



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:45 PM BST

PDB ID : 3J0K  
EMDB ID: : EMD-5343  
Title : Orientation of RNA polymerase II within the human VP16-Mediator-pol II-TFIIF assembly  
Authors : Bernecky, C.; Grob, P.; Ebmeier, C.C.; Nogales, E.; Taatjes, D.J.  
Deposited on : 2011-10-04  
Resolution : 36.00 Å(reported)  
Based on PDB ID : 1Y1V

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

---

MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

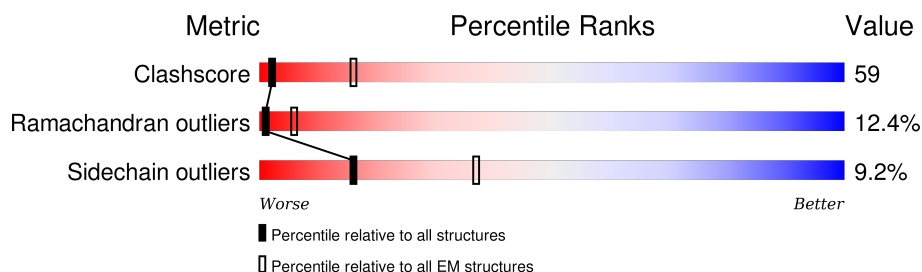
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 36.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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  $\geq 3$ , 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	1455	26% 55% 16% ..
2	B	1224	25% 52% 13% • 9%
3	C	268	26% 56% 15% ..
4	D	221	31% 42% 7% 20%
5	E	215	35% 54% 11%
6	F	84	29% 56% 15%
7	G	171	33% 59% 8%
8	H	146	29% 53% 9% 9%
9	I	122	30% 49% 13% 5% •

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	J	70	<div><div></div><div>20%54%17%• 7%</div></div>
11	K	120	<div><div></div><div>39%50%5%• 5%</div></div>
12	L	46	<div><div></div><div>9%63%26%•</div></div>

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 31137 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II largest subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1426	Total	C	N	O	S	0	0
			11214	7069	1959	2124	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1112	Total	C	N	O	S	0	0
			8837	5594	1548	1640	55		

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	266	Total	C	N	O	S	0	0
			2095	1317	348	417	13		

- Molecule 4 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	177	Total	C	N	O	S	0	0
			1356	840	241	273	2		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total	C	N	O	S	0	0
			679	434	115	127	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1068	673	180	211	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	119	Total	C	N	O	S	0	0
			971	596	179	186	10		

- Molecule 10 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	114	Total	C	N	O	S	0	0
			919	590	156	171	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			364	224	72	64	4		

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total	Mg	0
			1	1	

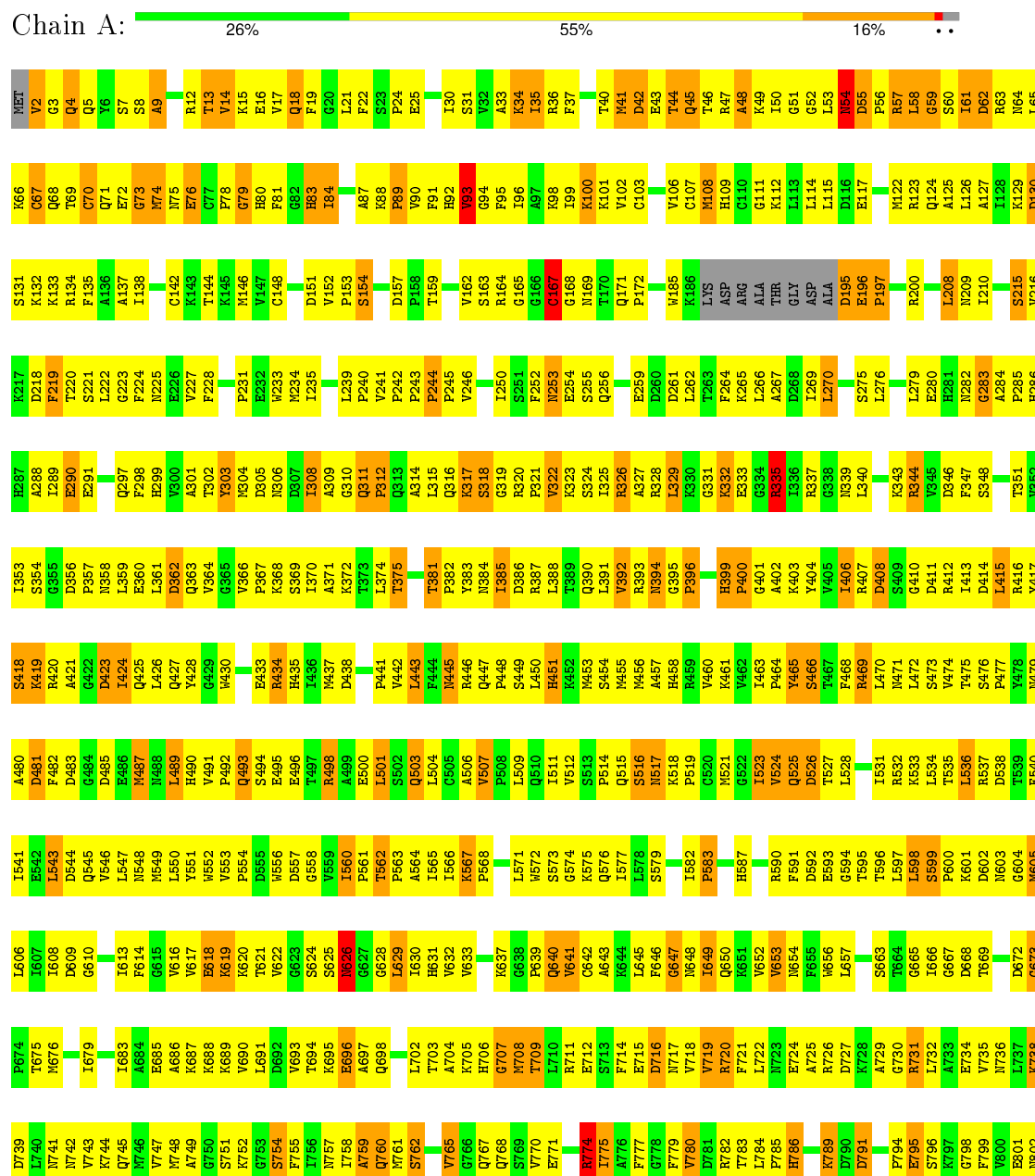
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

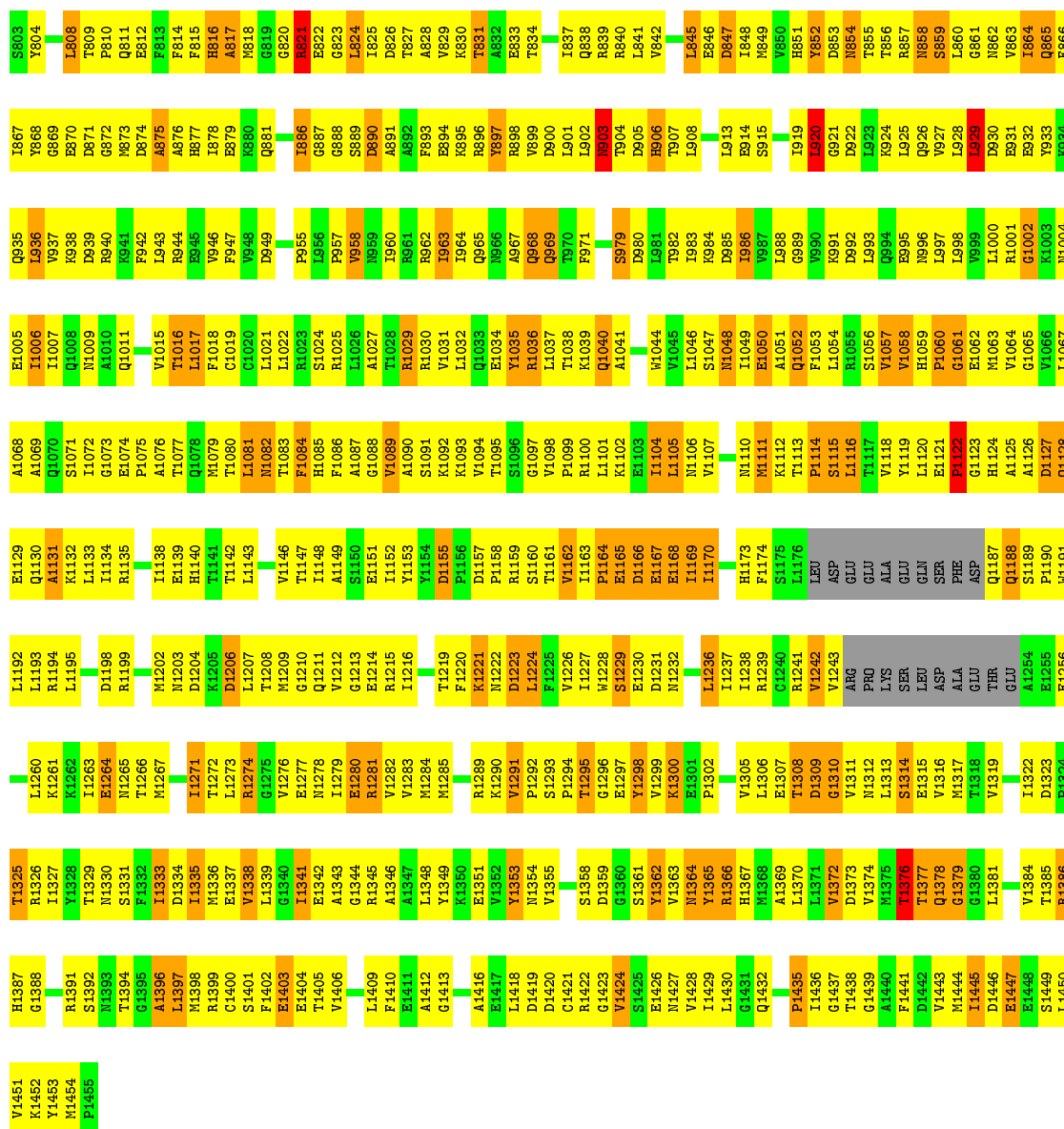
Mol	Chain	Residues	Atoms		AltConf
14	J	1	Total	Zn	0
			1	1	
14	B	1	Total	Zn	0
			1	1	
14	I	2	Total	Zn	0
			2	2	
14	C	1	Total	Zn	0
			1	1	
14	A	3	Total	Zn	0
			3	3	
14	L	1	Total	Zn	0
			1	1	

