	CB-CG	-6.21	1.35	1.52
2	M	12	GLN	CB-CG	-6.20	1.35	1.52
2	N	12	GLN	CB-CG	-6.20	1.35	1.52
2	J	52	ASN	CB-CG	5.38	1.63	1.51
2	L	52	ASN	CB-CG	5.38	1.63	1.51
2	I	52	ASN	CB-CG	5.38	1.63	1.51
2	K	52	ASN	CB-CG	5.37	1.63	1.51
2	N	52	ASN	CB-CG	5.37	1.63	1.51
2	H	52	ASN	CB-CG	5.37	1.63	1.51
2	M	52	ASN	CB-CG	5.37	1.63	1.51
1	G	396	PRO	N-CD	5.09	1.54	1.47
1	F	396	PRO	N-CD	5.08	1.54	1.47
1	E	396	PRO	N-CD	5.07	1.54	1.47
1	D	396	PRO	N-CD	5.07	1.54	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	396	PRO	N-CD	5.06	1.54	1.47
1	C	396	PRO	N-CD	5.03	1.54	1.47
1	A	396	PRO	N-CD	5.02	1.54	1.47

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	11	VAL	CG1-CB-CG2	-15.51	86.09	110.90
2	M	11	VAL	CG1-CB-CG2	-15.49	86.11	110.90
2	H	11	VAL	CG1-CB-CG2	-15.49	86.12	110.90
2	N	11	VAL	CG1-CB-CG2	-15.49	86.12	110.90
2	K	11	VAL	CG1-CB-CG2	-15.48	86.14	110.90
2	J	11	VAL	CG1-CB-CG2	-15.48	86.14	110.90
2	L	11	VAL	CG1-CB-CG2	-15.47	86.14	110.90
2	L	52	ASN	CB-CG-OD1	-12.31	96.98	121.60
2	N	52	ASN	CB-CG-OD1	-12.31	96.98	121.60
2	H	52	ASN	CB-CG-OD1	-12.31	96.99	121.60
2	K	52	ASN	CB-CG-OD1	-12.30	97.00	121.60
2	J	52	ASN	CB-CG-OD1	-12.30	97.00	121.60
2	M	52	ASN	CB-CG-OD1	-12.29	97.01	121.60
2	I	52	ASN	CB-CG-OD1	-12.29	97.03	121.60
1	E	1175	THR	C-N-CA	-8.28	101.01	121.70
1	A	1175	THR	C-N-CA	-8.27	101.02	121.70
1	G	1175	THR	C-N-CA	-8.27	101.03	121.70
1	B	1175	THR	C-N-CA	-8.26	101.05	121.70
1	C	1175	THR	C-N-CA	-8.26	101.05	121.70
1	D	1175	THR	C-N-CA	-8.25	101.07	121.70
1	F	1175	THR	C-N-CA	-8.25	101.07	121.70
1	C	588	VAL	CA-C-N	-8.00	99.61	117.20
1	F	588	VAL	CA-C-N	-7.99	99.61	117.20
1	D	588	VAL	CA-C-N	-7.99	99.62	117.20
1	A	588	VAL	CA-C-N	-7.99	99.62	117.20
1	G	588	VAL	CA-C-N	-7.99	99.62	117.20
1	B	588	VAL	CA-C-N	-7.99	99.63	117.20
1	E	588	VAL	CA-C-N	-7.99	99.63	117.20
2	N	12	GLN	CA-CB-CG	7.60	130.11	113.40
2	H	12	GLN	CA-CB-CG	7.59	130.09	113.40
2	J	12	GLN	CA-CB-CG	7.59	130.09	113.40
2	M	12	GLN	CA-CB-CG	7.58	130.09	113.40
2	I	12	GLN	CA-CB-CG	7.58	130.07	113.40
2	K	12	GLN	CA-CB-CG	7.58	130.07	113.40
2	L	12	GLN	CA-CB-CG	7.58	130.07	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	588	VAL	O-C-N	-7.49	110.72	122.70
1	D	588	VAL	O-C-N	-7.48	110.73	122.70
1	E	588	VAL	O-C-N	-7.48	110.73	122.70
1	A	588	VAL	O-C-N	-7.47	110.75	122.70
1	G	588	VAL	O-C-N	-7.46	110.77	122.70
1	B	588	VAL	O-C-N	-7.46	110.77	122.70
1	F	588	VAL	O-C-N	-7.45	110.79	122.70
1	F	1163	HIS	C-N-CA	6.42	137.74	121.70
1	B	1163	HIS	C-N-CA	6.41	137.72	121.70
1	A	1163	HIS	C-N-CA	6.41	137.71	121.70
1	E	1163	HIS	C-N-CA	6.40	137.71	121.70
1	C	1163	HIS	C-N-CA	6.40	137.70	121.70
1	G	1163	HIS	C-N-CA	6.40	137.70	121.70
1	D	1163	HIS	C-N-CA	6.40	137.70	121.70
1	D	588	VAL	CA-C-O	6.31	133.35	120.10
1	A	588	VAL	CA-C-O	6.30	133.33	120.10
1	C	588	VAL	CA-C-O	6.30	133.33	120.10
1	B	588	VAL	CA-C-O	6.30	133.32	120.10
1	E	588	VAL	CA-C-O	6.29	133.31	120.10
1	G	588	VAL	CA-C-O	6.29	133.30	120.10
1	F	588	VAL	CA-C-O	6.28	133.30	120.10
1	D	562	ASN	N-CA-C	-5.45	96.28	111.00
1	E	562	ASN	N-CA-C	-5.45	96.29	111.00
1	B	562	ASN	N-CA-C	-5.44	96.31	111.00
1	F	562	ASN	N-CA-C	-5.44	96.31	111.00
1	C	562	ASN	N-CA-C	-5.44	96.31	111.00
1	G	562	ASN	N-CA-C	-5.44	96.32	111.00
1	A	562	ASN	N-CA-C	-5.43	96.33	111.00
1	A	126	PHE	CA-C-N	-5.28	105.59	117.20
1	D	126	PHE	CA-C-N	-5.27	105.61	117.20
1	E	126	PHE	CA-C-N	-5.26	105.62	117.20
1	B	126	PHE	CA-C-N	-5.26	105.62	117.20
1	G	126	PHE	CA-C-N	-5.26	105.63	117.20
1	C	126	PHE	CA-C-N	-5.26	105.63	117.20
1	F	126	PHE	CA-C-N	-5.26	105.63	117.20
1	C	1161	LEU	N-CA-C	5.03	124.59	111.00
1	F	1161	LEU	N-CA-C	5.03	124.59	111.00
1	D	1161	LEU	N-CA-C	5.03	124.58	111.00
1	B	1161	LEU	N-CA-C	5.03	124.57	111.00
1	G	1161	LEU	N-CA-C	5.03	124.57	111.00
1	E	1161	LEU	N-CA-C	5.02	124.56	111.00
1	A	1161	LEU	N-CA-C	5.02	124.56	111.00

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	361	TYR	Mainchain
1	A	588	VAL	Mainchain
1	B	361	TYR	Mainchain
1	B	588	VAL	Mainchain
1	C	361	TYR	Mainchain
1	C	588	VAL	Mainchain
1	D	361	TYR	Mainchain
1	D	588	VAL	Mainchain
1	E	361	TYR	Mainchain
1	E	588	VAL	Mainchain
1	F	361	TYR	Mainchain
1	F	588	VAL	Mainchain
1	G	361	TYR	Mainchain
1	G	588	VAL	Mainchain
2	H	52	ASN	Sidechain
2	I	52	ASN	Sidechain
2	J	52	ASN	Sidechain
2	K	52	ASN	Sidechain
2	L	52	ASN	Sidechain
2	M	52	ASN	Sidechain
2	N	52	ASN	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9139	0	8998	336	0
1	B	9139	0	8998	330	0
1	C	9139	0	8998	333	0
1	D	9139	0	8998	337	0
1	E	9139	0	8998	336	0
1	F	9139	0	8998	338	0
1	G	9139	0	8998	337	0
2	H	814	0	833	92	0
2	I	814	0	833	90	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	814	0	833	90	0
2	K	814	0	833	88	0
2	L	814	0	833	88	0
2	M	814	0	833	91	0
2	N	814	0	833	91	0
3	A	31	0	12	1	0
3	B	31	0	12	2	0
3	C	31	0	12	1	0
3	D	31	0	12	1	0
3	E	31	0	12	1	0
3	F	31	0	12	2	0
3	G	31	0	12	1	0
4	H	43	0	30	7	0
4	I	43	0	30	10	0
4	J	43	0	30	7	0
4	K	43	0	30	6	0
4	L	43	0	30	6	0
4	M	43	0	30	8	0
4	N	43	0	30	7	0
All	All	70189	0	69111	2213	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 16.

All (2213) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1063:PHE:CE2	2:L:86:LYS:HG3	1.14	1.66
1:D:1063:PHE:CE2	2:K:86:LYS:HG3	1.14	1.65
1:F:1063:PHE:CE2	2:M:86:LYS:HG3	1.14	1.64
1:A:1063:PHE:CE2	2:H:86:LYS:HG3	1.14	1.62
1:B:1063:PHE:CE2	2:I:86:LYS:HG3	1.14	1.61
1:C:1063:PHE:CE2	2:J:86:LYS:HG3	1.15	1.61
1:G:1063:PHE:CE2	2:N:86:LYS:HG3	1.14	1.60
1:A:1063:PHE:HE2	2:H:86:LYS:CG	1.16	1.57
1:B:1169:SER:HB3	1:B:1170:GLU:CB	1.35	1.56
1:C:1169:SER:HB3	1:C:1170:GLU:CB	1.35	1.56
1:A:1169:SER:HB3	1:A:1170:GLU:CB	1.35	1.56
1:D:1169:SER:HB3	1:D:1170:GLU:CB	1.35	1.55
1:E:1169:SER:HB3	1:E:1170:GLU:CB	1.35	1.55
1:F:1063:PHE:HE2	2:M:86:LYS:CG	1.16	1.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1169:SER:HB3	1:F:1170:GLU:CB	1.35	1.55
1:B:1063:PHE:HE2	2:I:86:LYS:CG	1.16	1.54
1:G:1169:SER:HB3	1:G:1170:GLU:CB	1.35	1.54
1:G:1063:PHE:HE2	2:N:86:LYS:CG	1.16	1.53
1:D:558:GLN:HG2	1:D:1171:GLU:CG	1.38	1.53
1:D:1169:SER:CB	1:D:1170:GLU:HB2	1.37	1.53
1:E:1169:SER:CB	1:E:1170:GLU:HB2	1.37	1.53
1:C:1063:PHE:HE2	2:J:86:LYS:CG	1.16	1.53
1:E:1063:PHE:HE2	2:L:86:LYS:CG	1.16	1.53
1:B:1169:SER:CB	1:B:1170:GLU:HB2	1.37	1.52
1:E:558:GLN:HG2	1:E:1171:GLU:CG	1.38	1.52
1:C:558:GLN:HG2	1:C:1171:GLU:CG	1.38	1.52
1:D:1063:PHE:HE2	2:K:86:LYS:CG	1.16	1.52
1:A:558:GLN:HG2	1:A:1171:GLU:CG	1.38	1.51
1:D:340:TYR:CE1	1:E:409:GLU:OE2	1.64	1.51
1:G:558:GLN:HG2	1:G:1171:GLU:CG	1.38	1.51
1:C:1169:SER:CB	1:C:1170:GLU:HB2	1.37	1.50
1:G:1169:SER:CB	1:G:1170:GLU:HB2	1.37	1.50
1:A:565:GLN:NE2	1:A:592:MET:HE3	1.18	1.50
1:F:340:TYR:CE1	1:G:409:GLU:OE2	1.64	1.50
1:A:1169:SER:CB	1:A:1170:GLU:HB2	1.37	1.49
1:B:558:GLN:HG2	1:B:1171:GLU:CG	1.38	1.49
1:A:565:GLN:NE2	1:A:592:MET:CE	1.76	1.49
1:E:340:TYR:CE1	1:F:409:GLU:OE2	1.64	1.49
1:A:340:TYR:CE1	1:B:409:GLU:OE2	1.64	1.49
1:A:409:GLU:OE2	1:G:340:TYR:CE1	1.64	1.49
1:C:340:TYR:CE1	1:D:409:GLU:OE2	1.64	1.49
1:A:558:GLN:CG	1:A:1171:GLU:HG3	1.42	1.48
1:E:565:GLN:NE2	1:E:592:MET:CE	1.76	1.48
1:B:340:TYR:CE1	1:C:409:GLU:OE2	1.64	1.48
1:D:558:GLN:CG	1:D:1171:GLU:HG3	1.42	1.48
1:D:565:GLN:NE2	1:D:592:MET:CE	1.76	1.48
1:G:565:GLN:NE2	1:G:592:MET:HE3	1.19	1.48
1:B:558:GLN:CG	1:B:1171:GLU:HG3	1.42	1.48
1:F:1169:SER:CB	1:F:1170:GLU:HB2	1.37	1.48
1:G:565:GLN:NE2	1:G:592:MET:CE	1.76	1.48
1:B:565:GLN:NE2	1:B:592:MET:CE	1.76	1.48
1:F:558:GLN:CG	1:F:1171:GLU:HG3	1.42	1.47
1:E:558:GLN:CG	1:E:1171:GLU:HG3	1.42	1.46
1:G:558:GLN:CG	1:G:1171:GLU:HG3	1.42	1.46
1:C:565:GLN:NE2	1:C:592:MET:CE	1.76	1.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:558:GLN:CG	1:C:1171:GLU:HG3	1.42	1.45
1:F:558:GLN:HG2	1:F:1171:GLU:CG	1.38	1.45
1:C:565:GLN:NE2	1:C:592:MET:HE3	1.20	1.45
1:F:565:GLN:NE2	1:F:592:MET:HE3	1.17	1.45
1:F:565:GLN:NE2	1:F:592:MET:CE	1.76	1.45
1:E:565:GLN:NE2	1:E:592:MET:HE3	1.22	1.44
1:D:565:GLN:NE2	1:D:592:MET:HE3	1.17	1.42
1:F:559:PRO:CB	1:F:1174:ALA:HA	1.53	1.38
1:A:559:PRO:CB	1:A:1174:ALA:HA	1.53	1.38
1:G:559:PRO:CB	1:G:1174:ALA:HA	1.53	1.38
1:E:559:PRO:CB	1:E:1174:ALA:HA	1.53	1.37
1:D:559:PRO:CB	1:D:1174:ALA:HA	1.53	1.36
1:B:1007:TRP:CZ2	2:I:73:LYS:NZ	1.94	1.36
1:B:559:PRO:CB	1:B:1174:ALA:HA	1.53	1.36
1:G:1007:TRP:CZ2	2:N:73:LYS:NZ	1.94	1.36
1:C:559:PRO:CB	1:C:1174:ALA:HA	1.53	1.36
1:E:1007:TRP:CZ2	2:L:73:LYS:NZ	1.94	1.35
1:C:1007:TRP:CZ2	2:J:73:LYS:NZ	1.94	1.35
1:A:1007:TRP:CZ2	2:H:73:LYS:NZ	1.94	1.35
1:E:555:LEU:CD2	1:E:560:PHE:HE1	1.41	1.34
1:F:1007:TRP:CZ2	2:M:73:LYS:NZ	1.94	1.34
1:C:555:LEU:CD2	1:C:560:PHE:HE1	1.41	1.34
1:D:1007:TRP:CZ2	2:K:73:LYS:NZ	1.94	1.34
1:A:555:LEU:CD2	1:A:560:PHE:HE1	1.41	1.34
1:G:555:LEU:CD2	1:G:560:PHE:HE1	1.40	1.34
1:B:555:LEU:CD2	1:B:560:PHE:HE1	1.41	1.33
1:F:555:LEU:CD2	1:F:560:PHE:HE1	1.41	1.32
1:D:555:LEU:CD2	1:D:560:PHE:HE1	1.41	1.32
1:D:1169:SER:CA	1:D:1170:GLU:HB2	1.62	1.30
1:E:1169:SER:CA	1:E:1170:GLU:HB2	1.62	1.29
1:B:1063:PHE:CE2	2:I:86:LYS:CG	1.99	1.29
1:C:1169:SER:CA	1:C:1170:GLU:HB2	1.62	1.29
1:E:555:LEU:CD2	1:E:560:PHE:CE1	2.15	1.29
1:A:555:LEU:CD2	1:A:560:PHE:CE1	2.15	1.29
1:C:555:LEU:CD2	1:C:560:PHE:CE1	2.15	1.28
1:F:1169:SER:CA	1:F:1170:GLU:HB2	1.62	1.28
1:F:555:LEU:CD2	1:F:560:PHE:CE1	2.15	1.28
1:G:555:LEU:CD2	1:G:560:PHE:CE1	2.15	1.28
1:G:1063:PHE:CE2	2:N:86:LYS:CG	1.99	1.28
1:B:1169:SER:CA	1:B:1170:GLU:HB2	1.62	1.28
1:D:560:PHE:CD1	1:D:561:PRO:HD2	1.69	1.28

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:555:LEU:CD2	1:D:560:PHE:CE1	2.15	1.28
1:G:1169:SER:CA	1:G:1170:GLU:HB2	1.62	1.27
1:A:1169:SER:CA	1:A:1170:GLU:HB2	1.62	1.27
1:B:555:LEU:CD2	1:B:560:PHE:CE1	2.15	1.27
1:C:560:PHE:CD1	1:C:561:PRO:HD2	1.69	1.27
1:F:560:PHE:CD1	1:F:561:PRO:HD2	1.69	1.27
1:A:1063:PHE:CE2	2:H:86:LYS:CG	1.99	1.26
1:E:560:PHE:CD1	1:E:561:PRO:HD2	1.69	1.26
1:B:560:PHE:CD1	1:B:561:PRO:HD2	1.69	1.26
1:E:340:TYR:HE1	1:F:409:GLU:OE2	0.96	1.26
1:B:340:TYR:HE1	1:C:409:GLU:OE2	0.96	1.26
1:G:560:PHE:CD1	1:G:561:PRO:HD2	1.69	1.25
1:A:560:PHE:CD1	1:A:561:PRO:HD2	1.69	1.25
1:C:340:TYR:HE1	1:D:409:GLU:OE2	0.96	1.25
1:B:565:GLN:NE2	1:B:592:MET:HE3	1.34	1.24
1:A:340:TYR:HE1	1:B:409:GLU:OE2	0.96	1.24
1:C:555:LEU:HD23	1:C:560:PHE:CE1	1.74	1.23
1:E:555:LEU:HD23	1:E:560:PHE:CE1	1.74	1.22
1:D:1004:LYS:NZ	2:K:73:LYS:HG2	1.55	1.21
1:C:1004:LYS:NZ	2:J:73:LYS:HG2	1.55	1.21
1:A:555:LEU:HD23	1:A:560:PHE:CE1	1.74	1.21
1:A:409:GLU:OE2	1:G:340:TYR:HE1	0.96	1.21
1:E:1004:LYS:NZ	2:L:73:LYS:HG2	1.55	1.20
1:A:1173:ALA:HB1	1:A:1211:GLN:OE1	1.42	1.20
1:G:555:LEU:HD23	1:G:560:PHE:CE1	1.74	1.20
1:C:1007:TRP:HZ2	2:J:73:LYS:NZ	1.34	1.20
1:C:1063:PHE:CE2	2:J:86:LYS:CG	1.99	1.20
1:F:1063:PHE:CE2	2:M:86:LYS:CG	1.99	1.20
1:F:555:LEU:HD23	1:F:560:PHE:CE1	1.74	1.20
1:B:1173:ALA:HB1	1:B:1211:GLN:OE1	1.42	1.20
1:D:340:TYR:HE1	1:E:409:GLU:OE2	0.96	1.20
1:D:555:LEU:HD23	1:D:560:PHE:CE1	1.74	1.19
1:B:555:LEU:HD23	1:B:560:PHE:CE1	1.74	1.19
1:B:1004:LYS:NZ	2:I:73:LYS:HG2	1.55	1.19
1:F:1173:ALA:HB1	1:F:1211:GLN:OE1	1.42	1.19
1:F:1004:LYS:NZ	2:M:73:LYS:HG2	1.55	1.19
1:F:1088:VAL:O	2:M:86:LYS:HE3	1.44	1.18
1:D:1173:ALA:HB1	1:D:1211:GLN:OE1	1.42	1.17
1:E:1007:TRP:HZ2	2:L:73:LYS:NZ	1.34	1.17
1:B:565:GLN:HE21	1:B:592:MET:HE2	1.02	1.17
1:A:1004:LYS:NZ	2:H:73:LYS:HG2	1.55	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1173:ALA:HB1	1:C:1211:GLN:OE1	1.42	1.17
1:F:559:PRO:HB3	1:F:1175:THR:H	1.00	1.17
1:G:1007:TRP:HZ2	2:N:73:LYS:NZ	1.34	1.17
1:E:559:PRO:HB3	1:E:1175:THR:N	1.59	1.17
1:G:559:PRO:HB3	1:G:1175:THR:H	1.00	1.17
1:D:1088:VAL:O	2:K:86:LYS:HE3	1.44	1.17
1:D:1063:PHE:CE2	2:K:86:LYS:CG	1.99	1.17
1:D:559:PRO:HB3	1:D:1175:THR:N	1.59	1.17
1:G:1004:LYS:NZ	2:N:73:LYS:HG2	1.55	1.17
1:B:1088:VAL:O	2:I:86:LYS:HE3	1.44	1.17
1:E:559:PRO:HB3	1:E:1175:THR:H	1.00	1.16
1:A:1088:VAL:O	2:H:86:LYS:HE3	1.44	1.16
1:B:520:ALA:HB1	1:B:646:THR:OG1	1.45	1.16
1:G:1173:ALA:HB1	1:G:1211:GLN:OE1	1.42	1.16
2:K:14:CYS:SG	4:K:500:HEM:HAB	1.85	1.16
1:E:1063:PHE:CE2	2:L:86:LYS:CG	1.99	1.16
1:C:559:PRO:HB3	1:C:1175:THR:N	1.59	1.16
1:F:559:PRO:HB3	1:F:1175:THR:N	1.59	1.16
1:E:1088:VAL:O	2:L:86:LYS:HE3	1.44	1.16
1:D:348:LYS:HG3	1:D:352:ARG:CD	1.76	1.16
1:E:348:LYS:HG3	1:E:352:ARG:CD	1.76	1.16
2:I:14:CYS:SG	4:I:500:HEM:HAB	1.85	1.16
1:D:559:PRO:HB3	1:D:1175:THR:H	1.00	1.16
1:C:520:ALA:HB1	1:C:646:THR:OG1	1.45	1.16
2:N:14:CYS:SG	4:N:500:HEM:HAB	1.85	1.16
1:C:701:GLN:CD	2:J:25:LYS:HD3	1.67	1.15
1:D:701:GLN:CD	2:K:25:LYS:HD3	1.67	1.15
1:F:340:TYR:HE1	1:G:409:GLU:OE2	0.96	1.15
2:J:14:CYS:SG	4:J:500:HEM:HAB	1.85	1.15
2:M:14:CYS:SG	4:M:500:HEM:HAB	1.85	1.15
1:E:1173:ALA:HB1	1:E:1211:GLN:OE1	1.42	1.15
1:F:348:LYS:HG3	1:F:352:ARG:CD	1.76	1.15
1:B:701:GLN:CD	2:I:25:LYS:HD3	1.67	1.15
1:E:1004:LYS:HZ3	2:L:73:LYS:HG2	1.00	1.15
1:A:520:ALA:HB1	1:A:646:THR:OG1	1.45	1.15
1:C:348:LYS:HG3	1:C:352:ARG:CD	1.76	1.15
1:C:1088:VAL:O	2:J:86:LYS:HE3	1.44	1.15
1:G:348:LYS:HG3	1:G:352:ARG:CD	1.76	1.15
1:A:348:LYS:HG3	1:A:352:ARG:CD	1.76	1.15
1:E:701:GLN:CD	2:L:25:LYS:HD3	1.67	1.15
1:B:559:PRO:HB3	1:B:1175:THR:N	1.59	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:14:CYS:SG	4:H:500:HEM:HAB	1.85	1.15
1:A:559:PRO:HB3	1:A:1175:THR:H	1.00	1.15
1:A:559:PRO:HB3	1:A:1175:THR:N	1.59	1.15
2:L:14:CYS:SG	4:L:500:HEM:HAB	1.85	1.15
1:B:1007:TRP:HZ2	2:I:73:LYS:NZ	1.34	1.14
1:D:558:GLN:HA	1:D:1171:GLU:HG2	1.27	1.14
1:G:1088:VAL:O	2:N:86:LYS:HE3	1.44	1.14
1:G:559:PRO:HB3	1:G:1175:THR:N	1.59	1.14
1:D:520:ALA:HB1	1:D:646:THR:OG1	1.45	1.14
1:G:701:GLN:CD	2:N:25:LYS:HD3	1.67	1.14
1:B:348:LYS:HG3	1:B:352:ARG:CD	1.76	1.14
1:C:559:PRO:HB3	1:C:1175:THR:H	1.00	1.14
1:A:1089:LEU:HA	2:H:86:LYS:HE2	1.14	1.14
1:A:208:GLN:HG2	1:B:229:ILE:CD1	1.78	1.14
1:C:208:GLN:HG2	1:D:229:ILE:CD1	1.78	1.14
1:C:558:GLN:HA	1:C:1171:GLU:HG2	1.27	1.14
1:A:701:GLN:CD	2:H:25:LYS:HD3	1.67	1.13
1:B:559:PRO:HB3	1:B:1175:THR:H	1.00	1.13
1:E:1089:LEU:HA	2:L:86:LYS:HE2	1.14	1.13
1:B:1004:LYS:HZ3	2:I:73:LYS:HG2	0.96	1.13
1:D:208:GLN:HG2	1:E:229:ILE:CD1	1.78	1.13
1:G:520:ALA:HB1	1:G:646:THR:OG1	1.45	1.13
1:G:1089:LEU:HA	2:N:86:LYS:HE2	1.14	1.13
1:F:701:GLN:CD	2:M:25:LYS:HD3	1.67	1.13
1:E:520:ALA:HB1	1:E:646:THR:OG1	1.45	1.12
1:B:1089:LEU:HA	2:I:86:LYS:HE2	1.14	1.12
1:B:208:GLN:HG2	1:C:229:ILE:CD1	1.78	1.12
1:E:558:GLN:HA	1:E:1171:GLU:HG2	1.27	1.12
1:F:1089:LEU:HA	2:M:86:LYS:HE2	1.14	1.12
1:F:208:GLN:HG2	1:G:229:ILE:CD1	1.78	1.12
1:D:1089:LEU:HA	2:K:86:LYS:HE2	1.14	1.12
1:F:520:ALA:HB1	1:F:646:THR:OG1	1.45	1.12
1:A:229:ILE:CD1	1:G:208:GLN:HG2	1.78	1.12
1:E:208:GLN:HG2	1:F:229:ILE:CD1	1.78	1.11
1:E:208:GLN:HG2	1:F:229:ILE:HD11	1.31	1.11
1:A:229:ILE:HD11	1:G:208:GLN:HG2	1.31	1.11
1:C:1089:LEU:HA	2:J:86:LYS:HE2	1.14	1.11
1:B:557:ARG:O	1:B:1171:GLU:OE2	1.69	1.11