### 3 Residue-property plots

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

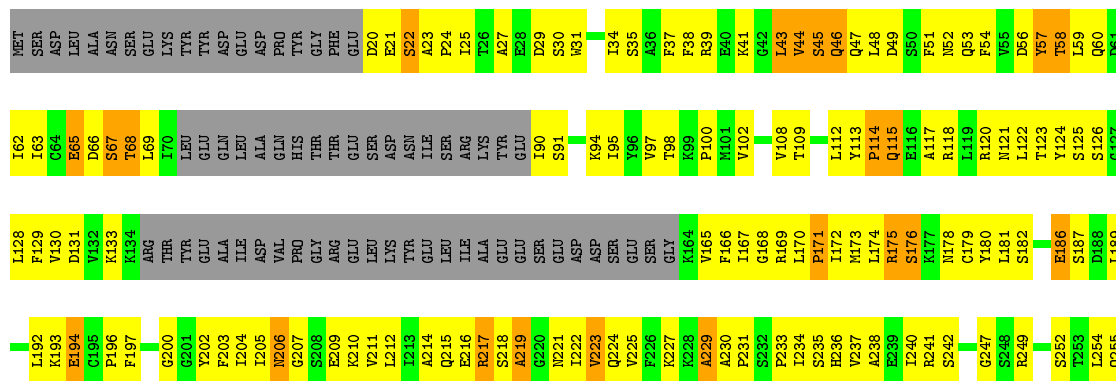
- Molecule 1: DNA-directed RNA polymerase II largest subunit



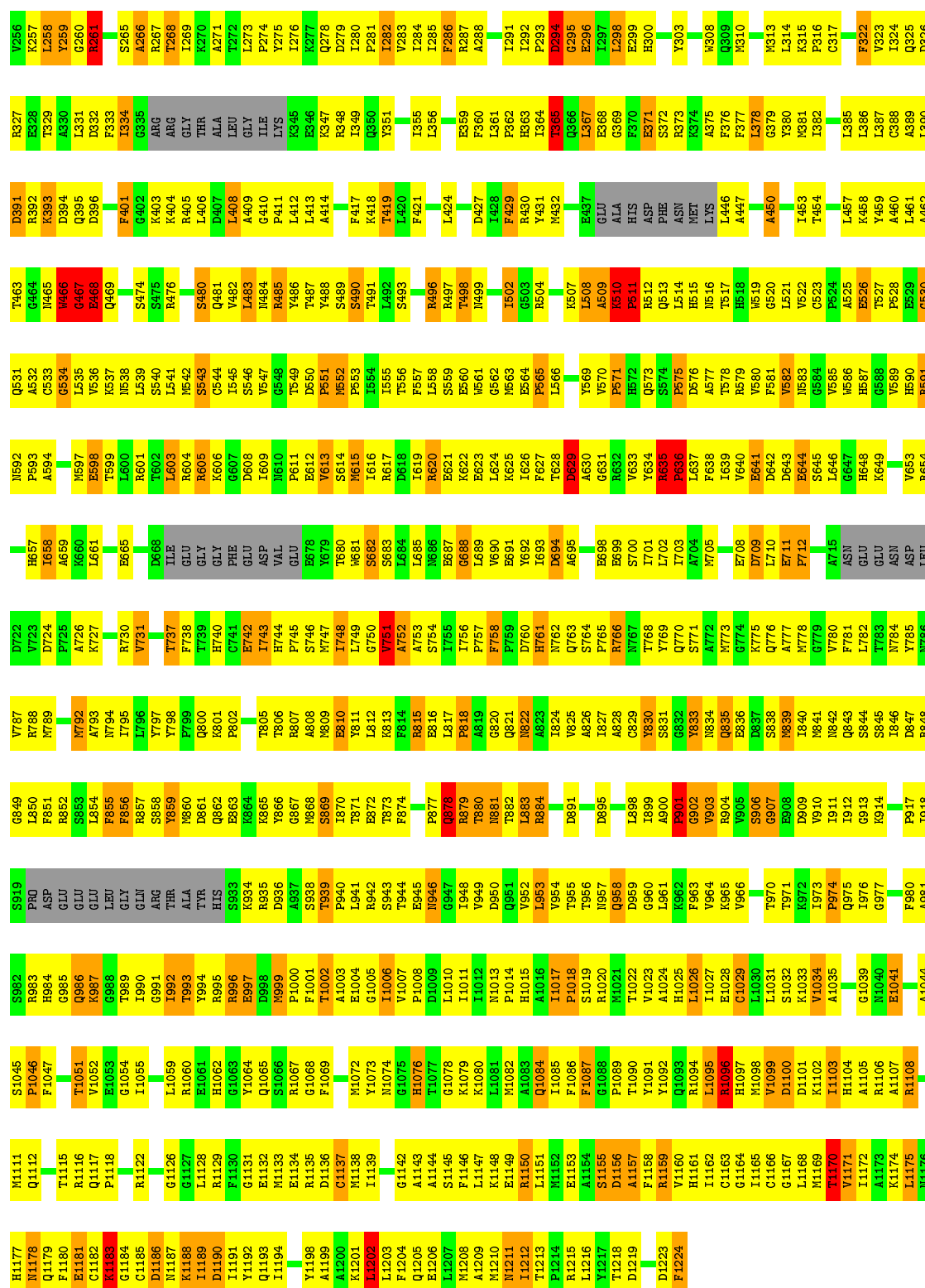


• Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide

Chain B:



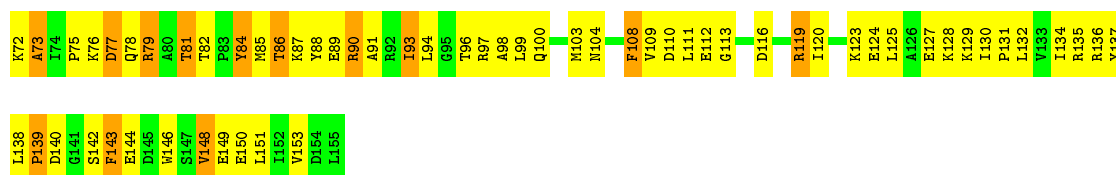




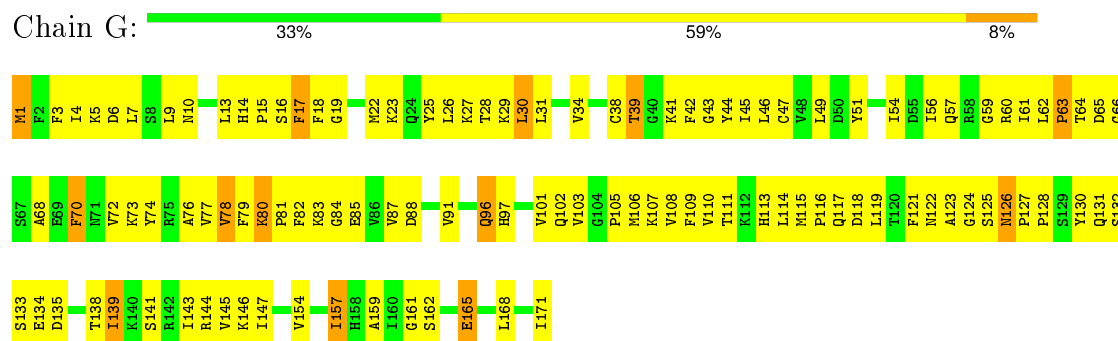
● Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C: 26% 56% 15% ..

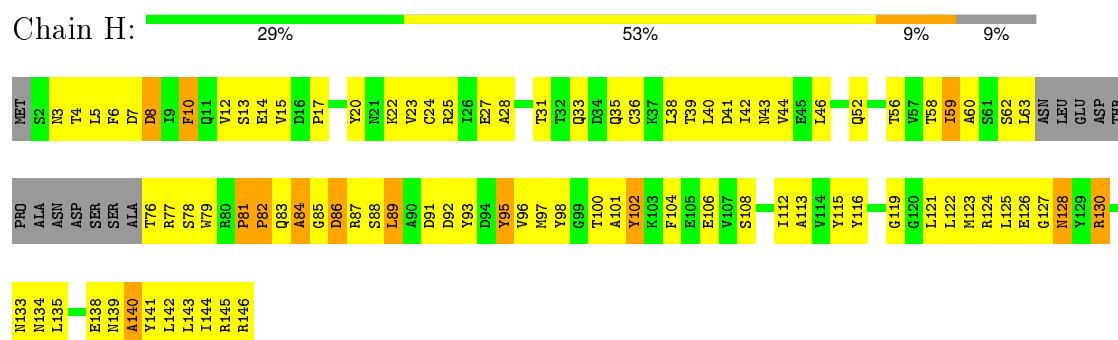




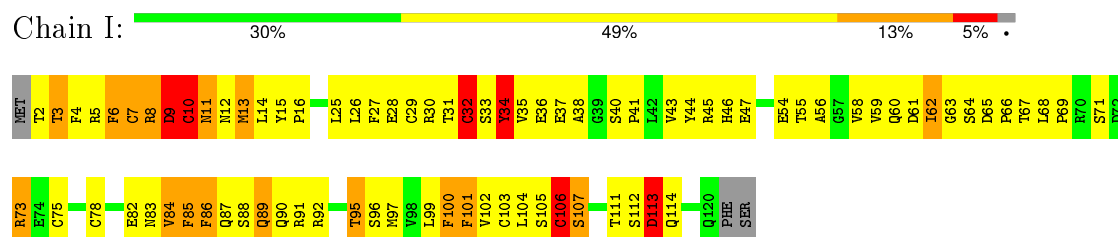
- Molecule 7: DNA-directed RNA polymerase II 19 kDa polypeptide



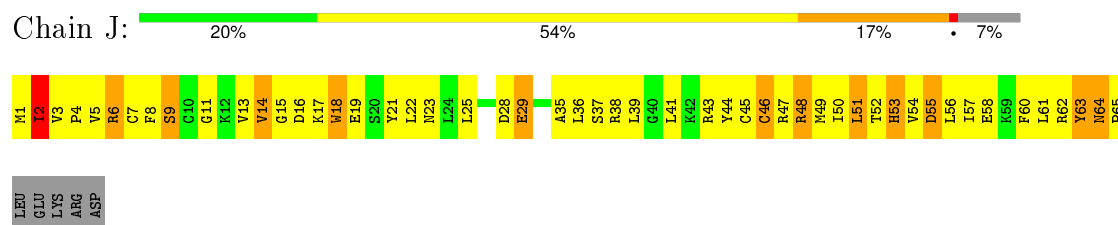
- Molecule 8: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



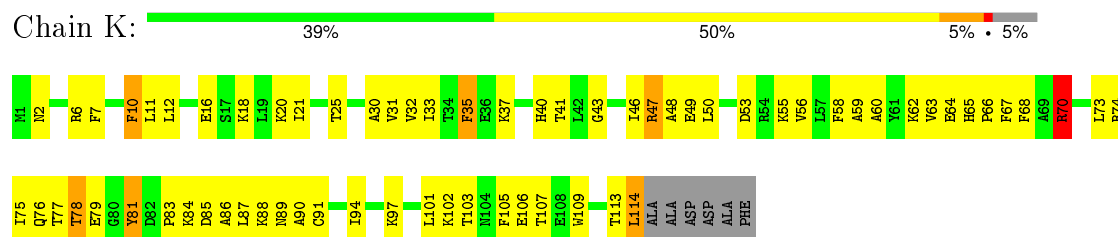
- Molecule 9: DNA-directed RNA polymerase II subunit 9



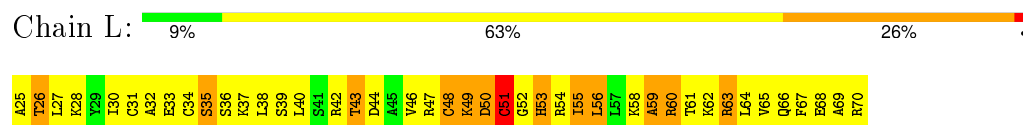
- Molecule 10: DNA-directed RNA polymerases I/II/III subunit 10



- Molecule 11: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- Molecule 12: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	3146	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	each micrograph	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	29000	Depositor
Image detector	Kodak SO-163 film	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.50	2/11417 (0.0%)	0.78	4/15442 (0.0%)
10	J	0.48	0/541	0.75	0/727
11	K	0.45	0/937	0.67	0/1265
12	L	0.54	0/366	0.79	0/485
2	B	0.52	4/9009 (0.0%)	0.76	8/12146 (0.1%)
3	C	0.48	0/2133	0.77	1/2891 (0.0%)
4	D	0.41	0/1365	0.64	0/1837
5	E	0.43	0/1788	0.66	0/2406
6	F	0.52	0/691	0.77	0/933
7	G	0.49	0/1368	0.72	0/1844
8	H	0.38	0/1086	0.65	1/1470 (0.1%)
9	I	0.46	0/989	0.77	1/1331 (0.1%)
All	All	0.49	6/31690 (0.0%)	0.75	15/42777 (0.0%)

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
2	B	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	467	GLY	C-O	-11.91	1.04	1.23
2	B	468	GLU	CB-CG	8.45	1.68	1.52
2	B	510	LYS	CB-CG	5.58	1.67	1.52
1	A	195	ASP	N-CA	5.49	1.57	1.46
2	B	468	GLU	CG-CD	5.21	1.59	1.51
1	A	196	GLU	CB-CG	5.09	1.61	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ASP	N-CA-C	9.36	136.28	111.00
2	B	510	LYS	CB-CA-C	-7.65	95.10	110.40
2	B	510	LYS	C-N-CD	-7.45	104.21	120.60
3	C	92	CYS	CA-CB-SG	-6.78	101.80	114.00
1	A	1310	GLY	N-CA-C	-6.49	96.88	113.10
9	I	10	CYS	CA-CB-SG	6.24	125.24	114.00
2	B	468	GLU	N-CA-C	5.97	127.11	111.00
2	B	467	GLY	CA-C-N	5.87	130.12	117.20
2	B	511	PRO	CA-N-CD	-5.80	103.38	111.50
2	B	508	LEU	C-N-CA	-5.72	107.41	121.70
1	A	344	ARG	N-CA-C	-5.59	95.90	111.00
2	B	510	LYS	C-N-CA	5.57	145.39	122.00
1	A	865	GLN	N-CA-C	-5.40	96.43	111.00
8	H	89	LEU	CA-CB-CG	5.40	127.72	115.30
2	B	296	GLU	N-CA-C	-5.28	96.76	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	510	LYS	Mainchain
2	B	833	TYR	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	11214	0	11281	1475	0
2	B	8837	0	8871	1203	0
3	C	2095	0	2052	263	0
4	D	1356	0	1319	106	0
5	E	1752	0	1776	189	0
6	F	679	0	701	84	0
7	G	1340	0	1357	161	0
8	H	1068	0	1040	120	0
9	I	971	0	929	113	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	532	0	542	110	0
11	K	919	0	929	97	0
12	L	364	0	387	68	0
13	A	1	0	0	0	0
14	A	3	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
All	All	31137	0	31184	3684	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 59.

All (3684) 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)
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.28	1.13
4:D:40:HIS:HB3	7:G:73:LYS:HZ3	1.10	1.12
7:G:138:THR:HG22	7:G:139:ILE:H	1.11	1.11
1:A:913:LEU:HD12	1:A:914:GLU:H	1.15	1.11
6:F:82:THR:HG22	6:F:84:TYR:H	1.15	1.11
1:A:1017:LEU:HB2	5:E:206:GLY:H	1.11	1.10
1:A:225:ASN:ND2	1:A:228:PHE:H	1.47	1.10
1:A:855:THR:HG21	1:A:857:ARG:HE	1.10	1.10
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.33	1.09
1:A:590:ARG:NH2	1:A:620:LYS:HB3	1.66	1.09
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.14	1.09
1:A:794:PRO:HG2	1:A:795:GLU:OE2	1.49	1.08
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.15	1.08
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.88	1.07
2:B:1095:LEU:HD12	2:B:1095:LEU:H	1.11	1.07
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.02	1.07
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.31	1.07
7:G:14:HIS:HD2	7:G:16:SER:HB2	1.15	1.06
4:D:40:HIS:HB3	7:G:73:LYS:NZ	1.69	1.05
10:J:64:ASN:HB3	10:J:65:PRO:CD	1.87	1.05
2:B:508:LEU:CB	2:B:510:LYS:H	1.70	1.05
2:B:112:LEU:HD12	2:B:113:TYR:H	1.18	1.04
1:A:901:LEU:H	1:A:926:GLN:NE2	1.54	1.04

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.39	1.03
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.19	1.03
2:B:839:MET:CG	2:B:1010:LEU:HD11	1.87	1.02
3:C:133:ILE:HD11	3:C:237:SER:HA	1.39	1.02
1:A:834:THR:HG21	1:A:1077:THR:HG23	1.39	1.02
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.19	1.02
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.42	1.02
7:G:111:THR:HG22	7:G:113:HIS:H	1.19	1.02
2:B:510:LYS:HD2	2:B:510:LYS:O	1.60	1.02
1:A:47:ARG:HH12	1:A:254:GLU:HB3	1.21	1.01
2:B:839:MET:HG3	2:B:1010:LEU:HD11	1.01	1.01
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.58	1.01
1:A:53:LEU:HD23	1:A:54:ASN:N	1.76	1.01
1:A:63:ARG:HA	1:A:74:MET:SD	2.02	1.00
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.25	1.00
2:B:65:GLU:HG3	2:B:66:ASP:H	1.27	0.99
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.27	0.99
11:K:65:HIS:CD2	11:K:67:PHE:H	1.81	0.98
2:B:589:VAL:HG12	2:B:590:HIS:H	1.24	0.98
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.43	0.98
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	1.78	0.98
1:A:490:HIS:HB3	2:B:1150:ARG:NH1	1.79	0.98
1:A:853:ASP:OD1	1:A:855:THR:HB	1.62	0.98
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.05	0.97
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.45	0.97
2:B:918:ILE:HD12	2:B:935:ARG:HD2	1.42	0.97
3:C:56:THR:HG21	3:C:145:CYS:SG	2.03	0.97
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.44	0.97
2:B:882:THR:HG22	2:B:884:ARG:H	1.29	0.97
1:A:164:ARG:HG3	1:A:165:GLY:H	1.26	0.97
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.44	0.96
2:B:863:GLU:OE2	2:B:873:THR:HA	1.64	0.96
2:B:211:VAL:O	2:B:480:SER:HA	1.65	0.96
2:B:295:GLY:H	2:B:298:LEU:HD23	1.27	0.96
11:K:65:HIS:HD2	11:K:67:PHE:H	1.10	0.96
2:B:583:ASN:HD21	2:B:628:THR:HB	1.29	0.96
1:A:1081:LEU:HD12	1:A:1082:ASN:OD1	1.66	0.96
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.45	0.96
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.46	0.96
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.48	0.96
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.00	0.95

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:LEU:HD12	1:A:914:GLU:N	1.81	0.95
2:B:824:ILE:HG12	10:J:48:ARG:HH12	1.31	0.94
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.66	0.94
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.49	0.94
1:A:1341:ILE:HG23	1:A:1342:GLU:H	1.32	0.93
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.03	0.93
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.51	0.93
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.67	0.93
3:C:167:HIS:HD2	3:C:169:LYS:H	1.17	0.93
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.48	0.93
1:A:337:ARG:CZ	1:A:839:ARG:HH12	1.81	0.93
7:G:14:HIS:CD2	7:G:16:SER:HB2	2.04	0.93
1:A:49:LYS:NZ	1:A:61:ILE:HG13	1.84	0.93
3:C:73:GLN:HE21	3:C:75:MET:H	1.03	0.92
1:A:1362:TYR:HD1	1:A:1363:VAL:H	1.18	0.92
1:A:225:ASN:HD22	1:A:228:PHE:H	1.03	0.92
2:B:1183:LYS:HE3	2:B:1183:LYS:N	1.85	0.92
2:B:1002:THR:HG21	2:B:1006:ILE:HD12	1.49	0.92
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.51	0.92
5:E:153:HIS:O	5:E:154:ILE:HG13	1.69	0.91
1:A:70:CYS:O	1:A:72:GLU:HG2	1.68	0.91
6:F:76:LYS:O	6:F:79:ARG:HD3	1.70	0.91
3:C:63:ILE:HA	3:C:66:ARG:HG3	1.50	0.91
1:A:666:ILE:HD12	1:A:667:GLY:H	1.35	0.91
9:I:85:PHE:HD2	9:I:85:PHE:H	0.93	0.90
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.52	0.90
2:B:839:MET:HG3	2:B:1010:LEU:CD1	1.98	0.90
2:B:168:GLY:H	2:B:450:ALA:HB1	1.34	0.90
1:A:1329:THR:HG22	1:A:1331:SER:H	1.36	0.90
1:A:1329:THR:N	1:A:1335:ILE:HD11	1.87	0.90
2:B:549:THR:HG22	2:B:550:ASP:H	1.35	0.90
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.53	0.89
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.54	0.89
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.52	0.89
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.37	0.89
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.55	0.89
5:E:22:MET:HE3	5:E:26:ARG:HE	1.37	0.89
2:B:835:GLN:HA	2:B:1013:ASN:HD22	1.35	0.89
2:B:35:SER:HA	2:B:811:TYR:HE2	1.36	0.88
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.55	0.88
7:G:1:MET:HG3	7:G:85:GLU:CD	1.93	0.88