1:E:557:ARG:O	1:E:1171:GLU:OE2	1.69	1.11
1:F:208:GLN:HG2	1:G:229:ILE:HD11	1.31	1.10
1:D:557:ARG:O	1:D:1171:GLU:OE2	1.69	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:14:CYS:SG	4:L:500:HEM:CAB	2.39	1.10
1:C:557:ARG:O	1:C:1171:GLU:OE2	1.69	1.10
2:I:14:CYS:SG	4:I:500:HEM:CAB	2.39	1.10
1:A:557:ARG:O	1:A:1171:GLU:OE2	1.69	1.10
1:F:557:ARG:O	1:F:1171:GLU:OE2	1.69	1.10
2:K:14:CYS:SG	4:K:500:HEM:CAB	2.39	1.10
1:B:558:GLN:HA	1:B:1171:GLU:HG2	1.27	1.10
2:J:14:CYS:SG	4:J:500:HEM:CAB	2.39	1.10
1:F:348:LYS:HG3	1:F:352:ARG:HD3	1.29	1.10
2:N:14:CYS:SG	4:N:500:HEM:CAB	2.39	1.10
1:C:340:TYR:OH	1:D:409:GLU:CD	1.91	1.10
1:E:340:TYR:OH	1:F:409:GLU:CD	1.91	1.09
2:H:14:CYS:SG	4:H:500:HEM:CAB	2.39	1.09
1:A:581:LYS:HZ1	1:A:1247:LEU:HD21	1.16	1.09
1:G:557:ARG:O	1:G:1171:GLU:OE2	1.69	1.09
1:C:1004:LYS:HZ3	2:J:73:LYS:HG2	1.06	1.09
1:E:348:LYS:HG3	1:E:352:ARG:HD3	1.28	1.09
1:C:1023:ASP:OD2	2:J:73:LYS:HD3	1.53	1.09
1:F:1023:ASP:OD2	2:M:73:LYS:HD3	1.53	1.09
1:A:340:TYR:OH	1:B:409:GLU:CD	1.91	1.09
1:D:1007:TRP:HZ2	2:K:73:LYS:NZ	1.33	1.09
1:F:558:GLN:HA	1:F:1171:GLU:HG2	1.27	1.09
1:F:340:TYR:OH	1:G:409:GLU:CD	1.91	1.09
1:G:1023:ASP:OD2	2:N:73:LYS:HD3	1.53	1.09
1:A:409:GLU:CD	1:G:340:TYR:OH	1.91	1.09
1:D:1088:VAL:O	2:K:86:LYS:CE	2.00	1.09
1:D:340:TYR:OH	1:E:409:GLU:CD	1.91	1.08
1:A:1007:TRP:HZ2	2:H:73:LYS:NZ	1.34	1.08
1:G:1088:VAL:O	2:N:86:LYS:CE	2.01	1.08
1:A:1023:ASP:CG	2:H:73:LYS:HD3	1.74	1.08
1:E:1088:VAL:O	2:L:86:LYS:CE	2.00	1.08
2:M:14:CYS:SG	4:M:500:HEM:CAB	2.39	1.08
1:A:1088:VAL:O	2:H:86:LYS:CE	2.01	1.08
1:G:1023:ASP:CG	2:N:73:LYS:HD3	1.74	1.08
1:A:208:GLN:HG2	1:B:229:ILE:HD11	1.31	1.08
1:B:340:TYR:OH	1:C:409:GLU:CD	1.91	1.08
1:B:1023:ASP:OD2	2:I:73:LYS:HD3	1.53	1.08
1:C:1088:VAL:O	2:J:86:LYS:CE	2.01	1.08
1:E:1023:ASP:OD2	2:L:73:LYS:HD3	1.53	1.08
1:F:1088:VAL:O	2:M:86:LYS:CE	2.00	1.08
1:D:208:GLN:HG2	1:E:229:ILE:HD11	1.31	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1088:VAL:O	2:I:86:LYS:CE	2.00	1.08
1:G:348:LYS:HG3	1:G:352:ARG:HD3	1.29	1.08
1:B:1023:ASP:CG	2:I:73:LYS:HD3	1.74	1.08
1:F:1023:ASP:CG	2:M:73:LYS:HD3	1.74	1.07
1:A:558:GLN:HA	1:A:1171:GLU:HG2	1.27	1.07
1:B:208:GLN:HG2	1:C:229:ILE:HD11	1.31	1.07
1:C:208:GLN:HG2	1:D:229:ILE:HD11	1.31	1.07
1:A:1023:ASP:OD2	2:H:73:LYS:HD3	1.53	1.07
1:C:1169:SER:CB	1:C:1170:GLU:CB	2.11	1.07
1:D:1023:ASP:OD2	2:K:73:LYS:HD3	1.53	1.07
1:C:1023:ASP:CG	2:J:73:LYS:HD3	1.74	1.07
1:E:1023:ASP:CG	2:L:73:LYS:HD3	1.74	1.07
1:C:348:LYS:HG3	1:C:352:ARG:HD3	1.29	1.07
1:F:1007:TRP:HZ2	2:M:73:LYS:NZ	1.34	1.07
1:C:348:LYS:HE3	1:C:447:GLU:HG2	1.37	1.06
1:D:348:LYS:HG3	1:D:352:ARG:HD3	1.29	1.06
1:D:1023:ASP:CG	2:K:73:LYS:HD3	1.74	1.06
1:B:348:LYS:HE3	1:B:447:GLU:HG2	1.37	1.06
1:D:348:LYS:HE3	1:D:447:GLU:HG2	1.37	1.06
1:G:558:GLN:HA	1:G:1171:GLU:HG2	1.27	1.06
1:G:1048:LYS:HD2	2:N:86:LYS:NZ	1.71	1.06
1:A:348:LYS:HG3	1:A:352:ARG:HD3	1.28	1.05
1:F:1048:LYS:HD2	2:M:86:LYS:NZ	1.71	1.05
1:G:559:PRO:HB2	1:G:1174:ALA:HA	1.08	1.05
1:B:1048:LYS:HD2	2:I:86:LYS:NZ	1.71	1.05
1:D:205:ARG:NH1	1:E:225:ASP:OD1	1.90	1.05
1:E:205:ARG:NH1	1:F:225:ASP:OD1	1.89	1.05
1:A:559:PRO:HB2	1:A:1174:ALA:HA	1.08	1.05
1:C:1048:LYS:HD2	2:J:86:LYS:NZ	1.71	1.05
1:B:348:LYS:HG3	1:B:352:ARG:HD3	1.29	1.05
1:A:225:ASP:OD1	1:G:205:ARG:NH1	1.89	1.05
1:B:565:GLN:HE22	1:B:592:MET:CE	1.53	1.05
1:C:205:ARG:NH1	1:D:225:ASP:OD1	1.89	1.05
1:F:559:PRO:HB2	1:F:1174:ALA:HA	1.08	1.05
1:E:1048:LYS:HD2	2:L:86:LYS:NZ	1.71	1.05
1:F:1004:LYS:HZ3	2:M:73:LYS:HG2	1.03	1.05
1:B:1169:SER:HB3	1:B:1170:GLU:CA	1.87	1.04
1:A:205:ARG:NH1	1:B:225:ASP:OD1	1.90	1.04
1:C:1169:SER:HB3	1:C:1170:GLU:CA	1.87	1.04
1:B:205:ARG:NH1	1:C:225:ASP:OD1	1.89	1.04
1:E:348:LYS:HE3	1:E:447:GLU:HG2	1.37	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:559:PRO:HB2	1:E:1174:ALA:HA	1.08	1.04
1:F:205:ARG:NH1	1:G:225:ASP:OD1	1.89	1.04
1:A:348:LYS:HE3	1:A:447:GLU:HG2	1.37	1.04
1:D:1048:LYS:HD2	2:K:86:LYS:NZ	1.71	1.04
1:D:581:LYS:HZ1	1:D:1247:LEU:HD21	1.18	1.04
1:A:1169:SER:HB3	1:A:1170:GLU:CA	1.87	1.04
1:D:1169:SER:HB3	1:D:1170:GLU:CA	1.87	1.03
1:A:1048:LYS:HD2	2:H:86:LYS:NZ	1.71	1.03
1:B:559:PRO:HB2	1:B:1174:ALA:HA	1.08	1.03
1:D:559:PRO:HB2	1:D:1174:ALA:HA	1.08	1.03
1:D:559:PRO:HB3	1:D:1174:ALA:HA	1.38	1.03
1:E:559:PRO:HB3	1:E:1174:ALA:HA	1.38	1.03
1:G:646:THR:HG23	1:G:648:GLU:H	1.23	1.03
1:C:559:PRO:HB2	1:C:1174:ALA:HA	1.08	1.02
1:D:1169:SER:CB	1:D:1170:GLU:CB	2.11	1.02
1:B:1169:SER:CB	1:B:1170:GLU:CB	2.11	1.02
1:F:348:LYS:HE3	1:F:447:GLU:HG2	1.37	1.02
1:G:1169:SER:HB3	1:G:1170:GLU:CA	1.87	1.02
1:G:348:LYS:HE3	1:G:447:GLU:HG2	1.37	1.02
1:E:565:GLN:HE21	1:E:592:MET:HE2	1.23	1.02
1:D:1004:LYS:HZ3	2:K:73:LYS:HG2	1.04	1.02
1:G:581:LYS:HZ1	1:G:1247:LEU:HD21	1.24	1.02
1:E:1169:SER:HB3	1:E:1170:GLU:CA	1.87	1.02
1:F:1169:SER:HB3	1:F:1170:GLU:CA	1.87	1.01
1:B:1169:SER:N	1:B:1170:GLU:HB2	1.76	1.01
1:G:1169:SER:CB	1:G:1170:GLU:CB	2.11	1.01
1:A:1004:LYS:HZ3	2:H:73:LYS:HG2	1.07	1.01
1:C:1169:SER:N	1:C:1170:GLU:HB2	1.76	1.01
1:A:646:THR:HG23	1:A:648:GLU:H	1.24	1.01
1:D:557:ARG:C	1:D:1171:GLU:OE2	1.99	1.01
1:A:1169:SER:N	1:A:1170:GLU:HB2	1.76	1.01
1:F:205:ARG:CZ	1:G:225:ASP:OD2	2.09	1.01
1:C:557:ARG:C	1:C:1171:GLU:OE2	1.99	1.01
1:E:1169:SER:CB	1:E:1170:GLU:CB	2.11	1.01
1:E:205:ARG:CZ	1:F:225:ASP:OD2	2.09	1.01
1:C:559:PRO:HB3	1:C:1174:ALA:HA	1.38	1.00
1:D:205:ARG:CZ	1:E:225:ASP:OD2	2.09	1.00
1:F:1048:LYS:CD	2:M:86:LYS:NZ	2.25	1.00
1:G:557:ARG:C	1:G:1171:GLU:OE2	1.99	1.00
1:D:1169:SER:N	1:D:1170:GLU:HB2	1.76	1.00
1:E:1169:SER:N	1:E:1170:GLU:HB2	1.76	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:557:ARG:C	1:E:1171:GLU:OE2	1.99	1.00
1:F:1169:SER:N	1:F:1170:GLU:HB2	1.75	1.00
1:A:225:ASP:OD2	1:G:205:ARG:CZ	2.09	1.00
1:A:1169:SER:CB	1:A:1170:GLU:CB	2.11	1.00
1:A:557:ARG:C	1:A:1171:GLU:OE2	1.99	1.00
1:C:646:THR:HG23	1:C:648:GLU:H	1.23	1.00
1:E:1048:LYS:HG3	2:L:86:LYS:NZ	1.76	1.00
1:F:1169:SER:CB	1:F:1170:GLU:CB	2.11	1.00
1:G:1048:LYS:CD	2:N:86:LYS:NZ	2.25	1.00
1:B:557:ARG:C	1:B:1171:GLU:OE2	1.99	0.99
1:D:1048:LYS:CD	2:K:86:LYS:NZ	2.25	0.99
1:D:1048:LYS:HG3	2:K:86:LYS:NZ	1.76	0.99
1:F:1048:LYS:HG3	2:M:86:LYS:NZ	1.76	0.99
1:G:1169:SER:N	1:G:1170:GLU:HB2	1.76	0.99
1:A:1048:LYS:CD	2:H:86:LYS:NZ	2.25	0.99
1:G:565:GLN:HE22	1:G:592:MET:CE	1.53	0.99
1:A:205:ARG:CZ	1:B:225:ASP:OD2	2.09	0.99
1:C:581:LYS:HZ1	1:C:1247:LEU:HD21	1.23	0.99
1:E:214:GLN:OE1	1:F:213:SER:OG	1.73	0.99
1:G:1048:LYS:HG3	2:N:86:LYS:NZ	1.76	0.99
1:B:1048:LYS:CD	2:I:86:LYS:NZ	2.25	0.99
1:C:205:ARG:CZ	1:D:225:ASP:OD2	2.09	0.99
1:G:559:PRO:HB3	1:G:1174:ALA:HA	1.38	0.99
1:C:1048:LYS:CD	2:J:86:LYS:NZ	2.25	0.99
1:E:559:PRO:CB	1:E:1174:ALA:CA	2.41	0.99
1:F:559:PRO:CB	1:F:1174:ALA:CA	2.41	0.99
1:B:559:PRO:HB3	1:B:1174:ALA:HA	1.38	0.99
1:B:205:ARG:CZ	1:C:225:ASP:OD2	2.09	0.99
1:E:1048:LYS:CD	2:L:86:LYS:NZ	2.25	0.99
1:G:559:PRO:CB	1:G:1174:ALA:CA	2.41	0.99
1:A:1048:LYS:CG	2:H:86:LYS:NZ	2.26	0.99
1:F:565:GLN:HE22	1:F:592:MET:CE	1.53	0.99
1:A:559:PRO:CB	1:A:1174:ALA:CA	2.41	0.99
1:A:409:GLU:CD	1:G:340:TYR:HH	1.65	0.99
1:D:1169:SER:CA	1:D:1170:GLU:CB	2.39	0.99
1:D:646:THR:HG23	1:D:648:GLU:H	1.23	0.99
1:E:646:THR:HG23	1:E:648:GLU:H	1.23	0.99
1:D:559:PRO:CB	1:D:1174:ALA:CA	2.41	0.99
1:F:557:ARG:C	1:F:1171:GLU:OE2	1.99	0.99
1:G:1048:LYS:CG	2:N:86:LYS:NZ	2.26	0.99
1:F:646:THR:HG23	1:F:648:GLU:H	1.24	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:PRO:HB3	1:A:1174:ALA:HA	1.38	0.98
1:B:1004:LYS:HZ3	2:I:73:LYS:CG	1.75	0.98
1:D:1048:LYS:CG	2:K:86:LYS:NZ	2.26	0.98
1:B:559:PRO:CB	1:B:1174:ALA:CA	2.41	0.98
1:C:559:PRO:CB	1:C:1174:ALA:CA	2.41	0.98
1:A:581:LYS:HZ1	1:A:1247:LEU:CD2	1.76	0.98
1:C:1048:LYS:HG3	2:J:86:LYS:NZ	1.76	0.98
1:F:581:LYS:HZ1	1:F:1247:LEU:HD21	1.26	0.98
1:C:1169:SER:CA	1:C:1170:GLU:CB	2.39	0.98
1:A:565:GLN:HE22	1:A:592:MET:CE	1.53	0.98
1:B:1048:LYS:CG	2:I:86:LYS:NZ	2.26	0.97
1:B:1169:SER:CA	1:B:1170:GLU:CB	2.39	0.97
1:B:581:LYS:HZ1	1:B:1247:LEU:HD21	1.24	0.97
1:E:565:GLN:HE22	1:E:592:MET:CE	1.53	0.97
1:A:1048:LYS:HG3	2:H:86:LYS:NZ	1.76	0.97
1:B:646:THR:HG23	1:B:648:GLU:H	1.23	0.97
1:F:1048:LYS:CG	2:M:86:LYS:NZ	2.26	0.97
1:B:1048:LYS:HG3	2:I:86:LYS:NZ	1.76	0.97
1:E:1048:LYS:HG3	2:L:86:LYS:HZ1	1.29	0.97
1:A:214:GLN:OE1	1:B:213:SER:OG	1.73	0.97
1:D:214:GLN:OE1	1:E:213:SER:OG	1.73	0.97
1:A:213:SER:OG	1:G:214:GLN:OE1	1.74	0.97
1:C:1048:LYS:CG	2:J:86:LYS:NZ	2.26	0.97
1:F:214:GLN:OE1	1:G:213:SER:OG	1.74	0.97
1:B:340:TYR:HH	1:C:409:GLU:CD	1.65	0.97
1:D:560:PHE:CG	1:D:561:PRO:HD2	2.00	0.97
1:C:565:GLN:HE21	1:C:592:MET:HE2	1.30	0.96
1:D:581:LYS:HZ1	1:D:1247:LEU:CD2	1.76	0.96
1:E:558:GLN:CB	1:E:1171:GLU:HG3	1.95	0.96
1:E:520:ALA:O	1:E:524:HIS:CD2	2.19	0.96
1:F:520:ALA:O	1:F:524:HIS:CD2	2.19	0.96
1:C:560:PHE:CG	1:C:561:PRO:HD2	2.00	0.96
1:G:520:ALA:O	1:G:524:HIS:CD2	2.19	0.96
1:E:1048:LYS:CG	2:L:86:LYS:NZ	2.26	0.96
1:C:558:GLN:CB	1:C:1171:GLU:HG3	1.95	0.96
1:E:560:PHE:CG	1:E:561:PRO:HD2	2.00	0.96
1:F:559:PRO:HB3	1:F:1174:ALA:HA	1.38	0.96
1:D:520:ALA:O	1:D:524:HIS:CD2	2.18	0.96
1:A:1048:LYS:HG3	2:H:86:LYS:HZ1	1.27	0.96
1:C:565:GLN:HE22	1:C:592:MET:CE	1.53	0.96
1:D:565:GLN:HE22	1:D:592:MET:CE	1.53	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:560:PHE:CG	1:F:561:PRO:HD2	2.00	0.96
1:E:581:LYS:HZ1	1:E:1247:LEU:HD21	1.29	0.96
1:A:520:ALA:O	1:A:524:HIS:CD2	2.18	0.96
1:D:558:GLN:CB	1:D:1171:GLU:HG3	1.95	0.96
1:G:560:PHE:CG	1:G:561:PRO:HD2	2.00	0.96
1:G:1004:LYS:HZ2	2:N:73:LYS:CG	1.79	0.96
1:C:1048:LYS:HG3	2:J:86:LYS:HZ1	1.30	0.95
1:D:1048:LYS:HG3	2:K:86:LYS:HZ1	1.28	0.95
1:A:1048:LYS:CD	2:H:86:LYS:HZ3	1.78	0.95
1:A:558:GLN:CB	1:A:1171:GLU:HG3	1.95	0.95
1:F:558:GLN:CB	1:F:1171:GLU:HG3	1.95	0.95
1:G:1004:LYS:NZ	2:N:73:LYS:CG	2.29	0.95
1:B:560:PHE:CG	1:B:561:PRO:HD2	2.00	0.95
1:B:1004:LYS:NZ	2:I:73:LYS:CG	2.29	0.95
1:G:558:GLN:CB	1:G:1171:GLU:HG3	1.95	0.95
1:E:1004:LYS:NZ	2:L:73:LYS:CG	2.29	0.95
1:G:555:LEU:HD21	1:G:560:PHE:CE1	2.02	0.95
1:A:558:GLN:HG2	1:A:1171:GLU:CD	1.87	0.94
1:C:581:LYS:HZ1	1:C:1247:LEU:CD2	1.79	0.94
1:C:520:ALA:O	1:C:524:HIS:CD2	2.18	0.94
1:F:555:LEU:HD21	1:F:560:PHE:CE1	2.02	0.94
1:G:581:LYS:HZ1	1:G:1247:LEU:CD2	1.79	0.94
1:A:560:PHE:CG	1:A:561:PRO:HD2	2.00	0.94
1:B:558:GLN:HG2	1:B:1171:GLU:CD	1.86	0.94
1:C:348:LYS:HE3	1:C:447:GLU:CG	1.97	0.94
1:B:520:ALA:O	1:B:524:HIS:CD2	2.19	0.94
1:D:1048:LYS:CD	2:K:86:LYS:HZ3	1.80	0.94
1:B:558:GLN:CB	1:B:1171:GLU:HG3	1.95	0.94
1:D:1004:LYS:NZ	2:K:73:LYS:CG	2.29	0.94
1:D:1048:LYS:HD2	2:K:86:LYS:HZ3	1.32	0.94
1:G:1004:LYS:HZ2	2:N:73:LYS:HG2	1.33	0.94
1:G:558:GLN:HG2	1:G:1171:GLU:CD	1.87	0.94
1:C:558:GLN:HG2	1:C:1171:GLU:CD	1.87	0.94
1:D:348:LYS:HE3	1:D:447:GLU:CG	1.97	0.94
1:A:1004:LYS:NZ	2:H:73:LYS:CG	2.29	0.94
1:F:1004:LYS:NZ	2:M:73:LYS:CG	2.29	0.94
1:B:214:GLN:OE1	1:C:213:SER:OG	1.73	0.94
1:B:348:LYS:HE3	1:B:447:GLU:CG	1.97	0.94
1:D:1169:SER:HB3	1:D:1170:GLU:CG	1.98	0.94
1:E:1169:SER:HB3	1:E:1170:GLU:CG	1.98	0.94
1:F:581:LYS:HZ1	1:F:1247:LEU:CD2	1.80	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1089:LEU:HA	2:I:86:LYS:CE	1.97	0.94
1:C:1089:LEU:HA	2:J:86:LYS:CE	1.98	0.94
1:D:1089:LEU:HA	2:K:86:LYS:CE	1.97	0.94
1:E:1004:LYS:HZ3	2:L:73:LYS:CG	1.80	0.94
1:B:581:LYS:HZ1	1:B:1247:LEU:CD2	1.79	0.94
1:C:1169:SER:HB3	1:C:1170:GLU:CG	1.98	0.94
1:D:558:GLN:HG2	1:D:1171:GLU:CD	1.87	0.93
1:E:1169:SER:CA	1:E:1170:GLU:CB	2.39	0.93
1:F:558:GLN:HG2	1:F:1171:GLU:CD	1.87	0.93
1:G:565:GLN:HE21	1:G:592:MET:CE	1.58	0.93
1:A:1089:LEU:HA	2:H:86:LYS:CE	1.98	0.93
1:C:555:LEU:HD21	1:C:560:PHE:CE1	2.02	0.93
1:E:1089:LEU:HA	2:L:86:LYS:CE	1.98	0.93
1:E:555:LEU:HD21	1:E:560:PHE:CE1	2.02	0.93
1:E:558:GLN:HG2	1:E:1171:GLU:CD	1.87	0.93
1:A:1169:SER:HB3	1:A:1170:GLU:CG	1.98	0.93
1:C:1004:LYS:NZ	2:J:73:LYS:CG	2.29	0.93
1:E:348:LYS:HE3	1:E:447:GLU:CG	1.97	0.93
1:D:555:LEU:HD21	1:D:560:PHE:CE1	2.02	0.93
1:F:1169:SER:HB3	1:F:1170:GLU:CG	1.98	0.93
1:G:348:LYS:HE3	1:G:447:GLU:CG	1.97	0.93
1:E:1048:LYS:CD	2:L:86:LYS:HZ3	1.82	0.93
1:A:555:LEU:HD21	1:A:560:PHE:CE1	2.02	0.93
1:F:348:LYS:HE3	1:F:447:GLU:CG	1.97	0.93
1:A:348:LYS:HE3	1:A:447:GLU:CG	1.97	0.92
1:F:1089:LEU:HA	2:M:86:LYS:CE	1.98	0.92
1:G:1169:SER:HB3	1:G:1170:GLU:CG	1.98	0.92
1:G:581:LYS:NZ	1:G:1247:LEU:CD2	2.33	0.92
1:C:1169:SER:CB	1:C:1170:GLU:CA	2.47	0.92
1:F:1023:ASP:CG	2:M:73:LYS:CD	2.38	0.92
1:F:581:LYS:NZ	1:F:1247:LEU:CD2	2.33	0.92
1:F:208:GLN:CB	1:G:229:ILE:HD13	1.99	0.92
1:A:1169:SER:CA	1:A:1170:GLU:CB	2.39	0.92
1:A:229:ILE:HD13	1:G:208:GLN:CB	1.99	0.92
1:G:1048:LYS:HD2	2:N:86:LYS:HZ1	1.29	0.92
1:E:565:GLN:HE21	1:E:592:MET:CE	1.58	0.92
1:G:1004:LYS:HZ3	2:N:73:LYS:HG2	1.22	0.92
1:B:1169:SER:HB3	1:B:1170:GLU:CG	1.98	0.92
1:C:1048:LYS:CD	2:J:86:LYS:HZ3	1.82	0.92
1:C:565:GLN:HE21	1:C:592:MET:CE	1.58	0.92
1:C:208:GLN:CB	1:D:229:ILE:HD13	1.99	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:LYS:HD2	2:H:86:LYS:HZ3	1.29	0.92
1:D:1023:ASP:CG	2:K:73:LYS:CD	2.38	0.92
1:E:208:GLN:CB	1:F:229:ILE:HD13	1.99	0.92
1:F:1169:SER:CA	1:F:1170:GLU:CB	2.39	0.92
1:A:581:LYS:NZ	1:A:1247:LEU:CD2	2.33	0.91
1:B:555:LEU:HD21	1:B:560:PHE:CE1	2.02	0.91
1:E:1023:ASP:CG	2:L:73:LYS:CD	2.38	0.91
1:E:581:LYS:NZ	1:E:1247:LEU:CD2	2.33	0.91
1:B:581:LYS:NZ	1:B:1247:LEU:CD2	2.33	0.91
1:C:581:LYS:NZ	1:C:1247:LEU:CD2	2.33	0.91
1:D:208:GLN:CB	1:E:229:ILE:HD13	1.99	0.91
1:D:558:GLN:HA	1:D:1171:GLU:CG	2.00	0.91
1:A:1023:ASP:CG	2:H:73:LYS:CD	2.38	0.91
1:E:581:LYS:HZ1	1:E:1247:LEU:CD2	1.82	0.91
1:G:1023:ASP:CG	2:N:73:LYS:CD	2.38	0.91
1:G:1089:LEU:HA	2:N:86:LYS:CE	1.98	0.91
1:G:565:GLN:HE21	1:G:592:MET:HE2	1.35	0.91
1:C:558:GLN:HA	1:C:1171:GLU:CG	2.00	0.91
1:C:1023:ASP:CG	2:J:73:LYS:CD	2.38	0.91
1:A:208:GLN:CB	1:B:229:ILE:HD13	1.99	0.91
1:D:559:PRO:CB	1:D:1175:THR:H	1.84	0.91
1:C:340:TYR:HH	1:D:409:GLU:CD	1.73	0.91
1:F:559:PRO:CB	1:F:1175:THR:H	1.84	0.91
1:G:559:PRO:CB	1:G:1175:THR:H	1.84	0.91
1:A:565:GLN:HE21	1:A:592:MET:HE2	1.36	0.91
1:C:559:PRO:HB3	1:C:1174:ALA:CA	2.01	0.91
1:E:558:GLN:HA	1:E:1171:GLU:CG	2.00	0.91
1:F:559:PRO:HB2	1:F:1174:ALA:CA	2.01	0.91
1:B:1088:VAL:C	2:I:86:LYS:HE3	1.91	0.90
1:B:208:GLN:CB	1:C:229:ILE:HD13	1.99	0.90
1:C:1088:VAL:C	2:J:86:LYS:HE3	1.91	0.90
1:A:558:GLN:HA	1:A:1171:GLU:CG	2.00	0.90
1:F:565:GLN:HE21	1:F:592:MET:CE	1.58	0.90
1:G:558:GLN:HA	1:G:1171:GLU:CG	2.00	0.90
1:D:558:GLN:CG	1:D:1171:GLU:CG	2.21	0.90
1:F:1048:LYS:HG3	2:M:86:LYS:HZ1	1.32	0.90
1:G:1169:SER:CB	1:G:1170:GLU:CA	2.47	0.90
1:B:1023:ASP:CG	2:I:73:LYS:CD	2.38	0.90
1:A:559:PRO:HB3	1:A:1174:ALA:CA	2.01	0.90
1:B:559:PRO:CB	1:B:1175:THR:H	1.84	0.90
1:D:581:LYS:NZ	1:D:1247:LEU:CD2	2.33	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1169:SER:CB	1:E:1170:GLU:CA	2.47	0.90
1:C:1063:PHE:CZ	2:J:86:LYS:HG3	2.06	0.90
1:A:559:PRO:HB2	1:A:1174:ALA:CA	2.01	0.90
1:A:581:LYS:NZ	1:A:1247:LEU:HD21	1.87	0.90
1:B:581:LYS:NZ	1:B:1247:LEU:HD21	1.87	0.90
1:E:559:PRO:HB3	1:E:1174:ALA:CA	2.01	0.90
1:A:1088:VAL:C	2:H:86:LYS:HE3	1.91	0.90
1:B:558:GLN:HA	1:B:1171:GLU:CG	2.00	0.90
1:F:558:GLN:HA	1:F:1171:GLU:CG	2.00	0.90
1:A:559:PRO:CB	1:A:1175:THR:H	1.84	0.90
1:D:559:PRO:HB3	1:D:1174:ALA:CA	2.01	0.90
1:E:559:PRO:CB	1:E:1175:THR:H	1.84	0.90
1:F:1088:VAL:C	2:M:86:LYS:HE3	1.91	0.90
1:G:559:PRO:HB3	1:G:1174:ALA:CA	2.01	0.90
1:B:1048:LYS:HG3	2:I:86:LYS:HZ1	1.36	0.90
1:D:1088:VAL:C	2:K:86:LYS:HE3	1.91	0.89
1:F:559:PRO:HB3	1:F:1174:ALA:CA	2.01	0.89
1:B:1169:SER:CB	1:B:1170:GLU:CA	2.47	0.89
1:C:581:LYS:NZ	1:C:1247:LEU:HD21	1.87	0.89
1:A:565:GLN:HE21	1:A:592:MET:CE	1.58	0.89
1:C:559:PRO:CB	1:C:1175:THR:H	1.84	0.89
1:G:1088:VAL:C	2:N:86:LYS:HE3	1.91	0.89
1:G:581:LYS:NZ	1:G:1247:LEU:HD21	1.87	0.89
1:B:565:GLN:HE22	1:B:592:MET:HE3	0.73	0.89
1:C:1023:ASP:HB2	2:J:73:LYS:HZ3	1.37	0.89
1:D:1023:ASP:HB2	2:K:73:LYS:HZ3	1.37	0.89
1:E:1088:VAL:C	2:L:86:LYS:HE3	1.91	0.89
1:B:559:PRO:HB3	1:B:1174:ALA:CA	2.01	0.89
1:C:559:PRO:HB2	1:C:1174:ALA:CA	2.01	0.89
1:B:1063:PHE:CZ	2:I:86:LYS:HG3	2.06	0.89
1:F:1048:LYS:CD	2:M:86:LYS:HZ3	1.86	0.89
1:F:581:LYS:NZ	1:F:1247:LEU:HD21	1.87	0.89
1:D:559:PRO:HB2	1:D:1174:ALA:CA	2.01	0.88
1:C:1048:LYS:HD2	2:J:86:LYS:HZ3	1.35	0.88
1:D:581:LYS:NZ	1:D:1247:LEU:HD21	1.87	0.88
1:E:581:LYS:NZ	1:E:1247:LEU:HD21	1.87	0.88
1:F:340:TYR:CE1	1:G:409:GLU:CD	2.47	0.88
1:G:1169:SER:CA	1:G:1170:GLU:CB	2.39	0.88
1:G:559:PRO:HB2	1:G:1174:ALA:CA	2.01	0.88
1:C:340:TYR:CE1	1:D:409:GLU:CD	2.47	0.88
1:A:340:TYR:HH	1:B:409:GLU:CD	1.73	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:TYR:CE1	1:E:409:GLU:CD	2.47	0.88
1:E:340:TYR:CE1	1:F:409:GLU:CD	2.47	0.87
1:B:559:PRO:HB2	1:B:1174:ALA:CA	2.01	0.87
1:A:409:GLU:CD	1:G:340:TYR:CE1	2.47	0.87
1:A:409:GLU:OE2	1:G:340:TYR:CZ	2.28	0.87
1:B:340:TYR:CZ	1:C:409:GLU:OE2	2.28	0.87
1:C:214:GLN:OE1	1:D:213:SER:OG	1.74	0.87
1:A:348:LYS:HG3	1:A:352:ARG:HD2	1.57	0.87
1:E:340:TYR:CZ	1:F:409:GLU:OE2	2.28	0.87
1:A:1063:PHE:CZ	2:H:86:LYS:HG3	2.06	0.87
1:D:340:TYR:CZ	1:E:409:GLU:OE2	2.28	0.87
1:B:348:LYS:HG3	1:B:352:ARG:HD2	1.57	0.86
1:A:340:TYR:CZ	1:B:409:GLU:OE2	2.28	0.86
1:C:340:TYR:CZ	1:D:409:GLU:OE2	2.28	0.86
1:E:340:TYR:HH	1:F:409:GLU:CD	1.76	0.86
1:C:348:LYS:HG3	1:C:352:ARG:HD2	1.57	0.86
1:F:340:TYR:HH	1:G:409:GLU:CD	1.73	0.86
1:A:340:TYR:CE1	1:B:409:GLU:CD	2.47	0.86
1:E:348:LYS:HG3	1:E:352:ARG:HD2	1.57	0.86
1:F:340:TYR:CZ	1:G:409:GLU:OE2	2.28	0.86
1:F:1004:LYS:HZ3	2:M:73:LYS:CG	1.83	0.86
1:C:1089:LEU:CA	2:J:86:LYS:HE2	2.04	0.86
1:B:340:TYR:CE1	1:C:409:GLU:CD	2.47	0.86
1:G:1063:PHE:CZ	2:N:86:LYS:HG3	2.06	0.86
1:A:1048:LYS:CG	2:H:86:LYS:HZ1	1.88	0.85
1:D:1169:SER:CB	1:D:1170:GLU:CA	2.47	0.85
1:F:1048:LYS:CG	2:M:86:LYS:HZ1	1.88	0.85
1:F:560:PHE:CD2	1:F:561:PRO:O	2.30	0.85
1:G:348:LYS:HG3	1:G:352:ARG:HD2	1.57	0.85
1:D:1089:LEU:CA	2:K:86:LYS:HE2	2.04	0.85
1:D:588:VAL:HG12	1:D:589:ASP:N	1.92	0.85
1:C:560:PHE:CD2	1:C:561:PRO:O	2.30	0.85
1:F:348:LYS:HG3	1:F:352:ARG:HD2	1.57	0.85
2:I:14:CYS:HG	4:I:500:HEM:HAB	1.41	0.85
1:D:340:TYR:HH	1:E:409:GLU:CD	1.76	0.85
1:F:1063:PHE:CZ	2:M:86:LYS:HG3	2.06	0.85
1:B:558:GLN:CG	1:B:1171:GLU:CG	2.21	0.85
1:G:560:PHE:CD2	1:G:561:PRO:O	2.30	0.85
1:C:588:VAL:HG12	1:C:589:ASP:N	1.92	0.85
1:B:1089:LEU:CA	2:I:86:LYS:HE2	2.04	0.85
1:C:1048:LYS:CG	2:J:86:LYS:HZ1	1.88	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:VAL:HG12	1:A:589:ASP:N	1.92	0.85
1:D:560:PHE:CD2	1:D:561:PRO:O	2.30	0.85
1:A:1169:SER:CB	1:A:1170:GLU:CA	2.47	0.84
1:E:560:PHE:CD2	1:E:561:PRO:O	2.30	0.84
1:F:1169:SER:CB	1:F:1170:GLU:CA	2.47	0.84
1:B:560:PHE:CD2	1:B:561:PRO:O	2.30	0.84
1:E:208:GLN:CG	1:F:229:ILE:CD1	2.55	0.84
1:F:208:GLN:CG	1:G:229:ILE:CD1	2.55	0.84
1:F:588:VAL:HG12	1:F:589:ASP:N	1.92	0.84
1:A:560:PHE:CD2	1:A:561:PRO:O	2.30	0.84
1:E:558:GLN:CG	1:E:1171:GLU:CG	2.21	0.84
1:E:588:VAL:HG12	1:E:589:ASP:N	1.92	0.84
1:F:1089:LEU:CA	2:M:86:LYS:HE2	2.04	0.84
1:A:409:GLU:CD	1:G:340:TYR:CZ	2.51	0.84
1:B:208:GLN:CG	1:C:229:ILE:CD1	2.55	0.84
1:D:348:LYS:HG3	1:D:352:ARG:HD2	1.57	0.84
1:D:565:GLN:HE21	1:D:592:MET:CE	1.58	0.84
1:B:1048:LYS:CD	2:I:86:LYS:HZ3	1.90	0.84
1:B:1169:SER:N	1:B:1170:GLU:CB	2.41	0.84
1:E:340:TYR:CZ	1:F:409:GLU:CD	2.51	0.84
1:A:229:ILE:CD1	1:G:208:GLN:CG	2.55	0.84
1:G:1048:LYS:CD	2:N:86:LYS:HZ1	1.84	0.84
1:A:1169:SER:N	1:A:1170:GLU:CB	2.41	0.84
1:B:588:VAL:HG12	1:B:589:ASP:N	1.92	0.84
1:F:558:GLN:CG	1:F:1171:GLU:CG	2.21	0.84
1:E:1023:ASP:HB2	2:L:73:LYS:NZ	1.93	0.84
1:C:168:VAL:HG12	1:C:168:VAL:O	1.78	0.84
1:E:1063:PHE:CZ	2:L:86:LYS:HG3	2.06	0.84
1:C:208:GLN:CG	1:D:229:ILE:CD1	2.55	0.83
1:G:1089:LEU:CA	2:N:86:LYS:HE2	2.04	0.83
1:A:208:GLN:CG	1:B:229:ILE:CD1	2.55	0.83
1:E:565:GLN:HE22	1:E:592:MET:HE3	0.78	0.83
1:D:1023:ASP:HB2	2:K:73:LYS:NZ	1.93	0.83
1:E:1089:LEU:CA	2:L:86:LYS:HE2	2.04	0.83
1:D:208:GLN:CG	1:E:229:ILE:CD1	2.55	0.83
1:F:1023:ASP:HB2	2:M:73:LYS:NZ	1.93	0.83
1:E:1048:LYS:CG	2:L:86:LYS:HZ1	1.88	0.83
1:G:1169:SER:N	1:G:1170:GLU:CB	2.41	0.83
1:F:1169:SER:N	1:F:1170:GLU:CB	2.41	0.83
1:G:588:VAL:HG12	1:G:589:ASP:N	1.92	0.83
1:A:1089:LEU:CA	2:H:86:LYS:HE2	2.04	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:558:GLN:CG	1:C:1171:GLU:CG	2.21	0.83
1:C:565:GLN:HE22	1:C:592:MET:HE3	0.82	0.83
1:A:340:TYR:CZ	1:B:409:GLU:CD	2.51	0.83
1:C:1169:SER:N	1:C:1170:GLU:CB	2.41	0.83
1:D:1169:SER:N	1:D:1170:GLU:CB	2.41	0.83
1:D:340:TYR:CZ	1:E:409:GLU:CD	2.51	0.83
1:C:1004:LYS:HZ3	2:J:73:LYS:CG	1.87	0.83
1:E:1169:SER:N	1:E:1170:GLU:CB	2.41	0.83
1:F:340:TYR:CZ	1:G:409:GLU:CD	2.51	0.83
1:A:168:VAL:O	1:A:168:VAL:HG12	1.77	0.82
1:B:340:TYR:CZ	1:C:409:GLU:CD	2.51	0.82
1:C:588:VAL:HG12	1:C:589:ASP:H	1.44	0.82
1:D:168:VAL:HG12	1:D:168:VAL:O	1.77	0.82
1:G:1048:LYS:HG3	2:N:86:LYS:HZ1	1.40	0.82
1:E:168:VAL:HG12	1:E:168:VAL:O	1.77	0.82
1:F:565:GLN:HE21	1:F:592:MET:HE2	1.43	0.82
1:G:168:VAL:O	1:G:168:VAL:HG12	1.77	0.82
1:B:1048:LYS:CD	2:I:86:LYS:HZ1	1.89	0.82
1:E:588:VAL:HG12	1:E:589:ASP:H	1.44	0.82
1:C:1023:ASP:HB2	2:J:73:LYS:NZ	1.93	0.82
1:C:1063:PHE:CE2	2:J:86:LYS:HG2	2.14	0.82
1:D:1004:LYS:HZ3	2:K:73:LYS:CG	1.85	0.82
1:C:340:TYR:CZ	1:D:409:GLU:CD	2.51	0.82
1:D:1063:PHE:CE2	2:K:86:LYS:HG2	2.14	0.82
1:B:1048:LYS:HD2	2:I:86:LYS:HZ1	1.36	0.82
1:D:588:VAL:HG12	1:D:589:ASP:H	1.44	0.82
1:F:168:VAL:HG12	1:F:168:VAL:O	1.78	0.82
1:G:1023:ASP:HB2	2:N:73:LYS:NZ	1.93	0.82
1:B:588:VAL:HG12	1:B:589:ASP:H	1.44	0.82
1:A:558:GLN:CG	1:A:1171:GLU:CG	2.21	0.82
1:A:588:VAL:HG12	1:A:589:ASP:H	1.44	0.82
1:D:1063:PHE:CZ	2:K:86:LYS:HG3	2.06	0.82
1:B:1023:ASP:HB2	2:I:73:LYS:NZ	1.93	0.82
1:B:168:VAL:O	1:B:168:VAL:HG12	1.77	0.81
1:A:1004:LYS:HZ3	2:H:73:LYS:CG	1.88	0.81
1:E:565:GLN:NE2	1:E:592:MET:HE2	1.82	0.81
1:B:1063:PHE:CE2	2:I:86:LYS:HG2	2.14	0.81
1:A:1023:ASP:HB2	2:H:73:LYS:NZ	1.93	0.81
1:G:588:VAL:HG12	1:G:589:ASP:H	1.44	0.81
1:G:1023:ASP:HB2	2:N:73:LYS:HZ3	1.45	0.81
2:N:17:CYS:HG	4:N:500:HEM:CAC	1.93	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1048:LYS:CG	2:N:86:LYS:HZ1	1.90	0.81
1:E:1063:PHE:CE2	2:L:86:LYS:HG2	2.14	0.81
1:F:1048:LYS:HD2	2:M:86:LYS:HZ1	1.42	0.81
1:F:588:VAL:HG12	1:F:589:ASP:H	1.44	0.81
1:D:1048:LYS:CG	2:K:86:LYS:HZ1	1.88	0.80
1:C:1023:ASP:OD2	2:J:73:LYS:CD	2.30	0.80
1:F:1048:LYS:CD	2:M:86:LYS:HZ1	1.93	0.80
1:E:559:PRO:HB2	1:E:1174:ALA:CA	2.01	0.80
1:F:1023:ASP:OD2	2:M:73:LYS:CD	2.30	0.80
1:B:1023:ASP:OD2	2:I:73:LYS:CD	2.30	0.80
1:C:565:GLN:NE2	1:C:592:MET:HE2	1.87	0.80
1:A:1023:ASP:OD2	2:H:73:LYS:CD	2.30	0.79
1:G:1023:ASP:OD2	2:N:73:LYS:CD	2.30	0.79
1:A:1063:PHE:CE2	2:H:86:LYS:HG2	2.14	0.79
2:H:14:CYS:HG	4:H:500:HEM:HAB	1.46	0.79
1:B:1048:LYS:CG	2:I:86:LYS:HZ1	1.89	0.79
1:B:340:TYR:OH	1:C:409:GLU:CG	2.31	0.79
1:C:340:TYR:OH	1:D:409:GLU:CG	2.31	0.79
1:B:588:VAL:CG1	1:B:589:ASP:H	1.96	0.79
1:D:340:TYR:OH	1:E:409:GLU:CG	2.31	0.79
1:G:588:VAL:CG1	1:G:589:ASP:H	1.96	0.79
1:F:1048:LYS:HD2	2:M:86:LYS:HZ3	1.41	0.78
1:G:1063:PHE:CE2	2:N:86:LYS:HG2	2.14	0.78
1:A:340:TYR:OH	1:B:409:GLU:CG	2.31	0.78
1:D:588:VAL:CG1	1:D:589:ASP:H	1.96	0.78
1:F:1063:PHE:CE2	2:M:86:LYS:HG2	2.14	0.78
1:E:588:VAL:CG1	1:E:589:ASP:H	1.96	0.78
1:A:588:VAL:CG1	1:A:589:ASP:H	1.96	0.78
1:E:340:TYR:OH	1:F:409:GLU:CG	2.31	0.78
1:E:1048:LYS:HD2	2:L:86:LYS:HZ3	1.35	0.78
1:F:588:VAL:CG1	1:F:589:ASP:H	1.96	0.78
1:F:565:GLN:NE2	1:F:592:MET:HE2	1.95	0.78
1:E:205:ARG:CZ	1:F:225:ASP:CG	2.53	0.77
1:G:1168:LEU:C	1:G:1170:GLU:OE1	2.23	0.77
1:C:1168:LEU:C	1:C:1170:GLU:OE1	2.23	0.77
1:C:348:LYS:CG	1:C:352:ARG:CD	2.62	0.77
1:C:588:VAL:CG1	1:C:589:ASP:H	1.96	0.77
1:A:409:GLU:CG	1:G:340:TYR:OH	2.31	0.77
1:B:1168:LEU:C	1:B:1170:GLU:OE1	2.23	0.77
1:B:205:ARG:CZ	1:C:225:ASP:CG	2.53	0.77
1:F:1168:LEU:C	1:F:1170:GLU:OE1	2.23	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:LYS:CG	1:B:352:ARG:CD	2.62	0.77
1:A:225:ASP:CG	1:G:205:ARG:CZ	2.53	0.77
1:A:565:GLN:HE22	1:A:592:MET:HE3	0.87	0.77
1:E:1168:LEU:C	1:E:1170:GLU:OE1	2.23	0.77
1:A:1023:ASP:HB2	2:H:73:LYS:HZ3	1.49	0.77
1:D:565:GLN:HE21	1:D:592:MET:HE2	1.49	0.77
1:D:565:GLN:HE22	1:D:592:MET:HE3	0.98	0.77
1:E:1173:ALA:O	1:E:1174:ALA:HB3	1.85	0.77
1:B:1048:LYS:HD2	2:I:86:LYS:HZ3	1.46	0.77
1:A:558:GLN:CA	1:A:1171:GLU:HG2	2.13	0.76
1:C:1004:LYS:HZ2	2:J:73:LYS:CG	1.98	0.76
1:D:1168:LEU:C	1:D:1170:GLU:OE1	2.23	0.76
1:F:340:TYR:OH	1:G:409:GLU:CG	2.31	0.76
1:B:565:GLN:NE2	1:B:592:MET:HE2	1.65	0.76
1:F:205:ARG:CZ	1:G:225:ASP:CG	2.53	0.76
1:G:558:GLN:CG	1:G:1171:GLU:CG	2.21	0.76
1:D:205:ARG:CZ	1:E:225:ASP:CG	2.53	0.76
1:G:1048:LYS:CD	2:N:86:LYS:HZ3	1.95	0.76
1:C:1173:ALA:O	1:C:1174:ALA:HB3	1.85	0.76
1:B:1173:ALA:O	1:B:1174:ALA:HB3	1.85	0.76
1:A:205:ARG:CZ	1:B:225:ASP:CG	2.53	0.76
1:E:1023:ASP:OD2	2:L:73:LYS:CD	2.30	0.76
1:A:1168:LEU:C	1:A:1170:GLU:OE1	2.23	0.76
1:C:205:ARG:CZ	1:D:225:ASP:CG	2.53	0.76
1:F:565:GLN:HE22	1:F:592:MET:HE3	0.93	0.76
1:C:555:LEU:HD22	1:C:560:PHE:HE1	1.50	0.75
1:A:1004:LYS:HZ2	2:H:73:LYS:CG	1.97	0.75
2:L:17:CYS:HG	4:L:500:HEM:CAC	1.98	0.75
1:G:565:GLN:HE22	1:G:592:MET:HE3	0.86	0.75
1:F:1173:ALA:O	1:F:1174:ALA:HB3	1.86	0.75
1:E:1048:LYS:HD2	2:L:86:LYS:HZ1	1.48	0.75
1:F:558:GLN:CA	1:F:1171:GLU:HG2	2.13	0.75
1:G:1173:ALA:O	1:G:1174:ALA:HB3	1.86	0.75
1:C:1004:LYS:HZ2	2:J:73:LYS:HG2	1.49	0.75
1:D:1023:ASP:OD2	2:K:73:LYS:CD	2.30	0.75
1:E:208:GLN:CA	1:F:229:ILE:HD13	2.17	0.75
1:G:559:PRO:HB3	1:G:1174:ALA:C	2.07	0.75
1:C:208:GLN:CA	1:D:229:ILE:HD13	2.17	0.75
1:D:1173:ALA:O	1:D:1174:ALA:HB3	1.86	0.75
1:D:559:PRO:HB3	1:D:1174:ALA:C	2.07	0.75
1:E:559:PRO:HB3	1:E:1174:ALA:C	2.07	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:GLN:CA	1:C:229:ILE:HD13	2.17	0.74
1:C:560:PHE:CE1	1:C:561:PRO:HD2	2.22	0.74
1:B:559:PRO:HB3	1:B:1174:ALA:C	2.07	0.74
1:F:348:LYS:CG	1:F:352:ARG:CD	2.62	0.74
1:A:1173:ALA:O	1:A:1174:ALA:HB3	1.86	0.74
1:B:555:LEU:HD23	1:B:560:PHE:CD1	2.22	0.74
1:D:560:PHE:CE1	1:D:561:PRO:HD2	2.22	0.74
1:F:208:GLN:CA	1:G:229:ILE:HD13	2.17	0.74
1:A:208:GLN:CA	1:B:229:ILE:HD13	2.17	0.74
1:C:558:GLN:CB	1:C:1171:GLU:CG	2.63	0.74
1:E:1023:ASP:HB2	2:L:73:LYS:HZ3	1.52	0.74
1:A:229:ILE:HD13	1:G:208:GLN:CA	2.17	0.74
1:C:558:GLN:CA	1:C:1171:GLU:HG2	2.13	0.74
1:C:555:LEU:HD23	1:C:560:PHE:CD1	2.22	0.74
1:D:565:GLN:HE21	1:D:592:MET:HE3	1.13	0.74
1:A:555:LEU:HD23	1:A:560:PHE:CD1	2.22	0.74
1:A:559:PRO:HB3	1:A:1174:ALA:C	2.07	0.74
1:D:348:LYS:CG	1:D:352:ARG:CD	2.62	0.74
1:F:559:PRO:HB3	1:F:1174:ALA:C	2.07	0.74
1:G:558:GLN:CB	1:G:1171:GLU:CG	2.63	0.74
1:F:558:GLN:CB	1:F:1171:GLU:CG	2.63	0.74
1:C:348:LYS:HE3	1:C:447:GLU:CD	2.09	0.73
1:D:208:GLN:CA	1:E:229:ILE:HD13	2.17	0.73
1:E:560:PHE:CE1	1:E:561:PRO:HD2	2.22	0.73
1:F:555:LEU:HD23	1:F:560:PHE:CD1	2.22	0.73
1:G:348:LYS:CG	1:G:352:ARG:CD	2.62	0.73
1:C:559:PRO:HB3	1:C:1174:ALA:C	2.07	0.73
1:A:348:LYS:HE3	1:A:447:GLU:CD	2.09	0.73
1:B:348:LYS:HE3	1:B:447:GLU:CD	2.09	0.73
1:D:348:LYS:HE3	1:D:447:GLU:CD	2.09	0.73
1:D:1004:LYS:HZ2	2:K:73:LYS:HG2	1.52	0.73
1:D:555:LEU:HD23	1:D:560:PHE:CD1	2.22	0.73
1:E:555:LEU:HD22	1:E:560:PHE:HE1	1.50	0.73
1:G:558:GLN:CA	1:G:1171:GLU:HG2	2.13	0.73
1:G:348:LYS:HE3	1:G:447:GLU:CD	2.09	0.73
1:A:565:GLN:HG2	1:A:594:TYR:OH	1.89	0.73
1:C:565:GLN:HG2	1:C:594:TYR:OH	1.89	0.73
1:G:1063:PHE:CD1	2:N:69:GLU:OE1	2.42	0.73
1:G:555:LEU:HD22	1:G:560:PHE:HE1	1.50	0.73
1:A:1063:PHE:CD1	2:H:69:GLU:OE1	2.42	0.73
1:A:565:GLN:HG2	1:A:594:TYR:CE2	2.24	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:GLN:HG2	1:B:594:TYR:CE2	2.24	0.73
1:C:565:GLN:HG2	1:C:594:TYR:CE2	2.24	0.73
1:E:348:LYS:HE3	1:E:447:GLU:CD	2.09	0.73
1:G:555:LEU:HD23	1:G:560:PHE:CD1	2.22	0.73
1:F:1063:PHE:CD1	2:M:69:GLU:OE1	2.42	0.73
1:E:1063:PHE:CD1	2:L:69:GLU:OE1	2.42	0.73
1:E:565:GLN:HG2	1:E:594:TYR:OH	1.89	0.73
1:F:348:LYS:HE3	1:F:447:GLU:CD	2.09	0.73
1:G:565:GLN:HG2	1:G:594:TYR:OH	1.89	0.73
1:G:565:GLN:HG2	1:G:594:TYR:CE2	2.24	0.73
1:B:565:GLN:HG2	1:B:594:TYR:OH	1.89	0.72
1:D:565:GLN:HG2	1:D:594:TYR:OH	1.89	0.72
1:F:560:PHE:CE1	1:F:561:PRO:HD2	2.22	0.72
1:F:1004:LYS:HZ2	2:M:73:LYS:HG2	1.53	0.72
2:H:17:CYS:SG	4:H:500:HEM:CAC	2.78	0.72
2:L:17:CYS:SG	4:L:500:HEM:CAC	2.78	0.72
1:B:558:GLN:CA	1:B:1171:GLU:HG2	2.13	0.72
1:G:565:GLN:NE2	1:G:592:MET:HE2	1.90	0.72
2:N:17:CYS:SG	4:N:500:HEM:CAC	2.77	0.72
1:D:558:GLN:CB	1:D:1171:GLU:CG	2.63	0.72
1:E:558:GLN:CG	1:E:1171:GLU:CD	2.55	0.72
1:F:1004:LYS:HZ2	2:M:73:LYS:CG	2.02	0.72
1:B:1063:PHE:CD1	2:I:69:GLU:OE1	2.42	0.72
1:D:565:GLN:HG2	1:D:594:TYR:CE2	2.24	0.72
2:I:17:CYS:SG	4:I:500:HEM:CAC	2.78	0.72
1:A:560:PHE:CE1	1:A:561:PRO:HD2	2.22	0.72
1:E:558:GLN:CB	1:E:1171:GLU:CG	2.63	0.72
1:D:565:GLN:NE2	1:D:592:MET:HE1	1.98	0.72
1:E:348:LYS:CG	1:E:352:ARG:CD	2.62	0.72
1:E:555:LEU:HD23	1:E:560:PHE:CD1	2.22	0.72
1:E:565:GLN:HG2	1:E:594:TYR:CE2	2.24	0.72
1:A:348:LYS:CG	1:A:352:ARG:CD	2.62	0.72
1:A:555:LEU:HD23	1:A:560:PHE:HE1	1.21	0.72
2:K:17:CYS:SG	4:K:500:HEM:CAC	2.77	0.72
1:B:560:PHE:CE1	1:B:561:PRO:HD2	2.22	0.72
2:J:17:CYS:SG	4:J:500:HEM:CAC	2.78	0.72
1:A:348:LYS:HG2	1:A:352:ARG:HB2	1.72	0.72
1:D:208:GLN:HA	1:E:229:ILE:HD13	1.72	0.72
1:A:1086:GLY:HA2	2:H:88:LYS:HB3	1.72	0.72
2:M:17:CYS:SG	4:M:500:HEM:CAC	2.78	0.72
1:F:1086:GLY:HA2	2:M:88:LYS:HB3	1.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1086:GLY:HA2	2:N:88:LYS:HB3	1.72	0.72
1:A:558:GLN:CB	1:A:1171:GLU:CG	2.63	0.71
1:E:1086:GLY:HA2	2:L:88:LYS:HB3	1.72	0.71
1:F:565:GLN:HG2	1:F:594:TYR:CE2	2.24	0.71
1:F:205:ARG:CZ	1:G:225:ASP:OD1	2.38	0.71
1:B:348:LYS:HG2	1:B:352:ARG:HB2	1.72	0.71
1:F:558:GLN:CG	1:F:1171:GLU:CD	2.55	0.71
1:G:348:LYS:HG2	1:G:352:ARG:HB2	1.72	0.71