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:ILE:O	1:A:865:GLN:HG3	1.72	0.88
2:B:1095:LEU:HD12	2:B:1095:LEU:N	1.88	0.88
7:G:23:LYS:HG3	7:G:56:ILE:HD11	1.55	0.88
1:A:560:ILE:HG13	8:H:78:SER:HB2	1.51	0.88
9:I:111:THR:HG22	9:I:112:SER:H	1.37	0.88
1:A:1118:VAL:O	1:A:1305:VAL:HG13	1.71	0.88
10:J:6:ARG:HG2	10:J:13:VAL:HA	1.55	0.88
1:A:490:HIS:HB3	2:B:1150:ARG:HH11	1.36	0.88
1:A:1029:ARG:HG3	1:A:1029:ARG:HH11	1.38	0.88
5:E:197:LYS:HE2	5:E:199:ILE:HD11	1.55	0.88
2:B:113:TYR:HB3	2:B:114:PRO:HD2	1.55	0.88
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.39	0.87
1:A:55:ASP:C	1:A:57:ARG:H	1.73	0.87
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	1.88	0.87
5:E:22:MET:HE3	5:E:26:ARG:NE	1.89	0.87
2:B:365:THR:HG23	2:B:367:LEU:HG	1.55	0.87
9:I:29:CYS:SG	9:I:32:CYS:N	2.48	0.87
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.56	0.87
2:B:579:ARG:HB2	2:B:586:TRP:NE1	1.90	0.87
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.09	0.87
1:A:1341:ILE:HG23	1:A:1342:GLU:N	1.89	0.87
1:A:524:VAL:HG12	1:A:525:GLN:H	1.38	0.87
2:B:39:ARG:NH2	2:B:665:GLU:HG2	1.89	0.87
3:C:213:PRO:O	3:C:214:ASN:HB2	1.74	0.87
2:B:493:SER:HA	2:B:751:VAL:HG21	1.57	0.86
7:G:138:THR:HG22	7:G:139:ILE:N	1.91	0.86
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.57	0.86
1:A:567:LYS:HB3	8:H:96:VAL:H	1.39	0.86
1:A:443:LEU:HG	2:B:1146:PHE:HE2	1.38	0.86
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.56	0.86
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.55	0.86
10:J:43:ARG:HG3	10:J:45:CYS:SG	2.16	0.86
2:B:467:GLY:O	2:B:468:GLU:HB2	1.73	0.86
2:B:880:THR:HB	2:B:934:LYS:HD2	1.56	0.86
7:G:1:MET:HG3	7:G:85:GLU:OE2	1.75	0.86
11:K:56:VAL:HA	11:K:77:THR:HG22	1.55	0.86
1:A:537:ARG:HD2	8:H:20:TYR:HE1	1.40	0.86
1:A:963:ILE:HD13	1:A:1049:ILE:HG13	1.58	0.86
1:A:855:THR:HG21	1:A:857:ARG:NE	1.89	0.85
3:C:244:VAL:O	3:C:248:ILE:HG13	1.76	0.85
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.05	0.85

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.44	0.85
1:A:708:MET:HE2	1:A:1089:VAL:HG13	1.58	0.85
2:B:955:THR:HG23	12:L:54:ARG:O	1.77	0.85
1:A:466:SER:O	2:B:1103:ILE:HD11	1.75	0.85
2:B:466:TRP:O	2:B:468:GLU:N	2.08	0.85
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.11	0.85
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.59	0.85
5:E:153:HIS:HB3	5:E:196:VAL:HG11	1.58	0.85
5:E:117:THR:HG22	5:E:119:SER:H	1.39	0.85
8:H:100:THR:HG23	8:H:138:GLU:HA	1.58	0.85
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	1.76	0.85
1:A:587:HIS:CD2	1:A:969:GLN:HG2	2.11	0.84
2:B:510:LYS:O	2:B:510:LYS:CD	2.25	0.84
2:B:510:LYS:HG2	2:B:512:ARG:H	1.43	0.84
2:B:37:PHE:HE2	2:B:542:MET:HA	1.40	0.84
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.58	0.84
1:A:540:PHE:HB3	1:A:571:LEU:HD23	1.59	0.84
1:A:849:MET:HE1	1:A:1061:GLY:HA2	1.60	0.84
1:A:1116:LEU:N	1:A:1308:THR:HG22	1.92	0.84
1:A:1239:ARG:HH22	1:A:1241:ARG:HH22	1.25	0.84
2:B:843:GLN:HB2	2:B:993:THR:HB	1.58	0.84
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.59	0.84
2:B:582:VAL:HG23	2:B:626:ILE:HB	1.57	0.84
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.12	0.84
2:B:1065:GLN:HE21	2:B:1067:ARG:H	0.86	0.84
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.57	0.84
1:A:1116:LEU:HD23	1:A:1311:VAL:HG22	1.60	0.84
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.40	0.84
1:A:472:LEU:HD11	2:B:835:GLN:NE2	1.93	0.83
2:B:295:GLY:N	2:B:298:LEU:HD23	1.94	0.83
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.60	0.83
2:B:1107:ALA:O	2:B:1108:ARG:HG2	1.77	0.83
1:A:49:LYS:HZ3	1:A:61:ILE:HG13	1.44	0.83
2:B:766:ARG:NH2	2:B:1020:ARG:HG2	1.92	0.83
1:A:901:LEU:H	1:A:926:GLN:HE21	1.22	0.83
9:I:85:PHE:N	9:I:85:PHE:CD2	2.45	0.83
9:I:111:THR:HG22	9:I:113:ASP:H	1.43	0.83
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.59	0.83
2:B:781:PHE:O	2:B:782:LEU:HG	1.78	0.83
1:A:743:VAL:O	1:A:747:VAL:HG23	1.79	0.83
1:A:665:GLY:HA2	2:B:1026:LEU:HD21	1.58	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:153:HIS:HB3	5:E:196:VAL:CG1	2.08	0.82
2:B:1095:LEU:CD1	2:B:1095:LEU:H	1.87	0.82
10:J:9:SER:OG	10:J:45:CYS:HB2	1.79	0.82
2:B:1020:ARG:HH11	2:B:1020:ARG:HG2	1.44	0.82
1:A:353:ILE:HD12	1:A:470:LEU:HD21	1.61	0.82
2:B:502:ILE:HG22	2:B:502:ILE:O	1.79	0.82
9:I:56:ALA:HB2	9:I:89:GLN:CG	2.10	0.82
2:B:589:VAL:HG12	2:B:590:HIS:N	1.95	0.82
1:A:503:GLN:HE21	6:F:90:ARG:HH21	1.25	0.82
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.09	0.82
1:A:1317:MET:O	1:A:1322:ILE:HD11	1.80	0.82
1:A:649:ILE:O	1:A:653:VAL:HG23	1.80	0.82
6:F:86:THR:OG1	6:F:89:GLU:HG3	1.80	0.81
1:A:1017:LEU:HB2	5:E:206:GLY:N	1.93	0.81
1:A:795:GLU:CD	1:A:795:GLU:H	1.84	0.81
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.41	0.81
1:A:669:THR:O	1:A:762:SER:HB3	1.81	0.81
9:I:6:PHE:HB3	9:I:12:ASN:O	1.80	0.81
1:A:628:GLY:O	1:A:632:VAL:HG23	1.80	0.81
7:G:111:THR:HG22	7:G:113:HIS:N	1.95	0.81
2:B:1169:MET:CE	2:B:1201:LYS:HA	2.11	0.81
2:B:509:ALA:O	2:B:510:LYS:HD2	1.81	0.81
2:B:1099:VAL:HG13	2:B:1100:ASP:H	1.43	0.81
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.10	0.81
3:C:73:GLN:NE2	3:C:75:MET:H	1.79	0.81
2:B:816:GLU:O	2:B:817:LEU:HD23	1.80	0.81
10:J:16:ASP:OD1	10:J:17:LYS:HD2	1.80	0.81
1:A:1372:VAL:O	1:A:1376:THR:HG22	1.81	0.81
2:B:510:LYS:HD2	2:B:510:LYS:C	1.98	0.81
1:A:14:VAL:HG23	1:A:1432:GLN:NE2	1.95	0.80
1:A:335:ARG:HE	1:A:339:ASN:ND2	1.79	0.80
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.62	0.80
11:K:65:HIS:HD2	11:K:67:PHE:N	1.79	0.80
1:A:399:HIS:O	1:A:401:GLY:N	2.14	0.80
1:A:471:ASN:O	1:A:474:VAL:HG12	1.81	0.80
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.63	0.80
2:B:39:ARG:HH21	2:B:665:GLU:HG2	1.46	0.80
2:B:862:GLN:HG2	2:B:963:PHE:HD1	1.45	0.80
3:C:133:ILE:CD1	3:C:237:SER:HA	2.11	0.80
1:A:78:PRO:HA	2:B:1201:LYS:NZ	1.96	0.80
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.44	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:359:GLU:O	2:B:362:PRO:HD3	1.82	0.80
1:A:1237:ILE:HG22	1:A:1238:ILE:N	1.96	0.80
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.63	0.80
2:B:1204:PHE:O	2:B:1208:MET:HG3	1.82	0.80
1:A:56:PRO:O	1:A:57:ARG:HG3	1.82	0.80
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.64	0.80
9:I:58:VAL:HG22	9:I:62:ILE:HD12	1.63	0.80
1:A:666:ILE:HD12	1:A:667:GLY:N	1.95	0.79
9:I:55:THR:HG23	9:I:100:PHE:HD2	1.48	0.79
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.47	0.79
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.64	0.79
2:B:1106:ARG:HG3	2:B:1107:ALA:N	1.96	0.79
1:A:1017:LEU:HB3	5:E:205:SER:HA	1.64	0.79
1:A:1435:PRO:HA	1:A:1439:GLY:O	1.82	0.79
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.18	0.79
1:A:164:ARG:HG3	1:A:165:GLY:N	1.98	0.79
1:A:1444:MET:HG2	7:G:60:ARG:HA	1.65	0.79
9:I:58:VAL:HG12	9:I:60:GLN:H	1.47	0.79
12:L:30:ILE:HD11	12:L:59:ALA:HB2	1.64	0.79
1:A:494:SER:O	1:A:498:ARG:HG2	1.83	0.79
1:A:299:HIS:HA	1:A:302:THR:HG22	1.65	0.79
7:G:9:LEU:HD12	7:G:10:ASN:H	1.48	0.79
2:B:510:LYS:HG2	2:B:512:ARG:HG3	1.64	0.78
1:A:537:ARG:HD2	8:H:20:TYR:CE1	2.18	0.78
7:G:1:MET:HE3	7:G:80:LYS:C	2.03	0.78
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.65	0.78
6:F:82:THR:HG22	6:F:84:TYR:N	1.97	0.78
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.63	0.78
2:B:1165:ILE:HG22	2:B:1166:CYS:N	1.99	0.78
1:A:825:ILE:HG21	2:B:510:LYS:HE3	1.64	0.78
2:B:593:PRO:HG2	2:B:617:ARG:NH2	1.99	0.78
5:E:124:VAL:HG13	5:E:132:ILE:HD12	1.64	0.78
4:D:35:LEU:H	4:D:35:LEU:HD12	1.48	0.78
2:B:508:LEU:HB3	2:B:510:LYS:H	1.48	0.78
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.48	0.78
1:A:767:GLN:OE1	1:A:799:PHE:HB2	1.83	0.78
1:A:225:ASN:HD22	1:A:228:PHE:N	1.80	0.78
2:B:613:VAL:HG13	2:B:627:PHE:O	1.84	0.78
2:B:112:LEU:HD12	2:B:113:TYR:N	1.96	0.78
2:B:508:LEU:C	2:B:510:LYS:H	1.81	0.78
1:A:1127:ASP:HB3	1:A:1130:GLN:CB	2.14	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:ALA:HA	1:A:1093:LYS:HE3	1.66	0.78
2:B:615:MET:HB3	2:B:626:ILE:HG12	1.66	0.78
2:B:1206:GLU:O	2:B:1209:ALA:HB3	1.83	0.78
2:B:882:THR:HG22	2:B:884:ARG:N	1.99	0.77
1:A:1224:LEU:HD12	1:A:1241:ARG:O	1.84	0.77
1:A:765:VAL:HG23	1:A:802:ASN:O	1.84	0.77
4:D:185:CYS:HA	4:D:190:GLU:OE1	1.84	0.77
10:J:45:CYS:O	10:J:48:ARG:HG3	1.85	0.77
8:H:4:THR:HA	8:H:60:ALA:HB2	1.66	0.77
2:B:515:HIS:CD2	2:B:517:THR:H	2.03	0.77
1:A:908:LEU:HD12	1:A:983:ILE:HD11	1.67	0.77
3:C:98:VAL:C	3:C:99:LEU:HD23	2.03	0.77
3:C:167:HIS:CD2	3:C:169:LYS:H	2.02	0.77
3:C:47:ASP:HA	12:L:69:ALA:CB	2.15	0.77
2:B:508:LEU:C	2:B:510:LYS:N	2.30	0.77
11:K:113:THR:O	11:K:114:LEU:HB2	1.84	0.77
7:G:87:VAL:HB	7:G:103:VAL:HG11	1.67	0.77
1:A:489:LEU:HD12	1:A:490:HIS:N	1.99	0.77
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.00	0.77
1:A:1079:MET:HE2	1:A:1101:LEU:HD23	1.67	0.76
1:A:587:HIS:HD2	1:A:969:GLN:HG2	1.48	0.76
1:A:590:ARG:HD3	1:A:604:GLY:HA2	1.67	0.76
2:B:583:ASN:ND2	2:B:628:THR:HB	2.00	0.76
1:A:826:ASP:O	1:A:830:LYS:HB3	1.85	0.76
2:B:806:THR:HG22	2:B:808:ALA:H	1.48	0.76
2:B:467:GLY:O	2:B:468:GLU:CB	2.29	0.76
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.21	0.76
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.67	0.76
2:B:98:THR:O	2:B:126:SER:HB2	1.86	0.76
2:B:1187:ASN:O	2:B:1188:LYS:HB2	1.84	0.76
1:A:963:ILE:HD11	1:A:1048:ASN:HB2	1.68	0.76
1:A:1406:VAL:HG12	1:A:1410:PHE:CE1	2.21	0.76
1:A:107:CYS:H	1:A:114:LEU:HD21	1.51	0.76
2:B:918:ILE:HD12	2:B:935:ARG:CD	2.15	0.76
1:A:515:GLN:O	1:A:516:SER:HB3	1.85	0.76
4:D:170:THR:CG2	4:D:172:LEU:HG	2.16	0.76
5:E:154:ILE:H	5:E:196:VAL:HG13	1.49	0.76
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.68	0.76
10:J:7:CYS:SG	10:J:49:MET:HE3	2.26	0.76
1:A:106:VAL:HG13	1:A:112:LYS:O	1.86	0.76
7:G:121:PHE:HB2	7:G:130:TYR:CE2	2.20	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:48:ILE:HG21	7:G:4:ILE:HD12	1.66	0.76
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.21	0.76
9:I:62:ILE:HG22	9:I:62:ILE:O	1.84	0.76
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.68	0.76
1:A:866:PHE:O	1:A:867:ILE:HD12	1.85	0.76
1:A:95:PHE:CD1	1:A:234:MET:HG2	2.20	0.76
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.68	0.75
1:A:899:VAL:CB	1:A:929:LEU:HD11	2.16	0.75
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.68	0.75
1:A:754:SER:H	1:A:757:ASN:HD22	1.35	0.75
9:I:34:TYR:CD2	9:I:35:VAL:N	2.54	0.75
2:B:745:PRO:O	2:B:748:ILE:HG12	1.86	0.75
1:A:858:ASN:HD22	1:A:858:ASN:C	1.90	0.75
2:B:510:LYS:HG2	2:B:512:ARG:CG	2.17	0.75
1:A:337:ARG:CZ	1:A:839:ARG:NH1	2.50	0.75
8:H:59:ILE:HG22	8:H:60:ALA:N	2.01	0.75
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.50	0.75
4:D:40:HIS:CB	7:G:73:LYS:HZ3	1.96	0.75
2:B:705:MET:HA	2:B:705:MET:CE	2.17	0.75
5:E:7:ARG:HG3	5:E:8:ASN:N	2.00	0.75
2:B:508:LEU:CB	2:B:510:LYS:N	2.50	0.75
3:C:73:GLN:HE21	3:C:75:MET:N	1.82	0.75
3:C:90:ASP:O	3:C:91:HIS:CD2	2.39	0.75
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.17	0.75
1:A:897:TYR:HD1	1:A:897:TYR:N	1.85	0.74
1:A:95:PHE:O	1:A:99:ILE:HG13	1.87	0.74
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.67	0.74
1:A:820:GLY:O	1:A:822:GLU:N	2.20	0.74
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.67	0.74
1:A:1027:ALA:HB3	1:A:1030:ARG:HB2	1.68	0.74
3:C:50:GLU:HG2	12:L:64:LEU:HD13	1.69	0.74
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.02	0.74
3:C:6:PRO:HB3	3:C:25:VAL:HG12	1.69	0.74
1:A:1445:ILE:HD12	1:A:1445:ILE:H	1.53	0.74
1:A:1107:VAL:HG12	1:A:1107:VAL:O	1.87	0.74
1:A:567:LYS:HB3	8:H:96:VAL:N	2.01	0.74
2:B:1084:GLN:NE2	2:B:1084:GLN:N	2.35	0.74
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.70	0.74
1:A:225:ASN:ND2	1:A:228:PHE:N	2.32	0.74
2:B:1084:GLN:HE21	2:B:1084:GLN:N	1.84	0.74
1:A:830:LYS:HB2	1:A:1081:LEU:HD23	1.67	0.74