1:B:558:GLN:HG2	1:B:1171:GLU:HG3	0.72	0.71
1:D:558:GLN:CA	1:D:1171:GLU:HG2	2.13	0.71
1:C:208:GLN:HA	1:D:229:ILE:HD13	1.72	0.71
1:E:205:ARG:NH1	1:F:225:ASP:CG	2.44	0.71
1:F:565:GLN:HG2	1:F:594:TYR:OH	1.89	0.71
1:F:208:GLN:HB3	1:G:229:ILE:HG21	1.73	0.71
1:D:1063:PHE:CD1	2:K:69:GLU:OE1	2.42	0.71
1:D:565:GLN:NE2	1:D:592:MET:HE2	1.98	0.71
1:E:208:GLN:HA	1:F:229:ILE:HD13	1.72	0.71
1:A:229:ILE:HG21	1:G:208:GLN:HB3	1.73	0.71
1:B:555:LEU:HD22	1:B:560:PHE:HE1	1.50	0.71
1:E:208:GLN:HB3	1:F:229:ILE:HG21	1.73	0.71
1:D:205:ARG:NH1	1:E:225:ASP:CG	2.44	0.71
1:F:348:LYS:HG2	1:F:352:ARG:HB2	1.72	0.71
1:G:560:PHE:CE1	1:G:561:PRO:HD2	2.22	0.71
1:C:1063:PHE:CD1	2:J:69:GLU:OE1	2.42	0.71
1:F:558:GLN:HG2	1:F:1171:GLU:HG3	0.72	0.71
1:F:1173:ALA:CB	1:F:1211:GLN:OE1	2.33	0.71
2:I:17:CYS:HG	4:I:500:HEM:CAC	2.03	0.71
1:D:558:GLN:HG2	1:D:1171:GLU:HG3	0.72	0.71
1:E:558:GLN:HG2	1:E:1171:GLU:HG3	0.72	0.71
1:B:208:GLN:HA	1:C:229:ILE:HD13	1.72	0.71
1:G:558:GLN:CA	1:G:1171:GLU:CG	2.69	0.71
1:A:701:GLN:CG	2:H:25:LYS:HD3	2.21	0.71
1:B:1086:GLY:HA2	2:I:88:LYS:HB3	1.72	0.71
1:A:225:ASP:OD1	1:G:205:ARG:CZ	2.38	0.71
1:A:205:ARG:CZ	1:B:225:ASP:OD1	2.38	0.71
1:F:558:GLN:CA	1:F:1171:GLU:CG	2.69	0.71
1:D:1004:LYS:HZ2	2:K:73:LYS:CG	2.01	0.71
1:B:701:GLN:CG	2:I:25:LYS:HD3	2.21	0.70
1:C:348:LYS:HG2	1:C:352:ARG:HB2	1.72	0.70
1:D:205:ARG:CZ	1:E:225:ASP:OD1	2.39	0.70
1:E:205:ARG:CZ	1:F:225:ASP:OD1	2.38	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1086:GLY:HA2	2:K:88:LYS:HB3	1.72	0.70
1:B:558:GLN:CA	1:B:1171:GLU:CG	2.69	0.70
1:D:208:GLN:HB3	1:E:229:ILE:HG21	1.73	0.70
1:G:701:GLN:CG	2:N:25:LYS:HD3	2.21	0.70
1:A:208:GLN:HB3	1:B:229:ILE:HG21	1.73	0.70
1:A:208:GLN:HA	1:B:229:ILE:HD13	1.72	0.70
1:C:1048:LYS:HD2	2:J:86:LYS:HZ1	1.48	0.70
1:E:701:GLN:CG	2:L:25:LYS:HD3	2.21	0.70
1:F:1023:ASP:HB2	2:M:73:LYS:HZ3	1.55	0.70
1:F:345:LEU:HG	1:F:349:GLN:HB3	1.74	0.70
1:A:225:ASP:CG	1:G:205:ARG:NH1	2.44	0.70
1:A:558:GLN:CA	1:A:1171:GLU:CG	2.69	0.70
1:B:588:VAL:O	1:B:589:ASP:C	2.30	0.70
1:E:558:GLN:CA	1:E:1171:GLU:HG2	2.13	0.70
1:F:205:ARG:NH1	1:G:225:ASP:CG	2.44	0.70
1:A:205:ARG:NH1	1:B:225:ASP:CG	2.44	0.70
1:C:588:VAL:CG1	1:C:589:ASP:N	2.55	0.70
1:C:205:ARG:CZ	1:D:225:ASP:OD1	2.38	0.70
1:F:208:GLN:HA	1:G:229:ILE:HD13	1.72	0.70
1:G:345:LEU:HG	1:G:349:GLN:HB3	1.74	0.70
1:A:229:ILE:HD13	1:G:208:GLN:HA	1.72	0.70
1:C:646:THR:HG23	1:C:648:GLU:N	2.04	0.70
1:C:1086:GLY:HA2	2:J:88:LYS:HB3	1.72	0.70
1:A:588:VAL:O	1:A:589:ASP:C	2.30	0.70
1:G:348:LYS:CG	1:G:352:ARG:HD2	2.21	0.70
1:A:348:LYS:CG	1:A:352:ARG:HD2	2.21	0.70
1:B:208:GLN:HB3	1:C:229:ILE:HG21	1.73	0.70
1:B:646:THR:HG23	1:B:648:GLU:N	2.04	0.70
1:E:345:LEU:HG	1:E:349:GLN:HB3	1.74	0.70
1:B:205:ARG:CZ	1:C:225:ASP:OD1	2.38	0.70
1:C:205:ARG:NH1	1:D:225:ASP:CG	2.44	0.70
1:C:208:GLN:HB3	1:D:229:ILE:HG21	1.73	0.70
1:E:1173:ALA:O	1:E:1174:ALA:CB	2.40	0.70
1:F:646:THR:HG23	1:F:648:GLU:N	2.04	0.70
1:C:558:GLN:HG2	1:C:1171:GLU:HG3	0.72	0.70
1:C:1173:ALA:CB	1:C:1211:GLN:OE1	2.33	0.70
1:C:701:GLN:CG	2:J:25:LYS:HD3	2.21	0.70
1:F:701:GLN:CG	2:M:25:LYS:HD3	2.21	0.70
1:A:345:LEU:HG	1:A:349:GLN:HB3	1.74	0.69
1:B:348:LYS:CG	1:B:352:ARG:HD2	2.21	0.69
1:B:205:ARG:NH1	1:C:225:ASP:CG	2.44	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:558:GLN:HG2	1:G:1171:GLU:HG3	0.72	0.69
1:C:348:LYS:CG	1:C:352:ARG:HD2	2.21	0.69
1:D:1048:LYS:HD2	2:K:86:LYS:HZ1	1.50	0.69
1:E:348:LYS:HG2	1:E:352:ARG:HB2	1.72	0.69
1:F:1173:ALA:O	1:F:1174:ALA:CB	2.40	0.69
1:F:555:LEU:HD23	1:F:560:PHE:HE1	1.21	0.69
1:A:1173:ALA:O	1:A:1174:ALA:CB	2.40	0.69
1:C:558:GLN:CA	1:C:1171:GLU:CG	2.69	0.69
1:C:588:VAL:O	1:C:589:ASP:C	2.30	0.69
1:E:558:GLN:CA	1:E:1171:GLU:CG	2.69	0.69
1:B:345:LEU:HG	1:B:349:GLN:HB3	1.74	0.69
1:D:1173:ALA:O	1:D:1174:ALA:CB	2.40	0.69
1:G:1169:SER:HB3	1:G:1170:GLU:HA	1.74	0.69
1:C:1007:TRP:HZ2	2:J:73:LYS:HZ1	0.72	0.69
1:B:1173:ALA:O	1:B:1174:ALA:CB	2.40	0.69
1:D:345:LEU:HG	1:D:349:GLN:HB3	1.74	0.69
1:G:1173:ALA:O	1:G:1174:ALA:CB	2.40	0.69
1:D:701:GLN:CG	2:K:25:LYS:HD3	2.21	0.69
1:F:558:GLN:OE1	1:F:1170:GLU:N	2.26	0.69
1:D:348:LYS:HG2	1:D:352:ARG:HB2	1.72	0.69
1:D:348:LYS:CG	1:D:352:ARG:HD2	2.21	0.69
1:A:588:VAL:CG1	1:A:589:ASP:N	2.55	0.69
1:D:558:GLN:OE1	1:D:1170:GLU:N	2.26	0.69
1:D:646:THR:HG23	1:D:648:GLU:N	2.04	0.69
1:E:348:LYS:CG	1:E:352:ARG:HD2	2.21	0.69
1:A:1077:LYS:O	1:A:1077:LYS:HD2	1.93	0.69
1:C:345:LEU:HG	1:C:349:GLN:HB3	1.74	0.69
1:D:588:VAL:O	1:D:589:ASP:C	2.30	0.69
1:F:348:LYS:CG	1:F:352:ARG:HD2	2.21	0.69
1:D:558:GLN:CA	1:D:1171:GLU:CG	2.69	0.69
1:D:1173:ALA:CB	1:D:1211:GLN:OE1	2.33	0.69
1:G:558:GLN:CG	1:G:1171:GLU:CD	2.55	0.69
1:C:1077:LYS:HD2	1:C:1077:LYS:O	1.93	0.69
1:C:558:GLN:OE1	1:C:1170:GLU:N	2.26	0.69
1:E:588:VAL:O	1:E:589:ASP:C	2.30	0.69
1:G:1048:LYS:HG3	2:N:86:LYS:HZ2	1.56	0.69
1:C:1048:LYS:CD	2:J:86:LYS:HZ1	1.97	0.69
1:D:1087:THR:H	2:K:88:LYS:H	1.40	0.69
1:F:1077:LYS:HD2	1:F:1077:LYS:O	1.93	0.68
1:F:1169:SER:HB3	1:F:1170:GLU:HA	1.74	0.68
1:G:558:GLN:OE1	1:G:1170:GLU:N	2.26	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLN:HB3	1:B:229:ILE:HD13	1.76	0.68
1:B:208:GLN:HB3	1:C:229:ILE:HD13	1.76	0.68
1:D:1169:SER:HB3	1:D:1170:GLU:HA	1.74	0.68
1:G:588:VAL:O	1:G:589:ASP:C	2.30	0.68
1:A:558:GLN:CG	1:A:1171:GLU:CD	2.55	0.68
1:A:565:GLN:NE2	1:A:592:MET:HE2	1.90	0.68
1:B:558:GLN:OE1	1:B:1170:GLU:N	2.26	0.68
1:C:1173:ALA:O	1:C:1174:ALA:CB	2.40	0.68
1:A:558:GLN:OE1	1:A:1170:GLU:N	2.26	0.68
1:C:1169:SER:HB3	1:C:1170:GLU:HA	1.74	0.68
1:E:1169:SER:HB3	1:E:1170:GLU:HA	1.74	0.68
1:E:558:GLN:OE1	1:E:1170:GLU:N	2.26	0.68
1:B:558:GLN:CB	1:B:1171:GLU:CG	2.63	0.68
1:E:560:PHE:CD1	1:E:561:PRO:CD	2.64	0.68
1:G:1087:THR:H	2:N:88:LYS:H	1.40	0.68
1:B:565:GLN:HE21	1:B:592:MET:CE	1.58	0.68
1:C:560:PHE:CD1	1:C:561:PRO:CD	2.64	0.68
1:F:588:VAL:O	1:F:589:ASP:C	2.30	0.68
1:C:208:GLN:HB3	1:D:229:ILE:HD13	1.76	0.68
1:A:229:ILE:HD13	1:G:208:GLN:HB3	1.76	0.68
1:A:558:GLN:HG2	1:A:1171:GLU:HG3	0.72	0.68
1:C:560:PHE:CG	1:C:561:PRO:CD	2.76	0.68
1:D:560:PHE:CG	1:D:561:PRO:CD	2.76	0.68
1:B:1087:THR:H	2:I:88:LYS:H	1.40	0.68
1:E:1048:LYS:CD	2:L:86:LYS:HZ1	1.97	0.67
1:B:1077:LYS:O	1:B:1077:LYS:HD2	1.93	0.67
1:D:1077:LYS:HD2	1:D:1077:LYS:O	1.93	0.67
1:D:555:LEU:HD22	1:D:560:PHE:HE1	1.50	0.67
1:A:560:PHE:CG	1:A:561:PRO:CD	2.76	0.67
1:B:558:GLN:CG	1:B:1171:GLU:CD	2.55	0.67
1:E:1077:LYS:O	1:E:1077:LYS:HD2	1.93	0.67
1:G:1077:LYS:O	1:G:1077:LYS:HD2	1.93	0.67
1:A:1087:THR:H	2:H:88:LYS:H	1.40	0.67
1:A:1048:LYS:HD2	2:H:86:LYS:HZ1	1.53	0.67
1:A:646:THR:HG23	1:A:648:GLU:N	2.04	0.67
1:D:208:GLN:HB3	1:E:229:ILE:HD13	1.75	0.67
1:E:1087:THR:H	2:L:88:LYS:H	1.40	0.67
1:F:1087:THR:H	2:M:88:LYS:H	1.40	0.67
1:B:560:PHE:CG	1:B:561:PRO:CD	2.76	0.67
1:C:588:VAL:O	1:C:590:ASN:CG	2.33	0.67
1:F:208:GLN:HB3	1:G:229:ILE:HD13	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:560:PHE:CG	1:G:561:PRO:CD	2.76	0.67
1:A:588:VAL:O	1:A:590:ASN:CG	2.33	0.67
1:B:588:VAL:O	1:B:590:ASN:CG	2.33	0.67
1:F:560:PHE:CG	1:F:561:PRO:CD	2.76	0.67
1:B:1169:SER:HB3	1:B:1170:GLU:HA	1.74	0.67
1:C:581:LYS:NZ	1:C:1247:LEU:HD22	2.10	0.67
1:F:588:VAL:O	1:F:590:ASN:CG	2.33	0.67
1:E:208:GLN:HB3	1:F:229:ILE:HD13	1.76	0.67
1:D:560:PHE:CD1	1:D:561:PRO:CD	2.64	0.67
1:E:588:VAL:O	1:E:590:ASN:CG	2.33	0.67
1:B:1173:ALA:CB	1:B:1211:GLN:OE1	2.33	0.66
1:B:581:LYS:NZ	1:B:1247:LEU:HD22	2.10	0.66
1:E:560:PHE:CG	1:E:561:PRO:CD	2.76	0.66
1:D:588:VAL:O	1:D:590:ASN:CG	2.33	0.66
1:F:555:LEU:HD22	1:F:560:PHE:HE1	1.50	0.66
1:G:588:VAL:O	1:G:590:ASN:CG	2.33	0.66
1:A:581:LYS:NZ	1:A:1247:LEU:HD22	2.10	0.66
1:C:1087:THR:H	2:J:88:LYS:H	1.40	0.66
1:C:1063:PHE:CE2	2:J:86:LYS:NZ	2.61	0.66
1:D:208:GLN:CG	1:E:229:ILE:HD13	2.25	0.66
1:E:1004:LYS:HZ2	2:L:73:LYS:HG2	1.56	0.66
1:C:558:GLN:CG	1:C:1171:GLU:CD	2.55	0.66
2:M:17:CYS:HG	4:M:500:HEM:CAC	2.08	0.66
1:A:208:GLN:CG	1:B:229:ILE:HD13	2.25	0.66
1:F:1077:LYS:CG	1:F:1077:LYS:O	2.44	0.66
1:D:520:ALA:CB	1:D:646:THR:OG1	2.36	0.66
1:D:581:LYS:NZ	1:D:1247:LEU:HD22	2.10	0.66
1:A:1173:ALA:CB	1:A:1211:GLN:OE1	2.33	0.66
1:A:1063:PHE:CE2	2:H:86:LYS:NZ	2.61	0.65
1:A:1063:PHE:CD2	2:H:86:LYS:CG	2.77	0.65
1:C:1087:THR:N	2:J:88:LYS:H	1.94	0.65
1:D:1087:THR:N	2:K:88:LYS:H	1.94	0.65
1:D:558:GLN:CG	1:D:1171:GLU:CD	2.55	0.65
1:G:1087:THR:N	2:N:88:LYS:H	1.94	0.65
1:F:208:GLN:CG	1:G:229:ILE:HD13	2.25	0.65
1:C:208:GLN:HB3	1:D:229:ILE:CG2	2.27	0.65
1:F:1063:PHE:CD2	2:M:86:LYS:CG	2.77	0.65
1:E:1063:PHE:CE2	2:L:86:LYS:NZ	2.61	0.65
1:D:208:GLN:HB3	1:E:229:ILE:CG2	2.27	0.65
1:F:565:GLN:NE2	1:F:592:MET:HE1	2.01	0.65
1:B:1169:SER:CB	1:B:1170:GLU:HA	2.26	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1077:LYS:CG	1:D:1077:LYS:O	2.44	0.65
1:E:1077:LYS:CG	1:E:1077:LYS:O	2.44	0.65
1:E:1169:SER:CB	1:E:1170:GLU:HA	2.26	0.65
1:A:1077:LYS:O	1:A:1077:LYS:CG	2.44	0.65
1:A:1169:SER:HB3	1:A:1170:GLU:HA	1.74	0.65
1:A:229:ILE:HD13	1:G:208:GLN:CG	2.25	0.65
1:B:565:GLN:HG2	1:B:594:TYR:CZ	2.32	0.65
1:B:208:GLN:HB3	1:C:229:ILE:CG2	2.27	0.65
1:D:1007:TRP:HZ2	2:K:73:LYS:HZ1	0.73	0.65
1:D:1063:PHE:CD2	2:K:86:LYS:CG	2.77	0.65
1:A:565:GLN:HG2	1:A:594:TYR:CZ	2.32	0.65
1:F:1169:SER:CB	1:F:1170:GLU:HA	2.26	0.65
1:G:1077:LYS:O	1:G:1077:LYS:CG	2.44	0.65
1:A:555:LEU:HD22	1:A:560:PHE:HE1	1.50	0.65
1:B:1087:THR:N	2:I:88:LYS:H	1.94	0.65
1:C:1077:LYS:O	1:C:1077:LYS:CG	2.44	0.65
1:C:565:GLN:HG2	1:C:594:TYR:CZ	2.32	0.65
1:D:559:PRO:N	1:D:1175:THR:HG22	2.12	0.65
1:E:1087:THR:N	2:L:88:LYS:H	1.94	0.65
1:F:565:GLN:HG2	1:F:594:TYR:CZ	2.32	0.65
1:B:1077:LYS:CG	1:B:1077:LYS:O	2.44	0.65
1:B:559:PRO:N	1:B:1175:THR:HG22	2.12	0.64
1:C:559:PRO:N	1:C:1175:THR:HG22	2.12	0.64
1:E:565:GLN:HG2	1:E:594:TYR:CZ	2.32	0.64
1:F:581:LYS:NZ	1:F:1247:LEU:HD22	2.10	0.64
1:A:1077:LYS:CD	1:A:1077:LYS:O	2.46	0.64
1:A:208:GLN:HB3	1:B:229:ILE:CG2	2.27	0.64
1:G:560:PHE:CD1	1:G:561:PRO:CD	2.64	0.64
1:G:581:LYS:NZ	1:G:1247:LEU:HD22	2.10	0.64
1:A:559:PRO:N	1:A:1175:THR:HG22	2.12	0.64
1:G:1077:LYS:O	1:G:1077:LYS:CD	2.46	0.64
1:B:1077:LYS:O	1:B:1077:LYS:CD	2.46	0.64
1:E:1173:ALA:CB	1:E:1211:GLN:OE1	2.33	0.64
1:E:581:LYS:NZ	1:E:1247:LEU:HD22	2.10	0.64
1:G:1063:PHE:HE2	2:N:86:LYS:CD	2.06	0.64
1:G:1169:SER:CB	1:G:1170:GLU:HA	2.26	0.64
1:A:229:ILE:CG2	1:G:208:GLN:HB3	2.27	0.64
1:G:565:GLN:HG2	1:G:594:TYR:CZ	2.32	0.64
1:E:646:THR:HG23	1:E:648:GLU:N	2.04	0.64
1:G:1048:LYS:HD2	2:N:86:LYS:HZ3	1.53	0.64
1:C:208:GLN:CG	1:D:229:ILE:HD13	2.25	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1173:ALA:CB	1:G:1211:GLN:OE1	2.33	0.64
1:F:208:GLN:HB3	1:G:229:ILE:CG2	2.27	0.64
1:G:646:THR:HG23	1:G:648:GLU:N	2.04	0.64
1:B:1063:PHE:CD2	2:I:86:LYS:CG	2.77	0.64
1:D:565:GLN:HG2	1:D:594:TYR:CZ	2.32	0.64
1:B:1023:ASP:HB2	2:I:73:LYS:HZ3	1.60	0.64
1:A:1087:THR:N	2:H:88:LYS:H	1.94	0.64
1:D:1169:SER:CB	1:D:1170:GLU:HA	2.26	0.64
1:E:559:PRO:N	1:E:1175:THR:HG22	2.12	0.64
1:F:1063:PHE:CE2	2:M:86:LYS:NZ	2.61	0.64
1:F:1087:THR:N	2:M:88:LYS:H	1.94	0.64
1:B:1087:THR:HB	2:I:86:LYS:HG2	1.80	0.64
1:D:1088:VAL:O	2:K:86:LYS:NZ	2.31	0.64
1:C:1077:LYS:CD	1:C:1077:LYS:O	2.46	0.63
1:C:1088:VAL:O	2:J:86:LYS:NZ	2.31	0.63
1:D:1063:PHE:CE2	2:K:86:LYS:NZ	2.61	0.63
1:G:559:PRO:N	1:G:1175:THR:HG22	2.12	0.63
1:A:1004:LYS:HZ2	2:H:73:LYS:HG2	1.48	0.63
1:E:1087:THR:HB	2:L:86:LYS:HG2	1.80	0.63
1:A:1087:THR:HB	2:H:86:LYS:HG2	1.80	0.63
1:A:1169:SER:CB	1:A:1170:GLU:HA	2.26	0.63
1:D:1077:LYS:O	1:D:1077:LYS:CD	2.46	0.63
1:E:208:GLN:HB3	1:F:229:ILE:CG2	2.27	0.63
1:F:1007:TRP:CE2	2:M:73:LYS:NZ	2.63	0.63
1:B:1063:PHE:HE2	2:I:86:LYS:CD	2.06	0.63
1:E:1077:LYS:O	1:E:1077:LYS:CD	2.46	0.63
1:F:559:PRO:N	1:F:1175:THR:HG22	2.12	0.63
1:D:1087:THR:HB	2:K:86:LYS:HG2	1.80	0.63
1:B:1087:THR:H	2:I:88:LYS:N	1.96	0.63
1:C:1087:THR:H	2:J:88:LYS:N	1.97	0.63
1:C:520:ALA:CB	1:C:646:THR:OG1	2.36	0.63
1:F:1077:LYS:CD	1:F:1077:LYS:O	2.46	0.63
1:B:1088:VAL:O	2:I:86:LYS:NZ	2.31	0.63
1:G:1007:TRP:CE2	2:N:73:LYS:NZ	2.63	0.63
1:B:1048:LYS:HG3	2:I:86:LYS:HZ2	1.61	0.63
1:C:208:GLN:HG2	1:D:229:ILE:HD13	1.78	0.63
1:A:1063:PHE:HE2	2:H:86:LYS:CD	2.06	0.63
1:E:1088:VAL:O	2:L:86:LYS:NZ	2.31	0.63
1:G:1087:THR:H	2:N:88:LYS:N	1.96	0.63
1:A:1007:TRP:CE2	2:H:73:LYS:NZ	2.63	0.63
1:F:1087:THR:H	2:M:88:LYS:N	1.96	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1087:THR:HB	2:M:86:LYS:HG2	1.80	0.63
1:G:1087:THR:HB	2:N:86:LYS:HG2	1.80	0.63
1:D:1087:THR:H	2:K:88:LYS:N	1.96	0.62
1:G:1063:PHE:CE2	2:N:86:LYS:NZ	2.61	0.62
1:E:1004:LYS:HZ2	2:L:73:LYS:CG	2.06	0.62
1:A:1087:THR:H	2:H:88:LYS:N	1.97	0.62
1:E:701:GLN:NE2	2:L:25:LYS:HD3	2.14	0.62
1:A:565:GLN:CG	1:A:594:TYR:HE2	2.12	0.62
1:A:520:ALA:CB	1:A:646:THR:OG1	2.36	0.62
1:D:701:GLN:NE2	2:K:25:LYS:HD3	2.14	0.62
1:G:520:ALA:CB	1:G:646:THR:OG1	2.36	0.62
1:A:1048:LYS:CD	2:H:86:LYS:HZ1	2.02	0.62
1:E:1007:TRP:CE2	2:L:73:LYS:NZ	2.63	0.62
1:F:701:GLN:NE2	2:M:25:LYS:HD3	2.14	0.62
1:D:565:GLN:CG	1:D:594:TYR:HE2	2.12	0.62
1:D:565:GLN:HE22	1:D:592:MET:HE1	1.53	0.62
1:A:229:ILE:CD1	1:G:208:GLN:CB	2.77	0.62
1:B:1004:LYS:HZ2	2:I:73:LYS:CG	2.12	0.62
1:G:701:GLN:NE2	2:N:25:LYS:HD3	2.14	0.62
1:A:565:GLN:NE2	1:A:592:MET:HE1	2.04	0.62
1:C:1087:THR:HB	2:J:86:LYS:HG2	1.80	0.62
1:A:560:PHE:CD1	1:A:561:PRO:CD	2.64	0.62
1:A:701:GLN:NE2	2:H:25:LYS:HD3	2.14	0.62
1:A:1088:VAL:O	2:H:86:LYS:NZ	2.31	0.62
1:B:565:GLN:CG	1:B:594:TYR:HE2	2.12	0.62
1:B:520:ALA:CB	1:B:646:THR:OG1	2.36	0.62
1:C:1169:SER:CB	1:C:1170:GLU:HA	2.26	0.62
2:J:72:LYS:HD3	2:J:78:THR:HG22	1.82	0.62
1:E:1087:THR:H	2:L:88:LYS:N	1.96	0.62
1:E:208:GLN:CG	1:F:229:ILE:HD13	2.25	0.62
1:A:590:ASN:O	1:A:592:MET:HG2	2.00	0.62
1:C:565:GLN:CG	1:C:594:TYR:HE2	2.12	0.62
1:D:588:VAL:CG1	1:D:589:ASP:N	2.55	0.62
1:E:588:VAL:CG1	1:E:589:ASP:N	2.55	0.62
1:E:590:ASN:O	1:E:592:MET:HG2	2.00	0.62
1:F:1088:VAL:O	2:M:86:LYS:NZ	2.31	0.62
1:G:590:ASN:O	1:G:592:MET:HG2	2.00	0.62
1:B:559:PRO:CD	1:B:1175:THR:HG22	2.30	0.62
1:D:559:PRO:CD	1:D:1175:THR:HG22	2.30	0.62
1:F:588:VAL:CG1	1:F:589:ASP:N	2.55	0.62
1:C:701:GLN:NE2	2:J:25:LYS:HD3	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:590:ASN:O	1:D:592:MET:HG2	2.00	0.61
1:F:565:GLN:CG	1:F:594:TYR:HE2	2.12	0.61
2:I:72:LYS:HD3	2:I:78:THR:HG22	1.82	0.61
1:E:559:PRO:CD	1:E:1175:THR:HG22	2.30	0.61
1:F:565:GLN:HE21	1:F:592:MET:HE3	1.18	0.61
1:B:1007:TRP:CE2	2:I:73:LYS:NZ	2.63	0.61
2:K:72:LYS:HD3	2:K:78:THR:HG22	1.82	0.61
1:C:559:PRO:CD	1:C:1175:THR:HG22	2.31	0.61
1:E:565:GLN:CG	1:E:594:TYR:HE2	2.12	0.61
2:M:72:LYS:HD3	2:M:78:THR:HG22	1.82	0.61
1:C:1007:TRP:CE2	2:J:73:LYS:NZ	2.63	0.61
1:G:1088:VAL:O	2:N:86:LYS:NZ	2.31	0.61
1:A:558:GLN:OE1	1:A:1169:SER:O	2.19	0.61
1:A:565:GLN:CG	1:A:594:TYR:CE2	2.84	0.61
1:B:208:GLN:HG2	1:C:229:ILE:HD13	1.78	0.61
1:C:558:GLN:OE1	1:C:1169:SER:O	2.19	0.61
1:F:1048:LYS:HG3	2:M:86:LYS:HZ2	1.64	0.61
1:F:1063:PHE:HE2	2:M:86:LYS:CD	2.06	0.61
1:F:590:ASN:O	1:F:592:MET:HG2	2.00	0.61
1:G:559:PRO:CD	1:G:1175:THR:HG22	2.30	0.61
1:B:558:GLN:OE1	1:B:1169:SER:O	2.19	0.61
1:G:565:GLN:CG	1:G:594:TYR:HE2	2.12	0.61
1:C:1063:PHE:CD2	2:J:86:LYS:CG	2.77	0.61
2:N:72:LYS:HD3	2:N:78:THR:HG22	1.82	0.61
1:A:559:PRO:HD3	1:A:1175:THR:CG2	2.31	0.61
1:B:590:ASN:O	1:B:592:MET:HG2	2.00	0.61
1:E:559:PRO:HD3	1:E:1175:THR:CG2	2.31	0.61
1:F:559:PRO:HD3	1:F:1175:THR:CG2	2.31	0.61
1:F:520:ALA:CB	1:F:646:THR:OG1	2.36	0.61
2:H:72:LYS:HD3	2:H:78:THR:HG22	1.82	0.61
1:B:701:GLN:NE2	2:I:25:LYS:HD3	2.14	0.61
1:E:1063:PHE:CD2	2:L:86:LYS:CG	2.77	0.61
1:C:565:GLN:CG	1:C:594:TYR:CE2	2.84	0.61
1:E:581:LYS:HZ1	1:E:1247:LEU:CD1	2.13	0.61
1:F:565:GLN:CG	1:F:594:TYR:CE2	2.84	0.61
1:G:559:PRO:HD3	1:G:1175:THR:CG2	2.31	0.61
1:C:590:ASN:O	1:C:592:MET:HG2	2.00	0.60
1:B:565:GLN:CG	1:B:594:TYR:CE2	2.84	0.60
1:D:565:GLN:CG	1:D:594:TYR:CE2	2.84	0.60
1:B:208:GLN:CG	1:C:229:ILE:HD13	2.25	0.60
1:C:559:PRO:HD3	1:C:1175:THR:CG2	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1063:PHE:HE2	2:L:86:LYS:CD	2.06	0.60
1:E:565:GLN:CG	1:E:594:TYR:CE2	2.84	0.60
1:A:559:PRO:CD	1:A:1175:THR:HG22	2.30	0.60
1:D:558:GLN:OE1	1:D:1169:SER:O	2.19	0.60
1:D:559:PRO:HD3	1:D:1175:THR:CG2	2.31	0.60
1:G:558:GLN:OE1	1:G:1169:SER:O	2.19	0.60
1:D:1007:TRP:CE2	2:K:73:LYS:NZ	2.63	0.60
2:L:72:LYS:HD3	2:L:78:THR:HG22	1.82	0.60
1:C:208:GLN:CB	1:D:229:ILE:CD1	2.77	0.60
1:B:1063:PHE:CE2	2:I:86:LYS:NZ	2.61	0.60
1:G:565:GLN:CG	1:G:594:TYR:CE2	2.84	0.60
1:B:559:PRO:HD3	1:B:1175:THR:CG2	2.31	0.60
1:B:560:PHE:CD1	1:B:561:PRO:CD	2.64	0.60
1:C:1063:PHE:HE2	2:J:86:LYS:CD	2.06	0.60
1:F:559:PRO:CD	1:F:1175:THR:HG22	2.30	0.60
1:G:565:GLN:NE2	1:G:592:MET:HE1	2.05	0.60
1:A:565:GLN:HE21	1:A:592:MET:HE3	1.25	0.60
1:D:1063:PHE:HE2	2:K:86:LYS:CD	2.06	0.60
1:E:348:LYS:HE2	1:E:352:ARG:HB3	1.84	0.60
1:F:348:LYS:HE2	1:F:352:ARG:HB3	1.84	0.60
1:E:558:GLN:OE1	1:E:1169:SER:O	2.19	0.59
1:F:558:GLN:OE1	1:F:1169:SER:O	2.19	0.59
1:F:560:PHE:CD1	1:F:561:PRO:CD	2.64	0.59
1:G:1063:PHE:CD2	2:N:86:LYS:CG	2.77	0.59
1:B:1023:ASP:CB	2:I:73:LYS:HZ2	2.14	0.59
1:A:1007:TRP:HZ2	2:H:73:LYS:HZ1	0.65	0.59
1:A:348:LYS:HE2	1:A:352:ARG:HB3	1.84	0.59
1:C:560:PHE:CE2	1:C:561:PRO:O	2.56	0.59
1:G:348:LYS:HE2	1:G:352:ARG:HB3	1.84	0.59
1:E:560:PHE:CE2	1:E:561:PRO:O	2.56	0.59
1:G:560:PHE:CE2	1:G:561:PRO:O	2.56	0.59
1:A:208:GLN:HG2	1:B:229:ILE:HD13	1.78	0.59
1:D:348:LYS:HE2	1:D:352:ARG:HB3	1.84	0.59
1:C:1023:ASP:CB	2:J:73:LYS:NZ	2.65	0.59
1:B:348:LYS:HE2	1:B:352:ARG:HB3	1.84	0.59
1:A:560:PHE:CE2	1:A:561:PRO:O	2.56	0.59
1:C:348:LYS:HE2	1:C:352:ARG:HB3	1.84	0.59
1:E:1089:LEU:CA	2:L:86:LYS:CE	2.74	0.59
1:B:1023:ASP:CG	2:I:73:LYS:HZ2	2.05	0.58
1:B:1077:LYS:HG3	1:B:1077:LYS:O	2.03	0.58
1:D:560:PHE:CE2	1:D:561:PRO:O	2.56	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1007:TRP:HZ2	2:M:73:LYS:HZ1	0.62	0.58
1:F:560:PHE:CE2	1:F:561:PRO:O	2.56	0.58
1:G:1023:ASP:CB	2:N:73:LYS:NZ	2.66	0.58
1:C:1077:LYS:HG3	1:C:1077:LYS:O	2.03	0.58
1:D:1077:LYS:HG3	1:D:1077:LYS:O	2.03	0.58
1:E:1048:LYS:HG3	2:L:86:LYS:HZ2	1.68	0.58
1:F:1023:ASP:CB	2:M:73:LYS:NZ	2.65	0.58
1:B:559:PRO:CB	1:B:1175:THR:N	2.51	0.58
1:B:591:GLY:O	1:B:593:LEU:N	2.37	0.58
1:D:1023:ASP:CB	2:K:73:LYS:NZ	2.65	0.58
1:D:348:LYS:CE	1:D:447:GLU:CD	2.72	0.58
1:E:520:ALA:CB	1:E:646:THR:OG1	2.36	0.58
1:G:1077:LYS:HG3	1:G:1077:LYS:O	2.03	0.58
1:A:1023:ASP:CB	2:H:73:LYS:NZ	2.65	0.58
1:B:560:PHE:CE2	1:B:561:PRO:O	2.56	0.58
1:G:1007:TRP:HZ2	2:N:73:LYS:HZ1	0.67	0.58
1:E:348:LYS:CE	1:E:447:GLU:CD	2.72	0.58
1:C:348:LYS:CE	1:C:447:GLU:CD	2.72	0.58
1:F:1077:LYS:O	1:F:1077:LYS:HG3	2.03	0.58
1:D:1048:LYS:CD	2:K:86:LYS:HZ1	2.00	0.58
1:A:1077:LYS:O	1:A:1077:LYS:HG3	2.03	0.58
1:E:1023:ASP:CB	2:L:73:LYS:NZ	2.65	0.57
1:A:348:LYS:CE	1:A:447:GLU:CD	2.72	0.57
1:B:348:LYS:CE	1:B:447:GLU:CD	2.72	0.57
1:E:1077:LYS:O	1:E:1077:LYS:HG3	2.03	0.57
1:F:348:LYS:CE	1:F:447:GLU:CD	2.72	0.57
1:G:348:LYS:CE	1:G:447:GLU:CD	2.72	0.57
1:B:1004:LYS:HZ2	2:I:73:LYS:HG2	1.60	0.57
1:D:1089:LEU:CA	2:K:86:LYS:CE	2.74	0.57
1:A:557:ARG:O	1:A:1171:GLU:CD	2.43	0.57
1:A:591:GLY:O	1:A:593:LEU:N	2.37	0.57
1:C:591:GLY:O	1:C:593:LEU:N	2.37	0.57
1:D:591:GLY:O	1:D:593:LEU:N	2.37	0.57
1:A:1063:PHE:CD2	2:H:86:LYS:HG2	2.39	0.57
1:B:168:VAL:CG1	1:B:168:VAL:O	2.51	0.57
1:C:1048:LYS:HG3	2:J:86:LYS:HZ2	1.68	0.57
1:D:1128:GLY:O	1:D:1129:CYS:HB2	2.05	0.57
1:E:591:GLY:O	1:E:593:LEU:N	2.37	0.57
1:F:591:GLY:O	1:F:593:LEU:N	2.37	0.57
1:G:559:PRO:HD3	1:G:1175:THR:HG22	1.87	0.57
1:G:591:GLY:O	1:G:593:LEU:N	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1128:GLY:O	1:E:1129:CYS:HB2	2.05	0.57
1:G:1063:PHE:CD2	2:N:86:LYS:HG2	2.39	0.57
1:A:559:PRO:HD3	1:A:1175:THR:HG22	1.87	0.57
1:F:1023:ASP:CG	2:M:73:LYS:HZ2	2.07	0.57
1:F:1089:LEU:CA	2:M:86:LYS:CE	2.74	0.57
1:F:559:PRO:HD3	1:F:1175:THR:HG22	1.87	0.57
1:F:581:LYS:HZ1	1:F:1247:LEU:CD1	2.17	0.57
1:B:1063:PHE:CD2	2:I:86:LYS:HG2	2.39	0.57
1:D:946:LEU:C	1:D:946:LEU:HD12	2.26	0.57
1:E:946:LEU:C	1:E:946:LEU:HD12	2.26	0.57
1:F:557:ARG:O	1:F:1171:GLU:CD	2.43	0.57
1:B:1089:LEU:CA	2:I:86:LYS:CE	2.74	0.57
1:B:557:ARG:O	1:B:1171:GLU:CD	2.43	0.57
1:G:946:LEU:C	1:G:946:LEU:HD12	2.26	0.57
1:A:1089:LEU:CA	2:H:86:LYS:CE	2.74	0.56
1:F:946:LEU:C	1:F:946:LEU:HD12	2.26	0.56
1:A:946:LEU:HD12	1:A:946:LEU:C	2.25	0.56
1:B:1173:ALA:HB1	1:B:1211:GLN:CD	2.24	0.56
1:C:946:LEU:HD12	1:C:946:LEU:C	2.26	0.56
1:D:1048:LYS:HG3	2:K:86:LYS:HZ2	1.70	0.56
1:B:559:PRO:HD3	1:B:1175:THR:HG22	1.87	0.56
1:C:1128:GLY:O	1:C:1129:CYS:HB2	2.05	0.56
1:E:559:PRO:HD3	1:E:1175:THR:HG22	1.87	0.56
1:A:229:ILE:HD13	1:G:208:GLN:HG2	1.78	0.56
1:B:946:LEU:C	1:B:946:LEU:HD12	2.25	0.56
1:F:1063:PHE:CD2	2:M:86:LYS:HG2	2.39	0.56
1:A:1173:ALA:HB1	1:A:1211:GLN:CD	2.24	0.56
1:E:1063:PHE:CD2	2:L:86:LYS:O	2.59	0.56
1:E:1023:ASP:CG	2:L:73:LYS:HZ2	2.09	0.56
1:A:1128:GLY:O	1:A:1129:CYS:HB2	2.05	0.56
1:C:1063:PHE:CD2	2:J:86:LYS:HG2	2.39	0.56
1:F:1128:GLY:O	1:F:1129:CYS:HB2	2.05	0.56
1:A:1063:PHE:CD2	2:H:86:LYS:O	2.59	0.56
1:D:559:PRO:HD3	1:D:1175:THR:HG22	1.87	0.56
1:D:168:VAL:CG1	1:D:168:VAL:O	2.51	0.56
1:E:557:ARG:O	1:E:1171:GLU:CD	2.43	0.56
1:C:557:ARG:O	1:C:1171:GLU:CD	2.43	0.56
1:G:1128:GLY:O	1:G:1129:CYS:HB2	2.05	0.56
1:G:581:LYS:HZ1	1:G:1247:LEU:CD1	2.19	0.56
1:B:1063:PHE:CD2	2:I:86:LYS:O	2.59	0.56
1:D:1063:PHE:CD2	2:K:86:LYS:O	2.59	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1089:LEU:CA	2:N:86:LYS:CE	2.74	0.56
1:C:1173:ALA:HB1	1:C:1211:GLN:CD	2.24	0.56
1:E:348:LYS:CE	1:E:352:ARG:HB3	2.36	0.56
1:C:1063:PHE:CD2	2:J:86:LYS:O	2.59	0.56
1:B:1128:GLY:O	1:B:1129:CYS:HB2	2.05	0.55
1:C:559:PRO:HD3	1:C:1175:THR:HG22	1.87	0.55
1:F:1063:PHE:CD2	2:M:86:LYS:O	2.59	0.55
1:B:581:LYS:HZ1	1:B:1247:LEU:CD1	2.19	0.55
1:D:557:ARG:O	1:D:1171:GLU:CD	2.43	0.55
1:D:1169:SER:HB3	1:D:1170:GLU:HG3	1.87	0.55
1:D:348:LYS:CE	1:D:352:ARG:HB3	2.36	0.55
1:G:348:LYS:CE	1:G:352:ARG:HB3	2.36	0.55
1:G:677:VAL:HG22	2:N:25:LYS:HZ3	1.72	0.55
1:G:1063:PHE:CD2	2:N:86:LYS:O	2.59	0.55
1:C:348:LYS:CE	1:C:352:ARG:HB3	2.36	0.55
1:D:1063:PHE:CD2	2:K:86:LYS:HG2	2.39	0.55
1:C:1106:ASP:OD2	2:J:90:GLU:HG3	2.07	0.55
1:E:1063:PHE:CD2	2:L:86:LYS:HG2	2.39	0.55
1:C:898:LEU:HD12	1:C:898:LEU:O	2.07	0.55
1:G:1106:ASP:OD2	2:N:90:GLU:HG3	2.07	0.55
1:G:1113:SER:O	1:G:1114:PHE:HB2	2.06	0.55
1:A:1113:SER:O	1:A:1114:PHE:HB2	2.06	0.55
1:B:1106:ASP:OD2	2:I:90:GLU:HG3	2.07	0.55
1:E:898:LEU:O	1:E:898:LEU:HD12	2.07	0.55
1:D:1106:ASP:OD2	2:K:90:GLU:HG3	2.07	0.55
1:E:581:LYS:HZ1	1:E:1247:LEU:HD11	1.71	0.55
1:A:559:PRO:CB	1:A:1175:THR:N	2.51	0.55
1:E:581:LYS:HZ2	1:E:1247:LEU:CD2	2.20	0.55
1:G:1173:ALA:HB1	1:G:1211:GLN:CD	2.24	0.55
1:A:348:LYS:CE	1:A:352:ARG:HB3	2.36	0.55
1:C:1128:GLY:O	1:C:1129:CYS:CB	2.55	0.55
1:F:348:LYS:CE	1:F:352:ARG:HB3	2.36	0.55
1:E:1106:ASP:OD2	2:L:90:GLU:HG3	2.07	0.55
1:C:581:LYS:HZ1	1:C:1247:LEU:CD1	2.20	0.54
1:E:205:ARG:NE	1:F:225:ASP:OD2	2.41	0.54
1:A:225:ASP:OD2	1:G:205:ARG:NE	2.40	0.54
1:F:205:ARG:NE	1:G:225:ASP:OD2	2.41	0.54
1:B:1007:TRP:HZ2	2:I:73:LYS:HZ1	0.60	0.54
1:B:1128:GLY:O	1:B:1129:CYS:CB	2.55	0.54
1:E:1169:SER:HB3	1:E:1170:GLU:HG3	1.87	0.54
1:E:1007:TRP:HZ2	2:L:73:LYS:HZ1	0.63	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1106:ASP:OD2	2:H:90:GLU:HG3	2.07	0.54
1:A:1169:SER:HB3	1:A:1170:GLU:HG3	1.87	0.54
1:C:1113:SER:O	1:C:1114:PHE:HB2	2.07	0.54
1:D:1128:GLY:O	1:D:1129:CYS:CB	2.55	0.54
1:D:205:ARG:NE	1:E:225:ASP:OD2	2.40	0.54
1:G:588:VAL:CG1	1:G:589:ASP:N	2.55	0.54
1:F:1023:ASP:CB	2:M:73:LYS:HZ2	2.20	0.54
1:A:898:LEU:O	1:A:898:LEU:HD12	2.07	0.54
1:F:1113:SER:O	1:F:1114:PHE:HB2	2.06	0.54
1:A:208:GLN:CB	1:B:229:ILE:CD1	2.77	0.54
1:B:1113:SER:O	1:B:1114:PHE:HB2	2.06	0.54
1:B:348:LYS:CE	1:B:352:ARG:HB3	2.36	0.54
1:D:898:LEU:O	1:D:898:LEU:HD12	2.07	0.54
2:I:41:GLY:HA2	2:I:48:TYR:CZ	2.43	0.54
2:J:41:GLY:HA2	2:J:48:TYR:CZ	2.43	0.54
1:C:1169:SER:HB3	1:C:1170:GLU:HG3	1.87	0.54
1:D:1173:ALA:HB1	1:D:1211:GLN:CD	2.24	0.54
1:E:1128:GLY:O	1:E:1129:CYS:CB	2.55	0.54
1:E:1174:ALA:O	1:E:1200:LYS:NZ	2.41	0.54
1:F:1106:ASP:OD2	2:M:90:GLU:HG3	2.07	0.54
1:A:1128:GLY:O	1:A:1129:CYS:CB	2.56	0.54
1:F:1128:GLY:O	1:F:1129:CYS:CB	2.55	0.54
2:H:41:GLY:HA2	2:H:48:TYR:CZ	2.43	0.54
1:B:1170:GLU:HG2	1:B:1170:GLU:O	2.08	0.54
1:B:898:LEU:O	1:B:898:LEU:HD12	2.07	0.54
1:D:1113:SER:O	1:D:1114:PHE:HB2	2.06	0.54
1:E:1113:SER:O	1:E:1114:PHE:HB2	2.06	0.54
1:E:559:PRO:HA	1:E:1171:GLU:HG2	1.90	0.54
1:G:1174:ALA:O	1:G:1200:LYS:NZ	2.41	0.54
1:G:898:LEU:O	1:G:898:LEU:HD12	2.07	0.54
1:C:869:THR:O	1:C:870:ASP:HB2	2.08	0.54
1:F:208:GLN:HG2	1:G:229:ILE:HD13	1.78	0.54
1:F:898:LEU:HD12	1:F:898:LEU:O	2.07	0.54
1:A:1170:GLU:O	1:A:1170:GLU:HG2	2.08	0.53
1:A:168:VAL:O	1:A:168:VAL:CG1	2.51	0.53
1:A:282:VAL:O	1:A:282:VAL:HG12	2.08	0.53
1:F:559:PRO:HA	1:F:1171:GLU:HG2	1.90	0.53
1:G:869:THR:O	1:G:870:ASP:HB2	2.08	0.53
1:A:1023:ASP:CG	2:H:73:LYS:HZ2	2.11	0.53
1:D:559:PRO:HA	1:D:1171:GLU:HG2	1.90	0.53
1:D:869:THR:O	1:D:870:ASP:HB2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:869:THR:O	1:F:870:ASP:HB2	2.08	0.53
1:G:1128:GLY:O	1:G:1129:CYS:CB	2.55	0.53
2:N:41:GLY:HA2	2:N:48:TYR:CZ	2.43	0.53
1:B:869:THR:O	1:B:870:ASP:HB2	2.08	0.53
1:E:869:THR:O	1:E:870:ASP:HB2	2.09	0.53
2:K:41:GLY:HA2	2:K:48:TYR:CZ	2.43	0.53
1:A:869:THR:O	1:A:870:ASP:HB2	2.08	0.53
1:B:282:VAL:HG12	1:B:282:VAL:O	2.08	0.53
1:C:205:ARG:NE	1:D:225:ASP:OD2	2.40	0.53
1:C:1089:LEU:CA	2:J:86:LYS:CE	2.74	0.53
1:C:1170:GLU:HG2	1:C:1170:GLU:O	2.08	0.53
1:F:1173:ALA:HB1	1:F:1211:GLN:CD	2.24	0.53
1:B:1023:ASP:CB	2:I:73:LYS:NZ	2.65	0.53
1:C:168:VAL:O	1:C:168:VAL:CG1	2.51	0.53
1:A:1048:LYS:CE	2:H:86:LYS:HZ3	2.21	0.53
2:L:41:GLY:HA2	2:L:48:TYR:CZ	2.43	0.53
1:C:559:PRO:HA	1:C:1171:GLU:HG2	1.90	0.53
1:F:1169:SER:HB3	1:F:1170:GLU:HG3	1.87	0.53
1:G:1170:GLU:HG2	1:G:1170:GLU:O	2.08	0.53
1:F:168:VAL:CG1	1:F:168:VAL:O	2.51	0.53
1:G:1169:SER:HB3	1:G:1170:GLU:HG3	1.87	0.53
1:D:282:VAL:O	1:D:282:VAL:HG12	2.08	0.53
1:E:1170:GLU:O	1:E:1170:GLU:HG2	2.08	0.53
1:E:1173:ALA:HB1	1:E:1211:GLN:CD	2.24	0.53
1:E:208:GLN:CB	1:F:229:ILE:CD1	2.77	0.53
1:D:348:LYS:HG2	1:D:352:ARG:CB	2.40	0.53
1:G:282:VAL:O	1:G:282:VAL:HG12	2.08	0.53
1:B:565:GLN:CG	1:B:594:TYR:OH	2.57	0.52
1:C:282:VAL:O	1:C:282:VAL:HG12	2.08	0.52
1:F:1170:GLU:O	1:F:1170:GLU:HG2	2.08	0.52
1:G:559:PRO:HA	1:G:1171:GLU:HG2	1.90	0.52
1:G:555:LEU:HD21	1:G:560:PHE:CZ	2.44	0.52
1:A:565:GLN:CG	1:A:594:TYR:OH	2.57	0.52
1:E:282:VAL:HG12	1:E:282:VAL:O	2.08	0.52
1:C:1048:LYS:CE	2:J:86:LYS:HZ3	2.22	0.52
1:C:565:GLN:CG	1:C:594:TYR:OH	2.57	0.52
1:D:1170:GLU:HG2	1:D:1170:GLU:O	2.08	0.52
1:G:565:GLN:CG	1:G:594:TYR:OH	2.57	0.52
2:M:41:GLY:HA2	2:M:48:TYR:CZ	2.43	0.52
1:B:816:ALA:HB3	1:B:846:CYS:SG	2.50	0.52
1:F:282:VAL:HG12	1:F:282:VAL:O	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:701:GLN:HG2	2:M:25:LYS:HZ3	1.74	0.52
1:A:559:PRO:HA	1:A:1171:GLU:HG2	1.90	0.52
1:B:205:ARG:NE	1:C:225:ASP:OD2	2.40	0.52
1:C:1094:SER:O	1:C:1095:HIS:HB2	2.10	0.52
1:D:1094:SER:O	1:D:1095:HIS:HB2	2.10	0.52
1:D:565:GLN:CG	1:D:594:TYR:OH	2.57	0.52
1:E:555:LEU:HD21	1:E:560:PHE:CZ	2.44	0.52
1:A:1174:ALA:O	1:A:1200:LYS:NZ	2.41	0.52
1:A:555:LEU:HD21	1:A:560:PHE:CZ	2.44	0.52
1:E:1023:ASP:CB	2:L:73:LYS:HZ2	2.23	0.52
1:G:816:ALA:HB3	1:G:846:CYS:SG	2.50	0.52
1:D:1048:LYS:CE	2:K:86:LYS:HZ3	2.22	0.52
1:F:701:GLN:OE1	2:M:25:LYS:HB3	2.10	0.52
1:A:1169:SER:N	1:A:1170:GLU:HB3	2.25	0.52
1:A:816:ALA:HB3	1:A:846:CYS:SG	2.50	0.52
1:B:348:LYS:HG2	1:B:352:ARG:CB	2.39	0.52
1:C:1169:SER:N	1:C:1170:GLU:HB3	2.25	0.52
1:B:208:GLN:CD	1:C:229:ILE:HG12	2.30	0.52
1:F:565:GLN:HE22	1:F:592:MET:HE1	1.59	0.52
1:F:590:ASN:OD1	1:F:590:ASN:N	2.43	0.52
1:F:816:ALA:HB3	1:F:846:CYS:SG	2.50	0.52
1:G:520:ALA:O	1:G:524:HIS:HD2	1.89	0.52
1:E:1048:LYS:CE	2:L:86:LYS:HZ3	2.22	0.52
1:B:559:PRO:HA	1:B:1171:GLU:HG2	1.90	0.52
1:B:677:VAL:HG22	2:I:25:LYS:HZ3	1.75	0.52
1:E:208:GLN:CD	1:F:229:ILE:HG12	2.30	0.52
1:G:1094:SER:O	1:G:1095:HIS:HB2	2.10	0.52
1:A:229:ILE:HG12	1:G:208:GLN:CD	2.30	0.52
1:A:1094:SER:O	1:A:1095:HIS:HB2	2.10	0.52
1:A:591:GLY:O	1:A:592:MET:C	2.49	0.52
1:C:208:GLN:CD	1:D:229:ILE:HG12	2.30	0.52
1:D:591:GLY:O	1:D:592:MET:C	2.49	0.52
1:F:1174:ALA:O	1:F:1200:LYS:NZ	2.41	0.52
1:D:1174:ALA:O	1:D:1200:LYS:NZ	2.41	0.52
1:E:1094:SER:O	1:E:1095:HIS:HB2	2.10	0.52
1:E:701:GLN:OE1	2:L:25:LYS:HB3	2.10	0.52
1:E:816:ALA:HB3	1:E:846:CYS:SG	2.50	0.52
1:F:581:LYS:HZ1	1:F:1247:LEU:HD11	1.74	0.52
1:G:590:ASN:N	1:G:590:ASN:OD1	2.43	0.52
1:C:701:GLN:OE1	2:J:25:LYS:HB3	2.10	0.52
1:D:701:GLN:OE1	2:K:25:LYS:HB3	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:LYS:HG3	2:H:86:LYS:HZ2	1.71	0.51
1:C:1174:ALA:O	1:C:1200:LYS:NZ	2.41	0.51
1:C:816:ALA:HB3	1:C:846:CYS:SG	2.50	0.51
1:E:348:LYS:HG2	1:E:352:ARG:CB	2.40	0.51
1:B:701:GLN:OE1	2:I:25:LYS:HB3	2.10	0.51
1:A:205:ARG:NE	1:B:225:ASP:OD2	2.40	0.51
1:B:1094:SER:O	1:B:1095:HIS:HB2	2.10	0.51
1:E:590:ASN:N	1:E:590:ASN:OD1	2.43	0.51
1:F:581:LYS:HZ2	1:F:1247:LEU:CD2	2.22	0.51
1:F:555:LEU:HD21	1:F:560:PHE:CZ	2.44	0.51
1:G:565:GLN:NE2	1:G:594:TYR:OH	2.43	0.51
1:F:661:LEU:HD11	2:M:25:LYS:NZ	2.26	0.51
1:B:1174:ALA:O	1:B:1200:LYS:NZ	2.41	0.51
1:A:208:GLN:CD	1:B:229:ILE:HG12	2.30	0.51
1:B:591:GLY:O	1:B:592:MET:C	2.49	0.51
1:D:565:GLN:NE2	1:D:594:TYR:OH	2.44	0.51
1:F:208:GLN:CD	1:G:229:ILE:HG12	2.30	0.51
1:F:591:GLY:O	1:F:592:MET:C	2.49	0.51
1:F:565:GLN:NE2	1:F:594:TYR:OH	2.43	0.51
1:G:1023:ASP:CG	2:N:73:LYS:HZ2	2.13	0.51
1:G:581:LYS:NZ	1:G:1247:LEU:CD1	2.74	0.51
1:B:643:LYS:HD2	1:B:646:THR:HG22	1.92	0.51
1:C:643:LYS:HD2	1:C:646:THR:HG22	1.92	0.51