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:515:HIS:HD2	2:B:517:THR:H	1.35	0.74
1:A:853:ASP:OD1	1:A:855:THR:N	2.21	0.73
9:I:101:PHE:H	9:I:101:PHE:HD1	1.34	0.73
3:C:104:PHE:HD2	3:C:105:GLY:N	1.86	0.73
7:G:80:LYS:HG2	7:G:80:LYS:O	1.87	0.73
7:G:43:GLY:HA3	7:G:80:LYS:HB3	1.70	0.73
2:B:508:LEU:HB2	2:B:510:LYS:H	1.52	0.73
1:A:903:ASN:HD22	1:A:904:THR:N	1.87	0.73
4:D:145:MET:O	4:D:149:THR:HB	1.87	0.73
1:A:40:THR:HG21	1:A:259:GLU:OE2	1.88	0.73
6:F:111:LEU:HD12	6:F:111:LEU:H	1.54	0.73
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.70	0.73
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.53	0.73
1:A:1170:ILE:HG23	1:A:1174:PHE:CE1	2.22	0.73
10:J:41:LEU:HD11	10:J:50:ILE:HG13	1.70	0.73
8:H:36:CYS:HA	8:H:126:GLU:O	1.88	0.73
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.02	0.73
1:A:215:SER:HB3	1:A:218:ASP:OD2	1.89	0.73
1:A:68:GLN:HE22	1:A:80:HIS:CD2	2.06	0.73
2:B:873:THR:O	2:B:914:LYS:HA	1.88	0.73
1:A:1239:ARG:HH22	1:A:1241:ARG:NH2	1.85	0.73
2:B:1002:THR:CG2	2:B:1006:ILE:HD12	2.19	0.73
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.71	0.73
1:A:288:ALA:HA	1:A:291:GLU:OE2	1.89	0.73
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.52	0.73
1:A:31:SER:HA	1:A:81:PHE:O	1.87	0.73
2:B:1142:GLY:HA3	6:F:88:TYR:HE2	1.52	0.73
2:B:1180:PHE:HB3	2:B:1191:ILE:HD12	1.69	0.73
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.53	0.73
4:D:144:THR:O	4:D:148:LEU:HB2	1.89	0.73
1:A:1444:MET:CE	6:F:135:ARG:HB2	2.18	0.73
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.69	0.73
3:C:32:SER:O	3:C:36:VAL:HG23	1.89	0.73
7:G:91:VAL:HG23	7:G:141:SER:O	1.88	0.72
9:I:111:THR:HG22	9:I:112:SER:N	2.03	0.72
5:E:213:ILE:HG12	5:E:214:CYS:H	1.54	0.72
1:A:53:LEU:HD23	1:A:54:ASN:H	1.54	0.72
7:G:138:THR:CG2	7:G:139:ILE:H	1.95	0.72
9:I:101:PHE:N	9:I:101:PHE:CD1	2.55	0.72
1:A:265:LYS:HE2	1:A:322:VAL:CG1	2.19	0.72
1:A:364:VAL:HG12	1:A:458:HIS:HB3	1.71	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:LEU:N	1:A:926:GLN:NE2	2.36	0.72
2:B:637:LEU:O	2:B:690:VAL:HG13	1.90	0.72
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.72	0.72
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.52	0.72
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.30	0.72
1:A:741:ASN:HD22	1:A:744:LYS:H	1.35	0.72
2:B:976:ILE:HD11	2:B:992:ILE:HA	1.71	0.72
2:B:801:LYS:O	10:J:52:THR:HG23	1.89	0.72
2:B:1031:LEU:HA	2:B:1055:ILE:HD13	1.72	0.72
8:H:44:VAL:HG12	8:H:44:VAL:O	1.89	0.72
2:B:172:ILE:HD13	2:B:178:ASN:CB	2.19	0.72
1:A:90:VAL:HG12	1:A:91:PHE:N	2.03	0.72
2:B:957:ASN:O	2:B:959:ASP:N	2.22	0.72
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.70	0.72
2:B:604:ARG:NH2	2:B:613:VAL:O	2.23	0.72
1:A:1341:ILE:CG2	1:A:1342:GLU:H	2.03	0.72
2:B:1224:PHE:HE2	5:E:171:LYS:HG3	1.52	0.72
1:A:335:ARG:NH1	2:B:1206:GLU:OE2	2.22	0.72
9:I:59:VAL:O	9:I:60:GLN:HB2	1.88	0.72
1:A:1402:PHE:CE1	1:A:1403:GLU:HG3	2.24	0.72
1:A:310:GLY:O	1:A:312:PRO:HD2	1.90	0.72
1:A:648:ASN:O	1:A:652:VAL:HG23	1.88	0.71
1:A:1237:ILE:HG22	1:A:1238:ILE:H	1.55	0.71
2:B:123:THR:O	2:B:125:SER:N	2.22	0.71
7:G:145:VAL:HG12	7:G:146:LYS:N	2.03	0.71
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.69	0.71
1:A:71:GLN:C	1:A:73:GLY:H	1.91	0.71
2:B:953:LEU:O	2:B:953:LEU:HD23	1.89	0.71
1:A:13:THR:O	2:B:1218:THR:HG22	1.90	0.71
7:G:115:MET:HB2	7:G:116:PRO:HD2	1.69	0.71
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.53	0.71
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.25	0.71
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.72	0.71
2:B:114:PRO:HG2	2:B:115:GLN:H	1.54	0.71
1:A:897:TYR:CD1	1:A:897:TYR:N	2.56	0.71
6:F:86:THR:HG23	6:F:89:GLU:CD	2.10	0.71
4:D:54:GLU:O	4:D:58:VAL:HG23	1.89	0.71
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.71	0.71
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.06	0.71
1:A:1325:THR:O	5:E:148:GLU:HB2	1.90	0.71
1:A:256:GLN:HE21	2:B:918:ILE:HD11	1.54	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:56:ALA:HB2	9:I:89:GLN:HG3	1.72	0.71
2:B:758:PHE:HE1	2:B:1027:ILE:HG22	1.56	0.71
2:B:261:ARG:O	2:B:267:ARG:HD3	1.90	0.71
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.25	0.71
1:A:351:THR:HB	2:B:1103:ILE:HD12	1.72	0.71
2:B:857:ARG:HG2	2:B:858:SER:H	1.55	0.71
9:I:71:SER:OG	9:I:83:ASN:HB2	1.90	0.71
2:B:898:LEU:HB2	12:L:58:LYS:HZ2	1.54	0.71
9:I:34:TYR:CE2	9:I:36:GLU:HB3	2.25	0.71
1:A:535:THR:HG21	1:A:616:VAL:HA	1.73	0.71
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.73	0.71
1:A:1057:VAL:HG12	1:A:1058:VAL:H	1.53	0.71
12:L:38:LEU:O	12:L:39:SER:HB3	1.91	0.71
8:H:102:TYR:N	8:H:102:TYR:CD2	2.58	0.71
1:A:1279:ILE:HD11	1:A:1316:VAL:HG21	1.72	0.71
1:A:339:ASN:HB3	2:B:1117:GLN:NE2	2.05	0.71
1:A:1362:TYR:HD1	1:A:1363:VAL:N	1.85	0.70
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.72	0.70
2:B:510:LYS:HB2	2:B:511:PRO:CD	2.21	0.70
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.30	0.70
2:B:541:LEU:HB2	2:B:747:MET:HE3	1.71	0.70
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.56	0.70
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.05	0.70
2:B:496:ARG:HH11	2:B:496:ARG:HB3	1.56	0.70
1:A:666:ILE:HD11	2:B:1067:ARG:O	1.90	0.70
1:A:1435:PRO:O	1:A:1436:ILE:HG13	1.92	0.70
1:A:367:PRO:HB3	1:A:465:TYR:O	1.91	0.70
1:A:1261:LYS:HA	1:A:1264:GLU:HB3	1.74	0.70
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.71	0.70
9:I:56:ALA:HB2	9:I:89:GLN:HG2	1.72	0.70
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.73	0.70
2:B:794:ASN:C	2:B:795:ILE:HD12	2.11	0.70
1:A:888:GLY:O	1:A:940:ARG:NH2	2.24	0.70
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.74	0.70
3:C:191:TYR:HD2	3:C:201:TRP:CD1	2.09	0.70
2:B:1166:CYS:O	2:B:1168:LEU:N	2.22	0.70
5:E:135:PHE:CD2	5:E:140:LEU:HD21	2.27	0.70
1:A:1280:GLU:O	1:A:1281:ARG:O	2.10	0.70
2:B:563:MET:CE	2:B:580:VAL:HB	2.21	0.70
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.72	0.70
1:A:375:THR:OG1	1:A:433:GLU:HB3	1.91	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1443:VAL:O	1:A:1444:MET:HG3	1.91	0.70
1:A:265:LYS:HD2	1:A:265:LYS:N	2.06	0.70
1:A:852:TYR:CD1	6:F:136:ARG:HB3	2.27	0.70
1:A:1147:THR:HG22	1:A:1149:ALA:H	1.56	0.70
2:B:510:LYS:CB	2:B:511:PRO:HD2	2.21	0.70
8:H:81:PRO:HB2	8:H:82:PRO:HD2	1.74	0.70
1:A:370:ILE:HG22	1:A:374:LEU:CD1	2.21	0.70
2:B:986:GLN:OE1	2:B:986:GLN:HA	1.92	0.70
1:A:414:ASP:OD1	1:A:416:ARG:HG3	1.91	0.70
1:A:698:GLN:HA	9:I:97:MET:O	1.91	0.70
1:A:1385:THR:O	1:A:1388:GLY:N	2.21	0.70
1:A:1116:LEU:N	1:A:1308:THR:CG2	2.54	0.70
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.72	0.70
1:A:1104:ILE:O	1:A:1107:VAL:N	2.23	0.70
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.27	0.69
3:C:73:GLN:NE2	3:C:74:SER:H	1.89	0.69
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.07	0.69
1:A:384:ASN:OD1	1:A:388:LEU:HD12	1.92	0.69
12:L:32:ALA:HB3	12:L:55:ILE:CD1	2.21	0.69
5:E:202:SER:OG	5:E:204:THR:HG22	1.91	0.69
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.22	0.69
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.73	0.69
1:A:92:HIS:O	1:A:94:GLY:N	2.25	0.69
2:B:857:ARG:HH21	2:B:942:ARG:CZ	2.04	0.69
2:B:773:MET:C	2:B:775:LYS:H	1.95	0.69
1:A:1334:ASP:C	1:A:1336:MET:H	1.93	0.69
2:B:510:LYS:HB2	2:B:511:PRO:HD2	1.74	0.69
2:B:281:PRO:HG2	2:B:284:ILE:HG13	1.75	0.69
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.06	0.69
7:G:123:ALA:C	7:G:125:SER:H	1.96	0.69
1:A:370:ILE:HG23	2:B:1105:ALA:HB2	1.72	0.69
1:A:1334:ASP:O	1:A:1336:MET:N	2.25	0.69
5:E:164:LEU:HD13	5:E:211:TYR:CE2	2.28	0.69
1:A:1283:VAL:HG12	1:A:1284:MET:H	1.58	0.69
2:B:292:ILE:HD13	2:B:326:ASP:HA	1.73	0.69
1:A:347:PHE:H	2:B:1107:ALA:HA	1.57	0.69
3:C:147:LEU:HD12	3:C:151:GLN:O	1.91	0.69
1:A:367:PRO:HG2	1:A:370:ILE:HG13	1.74	0.69
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.57	0.69