1:D:816:ALA:HB3	1:D:846:CYS:SG	2.50	0.51
1:E:208:GLN:HG2	1:F:229:ILE:HD13	1.78	0.51
1:A:661:LEU:HD11	2:H:25:LYS:NZ	2.26	0.51
1:B:661:LEU:HD11	2:I:25:LYS:NZ	2.26	0.51
1:E:661:LEU:HD11	2:L:25:LYS:NZ	2.26	0.51
1:G:661:LEU:HD11	2:N:25:LYS:NZ	2.26	0.51
1:C:661:LEU:HD11	2:J:25:LYS:NZ	2.26	0.51
1:G:701:GLN:OE1	2:N:25:LYS:HB3	2.10	0.51
1:A:643:LYS:HD2	1:A:646:THR:HG22	1.92	0.51
1:B:208:GLN:CB	1:C:229:ILE:CD1	2.77	0.51
1:B:581:LYS:NZ	1:B:1247:LEU:CD1	2.74	0.51
1:D:208:GLN:CD	1:E:229:ILE:HG12	2.30	0.51
2:I:41:GLY:CA	2:I:52:ASN:ND2	2.74	0.51
1:G:800:ILE:CD1	2:N:47:SER:HB3	2.41	0.51
1:B:1169:SER:HB3	1:B:1170:GLU:HG3	1.87	0.51
1:C:565:GLN:NE2	1:C:594:TYR:OH	2.44	0.51
1:C:590:ASN:N	1:C:590:ASN:OD1	2.43	0.51
1:C:800:ILE:CD1	2:J:47:SER:HB3	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:581:LYS:NZ	1:D:1247:LEU:CD1	2.74	0.51
1:E:588:VAL:O	1:E:590:ASN:N	2.44	0.51
1:E:591:GLY:O	1:E:592:MET:C	2.49	0.51
1:D:661:LEU:HD11	2:K:25:LYS:NZ	2.26	0.51
1:D:800:ILE:CD1	2:K:47:SER:HB3	2.41	0.51
1:A:565:GLN:NE2	1:A:594:TYR:OH	2.43	0.51
1:D:1169:SER:N	1:D:1170:GLU:HB3	2.25	0.51
1:D:588:VAL:O	1:D:590:ASN:N	2.44	0.51
1:G:557:ARG:O	1:G:1171:GLU:CD	2.43	0.51
1:G:591:GLY:O	1:G:592:MET:C	2.49	0.51
2:L:41:GLY:CA	2:L:52:ASN:ND2	2.74	0.51
1:C:581:LYS:NZ	1:C:1247:LEU:CD1	2.74	0.51
1:G:565:GLN:HE21	1:G:592:MET:HE3	1.26	0.51
1:C:555:LEU:HD21	1:C:560:PHE:CZ	2.44	0.51
1:E:559:PRO:CB	1:E:1175:THR:N	2.51	0.51
1:E:565:GLN:NE2	1:E:594:TYR:OH	2.43	0.51
1:F:1094:SER:O	1:F:1095:HIS:HB2	2.10	0.51
2:H:41:GLY:CA	2:H:52:ASN:ND2	2.74	0.51
2:J:41:GLY:CA	2:J:52:ASN:ND2	2.74	0.51
1:B:565:GLN:NE2	1:B:594:TYR:OH	2.43	0.50
1:E:581:LYS:NZ	1:E:1247:LEU:CD1	2.74	0.50
1:F:643:LYS:HD2	1:F:646:THR:HG22	1.92	0.50
1:G:348:LYS:HG2	1:G:352:ARG:CB	2.40	0.50
1:A:701:GLN:OE1	2:H:25:LYS:HB3	2.10	0.50
1:B:800:ILE:CD1	2:I:47:SER:HB3	2.41	0.50
1:A:590:ASN:OD1	1:A:590:ASN:N	2.43	0.50
1:B:555:LEU:HD21	1:B:560:PHE:CZ	2.44	0.50
1:A:800:ILE:CD1	2:H:47:SER:HB3	2.41	0.50
2:M:41:GLY:CA	2:M:52:ASN:ND2	2.74	0.50
1:G:1023:ASP:CB	2:N:73:LYS:HD3	2.42	0.50
1:A:345:LEU:HA	1:A:349:GLN:HA	1.94	0.50
1:D:590:ASN:N	1:D:590:ASN:OD1	2.43	0.50
1:E:800:ILE:CD1	2:L:47:SER:HB3	2.41	0.50
1:F:1048:LYS:CE	2:M:86:LYS:HZ3	2.23	0.50
1:A:348:LYS:HG2	1:A:352:ARG:CB	2.39	0.50
1:A:565:GLN:HE22	1:A:592:MET:HE1	1.66	0.50
1:A:581:LYS:NZ	1:A:1247:LEU:CD1	2.74	0.50
1:B:590:ASN:OD1	1:B:590:ASN:N	2.43	0.50
1:E:643:LYS:HD2	1:E:646:THR:HG22	1.92	0.50
1:G:345:LEU:HA	1:G:349:GLN:HA	1.94	0.50
1:G:643:LYS:HD2	1:G:646:THR:HG22	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:701:GLN:OE1	2:J:25:LYS:HD3	2.10	0.50
1:F:800:ILE:CD1	2:M:47:SER:HB3	2.41	0.50
1:F:1023:ASP:CB	2:M:73:LYS:HD3	2.42	0.50
1:B:581:LYS:HZ1	1:B:1247:LEU:HD11	1.77	0.50
1:B:588:VAL:O	1:B:590:ASN:N	2.44	0.50
1:C:603:ILE:HD12	1:C:603:ILE:C	2.32	0.50
1:F:348:LYS:O	1:F:349:GLN:O	2.30	0.50
1:G:1168:LEU:O	1:G:1169:SER:HB2	2.11	0.50
1:G:588:VAL:O	1:G:590:ASN:N	2.44	0.50
2:N:41:GLY:CA	2:N:52:ASN:ND2	2.74	0.50
1:B:348:LYS:O	1:B:349:GLN:O	2.30	0.50
1:C:348:LYS:O	1:C:349:GLN:O	2.30	0.50
1:D:555:LEU:HD21	1:D:560:PHE:CZ	2.44	0.50
1:D:643:LYS:HD2	1:D:646:THR:HG22	1.92	0.50
1:A:348:LYS:O	1:A:349:GLN:O	2.30	0.50
1:C:348:LYS:HG2	1:C:352:ARG:CB	2.40	0.50
1:C:591:GLY:O	1:C:592:MET:C	2.49	0.50
1:E:1168:LEU:O	1:E:1169:SER:HB2	2.11	0.50
1:F:348:LYS:HG2	1:F:352:ARG:CB	2.39	0.50
1:F:581:LYS:NZ	1:F:1247:LEU:CD1	2.74	0.50
1:G:588:VAL:O	1:G:590:ASN:OD1	2.30	0.50
1:A:1023:ASP:CB	2:H:73:LYS:HD3	2.42	0.50
2:K:41:GLY:CA	2:K:52:ASN:ND2	2.74	0.50
1:A:588:VAL:O	1:A:590:ASN:N	2.44	0.50
1:B:205:ARG:NH1	1:C:228:ARG:HH22	2.10	0.50
1:E:565:GLN:CG	1:E:594:TYR:OH	2.57	0.50
1:F:588:VAL:O	1:F:590:ASN:N	2.44	0.50
1:G:1004:LYS:HZ2	2:N:73:LYS:CD	2.24	0.50
1:G:348:LYS:O	1:G:349:GLN:O	2.30	0.50
2:K:41:GLY:HA2	2:K:48:TYR:CE1	2.47	0.50
1:A:1171:GLU:O	1:A:1173:ALA:N	2.45	0.50
1:A:588:VAL:O	1:A:590:ASN:OD1	2.30	0.50
1:B:1168:LEU:O	1:B:1169:SER:HB2	2.11	0.50
1:C:1168:LEU:O	1:C:1169:SER:HB2	2.11	0.50
1:D:1168:LEU:O	1:D:1169:SER:HB2	2.11	0.50
1:D:1171:GLU:O	1:D:1173:ALA:N	2.45	0.50
1:F:345:LEU:HA	1:F:349:GLN:HA	1.94	0.50
1:A:701:GLN:OE1	2:H:25:LYS:HD3	2.10	0.50
1:A:1168:LEU:O	1:A:1169:SER:HB2	2.11	0.49
1:B:1077:LYS:C	1:B:1077:LYS:HD2	2.33	0.49
1:B:1171:GLU:O	1:B:1173:ALA:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:LEU:HA	1:B:349:GLN:HA	1.94	0.49
1:F:1077:LYS:HD2	1:F:1077:LYS:C	2.33	0.49
1:F:1168:LEU:O	1:F:1169:SER:HB2	2.11	0.49
1:F:588:VAL:O	1:F:590:ASN:OD1	2.30	0.49
1:G:1077:LYS:C	1:G:1077:LYS:HD2	2.33	0.49
1:C:1023:ASP:CB	2:J:73:LYS:HD3	2.42	0.49
2:L:41:GLY:HA2	2:L:48:TYR:CE1	2.47	0.49
1:A:205:ARG:NH1	1:B:228:ARG:HH22	2.10	0.49
1:D:208:GLN:CB	1:E:229:ILE:CD1	2.77	0.49
1:C:205:ARG:NH1	1:D:228:ARG:HH22	2.10	0.49
1:D:348:LYS:O	1:D:349:GLN:O	2.30	0.49
1:E:348:LYS:O	1:E:349:GLN:O	2.30	0.49
1:G:559:PRO:CB	1:G:1175:THR:N	2.51	0.49
1:B:1023:ASP:CB	2:I:73:LYS:HD3	2.42	0.49
1:D:348:LYS:HA	1:D:352:ARG:HD2	1.95	0.49
1:G:581:LYS:HZ1	1:G:1247:LEU:HD11	1.77	0.49
1:E:1023:ASP:CB	2:L:73:LYS:HD3	2.42	0.49
1:C:348:LYS:HA	1:C:352:ARG:HD2	1.95	0.49
1:E:1171:GLU:O	1:E:1173:ALA:N	2.45	0.49
1:G:603:ILE:HD12	1:G:603:ILE:C	2.32	0.49
1:E:348:LYS:HA	1:E:352:ARG:HD2	1.95	0.49
1:E:603:ILE:C	1:E:603:ILE:HD12	2.32	0.49
1:A:603:ILE:HD12	1:A:603:ILE:C	2.32	0.49
1:B:1169:SER:N	1:B:1170:GLU:HB3	2.25	0.49
1:C:1077:LYS:HD2	1:C:1077:LYS:C	2.33	0.49
1:C:588:VAL:O	1:C:590:ASN:N	2.44	0.49
1:D:1077:LYS:HD2	1:D:1077:LYS:C	2.33	0.49
1:D:208:GLN:HG2	1:E:229:ILE:HD13	1.78	0.49
1:D:588:VAL:O	1:D:590:ASN:OD1	2.30	0.49
1:E:701:GLN:HG2	2:L:25:LYS:HZ3	1.78	0.49
1:F:1089:LEU:O	1:F:1090:SER:HB3	2.13	0.49
1:F:898:LEU:HD12	1:F:898:LEU:C	2.33	0.49
1:G:1128:GLY:C	1:G:1129:CYS:SG	2.91	0.49
1:G:1171:GLU:O	1:G:1173:ALA:N	2.45	0.49
1:A:898:LEU:HD12	1:A:898:LEU:C	2.33	0.49
1:C:701:GLN:HG2	2:J:25:LYS:HZ3	1.77	0.49
1:E:1169:SER:N	1:E:1170:GLU:HB3	2.25	0.49
1:E:898:LEU:C	1:E:898:LEU:HD12	2.33	0.49
1:F:348:LYS:HA	1:F:352:ARG:HD2	1.95	0.49
1:F:603:ILE:C	1:F:603:ILE:HD12	2.32	0.49
2:I:41:GLY:HA2	2:I:48:TYR:CE1	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:70:ASN:HD22	2:L:70:ASN:C	2.16	0.49
1:B:588:VAL:O	1:B:590:ASN:OD1	2.30	0.49
1:C:898:LEU:HD12	1:C:898:LEU:C	2.33	0.49
1:E:168:VAL:CG1	1:E:168:VAL:O	2.51	0.49
1:F:565:GLN:CG	1:F:594:TYR:OH	2.57	0.49
2:N:70:ASN:C	2:N:70:ASN:HD22	2.16	0.49
1:A:1128:GLY:C	1:A:1129:CYS:SG	2.91	0.49
1:A:520:ALA:O	1:A:524:HIS:HD2	1.89	0.49
1:B:1128:GLY:C	1:B:1129:CYS:SG	2.91	0.49
1:B:565:GLN:CD	1:B:594:TYR:CE2	2.87	0.49
1:C:1128:GLY:C	1:C:1129:CYS:SG	2.91	0.49
1:C:1171:GLU:O	1:C:1173:ALA:N	2.45	0.49
1:C:345:LEU:HA	1:C:349:GLN:HA	1.94	0.49
1:E:345:LEU:HA	1:E:349:GLN:HA	1.94	0.49
1:E:588:VAL:O	1:E:590:ASN:OD1	2.30	0.49
1:F:1171:GLU:O	1:F:1173:ALA:N	2.45	0.49
1:G:348:LYS:HA	1:G:352:ARG:HD2	1.95	0.49
1:G:898:LEU:C	1:G:898:LEU:HD12	2.33	0.49
2:N:41:GLY:HA2	2:N:48:TYR:CE1	2.47	0.49
1:B:348:LYS:HA	1:B:352:ARG:HD2	1.95	0.49
1:C:565:GLN:CD	1:C:594:TYR:CE2	2.87	0.49
1:D:205:ARG:NH1	1:E:228:ARG:HH22	2.10	0.49
1:D:345:LEU:HA	1:D:349:GLN:HA	1.94	0.49
1:E:565:GLN:CD	1:E:594:TYR:CE2	2.87	0.49
1:A:1004:LYS:HG3	2:H:73:LYS:HD3	1.94	0.49
2:J:41:GLY:HA2	2:J:48:TYR:CE1	2.47	0.49
1:D:701:GLN:HG2	2:K:25:LYS:HZ3	1.78	0.49
1:G:1004:LYS:HG3	2:N:73:LYS:HD3	1.94	0.49
1:A:348:LYS:HA	1:A:352:ARG:HD2	1.95	0.48
1:B:1168:LEU:CA	1:B:1170:GLU:OE1	2.61	0.48
1:C:581:LYS:HZ1	1:C:1247:LEU:HD11	1.78	0.48
1:E:1077:LYS:C	1:E:1077:LYS:HD2	2.33	0.48
1:E:205:ARG:NH1	1:F:228:ARG:HH22	2.10	0.48
1:G:1089:LEU:O	1:G:1090:SER:HB3	2.13	0.48
2:H:41:GLY:HA2	2:H:48:TYR:CE1	2.47	0.48
1:B:603:ILE:HD12	1:B:603:ILE:C	2.32	0.48
1:C:588:VAL:O	1:C:590:ASN:OD1	2.30	0.48
1:D:603:ILE:C	1:D:603:ILE:HD12	2.32	0.48
2:I:70:ASN:HD22	2:I:70:ASN:C	2.16	0.48
2:J:70:ASN:HD22	2:J:70:ASN:C	2.16	0.48
1:A:1023:ASP:CB	2:H:73:LYS:HZ2	2.25	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1077:LYS:HD2	1:A:1077:LYS:C	2.33	0.48
1:A:1168:LEU:C	1:A:1170:GLU:HB2	2.34	0.48
1:A:565:GLN:CD	1:A:594:TYR:CE2	2.87	0.48
1:D:1168:LEU:CA	1:D:1170:GLU:OE1	2.61	0.48
1:F:205:ARG:NH1	1:G:228:ARG:HH22	2.10	0.48
1:E:1023:ASP:OD1	2:L:73:LYS:CD	2.62	0.48
2:M:41:GLY:HA2	2:M:48:TYR:CE1	2.47	0.48
1:B:1089:LEU:O	1:B:1090:SER:HB3	2.13	0.48
1:B:1168:LEU:C	1:B:1170:GLU:HB2	2.34	0.48
1:B:898:LEU:C	1:B:898:LEU:HD12	2.33	0.48
1:D:898:LEU:C	1:D:898:LEU:HD12	2.33	0.48
1:E:1089:LEU:O	1:E:1090:SER:HB3	2.13	0.48
1:F:1168:LEU:CA	1:F:1170:GLU:OE1	2.61	0.48
1:G:1168:LEU:CA	1:G:1170:GLU:OE1	2.61	0.48
1:A:1089:LEU:O	1:A:1090:SER:HB3	2.13	0.48
1:D:558:GLN:OE1	1:D:1169:SER:C	2.52	0.48
1:D:565:GLN:CD	1:D:594:TYR:CE2	2.87	0.48
1:D:581:LYS:HZ1	1:D:1247:LEU:CD1	2.26	0.48
1:E:1023:ASP:CG	2:L:73:LYS:HD2	2.32	0.48
1:E:1168:LEU:CA	1:E:1170:GLU:OE1	2.61	0.48
1:E:558:GLN:OE1	1:E:1169:SER:C	2.52	0.48
1:G:558:GLN:N	1:G:1171:GLU:OE2	2.47	0.48
1:D:1023:ASP:OD1	2:K:73:LYS:CD	2.62	0.48
1:G:1023:ASP:OD1	2:N:73:LYS:CD	2.62	0.48
1:C:122:ARG:HA	1:C:123:PRO:HD3	1.77	0.48
1:F:1004:LYS:HG3	2:M:73:LYS:HD3	1.94	0.48
1:F:1023:ASP:CG	2:M:73:LYS:HD2	2.32	0.48
1:F:559:PRO:CB	1:F:1175:THR:N	2.51	0.48
1:G:558:GLN:OE1	1:G:1169:SER:C	2.52	0.48
1:D:1023:ASP:CB	2:K:73:LYS:HD3	2.42	0.48
1:F:800:ILE:HD13	2:M:47:SER:HB3	1.95	0.48
1:F:1023:ASP:OD1	2:M:73:LYS:CD	2.62	0.48
1:A:1168:LEU:CA	1:A:1170:GLU:OE1	2.61	0.48
1:A:558:GLN:OE1	1:A:1169:SER:C	2.52	0.48
1:B:1048:LYS:CE	2:I:86:LYS:HZ3	2.25	0.48
1:C:1168:LEU:CA	1:C:1170:GLU:OE1	2.61	0.48
1:D:1128:GLY:C	1:D:1129:CYS:SG	2.91	0.48
1:E:1128:GLY:C	1:E:1129:CYS:SG	2.91	0.48
1:F:1128:GLY:C	1:F:1129:CYS:SG	2.91	0.48
1:A:228:ARG:HH22	1:G:205:ARG:NH1	2.10	0.48
1:G:565:GLN:CD	1:G:594:TYR:CE2	2.87	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1004:LYS:HG3	2:I:73:LYS:HD3	1.94	0.48
1:D:1004:LYS:HG3	2:K:73:LYS:HD3	1.94	0.48
2:M:70:ASN:C	2:M:70:ASN:HD22	2.16	0.48
1:A:520:ALA:C	1:A:524:HIS:CD2	2.88	0.48
1:C:1089:LEU:O	1:C:1090:SER:HB3	2.13	0.48
1:G:800:ILE:HD13	2:N:47:SER:CB	2.44	0.48
1:E:1004:LYS:HG3	2:L:73:LYS:HD3	1.94	0.48
1:G:168:VAL:CG1	1:G:168:VAL:O	2.51	0.48
1:E:1089:LEU:HD21	2:L:86:LYS:HB3	1.85	0.48
1:G:701:GLN:OE1	2:N:25:LYS:HD3	2.10	0.48
1:B:581:LYS:HZ2	1:B:1247:LEU:CD2	2.24	0.47
1:C:558:GLN:OE1	1:C:1169:SER:C	2.52	0.47
1:F:1169:SER:N	1:F:1170:GLU:HB3	2.25	0.47
1:F:565:GLN:CD	1:F:594:TYR:CE2	2.87	0.47
1:E:800:ILE:HD13	2:L:47:SER:CB	2.44	0.47
1:E:116:GLU:OE1	1:F:232:LEU:HD13	2.14	0.47
1:A:232:LEU:HD13	1:G:116:GLU:OE1	2.14	0.47
1:E:701:GLN:OE1	2:L:25:LYS:HD3	2.10	0.47
1:E:800:ILE:HD13	2:L:47:SER:HB3	1.95	0.47
1:G:800:ILE:HD13	2:N:47:SER:HB3	1.95	0.47
1:A:116:GLU:OE1	1:B:232:LEU:HD13	2.14	0.47
1:C:1004:LYS:HG3	2:J:73:LYS:HD3	1.94	0.47
1:D:1089:LEU:O	1:D:1090:SER:HB3	2.13	0.47
2:H:70:ASN:HD22	2:H:70:ASN:C	2.16	0.47
1:D:1048:LYS:HE2	1:D:1048:LYS:O	2.14	0.47
1:D:116:GLU:OE1	1:E:232:LEU:HD13	2.14	0.47
1:D:205:ARG:NH2	1:E:225:ASP:OD2	2.46	0.47
1:G:1048:LYS:O	1:G:1048:LYS:HE2	2.14	0.47
1:A:1048:LYS:O	1:A:1048:LYS:HE2	2.14	0.47
1:D:558:GLN:N	1:D:1171:GLU:OE2	2.47	0.47
3:D:1301:ATP:O2B	3:D:1301:ATP:O2G	2.33	0.47
1:E:205:ARG:NH2	1:F:225:ASP:OD2	2.46	0.47
1:F:558:GLN:OE1	1:F:1169:SER:C	2.52	0.47
1:G:520:ALA:C	1:G:524:HIS:CD2	2.87	0.47
1:C:800:ILE:HD13	2:J:47:SER:HB3	1.95	0.47
1:C:1023:ASP:OD1	2:J:73:LYS:CD	2.62	0.47
1:F:701:GLN:OE1	2:M:25:LYS:HD3	2.10	0.47
1:F:800:ILE:HD13	2:M:47:SER:CB	2.44	0.47
1:B:205:ARG:NH2	1:C:225:ASP:OD2	2.46	0.47
1:G:1106:ASP:OD2	2:N:90:GLU:CG	2.63	0.47
1:G:581:LYS:HZ2	1:G:1247:LEU:CD2	2.24	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:800:ILE:HD13	2:J:47:SER:CB	2.44	0.47
1:E:1106:ASP:OD2	2:L:90:GLU:CG	2.63	0.47
3:E:1301:ATP:O2G	3:E:1301:ATP:O2B	2.33	0.47
1:B:800:ILE:HD13	2:I:47:SER:HB3	1.96	0.47
1:C:1106:ASP:OD2	2:J:90:GLU:CG	2.63	0.47
1:D:800:ILE:HD13	2:K:47:SER:CB	2.44	0.47
1:E:1048:LYS:HE2	1:E:1048:LYS:O	2.14	0.47
1:F:1048:LYS:O	1:F:1048:LYS:HE2	2.14	0.47
1:A:409:GLU:OE1	1:G:340:TYR:OH	2.12	0.47
1:C:558:GLN:N	1:C:1171:GLU:OE2	2.47	0.47
1:D:1023:ASP:CG	2:K:73:LYS:HD2	2.32	0.47
1:F:558:GLN:N	1:F:1171:GLU:OE2	2.47	0.47
1:F:116:GLU:OE1	1:G:232:LEU:HD13	2.14	0.47
1:A:1106:ASP:OD2	2:H:90:GLU:CG	2.63	0.47
2:K:70:ASN:C	2:K:70:ASN:HD22	2.16	0.47
3:A:1301:ATP:O2G	3:A:1301:ATP:O2B	2.33	0.47
1:C:565:GLN:NE2	1:C:592:MET:HE1	2.07	0.47
1:A:800:ILE:HD13	2:H:47:SER:CB	2.44	0.47
1:B:701:GLN:OE1	2:I:25:LYS:HD3	2.10	0.47
1:F:1106:ASP:OD2	2:M:90:GLU:CG	2.63	0.47
1:B:116:GLU:OE1	1:C:232:LEU:HD13	2.14	0.47
1:B:558:GLN:OE1	1:B:1169:SER:C	2.52	0.47
1:D:520:ALA:C	1:D:524:HIS:CD2	2.87	0.47
1:D:800:ILE:HD13	2:K:47:SER:HB3	1.95	0.47
3:B:1301:ATP:O2B	3:B:1301:ATP:O2G	2.33	0.46
1:C:186:SER:HA	1:C:243:ASP:HB3	1.98	0.46
1:D:1106:ASP:OD2	2:K:90:GLU:CG	2.63	0.46
1:C:205:ARG:NH2	1:D:225:ASP:OD2	2.46	0.46
1:E:520:ALA:C	1:E:524:HIS:CD2	2.88	0.46
1:F:520:ALA:C	1:F:524:HIS:CD2	2.87	0.46
3:G:1301:ATP:O2B	3:G:1301:ATP:O2G	2.33	0.46
1:G:186:SER:HA	1:G:243:ASP:HB3	1.98	0.46
1:B:800:ILE:HD13	2:I:47:SER:CB	2.44	0.46
1:B:1048:LYS:O	1:B:1048:LYS:HE2	2.14	0.46
3:C:1301:ATP:O2G	3:C:1301:ATP:O2B	2.33	0.46
1:G:1023:ASP:CG	2:N:73:LYS:HD2	2.32	0.46
1:A:677:VAL:HG22	2:H:25:LYS:HZ3	1.80	0.46
1:B:1023:ASP:OD1	2:I:73:LYS:CD	2.62	0.46
1:C:1048:LYS:O	1:C:1048:LYS:HE2	2.14	0.46
1:G:1169:SER:N	1:G:1170:GLU:HB3	2.25	0.46
1:A:800:ILE:HD13	2:H:47:SER:HB3	1.95	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1023:ASP:CG	2:K:73:LYS:HZ2	2.19	0.46
1:B:1106:ASP:OD2	2:I:90:GLU:CG	2.63	0.46
1:C:116:GLU:OE1	1:D:232:LEU:HD13	2.14	0.46
1:D:186:SER:HA	1:D:243:ASP:HB3	1.98	0.46
1:G:1048:LYS:CE	2:N:86:LYS:HZ3	2.27	0.46
1:A:186:SER:HA	1:A:243:ASP:HB3	1.98	0.46
1:C:1023:ASP:CG	2:J:73:LYS:HZ2	2.19	0.46
3:F:1301:ATP:O2G	3:F:1301:ATP:O2B	2.33	0.46
1:F:205:ARG:NH2	1:G:225:ASP:OD2	2.46	0.46
1:B:186:SER:HA	1:B:243:ASP:HB3	1.98	0.46
1:D:565:GLN:CD	1:D:594:TYR:HE2	2.19	0.46
1:F:186:SER:HA	1:F:243:ASP:HB3	1.98	0.46
1:F:349:GLN:H	1:F:349:GLN:HG3	1.49	0.46
1:D:701:GLN:OE1	2:K:25:LYS:HD3	2.10	0.46
1:B:555:LEU:HD23	1:B:560:PHE:HE1	1.21	0.46
1:E:186:SER:HA	1:E:243:ASP:HB3	1.98	0.46
1:E:349:GLN:H	1:E:349:GLN:HG3	1.49	0.46
1:A:1023:ASP:OD1	2:H:73:LYS:CD	2.62	0.46
2:I:14:CYS:HG	4:I:500:HEM:CAB	2.08	0.46
1:F:559:PRO:HD3	1:F:1175:THR:HG23	1.98	0.46
1:G:752:SER:HB2	1:G:753:PRO:HD2	1.98	0.46
1:A:752:SER:HB2	1:A:753:PRO:HD2	1.98	0.45
1:B:558:GLN:N	1:B:1171:GLU:OE2	2.47	0.45
1:C:520:ALA:C	1:C:524:HIS:CD2	2.87	0.45
1:C:565:GLN:CD	1:C:594:TYR:HE2	2.19	0.45
1:D:1001:GLN:O	1:D:1002:HIS:HB2	2.16	0.45
1:F:1001:GLN:O	1:F:1002:HIS:HB2	2.16	0.45
1:F:558:GLN:HG3	1:F:1171:GLU:OE2	2.17	0.45
1:A:558:GLN:HG3	1:A:1171:GLU:OE2	2.17	0.45
1:B:345:LEU:O	1:B:349:GLN:HG3	2.17	0.45
1:B:565:GLN:CD	1:B:594:TYR:HE2	2.19	0.45
1:D:349:GLN:H	1:D:349:GLN:HG3	1.49	0.45
1:E:559:PRO:HD3	1:E:1175:THR:HG23	1.98	0.45
1:A:345:LEU:O	1:A:349:GLN:HG3	2.17	0.45
1:B:520:ALA:O	1:B:524:HIS:HD2	1.89	0.45
1:D:521:HIS:HA	1:D:524:HIS:HD2	1.82	0.45
1:D:558:GLN:HG3	1:D:1171:GLU:OE2	2.17	0.45
1:E:1001:GLN:O	1:E:1002:HIS:HB2	2.16	0.45
1:E:565:GLN:CD	1:E:594:TYR:HE2	2.19	0.45
1:F:345:LEU:O	1:F:349:GLN:HG3	2.17	0.45
1:G:559:PRO:HD3	1:G:1175:THR:HG23	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:PRO:HD3	1:A:1175:THR:HG23	1.98	0.45
1:B:1001:GLN:O	1:B:1002:HIS:HB2	2.16	0.45
1:B:208:GLN:HG2	1:C:229:ILE:CG1	2.44	0.45
1:C:558:GLN:CG	1:C:1171:GLU:OE2	2.65	0.45
1:E:521:HIS:HA	1:E:524:HIS:HD2	1.82	0.45
1:F:521:HIS:HA	1:F:524:HIS:HD2	1.82	0.45
1:G:1048:LYS:CG	2:N:86:LYS:HZ2	2.21	0.45
1:G:345:LEU:O	1:G:349:GLN:HG3	2.17	0.45
1:A:565:GLN:CD	1:A:594:TYR:HE2	2.19	0.45
1:B:521:HIS:HA	1:B:524:HIS:HD2	1.82	0.45
1:C:345:LEU:O	1:C:349:GLN:HG3	2.17	0.45
1:C:558:GLN:HG3	1:C:1171:GLU:OE2	2.17	0.45
1:E:345:LEU:O	1:E:349:GLN:HG3	2.17	0.45
1:F:208:GLN:HG2	1:G:229:ILE:CG1	2.44	0.45
1:A:1001:GLN:O	1:A:1002:HIS:HB2	2.16	0.45
1:A:225:ASP:OD2	1:G:205:ARG:NH2	2.46	0.45
1:B:1023:ASP:CG	2:I:73:LYS:HD2	2.33	0.45
1:B:752:SER:HB2	1:B:753:PRO:HD2	1.98	0.45
1:C:1001:GLN:O	1:C:1002:HIS:HB2	2.16	0.45
1:C:581:LYS:HZ2	1:C:1247:LEU:CD2	2.25	0.45
1:D:345:LEU:O	1:D:349:GLN:HG3	2.17	0.45
1:A:521:HIS:HA	1:A:524:HIS:HD2	1.82	0.45
1:B:1023:ASP:OD1	2:I:73:LYS:HD2	2.17	0.45
1:C:521:HIS:HA	1:C:524:HIS:HD2	1.82	0.45
1:D:559:PRO:HD3	1:D:1175:THR:HG23	1.98	0.45
1:G:565:GLN:CD	1:G:594:TYR:HE2	2.19	0.45
2:M:17:CYS:SG	4:M:500:HEM:C3C	3.10	0.45
1:B:1048:LYS:CG	2:I:86:LYS:HZ2	2.23	0.45
1:B:558:GLN:CG	1:B:1171:GLU:OE2	2.65	0.45
1:C:1023:ASP:CG	2:J:73:LYS:HD2	2.32	0.45
1:F:565:GLN:CD	1:F:594:TYR:HE2	2.19	0.45
1:C:1023:ASP:OD1	2:J:73:LYS:HD2	2.17	0.45
1:G:558:GLN:HG3	1:G:1171:GLU:OE2	2.17	0.45
1:A:205:ARG:NH2	1:B:225:ASP:OD2	2.46	0.45
1:D:677:VAL:HG22	2:K:25:LYS:NZ	2.32	0.45
1:E:558:GLN:HG3	1:E:1171:GLU:OE2	2.17	0.45
1:F:752:SER:HB2	1:F:753:PRO:HD2	1.98	0.45
1:G:521:HIS:HA	1:G:524:HIS:HD2	1.82	0.45
1:A:1023:ASP:OD1	2:H:73:LYS:HD2	2.17	0.45
1:C:559:PRO:HD3	1:C:1175:THR:HG23	1.98	0.44
1:C:677:VAL:HG22	2:J:25:LYS:NZ	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:752:SER:HB2	1:D:753:PRO:HD2	1.99	0.44
1:A:229:ILE:CG1	1:G:208:GLN:HG2	2.44	0.44
1:G:391:LYS:HA	1:G:392:ASP:HA	1.68	0.44
2:L:17:CYS:SG	4:L:500:HEM:C3C	3.10	0.44
1:B:677:VAL:HG22	2:I:25:LYS:NZ	2.32	0.44
1:D:558:GLN:CG	1:D:1171:GLU:OE2	2.65	0.44
1:E:1168:LEU:C	1:E:1170:GLU:HB2	2.34	0.44
1:E:208:GLN:HG2	1:F:229:ILE:CG1	2.44	0.44
1:G:701:GLN:CD	2:N:25:LYS:CD	2.61	0.44
1:G:677:VAL:HG22	2:N:25:LYS:NZ	2.32	0.44
1:C:1048:LYS:CG	2:J:86:LYS:HZ2	2.26	0.44
1:F:677:VAL:HG22	2:M:25:LYS:NZ	2.32	0.44
1:G:1023:ASP:OD1	2:N:73:LYS:HD2	2.17	0.44
1:B:122:ARG:HA	1:B:123:PRO:HD3	1.77	0.44
2:K:17:CYS:SG	4:K:500:HEM:C3C	3.10	0.44
1:A:1023:ASP:CG	2:H:73:LYS:HD2	2.32	0.44
1:A:558:GLN:CG	1:A:1171:GLU:OE2	2.65	0.44
1:B:520:ALA:C	1:B:524:HIS:CD2	2.87	0.44
1:E:558:GLN:N	1:E:1171:GLU:OE2	2.47	0.44
1:F:345:LEU:HG	1:F:349:GLN:CB	2.46	0.44
1:F:643:LYS:HB3	1:F:646:THR:HG22	1.99	0.44
1:A:677:VAL:HG22	2:H:25:LYS:NZ	2.32	0.44
1:B:643:LYS:HB3	1:B:646:THR:HG22	1.99	0.44
1:E:677:VAL:HG22	2:L:25:LYS:NZ	2.32	0.44
1:G:1171:GLU:C	1:G:1173:ALA:N	2.71	0.44
2:H:17:CYS:SG	4:H:500:HEM:C3C	3.10	0.44
1:A:701:GLN:HG2	2:H:25:LYS:HZ3	1.82	0.44
2:H:14:CYS:CB	4:H:500:HEM:HAB	2.47	0.44
2:K:14:CYS:CB	4:K:500:HEM:HAB	2.47	0.44
1:B:558:GLN:HG3	1:B:1171:GLU:OE2	2.17	0.44
1:B:559:PRO:HD3	1:B:1175:THR:HG23	1.98	0.44
1:C:752:SER:HB2	1:C:753:PRO:HD2	1.98	0.44
1:F:1168:LEU:C	1:F:1170:GLU:HB2	2.34	0.44
1:G:1023:ASP:CB	2:N:73:LYS:HZ2	2.30	0.44
1:G:558:GLN:CG	1:G:1171:GLU:OE2	2.65	0.44
1:D:1023:ASP:OD1	2:K:73:LYS:HD2	2.17	0.44
1:D:122:ARG:HA	1:D:123:PRO:HD3	1.77	0.44
1:E:1171:GLU:C	1:E:1173:ALA:N	2.71	0.44
1:E:391:LYS:HB2	1:E:392:ASP:HA	2.00	0.44
1:E:643:LYS:HB3	1:E:646:THR:HG22	1.99	0.44
1:G:1001:GLN:O	1:G:1002:HIS:HB2	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:17:CYS:SG	4:J:500:HEM:C3C	3.10	0.44
1:F:1023:ASP:OD1	2:M:73:LYS:HD2	2.17	0.44
1:A:643:LYS:HB3	1:A:646:THR:HG22	1.99	0.44
1:C:208:GLN:HG2	1:D:229:ILE:CG1	2.44	0.44
1:D:1171:GLU:C	1:D:1173:ALA:N	2.71	0.44
1:F:558:GLN:CG	1:F:1171:GLU:OE2	2.65	0.44
1:C:559:PRO:CB	1:C:1175:THR:N	2.51	0.43
1:E:1023:ASP:OD1	2:L:73:LYS:HD2	2.17	0.43
1:E:752:SER:HB2	1:E:753:PRO:HD2	1.99	0.43
1:F:391:LYS:HB2	1:F:392:ASP:HA	2.00	0.43
1:F:1089:LEU:HD21	2:M:86:LYS:HB3	1.85	0.43
1:A:558:GLN:N	1:A:1171:GLU:OE2	2.47	0.43
1:A:581:LYS:HZ1	1:A:1247:LEU:CD1	2.29	0.43
1:A:588:VAL:HG12	1:A:589:ASP:HB2	2.00	0.43
1:B:588:VAL:HG12	1:B:589:ASP:HB2	2.00	0.43
1:C:588:VAL:HG12	1:C:589:ASP:HB2	2.00	0.43
1:D:306:LEU:HA	1:D:307:PRO:HD3	1.82	0.43
1:D:588:VAL:HG12	1:D:589:ASP:HB2	2.00	0.43
1:D:1168:LEU:C	1:D:1170:GLU:HB2	2.34	0.43
1:D:559:PRO:CB	1:D:1175:THR:N	2.51	0.43
1:E:515:GLU:HG3	1:E:560:PHE:CZ	2.53	0.43
1:F:515:GLU:HG3	1:F:560:PHE:CZ	2.53	0.43
1:G:588:VAL:HG12	1:G:589:ASP:HB2	2.00	0.43
2:M:14:CYS:CB	4:M:500:HEM:HAB	2.47	0.43
1:A:515:GLU:HG3	1:A:560:PHE:CZ	2.53	0.43
1:A:704:CYS:SG	1:A:749:CYS:N	2.92	0.43
1:D:515:GLU:HG3	1:D:560:PHE:CZ	2.53	0.43
1:F:588:VAL:HG12	1:F:589:ASP:HB2	2.00	0.43
1:G:391:LYS:HB2	1:G:392:ASP:HA	2.00	0.43
1:G:515:GLU:HG3	1:G:560:PHE:CZ	2.53	0.43
1:G:643:LYS:HB3	1:G:646:THR:HG22	1.99	0.43
2:J:72:LYS:HD3	2:J:78:THR:CG2	2.48	0.43
1:A:345:LEU:HG	1:A:349:GLN:CB	2.46	0.43
1:C:643:LYS:HB3	1:C:646:THR:HG22	1.99	0.43
1:D:391:LYS:HB2	1:D:392:ASP:HA	2.00	0.43
1:D:590:ASN:O	1:D:592:MET:CG	2.64	0.43
1:E:558:GLN:CG	1:E:1171:GLU:OE2	2.65	0.43
1:G:1168:LEU:C	1:G:1170:GLU:HB2	2.34	0.43
1:G:349:GLN:H	1:G:349:GLN:HG3	1.49	0.43
2:M:72:LYS:HD3	2:M:78:THR:CG2	2.48	0.43
1:B:391:LYS:HB2	1:B:392:ASP:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:GLU:HG3	1:B:560:PHE:CZ	2.53	0.43
1:B:704:CYS:SG	1:B:749:CYS:N	2.92	0.43
1:C:515:GLU:HG3	1:C:560:PHE:CZ	2.53	0.43
1:C:704:CYS:SG	1:C:749:CYS:N	2.92	0.43
1:D:704:CYS:SG	1:D:749:CYS:N	2.92	0.43
1:E:588:VAL:HG12	1:E:589:ASP:HB2	2.00	0.43
1:F:1171:GLU:C	1:F:1173:ALA:N	2.71	0.43
2:I:17:CYS:SG	4:I:500:HEM:C3C	3.10	0.43
1:C:391:LYS:HB2	1:C:392:ASP:HA	2.00	0.43
1:D:643:LYS:HB3	1:D:646:THR:HG22	1.99	0.43
1:G:704:CYS:SG	1:G:749:CYS:N	2.92	0.43
2:L:72:LYS:HD3	2:L:78:THR:CG2	2.48	0.43
1:A:208:GLN:HG2	1:B:229:ILE:CG1	2.44	0.43
1:D:208:GLN:HG2	1:E:229:ILE:CG1	2.44	0.43
1:E:704:CYS:SG	1:E:749:CYS:N	2.92	0.43
1:F:668:ASP:O	1:F:669:ASP:HB2	2.19	0.43
1:G:1072:ILE:O	1:G:1073:ILE:HB	2.19	0.43
2:K:72:LYS:HD3	2:K:78:THR:CG2	2.48	0.43
1:A:1048:LYS:CG	2:H:86:LYS:HZ2	2.27	0.43
1:A:391:LYS:HB2	1:A:392:ASP:HA	2.00	0.43
1:E:345:LEU:HG	1:E:349:GLN:CB	2.46	0.43
1:F:1032:TRP:O	1:F:1033:GLN:HB3	2.19	0.43
1:G:345:LEU:HG	1:G:349:GLN:CB	2.46	0.43
2:I:14:CYS:CB	4:I:500:HEM:HAB	2.47	0.43
1:C:1171:GLU:C	1:C:1173:ALA:N	2.71	0.42
1:F:1096:ASP:O	1:F:1097:ALA:C	2.58	0.42
1:F:704:CYS:SG	1:F:749:CYS:N	2.92	0.42
2:N:72:LYS:HD3	2:N:78:THR:CG2	2.48	0.42
1:A:1004:LYS:HZ2	2:H:73:LYS:CD	2.32	0.42
1:B:1072:ILE:O	1:B:1073:ILE:HB	2.19	0.42
1:E:1164:LEU:HD12	1:E:1164:LEU:N	2.35	0.42
1:G:1032:TRP:O	1:G:1033:GLN:HB3	2.19	0.42
2:N:17:CYS:SG	4:N:500:HEM:C3C	3.10	0.42
1:D:1032:TRP:O	1:D:1033:GLN:HB3	2.19	0.42
1:D:1164:LEU:HD12	1:D:1164:LEU:N	2.35	0.42
1:F:1164:LEU:N	1:F:1164:LEU:HD12	2.35	0.42
1:A:1032:TRP:O	1:A:1033:GLN:HB3	2.19	0.42
1:A:229:ILE:HG12	1:G:208:GLN:CG	2.50	0.42
1:D:701:GLN:CD	2:K:25:LYS:CD	2.61	0.42
1:E:668:ASP:O	1:E:669:ASP:HB2	2.19	0.42
2:N:14:CYS:CB	4:N:500:HEM:HAB	2.47	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1096:ASP:O	1:A:1097:ALA:C	2.58	0.42
1:A:208:GLN:CG	1:B:229:ILE:HG12	2.50	0.42
1:B:1164:LEU:HD12	1:B:1164:LEU:N	2.35	0.42
1:D:1072:ILE:O	1:D:1073:ILE:HB	2.19	0.42
1:D:668:ASP:O	1:D:669:ASP:HB2	2.19	0.42
1:E:1072:ILE:O	1:E:1073:ILE:HB	2.19	0.42
1:F:208:GLN:CG	1:G:229:ILE:HG12	2.50	0.42
1:F:340:TYR:OH	1:G:409:GLU:OE1	2.12	0.42
1:G:1164:LEU:HD12	1:G:1164:LEU:N	2.35	0.42
1:C:1032:TRP:O	1:C:1033:GLN:HB3	2.19	0.42
1:E:340:TYR:OH	1:F:409:GLU:HG2	2.18	0.42
1:E:677:VAL:HG22	2:L:25:LYS:HZ3	1.85	0.42
1:G:668:ASP:O	1:G:669:ASP:HB2	2.19	0.42
2:H:68:LEU:HD21	4:H:500:HEM:HMB2	2.02	0.42
1:D:1088:VAL:C	2:K:86:LYS:CE	2.72	0.42
1:E:1096:ASP:O	1:E:1097:ALA:C	2.58	0.42
1:D:340:TYR:OH	1:E:409:GLU:OE1	2.12	0.42
2:N:68:LEU:HD21	4:N:500:HEM:HMB2	2.02	0.42
1:B:1032:TRP:O	1:B:1033:GLN:HB3	2.19	0.42
1:B:348:LYS:CA	1:B:352:ARG:HD2	2.50	0.42
1:C:208:GLN:CG	1:D:229:ILE:HG12	2.50	0.42
1:F:1072:ILE:O	1:F:1073:ILE:HB	2.19	0.42
1:F:348:LYS:CA	1:F:352:ARG:HD2	2.50	0.42
2:J:14:CYS:SG	4:J:500:HEM:CBB	3.05	0.42
1:C:348:LYS:CA	1:C:352:ARG:HD2	2.50	0.42
2:I:68:LEU:HD21	4:I:500:HEM:HMB2	2.02	0.42
2:M:17:CYS:SG	4:M:500:HEM:HAC	2.60	0.42
1:A:348:LYS:CA	1:A:352:ARG:HD2	2.50	0.42
1:B:1171:GLU:C	1:B:1173:ALA:N	2.71	0.42
1:C:1072:ILE:O	1:C:1073:ILE:HB	2.19	0.42
1:C:1168:LEU:C	1:C:1170:GLU:HB2	2.34	0.42
1:C:668:ASP:O	1:C:669:ASP:HB2	2.19	0.42
1:A:668:ASP:O	1:A:669:ASP:HB2	2.19	0.41
1:B:208:GLN:CG	1:C:229:ILE:HG12	2.50	0.41
1:B:668:ASP:O	1:B:669:ASP:HB2	2.19	0.41
1:D:581:LYS:HZ1	1:D:1247:LEU:HD11	1.84	0.41
1:E:208:GLN:CG	1:F:229:ILE:HG12	2.50	0.41
1:A:1072:ILE:O	1:A:1073:ILE:HB	2.19	0.41
1:B:1096:ASP:O	1:B:1097:ALA:C	2.58	0.41
2:I:17:CYS:SG	4:I:500:HEM:HAC	2.60	0.41
2:M:68:LEU:HD21	4:M:500:HEM:HMB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1171:GLU:C	1:A:1173:ALA:N	2.71	0.41
1:B:340:TYR:OH	1:C:409:GLU:HG2	2.18	0.41
1:C:1096:ASP:O	1:C:1097:ALA:C	2.58	0.41
1:C:391:LYS:CB	1:C:392:ASP:HA	2.49	0.41
1:D:1096:ASP:O	1:D:1097:ALA:C	2.58	0.41
1:D:122:ARG:HD3	1:D:122:ARG:H	1.86	0.41
1:D:348:LYS:CA	1:D:352:ARG:HD2	2.50	0.41
1:F:701:GLN:NE2	2:M:25:LYS:CD	2.83	0.41
1:G:122:ARG:HD3	1:G:122:ARG:H	1.86	0.41
2:J:14:CYS:CB	4:J:500:HEM:HAB	2.47	0.41
1:C:1164:LEU:N	1:C:1164:LEU:HD12	2.35	0.41
1:D:345:LEU:HG	1:D:349:GLN:CB	2.46	0.41
1:E:1032:TRP:O	1:E:1033:GLN:HB3	2.19	0.41
1:E:391:LYS:HA	1:E:392:ASP:HA	1.68	0.41
1:A:945:ARG:HD2	1:A:961:GLU:HB2	2.03	0.41
1:E:1094:SER:O	1:E:1096:ASP:N	2.53	0.41
1:G:348:LYS:CA	1:G:352:ARG:HD2	2.50	0.41
2:K:57:ILE:C	2:K:57:ILE:HD12	2.41	0.41
1:A:122:ARG:HD3	1:A:122:ARG:H	1.86	0.41
1:B:345:LEU:HG	1:B:349:GLN:CB	2.46	0.41
1:B:945:ARG:HD2	1:B:961:GLU:HB2	2.03	0.41
1:C:349:GLN:HG3	1:C:349:GLN:H	1.49	0.41
1:C:520:ALA:O	1:C:524:HIS:HD2	1.89	0.41
1:D:340:TYR:OH	1:E:409:GLU:HG2	2.18	0.41
1:G:945:ARG:HD2	1:G:961:GLU:HB2	2.03	0.41
2:J:68:LEU:HD21	4:J:500:HEM:HMB2	2.02	0.41
2:N:57:ILE:HD12	2:N:57:ILE:C	2.41	0.41
1:A:1164:LEU:HD12	1:A:1164:LEU:N	2.35	0.41
1:A:587:GLU:CB	1:A:590:ASN:HD21	2.34	0.41
1:C:122:ARG:H	1:C:122:ARG:HD3	1.86	0.41
1:D:1139:SER:O	1:D:1140:THR:HB	2.21	0.41
1:E:348:LYS:CA	1:E:352:ARG:HD2	2.50	0.41
1:F:945:ARG:HD2	1:F:961:GLU:HB2	2.03	0.41
2:H:57:ILE:C	2:H:57:ILE:HD12	2.41	0.41
1:C:677:VAL:HG22	2:J:25:LYS:HZ3	1.86	0.41
1:C:945:ARG:HD2	1:C:961:GLU:HB2	2.03	0.41
1:E:1139:SER:O	1:E:1140:THR:HB	2.21	0.41
1:F:587:GLU:HB3	1:F:590:ASN:ND2	2.36	0.41
1:G:1139:SER:O	1:G:1140:THR:HB	2.21	0.41
1:G:587:GLU:HB3	1:G:590:ASN:ND2	2.36	0.41
1:G:701:GLN:NE2	2:N:25:LYS:CD	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:57:ILE:HD12	2:I:57:ILE:C	2.41	0.41
1:A:122:ARG:HA	1:A:123:PRO:HD3	1.77	0.41
1:C:1004:LYS:HZ2	2:J:73:LYS:CD	2.33	0.41
1:C:345:LEU:HG	1:C:349:GLN:CB	2.46	0.41
1:D:208:GLN:CG	1:E:229:ILE:HG12	2.50	0.41
1:D:587:GLU:HB3	1:D:590:ASN:ND2	2.36	0.41
1:E:587:GLU:HB3	1:E:590:ASN:ND2	2.36	0.41
1:F:587:GLU:CB	1:F:590:ASN:HD21	2.34	0.41
1:B:587:GLU:CB	1:B:590:ASN:HD21	2.34	0.41
1:C:587:GLU:HB3	1:C:590:ASN:ND2	2.36	0.41
1:D:1094:SER:O	1:D:1096:ASP:N	2.53	0.41
1:D:587:GLU:CB	1:D:590:ASN:HD21	2.34	0.41
1:F:122:ARG:H	1:F:122:ARG:HD3	1.86	0.41
1:F:701:GLN:CD	2:M:25:LYS:CD	2.61	0.41
2:M:57:ILE:HD12	2:M:57:ILE:C	2.41	0.41
1:A:587:GLU:HB3	1:A:590:ASN:ND2	2.36	0.41
1:A:701:GLN:NE2	2:H:25:LYS:CD	2.83	0.41
1:B:1178:GLY:O	1:B:1179:TRP:HB3	2.21	0.41
1:B:587:GLU:HB3	1:B:590:ASN:ND2	2.36	0.41
1:C:340:TYR:OH	1:D:409:GLU:HG2	2.18	0.41
1:E:122:ARG:H	1:E:122:ARG:HD3	1.86	0.41
1:E:122:ARG:HA	1:E:123:PRO:HD3	1.77	0.41
1:G:1096:ASP:O	1:G:1097:ALA:C	2.58	0.41
2:H:72:LYS:HD3	2:H:78:THR:CG2	2.48	0.41
1:D:1178:GLY:O	1:D:1179:TRP:HB3	2.21	0.40
1:D:677:VAL:HG22	2:K:25:LYS:HZ3	1.85	0.40
1:F:581:LYS:NZ	1:F:1247:LEU:HD11	2.37	0.40
1:G:581:LYS:NZ	1:G:1247:LEU:HD11	2.37	0.40
1:G:587:GLU:CB	1:G:590:ASN:HD21	2.34	0.40
1:G:592:MET:O	1:G:593:LEU:HB3	2.22	0.40
1:A:1139:SER:O	1:A:1140:THR:HB	2.21	0.40
1:C:592:MET:O	1:C:593:LEU:HB3	2.22	0.40
1:D:716:LEU:HB2	1:D:730:LEU:HD21	2.03	0.40
1:D:945:ARG:HD2	1:D:961:GLU:HB2	2.03	0.40
1:E:945:ARG:HD2	1:E:961:GLU:HB2	2.03	0.40
1:F:1094:SER:O	1:F:1096:ASP:N	2.53	0.40
1:F:1139:SER:O	1:F:1140:THR:HB	2.21	0.40
1:G:1178:GLY:O	1:G:1179:TRP:HB3	2.21	0.40
2:K:68:LEU:HD21	4:K:500:HEM:HMB2	2.02	0.40
1:G:1089:LEU:HD21	2:N:86:LYS:HB3	1.85	0.40
1:B:122:ARG:H	1:B:122:ARG:HD3	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1178:GLY:O	1:E:1179:TRP:HB3	2.21	0.40
1:E:587:GLU:CB	1:E:590:ASN:HD21	2.34	0.40
2:J:57:ILE:C	2:J:57:ILE:HD12	2.41	0.40
1:A:208:GLN:CG	1:B:229:ILE:CG1	3.00	0.40
1:A:559:PRO:HA	1:A:1171:GLU:HA	2.04	0.40
1:B:1139:SER:O	1:B:1140:THR:HB	2.21	0.40
1:B:126:PHE:HA	3:B:1301:ATP:C2	2.57	0.40
1:B:235:HIS:N	1:B:236:PRO:CD	2.85	0.40
1:C:235:HIS:N	1:C:236:PRO:CD	2.85	0.40
1:D:208:GLN:CG	1:E:229:ILE:CG1	3.00	0.40
1:E:235:HIS:N	1:E:236:PRO:CD	2.85	0.40
1:F:126:PHE:HA	3:F:1301:ATP:C2	2.57	0.40
1:F:592:MET:O	1:F:593:LEU:HB3	2.22	0.40
1:A:235:HIS:N	1:A:236:PRO:CD	2.85	0.40
1:A:592:MET:O	1:A:593:LEU:HB3	2.22	0.40
1:A:701:GLN:CD	2:H:25:LYS:CD	2.61	0.40
1:C:581:LYS:NZ	1:C:1247:LEU:HD11	2.37	0.40
1:E:1202:TRP:HA	1:E:1208:GLU:HA	2.04	0.40
1:E:306:LEU:HA	1:E:307:PRO:HD3	1.82	0.40
1:F:559:PRO:HA	1:F:1171:GLU:HA	2.04	0.40
1:F:208:GLN:CB	1:G:229:ILE:CD1	2.77	0.40
1:F:520:ALA:O	1:F:524:HIS:HD2	1.89	0.40
1:G:1016:LYS:O	1:G:1017:THR:HB	2.22	0.40
1:C:1089:LEU:HD21	2:J:86:LYS:HB3	1.85	0.40
2:L:57:ILE:C	2:L:57:ILE:HD12	2.41	0.40
2:L:68:LEU:HD21	4:L:500:HEM:HMB2	2.02	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	1142/1263 (90%)	1048 (92%)	68 (6%)	26 (2%)	7	41
1	B	1142/1263 (90%)	1048 (92%)	68 (6%)	26 (2%)	7	41
1	C	1142/1263 (90%)	1048 (92%)	68 (6%)	26 (2%)	7	41
1	D	1142/1263 (90%)	1048 (92%)	68 (6%)	26 (2%)	7	41
1	E	1142/1263 (90%)	1048 (92%)	68 (6%)	26 (2%)	7	41
1	F	1142/1263 (90%)	1049 (92%)	67 (6%)	26 (2%)	7	41
1	G	1142/1263 (90%)	1048 (92%)	68 (6%)	26 (2%)	7	41
2	H	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
2	I	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
2	J	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