3:C:242:GLN:HA	3:C:245:VAL:HG23	1.73	0.69
1:A:1081:LEU:HD21	1:A:1098:VAL:HG21	1.74	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ARG:NH2	1:A:839:ARG:HH12	1.90	0.69
1:A:315:LEU:HD23	1:A:321:PRO:HA	1.73	0.69
2:B:1023:VAL:O	2:B:1027:ILE:HG13	1.93	0.69
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.74	0.69
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.23	0.69
2:B:769:TYR:CE2	2:B:987:LYS:NZ	2.55	0.69
2:B:839:MET:CE	2:B:1010:LEU:HD21	2.23	0.69
2:B:871:THR:HG22	2:B:872:GLU:O	1.93	0.69
2:B:1115:THR:O	2:B:1116:ARG:HB2	1.92	0.69
2:B:363:HIS:O	2:B:364:ILE:HB	1.91	0.69
1:A:390:GLN:HE21	1:A:394:ASN:ND2	1.91	0.69
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.00	0.69
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.23	0.69
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.27	0.69
1:A:1035:TYR:O	1:A:1037:LEU:N	2.25	0.69
2:B:510:LYS:CD	2:B:510:LYS:C	2.61	0.69
1:A:69:THR:O	1:A:71:GLN:N	2.25	0.69
2:B:948:ILE:HG22	2:B:949:VAL:O	1.93	0.69
1:A:95:PHE:HD1	1:A:234:MET:HG2	1.57	0.69
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.27	0.69
1:A:606:LEU:HG	1:A:613:ILE:HD12	1.74	0.69
5:E:2:ASP:O	5:E:3:GLN:HG2	1.92	0.69
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.73	0.69
1:A:608:ILE:HG23	1:A:969:GLN:OE1	1.91	0.68
2:B:37:PHE:CE2	2:B:542:MET:HA	2.27	0.68
6:F:111:LEU:C	6:F:113:GLY:H	1.96	0.68
2:B:1146:PHE:CD1	2:B:1146:PHE:O	2.47	0.68
1:A:289:ILE:C	1:A:291:GLU:H	1.95	0.68
2:B:606:LYS:HD2	2:B:608:ASP:OD2	1.92	0.68
2:B:821:GLN:HE22	2:B:851:PHE:H	1.42	0.68
1:A:979:SER:OG	1:A:980:ASP:N	2.22	0.68
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.76	0.68
1:A:49:LYS:NZ	1:A:60:SER:HA	2.08	0.68
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.07	0.68
2:B:1184:GLY:C	2:B:1186:ASP:H	1.96	0.68
1:A:709:THR:HG22	1:A:712:GLU:H	1.59	0.68
7:G:127:PRO:HG2	7:G:138:THR:HG21	1.74	0.68
10:J:2:ILE:HG12	10:J:57:ILE:HD12	1.74	0.68
7:G:96:GLN:HA	7:G:121:PHE:CE2	2.28	0.68
2:B:983:ARG:NH1	2:B:1028:GLU:OE1	2.27	0.68
6:F:97:ARG:NH2	6:F:108:PHE:HE1	1.92	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:LEU:CD1	2:B:113:TYR:H	2.03	0.68
1:A:768:GLN:CG	1:A:816:HIS:HA	2.22	0.68
1:A:1079:MET:CE	1:A:1101:LEU:HD23	2.23	0.68
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.74	0.68
11:K:12:LEU:H	11:K:12:LEU:HD12	1.58	0.68
3:C:45:ALA:CA	3:C:72:LEU:HD12	2.16	0.68
2:B:1159:ARG:HB3	2:B:1159:ARG:NH1	2.09	0.68
2:B:880:THR:O	2:B:881:ASN:HB2	1.94	0.68
2:B:282:ILE:CD1	2:B:382:ILE:HD13	2.23	0.68
2:B:546:SER:OG	2:B:631:GLY:N	2.22	0.68
1:A:1331:SER:OG	1:A:1333:ILE:HG22	1.94	0.68
2:B:172:ILE:HD13	2:B:178:ASN:HB2	1.76	0.68
4:D:130:LEU:C	4:D:132:GLN:H	1.97	0.68
5:E:143:ASN:HD22	5:E:146:HIS:CE1	2.12	0.68
5:E:207:ARG:HH11	5:E:207:ARG:HB3	1.58	0.68
2:B:831:SER:OG	2:B:840:ILE:HD11	1.93	0.68
1:A:41:MET:O	1:A:50:ILE:HG13	1.94	0.68
1:A:332:LYS:HG3	1:A:333:GLU:HG2	1.76	0.68
1:A:642:CYS:O	1:A:645:LEU:N	2.27	0.68
1:A:1410:PHE:HA	2:B:1212:ILE:HD11	1.75	0.68
2:B:654:ARG:H	2:B:657:HIS:HD2	1.41	0.68
1:A:853:ASP:OD1	1:A:855:THR:CB	2.40	0.68
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.24	0.68
1:A:1364:ASN:OD1	1:A:1366:ARG:HD2	1.94	0.68
1:A:135:PHE:C	1:A:137:ALA:H	1.97	0.68
1:A:837:ILE:HA	1:A:840:ARG:HD3	1.76	0.68
2:B:552:MET:HA	2:B:555:ILE:HB	1.75	0.67
1:A:1437:GLY:HA3	6:F:88:TYR:CD2	2.30	0.67
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.76	0.67
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	1.94	0.67
1:A:519:PRO:HG2	1:A:624:SER:O	1.94	0.67
7:G:73:LYS:HE2	7:G:74:TYR:O	1.95	0.67
7:G:13:LEU:HD23	7:G:14:HIS:N	2.10	0.67
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.25	0.67
2:B:622:LYS:HE3	9:I:59:VAL:HG22	1.76	0.67
1:A:982:THR:O	1:A:985:ASP:HB2	1.94	0.67
7:G:106:MET:HG3	7:G:157:ILE:O	1.93	0.67
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.10	0.67
3:C:105:GLY:HA3	3:C:149:LYS:O	1.92	0.67
5:E:210:SER:C	5:E:211:TYR:CD1	2.68	0.67
1:A:1192:LEU:HG	1:A:1193:LEU:N	2.08	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.74	0.67
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.77	0.67
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.29	0.67
2:B:900:ALA:O	2:B:903:VAL:HG23	1.95	0.67
1:A:997:LEU:HD13	1:A:1018:PHE:HE2	1.60	0.67
2:B:1010:LEU:HD12	2:B:1011:ILE:H	1.60	0.67
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.21	0.67
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.30	0.67
3:C:6:PRO:HB3	3:C:25:VAL:CG1	2.24	0.67
1:A:1083:THR:HG21	1:A:1085:HIS:CE1	2.30	0.67
2:B:378:LEU:HD12	2:B:378:LEU:O	1.94	0.67
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.25	0.67
2:B:97:VAL:HG12	2:B:178:ASN:ND2	2.09	0.67
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.76	0.67
1:A:886:ILE:CD1	1:A:943:LEU:HB3	2.22	0.67
2:B:546:SER:OG	2:B:630:ALA:HA	1.95	0.67
1:A:889:SER:HB3	1:A:1297:GLU:HG2	1.75	0.67
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.09	0.67
1:A:1447:GLU:OE2	7:G:23:LYS:HB2	1.94	0.67
2:B:1165:ILE:HG22	2:B:1166:CYS:H	1.59	0.67
2:B:899:ILE:CG2	2:B:903:VAL:HG21	2.25	0.67
1:A:858:ASN:ND2	1:A:860:LEU:H	1.92	0.67
1:A:75:ASN:O	1:A:76:GLU:HB3	1.95	0.67
1:A:1089:VAL:O	1:A:1089:VAL:HG12	1.94	0.67
3:C:86:CYS:O	3:C:88:CYS:N	2.27	0.67
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.77	0.67
2:B:854:LEU:HB3	2:B:856:PHE:HE1	1.60	0.67
1:A:829:VAL:HG13	2:B:507:LYS:HG2	1.76	0.66
1:A:34:LYS:HB2	1:A:36:ARG:HH21	1.60	0.66
2:B:1065:GLN:HB3	2:B:1069:PHE:O	1.95	0.66
2:B:237:VAL:HG22	2:B:257:LYS:HA	1.78	0.66
10:J:7:CYS:SG	10:J:46:CYS:HA	2.34	0.66
1:A:1161:THR:OG1	1:A:1170:ILE:HD11	1.95	0.66
12:L:61:THR:HG21	12:L:63:ARG:HG2	1.78	0.66
2:B:205:ILE:N	2:B:205:ILE:HD12	2.10	0.66
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.24	0.66
12:L:58:LYS:O	12:L:59:ALA:O	2.13	0.66
2:B:240:ILE:HG22	2:B:254:LEU:HB3	1.77	0.66
3:C:263:THR:C	3:C:265:MET:H	1.98	0.66
2:B:411:PRO:O	2:B:414:ALA:HB3	1.95	0.66
1:A:134:ARG:HG2	1:A:134:ARG:O	1.94	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:882:THR:CG2	2:B:884:ARG:HB2	2.25	0.66
2:B:1065:GLN:HB2	3:C:201:TRP:CZ3	2.31	0.66
1:A:55:ASP:N	1:A:56:PRO:HD3	2.11	0.66
1:A:1291:VAL:HG13	1:A:1292:PRO:CD	2.25	0.66
1:A:265:LYS:HD2	1:A:265:LYS:H	1.60	0.66
2:B:594:ALA:HA	2:B:617:ARG:HH12	1.61	0.66
7:G:91:VAL:HB	7:G:139:ILE:O	1.95	0.66
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.11	0.66
9:I:58:VAL:HG13	9:I:62:ILE:CG1	2.25	0.66
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.09	0.66
2:B:705:MET:H	2:B:710:LEU:CD1	2.09	0.66
2:B:773:MET:C	2:B:775:LYS:N	2.49	0.66
1:A:825:ILE:C	1:A:827:THR:H	1.96	0.66
2:B:579:ARG:HD2	2:B:586:TRP:CZ2	2.30	0.66
3:C:174:ALA:O	3:C:175:ALA:HB2	1.95	0.66
1:A:550:LEU:HD22	1:A:556:TRP:CE2	2.31	0.66
3:C:92:CYS:SG	3:C:94:LYS:HB3	2.36	0.66
2:B:616:ILE:HD12	2:B:616:ILE:N	2.11	0.66
2:B:820:GLY:N	2:B:1091:TYR:OH	2.29	0.66
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.26	0.66
1:A:254:GLU:HB2	2:B:935:ARG:HH22	1.60	0.66
2:B:1169:MET:HE1	2:B:1201:LYS:CA	2.25	0.66
2:B:862:GLN:HG2	2:B:963:PHE:CD1	2.28	0.66
1:A:115:LEU:HB2	1:A:122:MET:HE1	1.78	0.66
9:I:34:TYR:HE2	9:I:36:GLU:HB3	1.60	0.66
1:A:90:VAL:HG13	1:A:297:GLN:OE1	1.96	0.66
5:E:182:ASP:O	5:E:185:ALA:N	2.28	0.66
2:B:322:PHE:HZ	9:I:30:ARG:HB3	1.61	0.66
2:B:1223:ASP:O	2:B:1224:PHE:HB2	1.96	0.66
12:L:60:ARG:HG2	12:L:61:THR:H	1.60	0.66
6:F:103:MET:HE2	7:G:65:ASP:HB2	1.77	0.66
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.10	0.66
2:B:898:LEU:HB2	12:L:58:LYS:NZ	2.10	0.66
3:C:50:GLU:HG2	12:L:64:LEU:CD1	2.25	0.66
1:A:538:ASP:OD2	8:H:22:LYS:HB2	1.96	0.66
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.76	0.66
1:A:78:PRO:HA	2:B:1201:LYS:HZ1	1.61	0.66
1:A:1376:THR:OG1	1:A:1377:THR:N	2.23	0.66
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.75	0.66
2:B:365:THR:HG23	2:B:367:LEU:H	1.62	0.66
2:B:910:VAL:HG12	2:B:911:ILE:N	2.11	0.66