2	K	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
2	L	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
2	M	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
2	N	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
All	All	8708/9569 (91%)	8030 (92%)	496 (6%)	182 (2%)	12	43

All (182) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	348	LYS
1	A	349	GLN
1	A	591	GLY
1	A	592	MET
1	A	839	HIS
1	A	955	GLN
1	A	1107	LYS
1	A	1140	THR
1	A	1169	SER
1	A	1170	GLU
1	B	348	LYS
1	B	349	GLN
1	B	591	GLY
1	B	592	MET
1	B	839	HIS
1	B	955	GLN
1	B	1107	LYS
1	B	1140	THR
1	B	1169	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1170	GLU
1	C	348	LYS
1	C	349	GLN
1	C	591	GLY
1	C	592	MET
1	C	839	HIS
1	C	955	GLN
1	C	1107	LYS
1	C	1140	THR
1	C	1169	SER
1	C	1170	GLU
1	D	348	LYS
1	D	349	GLN
1	D	591	GLY
1	D	592	MET
1	D	839	HIS
1	D	955	GLN
1	D	1107	LYS
1	D	1140	THR
1	D	1169	SER
1	D	1170	GLU
1	E	348	LYS
1	E	349	GLN
1	E	591	GLY
1	E	592	MET
1	E	839	HIS
1	E	955	GLN
1	E	1107	LYS
1	E	1140	THR
1	E	1169	SER
1	E	1170	GLU
1	F	348	LYS
1	F	349	GLN
1	F	591	GLY
1	F	592	MET
1	F	839	HIS
1	F	955	GLN
1	F	1107	LYS
1	F	1140	THR
1	F	1169	SER
1	F	1170	GLU
1	G	348	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	349	GLN
1	G	591	GLY
1	G	592	MET
1	G	839	HIS
1	G	955	GLN
1	G	1107	LYS
1	G	1140	THR
1	G	1169	SER
1	G	1170	GLU
1	A	589	ASP
1	A	1098	THR
1	A	1174	ALA
1	B	589	ASP
1	B	1098	THR
1	B	1174	ALA
1	C	589	ASP
1	C	1098	THR
1	C	1174	ALA
1	D	589	ASP
1	D	1098	THR
1	D	1174	ALA
1	E	589	ASP
1	E	1098	THR
1	E	1174	ALA
1	F	589	ASP
1	F	1098	THR
1	F	1174	ALA
1	G	589	ASP
1	G	1098	THR
1	G	1174	ALA
1	A	963	GLN
1	A	1129	CYS
1	A	1139	SER
1	A	1222	LYS
1	B	963	GLN
1	B	1129	CYS
1	B	1139	SER
1	B	1222	LYS
1	C	963	GLN
1	C	1129	CYS
1	C	1139	SER
1	C	1222	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	963	GLN
1	D	1129	CYS
1	D	1139	SER
1	D	1222	LYS
1	E	963	GLN
1	E	1129	CYS
1	E	1139	SER
1	E	1222	LYS
1	F	963	GLN
1	F	1129	CYS
1	F	1139	SER
1	F	1222	LYS
1	G	963	GLN
1	G	1129	CYS
1	G	1139	SER
1	G	1222	LYS
1	A	593	LEU
1	A	604	THR
1	A	1205	VAL
1	B	593	LEU
1	B	604	THR
1	B	1205	VAL
1	C	593	LEU
1	C	604	THR
1	C	1205	VAL
1	D	593	LEU
1	D	604	THR
1	D	1205	VAL
1	E	593	LEU
1	E	604	THR
1	E	1205	VAL
1	F	593	LEU
1	F	604	THR
1	F	1205	VAL
1	G	593	LEU
1	G	604	THR
1	G	1205	VAL
1	A	1017	THR
1	A	1172	GLY
1	A	1206	THR
1	B	1017	THR
1	B	1172	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1206	THR
1	C	1017	THR
1	C	1172	GLY
1	C	1206	THR
1	D	1017	THR
1	D	1172	GLY
1	D	1206	THR
1	E	1017	THR
1	E	1172	GLY
1	E	1206	THR
1	F	1017	THR
1	F	1172	GLY
1	F	1206	THR
1	G	1017	THR
1	G	1172	GLY
1	G	1206	THR
1	A	1209	SER
1	B	1209	SER
1	C	1209	SER
1	D	1209	SER
1	E	1209	SER
1	F	1209	SER
1	G	1209	SER
1	A	880	GLY
1	B	880	GLY
1	D	880	GLY
1	E	880	GLY
1	F	880	GLY
1	G	880	GLY
1	A	1073	ILE
1	B	1073	ILE
1	C	880	GLY
1	C	1073	ILE
1	D	1073	ILE
1	E	1073	ILE
1	F	1073	ILE
1	G	1073	ILE

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	1027/1134 (91%)	1020 (99%)	7 (1%)	85	93
1	B	1027/1134 (91%)	1020 (99%)	7 (1%)	85	93
1	C	1027/1134 (91%)	1020 (99%)	7 (1%)	85	93
1	D	1027/1134 (91%)	1020 (99%)	7 (1%)	85	93
1	E	1027/1134 (91%)	1020 (99%)	7 (1%)	85	93
1	F	1027/1134 (91%)	1020 (99%)	7 (1%)	85	93
1	G	1027/1134 (91%)	1020 (99%)	7 (1%)	85	93
2	H	84/84 (100%)	82 (98%)	2 (2%)	52	75
2	I	84/84 (100%)	82 (98%)	2 (2%)	52	75
2	J	84/84 (100%)	82 (98%)	2 (2%)	52	75
2	K	84/84 (100%)	82 (98%)	2 (2%)	52	75
2	L	84/84 (100%)	82 (98%)	2 (2%)	52	75
2	M	84/84 (100%)	82 (98%)	2 (2%)	52	75
2	N	84/84 (100%)	82 (98%)	2 (2%)	52	75
All	All	7777/8526 (91%)	7714 (99%)	63 (1%)	84	92

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ARG
1	A	140	LEU
1	A	349	GLN
1	A	589	ASP
1	A	590	ASN
1	A	846	CYS
1	A	1077	LYS
1	B	122	ARG
1	B	140	LEU
1	B	349	GLN
1	B	589	ASP
1	B	590	ASN
1	B	846	CYS
1	B	1077	LYS
1	C	122	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	140	LEU
1	C	349	GLN
1	C	589	ASP
1	C	590	ASN
1	C	846	CYS
1	C	1077	LYS
1	D	122	ARG
1	D	140	LEU
1	D	349	GLN
1	D	589	ASP
1	D	590	ASN
1	D	846	CYS
1	D	1077	LYS
1	E	122	ARG
1	E	140	LEU
1	E	349	GLN
1	E	589	ASP
1	E	590	ASN
1	E	846	CYS
1	E	1077	LYS
1	F	122	ARG
1	F	140	LEU
1	F	349	GLN
1	F	589	ASP
1	F	590	ASN
1	F	846	CYS
1	F	1077	LYS
1	G	122	ARG
1	G	140	LEU
1	G	349	GLN
1	G	589	ASP
1	G	590	ASN
1	G	846	CYS
1	G	1077	LYS
2	H	52	ASN
2	H	70	ASN
2	I	52	ASN
2	I	70	ASN
2	J	52	ASN
2	J	70	ASN
2	K	52	ASN
2	K	70	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	52	ASN
2	L	70	ASN
2	M	52	ASN
2	M	70	ASN
2	N	52	ASN
2	N	70	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	441	GLN
1	A	565	GLN
1	A	583	GLN
1	A	693	HIS
1	A	712	HIS
1	B	441	GLN
1	B	565	GLN
1	B	583	GLN
1	B	693	HIS
1	B	712	HIS
1	C	441	GLN
1	C	565	GLN
1	C	583	GLN
1	C	693	HIS
1	C	712	HIS
1	D	441	GLN
1	D	565	GLN
1	D	583	GLN
1	D	693	HIS
1	D	712	HIS
1	E	441	GLN
1	E	565	GLN
1	E	583	GLN
1	E	693	HIS
1	E	712	HIS
1	F	441	GLN
1	F	565	GLN
1	F	583	GLN
1	F	693	HIS
1	F	712	HIS
1	G	441	GLN
1	G	565	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	583	GLN
1	G	693	HIS
1	G	712	HIS
2	H	52	ASN
2	H	54	ASN
2	H	70	ASN
2	I	52	ASN
2	I	54	ASN
2	I	70	ASN
2	J	52	ASN
2	J	54	ASN
2	J	70	ASN
2	K	52	ASN
2	K	54	ASN
2	K	70	ASN
2	L	52	ASN
2	L	54	ASN
2	L	70	ASN
2	M	52	ASN
2	M	54	ASN
2	M	70	ASN
2	N	52	ASN
2	N	54	ASN
2	N	70	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	A	1301	-	27,33,33	1.56	3 (11%)	27,52,52	1.91	4 (14%)
3	ATP	B	1301	-	27,33,33	1.55	3 (11%)	27,52,52	1.90	4 (14%)
3	ATP	C	1301	-	27,33,33	1.55	3 (11%)	27,52,52	1.91	4 (14%)
3	ATP	D	1301	-	27,33,33	1.55	3 (11%)	27,52,52	1.90	4 (14%)
3	ATP	E	1301	-	27,33,33	1.55	3 (11%)	27,52,52	1.90	4 (14%)
3	ATP	F	1301	-	27,33,33	1.56	3 (11%)	27,52,52	1.91	4 (14%)
3	ATP	G	1301	-	27,33,33	1.56	3 (11%)	27,52,52	1.91	4 (14%)
4	HEM	H	500	2	27,50,50	1.74	7 (25%)	17,82,82	2.88	11 (64%)
4	HEM	I	500	2	27,50,50	1.73	7 (25%)	17,82,82	2.88	11 (64%)
4	HEM	J	500	2	27,50,50	1.73	7 (25%)	17,82,82	2.88	11 (64%)
4	HEM	K	500	2	27,50,50	1.74	7 (25%)	17,82,82	2.88	11 (64%)
4	HEM	L	500	2	27,50,50	1.74	7 (25%)	17,82,82	2.88	11 (64%)
4	HEM	M	500	2	27,50,50	1.73	7 (25%)	17,82,82	2.88	11 (64%)
4	HEM	N	500	2	27,50,50	1.74	7 (25%)	17,82,82	2.89	11 (64%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	1301	-	-	0/18/38/38	0/3/3/3
3	ATP	B	1301	-	-	0/18/38/38	0/3/3/3
3	ATP	C	1301	-	-	0/18/38/38	0/3/3/3
3	ATP	D	1301	-	-	0/18/38/38	0/3/3/3
3	ATP	E	1301	-	-	0/18/38/38	0/3/3/3
3	ATP	F	1301	-	-	0/18/38/38	0/3/3/3
3	ATP	G	1301	-	-	0/18/38/38	0/3/3/3
4	HEM	H	500	2	-	0/6/54/54	0/0/8/8
4	HEM	I	500	2	-	0/6/54/54	0/0/8/8
4	HEM	J	500	2	-	0/6/54/54	0/0/8/8
4	HEM	K	500	2	-	0/6/54/54	0/0/8/8

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	L	500	2	-	0/6/54/54	0/0/8/8
4	HEM	M	500	2	-	0/6/54/54	0/0/8/8
4	HEM	N	500	2	-	0/6/54/54	0/0/8/8

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	500	HEM	C3C-CAC	-5.12	1.37	1.47
4	H	500	HEM	C3C-CAC	-5.11	1.37	1.47
4	N	500	HEM	C3C-CAC	-5.10	1.37	1.47
4	I	500	HEM	C3C-CAC	-5.10	1.37	1.47
4	L	500	HEM	C3C-CAC	-5.10	1.37	1.47
4	K	500	HEM	C3C-CAC	-5.09	1.37	1.47
4	J	500	HEM	C3C-CAC	-5.09	1.37	1.47
4	N	500	HEM	C3B-CAB	-2.89	1.42	1.47
4	J	500	HEM	C3B-CAB	-2.88	1.42	1.47
4	L	500	HEM	C3B-CAB	-2.88	1.42	1.47
4	H	500	HEM	C3B-CAB	-2.86	1.42	1.47
4	K	500	HEM	C3B-CAB	-2.86	1.42	1.47
4	M	500	HEM	C3B-CAB	-2.86	1.42	1.47
4	I	500	HEM	C3B-CAB	-2.84	1.42	1.47
4	M	500	HEM	C4A-CHB	-2.59	1.33	1.40
4	J	500	HEM	C4A-CHB	-2.58	1.33	1.40
4	L	500	HEM	C4A-CHB	-2.58	1.33	1.40
4	N	500	HEM	C4A-CHB	-2.57	1.33	1.40
4	H	500	HEM	C4A-CHB	-2.57	1.33	1.40
4	I	500	HEM	C4A-CHB	-2.57	1.33	1.40
4	K	500	HEM	C4A-CHB	-2.57	1.33	1.40
3	F	1301	ATP	PG-O1G	2.13	1.57	1.50
3	E	1301	ATP	PG-O1G	2.14	1.57	1.50
3	G	1301	ATP	PG-O1G	2.15	1.57	1.50
3	C	1301	ATP	PG-O1G	2.15	1.57	1.50
3	B	1301	ATP	PG-O1G	2.15	1.57	1.50
3	D	1301	ATP	PG-O1G	2.17	1.57	1.50
3	A	1301	ATP	PG-O1G	2.17	1.57	1.50
4	L	500	HEM	C1A-NA	2.23	1.40	1.36
4	K	500	HEM	C1A-NA	2.23	1.40	1.36
4	H	500	HEM	C1A-NA	2.24	1.40	1.36
4	N	500	HEM	C1A-NA	2.25	1.40	1.36
4	M	500	HEM	C1A-NA	2.25	1.40	1.36
4	I	500	HEM	C1A-NA	2.25	1.40	1.36
4	J	500	HEM	C1A-NA	2.25	1.40	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	500	HEM	C4B-NB	2.41	1.41	1.36
4	M	500	HEM	C4B-NB	2.42	1.41	1.36
4	I	500	HEM	C4B-NB	2.42	1.41	1.36
4	H	500	HEM	C4B-NB	2.44	1.41	1.36
4	L	500	HEM	C4B-NB	2.44	1.41	1.36
4	N	500	HEM	C4B-NB	2.44	1.41	1.36
4	K	500	HEM	C4B-NB	2.45	1.41	1.36
4	K	500	HEM	C4D-C3D	2.53	1.48	1.42
4	M	500	HEM	C4D-C3D	2.53	1.48	1.42
4	N	500	HEM	C4D-C3D	2.55	1.48	1.42
4	H	500	HEM	C4D-C3D	2.55	1.48	1.42
4	L	500	HEM	C4D-C3D	2.56	1.48	1.42
4	J	500	HEM	C4D-C3D	2.57	1.48	1.42
4	I	500	HEM	C4D-C3D	2.57	1.48	1.42
3	D	1301	ATP	C5-C4	2.73	1.46	1.40
3	E	1301	ATP	C5-C4	2.74	1.46	1.40
3	B	1301	ATP	C5-C4	2.74	1.46	1.40
3	C	1301	ATP	C5-C4	2.74	1.46	1.40
3	A	1301	ATP	C5-C4	2.75	1.46	1.40
3	F	1301	ATP	C5-C4	2.76	1.46	1.40
3	G	1301	ATP	C5-C4	2.78	1.46	1.40
4	M	500	HEM	C3B-C2B	3.29	1.44	1.40
4	L	500	HEM	C3B-C2B	3.30	1.44	1.40
4	J	500	HEM	C3B-C2B	3.30	1.44	1.40
4	H	500	HEM	C3B-C2B	3.32	1.45	1.40
4	N	500	HEM	C3B-C2B	3.33	1.45	1.40
4	I	500	HEM	C3B-C2B	3.33	1.45	1.40
4	K	500	HEM	C3B-C2B	3.36	1.45	1.40
3	C	1301	ATP	PG-O3B	5.80	1.68	1.60
3	A	1301	ATP	PG-O3B	5.82	1.68	1.60
3	D	1301	ATP	PG-O3B	5.84	1.69	1.60
3	B	1301	ATP	PG-O3B	5.84	1.69	1.60
3	E	1301	ATP	PG-O3B	5.86	1.69	1.60
3	G	1301	ATP	PG-O3B	5.86	1.69	1.60
3	F	1301	ATP	PG-O3B	5.88	1.69	1.60

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1301	ATP	N3-C2-N1	-6.95	122.91	128.86
3	A	1301	ATP	N3-C2-N1	-6.95	122.92	128.86
3	F	1301	ATP	N3-C2-N1	-6.93	122.93	128.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1301	ATP	N3-C2-N1	-6.92	122.94	128.86
3	B	1301	ATP	N3-C2-N1	-6.91	122.95	128.86
3	E	1301	ATP	N3-C2-N1	-6.91	122.95	128.86
3	D	1301	ATP	N3-C2-N1	-6.87	122.98	128.86
4	N	500	HEM	C4C-C3C-C2C	-5.52	103.04	106.90
4	I	500	HEM	C4C-C3C-C2C	-5.49	103.06	106.90
4	K	500	HEM	C4C-C3C-C2C	-5.48	103.07	106.90
4	H	500	HEM	C4C-C3C-C2C	-5.48	103.07	106.90
4	J	500	HEM	C4C-C3C-C2C	-5.46	103.08	106.90
4	M	500	HEM	C4C-C3C-C2C	-5.45	103.09	106.90
4	L	500	HEM	C4C-C3C-C2C	-5.45	103.09	106.90
4	I	500	HEM	CBD-CAD-C3D	-4.37	104.12	112.47
4	K	500	HEM	CBD-CAD-C3D	-4.37	104.13	112.47
4	J	500	HEM	CBD-CAD-C3D	-4.37	104.13	112.47
4	H	500	HEM	CBD-CAD-C3D	-4.37	104.13	112.47
4	L	500	HEM	CBD-CAD-C3D	-4.37	104.13	112.47
4	N	500	HEM	CBD-CAD-C3D	-4.37	104.14	112.47
4	M	500	HEM	CBD-CAD-C3D	-4.36	104.15	112.47
3	C	1301	ATP	PB-O3B-PG	-4.03	119.08	132.63
3	A	1301	ATP	PB-O3B-PG	-4.03	119.09	132.63
3	D	1301	ATP	PB-O3B-PG	-4.03	119.09	132.63
3	E	1301	ATP	PB-O3B-PG	-4.03	119.09	132.63
3	B	1301	ATP	PB-O3B-PG	-4.03	119.10	132.63
3	F	1301	ATP	PB-O3B-PG	-4.03	119.10	132.63
3	G	1301	ATP	PB-O3B-PG	-4.02	119.12	132.63
4	M	500	HEM	C1D-C2D-C3D	-3.38	104.65	107.00
4	N	500	HEM	C1D-C2D-C3D	-3.33	104.68	107.00
4	H	500	HEM	C1D-C2D-C3D	-3.32	104.68	107.00
4	K	500	HEM	C1D-C2D-C3D	-3.32	104.69	107.00
4	I	500	HEM	C1D-C2D-C3D	-3.31	104.69	107.00
4	J	500	HEM	C1D-C2D-C3D	-3.29	104.70	107.00
4	L	500	HEM	C1D-C2D-C3D	-3.28	104.71	107.00
4	N	500	HEM	CMA-C3A-C4A	-3.16	123.61	128.46
4	H	500	HEM	CMA-C3A-C4A	-3.13	123.65	128.46
4	J	500	HEM	CMA-C3A-C4A	-3.13	123.65	128.46
4	L	500	HEM	CMA-C3A-C4A	-3.13	123.66	128.46
4	K	500	HEM	CMA-C3A-C4A	-3.12	123.66	128.46
4	M	500	HEM	CMA-C3A-C4A	-3.12	123.67	128.46
4	I	500	HEM	CMA-C3A-C4A	-3.10	123.70	128.46
4	N	500	HEM	CMD-C2D-C1D	-2.82	124.13	128.46
4	K	500	HEM	CMD-C2D-C1D	-2.81	124.14	128.46
4	J	500	HEM	CMD-C2D-C1D	-2.80	124.16	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	500	HEM	CMD-C2D-C1D	-2.80	124.16	128.46
4	L	500	HEM	CMD-C2D-C1D	-2.80	124.16	128.46
4	H	500	HEM	CMD-C2D-C1D	-2.80	124.17	128.46
4	M	500	HEM	CMD-C2D-C1D	-2.77	124.21	128.46
3	G	1301	ATP	C4-C5-N7	-2.20	107.29	109.41
3	E	1301	ATP	C4-C5-N7	-2.17	107.31	109.41
3	B	1301	ATP	C4-C5-N7	-2.17	107.31	109.41
3	F	1301	ATP	C4-C5-N7	-2.17	107.31	109.41
3	C	1301	ATP	C4-C5-N7	-2.17	107.31	109.41
3	A	1301	ATP	C4-C5-N7	-2.15	107.34	109.41
3	D	1301	ATP	C4-C5-N7	-2.15	107.34	109.41
4	J	500	HEM	C3B-C4B-NB	2.12	111.95	109.21
4	I	500	HEM	C3B-C4B-NB	2.13	111.97	109.21
4	M	500	HEM	C3B-C4B-NB	2.13	111.97	109.21
4	L	500	HEM	C3B-C4B-NB	2.14	111.97	109.21
4	M	500	HEM	CAA-CBA-CGA	2.14	116.31	112.66
4	H	500	HEM	CAA-CBA-CGA	2.15	116.33	112.66
4	H	500	HEM	C3B-C4B-NB	2.15	111.98	109.21
4	L	500	HEM	CAA-CBA-CGA	2.15	116.33	112.66
4	J	500	HEM	CAA-CBA-CGA	2.15	116.33	112.66
4	K	500	HEM	CAA-CBA-CGA	2.16	116.35	112.66
4	I	500	HEM	CAA-CBA-CGA	2.16	116.35	112.66
4	N	500	HEM	CAA-CBA-CGA	2.16	116.35	112.66
4	N	500	HEM	C3B-C4B-NB	2.16	112.00	109.21
4	K	500	HEM	C3B-C4B-NB	2.18	112.03	109.21
3	D	1301	ATP	C2-N1-C6	2.47	122.94	118.75
3	B	1301	ATP	C2-N1-C6	2.48	122.97	118.75
3	E	1301	ATP	C2-N1-C6	2.48	122.97	118.75
3	A	1301	ATP	C2-N1-C6	2.48	122.97	118.75
3	F	1301	ATP	C2-N1-C6	2.49	122.98	118.75
3	G	1301	ATP	C2-N1-C6	2.50	122.99	118.75
3	C	1301	ATP	C2-N1-C6	2.50	123.00	118.75
4	J	500	HEM	CMB-C2B-C3B	2.60	129.61	124.88
4	H	500	HEM	CMB-C2B-C3B	2.60	129.61	124.88
4	L	500	HEM	CMB-C2B-C3B	2.60	129.62	124.88
4	K	500	HEM	CMB-C2B-C3B	2.61	129.62	124.88
4	N	500	HEM	CMB-C2B-C3B	2.61	129.63	124.88
4	I	500	HEM	CMB-C2B-C3B	2.61	129.63	124.88
4	M	500	HEM	CMB-C2B-C3B	2.62	129.65	124.88
4	I	500	HEM	C4A-C3A-C2A	2.99	109.08	107.00
4	K	500	HEM	C4A-C3A-C2A	3.00	109.08	107.00
4	N	500	HEM	C4A-C3A-C2A	3.03	109.10	107.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	500	HEM	C4A-C3A-C2A	3.03	109.10	107.00
4	H	500	HEM	C4A-C3A-C2A	3.03	109.10	107.00
4	M	500	HEM	C4A-C3A-C2A	3.05	109.12	107.00
4	L	500	HEM	C4A-C3A-C2A	3.06	109.13	107.00
4	L	500	HEM	CMD-C2D-C3D	3.27	131.11	124.94
4	J	500	HEM	CMD-C2D-C3D	3.28	131.12	124.94
4	M	500	HEM	CMD-C2D-C3D	3.28	131.12	124.94
4	H	500	HEM	CMD-C2D-C3D	3.28	131.13	124.94
4	I	500	HEM	CMD-C2D-C3D	3.28	131.13	124.94
4	K	500	HEM	CMD-C2D-C3D	3.29	131.15	124.94
4	N	500	HEM	CMD-C2D-C3D	3.31	131.18	124.94
4	I	500	HEM	CAD-CBD-CGD	4.47	120.30	112.66
4	M	500	HEM	CAD-CBD-CGD	4.48	120.32	112.66
4	K	500	HEM	CAD-CBD-CGD	4.48	120.32	112.66
4	N	500	HEM	CAD-CBD-CGD	4.49	120.33	112.66
4	H	500	HEM	CAD-CBD-CGD	4.49	120.33	112.66
4	L	500	HEM	CAD-CBD-CGD	4.49	120.33	112.66
4	J	500	HEM	CAD-CBD-CGD	4.50	120.34	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1301	ATP	1	0
3	B	1301	ATP	2	0
3	C	1301	ATP	1	0
3	D	1301	ATP	1	0
3	E	1301	ATP	1	0
3	F	1301	ATP	2	0
3	G	1301	ATP	1	0
4	H	500	HEM	7	0
4	I	500	HEM	10	0
4	J	500	HEM	7	0
4	K	500	HEM	6	0
4	L	500	HEM	6	0
4	M	500	HEM	8	0
4	N	500	HEM	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.