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1445:ILE:HD12	1:A:1445:ILE:N	2.11	0.66
5:E:157:SER:OG	5:E:160:GLU:HG3	1.96	0.66
1:A:908:LEU:CD1	1:A:983:ILE:HD11	2.25	0.65
1:A:1118:VAL:HG12	1:A:1327:ILE:HG13	1.77	0.65
2:B:1159:ARG:NE	2:B:1193:GLN:HE21	1.94	0.65
2:B:1198:TYR:CE1	2:B:1201:LYS:HD2	2.30	0.65
11:K:67:PHE:C	11:K:68:PHE:HD2	1.98	0.65
2:B:294:ASP:OD2	2:B:294:ASP:N	2.25	0.65
8:H:41:ASP:O	8:H:42:ILE:HG13	1.97	0.65
12:L:28:LYS:HB2	12:L:39:SER:HB2	1.78	0.65
7:G:143:ILE:HG22	7:G:144:ARG:N	2.11	0.65
3:C:5:GLY:O	3:C:7:GLN:HG3	1.96	0.65
3:C:73:GLN:HB3	3:C:131:HIS:H	1.60	0.65
3:C:241:ASP:O	3:C:245:VAL:HG23	1.96	0.65
1:A:709:THR:HB	1:A:712:GLU:HB2	1.77	0.65
1:A:550:LEU:HD22	1:A:556:TRP:NE1	2.11	0.65
4:D:137:ASN:HD22	4:D:137:ASN:C	2.00	0.65
1:A:886:ILE:HG22	1:A:887:GLY:N	2.11	0.65
2:B:955:THR:HG22	2:B:956:THR:N	2.12	0.65
2:B:117:ALA:HA	2:B:122:LEU:HD12	1.78	0.65
1:A:591:PHE:HA	1:A:595:THR:HG21	1.77	0.65
1:A:63:ARG:HG2	1:A:74:MET:SD	2.36	0.65
4:D:35:LEU:N	4:D:35:LEU:HD12	2.12	0.65
1:A:275:SER:O	1:A:279:LEU:HG	1.96	0.65
3:C:43:THR:HG22	3:C:44:LEU:N	2.10	0.65
2:B:1156:ASP:O	2:B:1157:ALA:O	2.15	0.65
9:I:85:PHE:HD2	9:I:85:PHE:N	1.78	0.65
2:B:794:ASN:O	2:B:795:ILE:HD12	1.96	0.65
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.61	0.65
2:B:825:VAL:HG22	2:B:1010:LEU:HB3	1.79	0.65
7:G:111:THR:CG2	7:G:113:HIS:H	2.04	0.65
2:B:1020:ARG:CG	2:B:1020:ARG:HH11	2.09	0.65
2:B:261:ARG:HB3	2:B:261:ARG:NH1	2.11	0.65
5:E:78:LEU:HD23	5:E:79:TRP:N	2.11	0.65
1:A:855:THR:CG2	1:A:857:ARG:HE	1.99	0.65
1:A:1283:VAL:O	1:A:1306:LEU:HA	1.96	0.65
1:A:1329:THR:H	1:A:1335:ILE:CD1	1.95	0.65
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.32	0.65
3:C:179:GLU:HG2	3:C:180:TYR:N	2.12	0.65
9:I:101:PHE:N	9:I:101:PHE:HD1	1.91	0.65
1:A:264:PHE:O	1:A:267:ALA:HB3	1.96	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:CYS:N	1:A:114:LEU:HD21	2.11	0.65
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.78	0.65
1:A:67:CYS:O	1:A:70:CYS:HB3	1.97	0.65
2:B:991:GLY:O	2:B:992:ILE:HB	1.95	0.65
2:B:227:LYS:HB2	2:B:395:GLN:OE1	1.97	0.65
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.29	0.65
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.79	0.65
2:B:541:LEU:HD12	2:B:747:MET:HE1	1.78	0.65
2:B:687:GLU:O	2:B:689:LEU:HG	1.96	0.65
2:B:322:PHE:CZ	9:I:30:ARG:HB3	2.32	0.65
1:A:689:LYS:HE2	1:A:721:PHE:CE2	2.32	0.65
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.77	0.65
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.08	0.65
1:A:443:LEU:HG	2:B:1146:PHE:CE2	2.27	0.65
2:B:953:LEU:CD2	2:B:965:LYS:HB2	2.26	0.65
1:A:55:ASP:CG	1:A:55:ASP:O	2.32	0.65
3:C:235:VAL:HG13	10:J:13:VAL:HG23	1.79	0.64
2:B:856:PHE:N	2:B:856:PHE:CD1	2.64	0.64
1:A:593:GLU:O	1:A:595:THR:N	2.30	0.64
1:A:903:ASN:HD22	1:A:903:ASN:C	2.00	0.64
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.32	0.64
5:E:177:ARG:C	5:E:212:ARG:HD3	2.18	0.64
8:H:89:LEU:HB3	8:H:91:ASP:OD1	1.97	0.64
2:B:770:GLN:HG2	2:B:983:ARG:O	1.96	0.64
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.78	0.64
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.78	0.64
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.80	0.64
2:B:508:LEU:HB2	2:B:510:LYS:N	2.10	0.64
1:A:243:PRO:O	1:A:246:VAL:HG23	1.98	0.64
1:A:704:ALA:O	1:A:705:LYS:HB2	1.97	0.64
4:D:47:LEU:HD13	4:D:48:ILE:H	1.63	0.64
2:B:952:VAL:HG12	2:B:953:LEU:N	2.11	0.64
6:F:97:ARG:HH22	6:F:108:PHE:HE1	1.45	0.64
2:B:446:LEU:O	2:B:447:ALA:HB3	1.97	0.64
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.80	0.64
7:G:14:HIS:ND1	7:G:15:PRO:HD2	2.12	0.64
2:B:508:LEU:HB2	2:B:510:LYS:CA	2.28	0.64
1:A:1409:LEU:O	1:A:1412:ALA:HB3	1.97	0.64
2:B:54:PHE:CE2	2:B:59:LEU:HD13	2.32	0.64
2:B:859:TYR:HD1	2:B:859:TYR:H	1.44	0.64
7:G:126:ASN:HD22	7:G:127:PRO:HA	1.63	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:ASP:O	2:B:296:GLU:N	2.30	0.64
1:A:1148:ILE:O	1:A:1148:ILE:HG22	1.98	0.64
1:A:1120:LEU:O	1:A:1323:ASP:HB2	1.98	0.64
2:B:23:ALA:HB1	2:B:24:PRO:CD	2.23	0.64
8:H:93:TYR:HB3	8:H:144:ILE:O	1.98	0.64
2:B:37:PHE:HD2	2:B:542:MET:SD	2.21	0.64
6:F:86:THR:HG23	6:F:89:GLU:OE1	1.97	0.64
2:B:737:THR:HG21	9:I:66:PRO:HA	1.79	0.64
1:A:996:ASN:C	1:A:998:LEU:HD12	2.18	0.64
2:B:54:PHE:HE1	2:B:414:ALA:HA	1.62	0.64
7:G:6:ASP:O	7:G:7:LEU:HD23	1.98	0.64
1:A:534:LEU:O	1:A:574:GLY:HA3	1.98	0.64
2:B:705:MET:H	2:B:710:LEU:HD12	1.61	0.64
2:B:1102:LYS:O	2:B:1103:ILE:C	2.34	0.64
1:A:1423:GLY:O	1:A:1426:GLU:N	2.31	0.64
1:A:370:ILE:HG22	1:A:374:LEU:HD11	1.80	0.64
1:A:47:ARG:NH2	1:A:255:SER:H	1.95	0.63
2:B:35:SER:HA	2:B:811:TYR:CE2	2.26	0.63
2:B:1060:ARG:HH11	2:B:1060:ARG:HG2	1.61	0.63
2:B:390:LEU:O	2:B:392:ARG:HG3	1.98	0.63
3:C:35:ARG:NH1	11:K:41:THR:H	1.96	0.63
1:A:845:LEU:HB3	1:A:848:ILE:HD12	1.80	0.63
1:A:55:ASP:C	1:A:57:ARG:N	2.46	0.63
1:A:61:ILE:O	1:A:63:ARG:N	2.32	0.63
9:I:113:ASP:O	9:I:114:GLN:HG3	1.98	0.63
11:K:47:ARG:NH1	11:K:47:ARG:HB3	2.12	0.63
1:A:283:GLY:O	1:A:285:PRO:HD3	1.99	0.63
2:B:315:LYS:N	2:B:316:PRO:HD2	2.11	0.63
2:B:859:TYR:CD1	2:B:859:TYR:N	2.67	0.63
7:G:14:HIS:CE1	7:G:15:PRO:HD2	2.34	0.63
2:B:511:PRO:C	2:B:513:GLN:N	2.51	0.63
2:B:604:ARG:NH2	2:B:614:SER:HA	2.13	0.63
2:B:294:ASP:C	2:B:296:GLU:H	2.01	0.63
8:H:123:MET:HE3	8:H:142:LEU:HD22	1.80	0.63
12:L:28:LYS:HB2	12:L:39:SER:CB	2.28	0.63
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.80	0.63
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.33	0.63
2:B:284:ILE:HD13	2:B:333:PHE:HD2	1.64	0.63
1:A:335:ARG:HE	1:A:339:ASN:HD22	1.45	0.63
1:A:367:PRO:HA	1:A:463:ILE:O	1.99	0.63
2:B:429:PHE:HA	2:B:432:MET:HE2	1.80	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.80	0.63
2:B:589:VAL:CG1	2:B:590:HIS:H	2.06	0.63
1:A:256:GLN:NE2	2:B:918:ILE:HD11	2.14	0.63
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.80	0.63
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.13	0.63
1:A:17:VAL:HG23	1:A:1421:CYS:SG	2.38	0.63
7:G:80:LYS:HE2	7:G:82:PHE:CZ	2.34	0.63
4:D:211:LEU:HD23	4:D:214:LEU:HD12	1.79	0.63
5:E:78:LEU:HD21	5:E:80:VAL:HG23	1.81	0.63
1:A:637:LYS:HB3	1:A:641:VAL:HG21	1.81	0.63
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.80	0.63
2:B:39:ARG:HH21	2:B:665:GLU:CG	2.10	0.63
1:A:546:VAL:HG21	1:A:572:TRP:CE3	2.34	0.63
1:A:1206:ASP:O	1:A:1274:ARG:NH1	2.31	0.63
1:A:922:ASP:OD1	1:A:924:LYS:N	2.32	0.63
1:A:1019:CYS:O	1:A:1022:LEU:HB3	1.99	0.63
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.28	0.63
2:B:1224:PHE:CE2	5:E:171:LYS:HG3	2.33	0.63
5:E:197:LYS:HG2	5:E:197:LYS:O	1.97	0.63
2:B:762:ASN:HD21	2:B:1024:ALA:HB3	1.64	0.63
1:A:1213:GLY:HA2	1:A:1216:ILE:HD12	1.81	0.63
2:B:526:GLU:OE2	2:B:752:ALA:HB2	1.98	0.63
5:E:168:TYR:HB3	5:E:170:LEU:HG	1.81	0.63
3:C:35:ARG:NH1	11:K:41:THR:N	2.47	0.63
1:A:244:PRO:HG2	1:A:245:PRO:HD3	1.81	0.62
8:H:42:ILE:HG23	8:H:95:TYR:CE1	2.34	0.62
1:A:1230:GLU:O	1:A:1232:ASN:N	2.32	0.62
2:B:601:ARG:O	2:B:605:ARG:HG3	1.99	0.62
2:B:129:PHE:HA	2:B:165:VAL:O	1.99	0.62
1:A:1081:LEU:HD11	1:A:1098:VAL:HB	1.81	0.62
1:A:1342:GLU:CD	5:E:198:ILE:HG21	2.18	0.62
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.28	0.62
1:A:265:LYS:HE2	1:A:322:VAL:HG13	1.81	0.62
1:A:1017:LEU:CB	5:E:205:SER:HA	2.29	0.62
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.33	0.62
3:C:235:VAL:HG21	10:J:6:ARG:NH2	2.14	0.62
7:G:1:MET:O	7:G:1:MET:HE1	1.99	0.62
7:G:80:LYS:HE2	7:G:82:PHE:HZ	1.64	0.62
1:A:691:LEU:O	1:A:694:THR:HB	1.99	0.62
2:B:204:ILE:C	2:B:205:ILE:HD12	2.19	0.62
1:A:1072:ILE:O	1:A:1075:PRO:HG2	1.98	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1080:THR:O	1:A:1081:LEU:HD22	1.98	0.62
1:A:90:VAL:CG1	1:A:91:PHE:N	2.63	0.62
3:C:147:LEU:HB2	3:C:151:GLN:CB	2.29	0.62
2:B:773:MET:O	2:B:776:GLN:N	2.28	0.62
7:G:23:LYS:HG3	7:G:56:ILE:CD1	2.28	0.62
2:B:292:ILE:CD1	2:B:326:ASP:HA	2.30	0.62
9:I:87:GLN:O	9:I:89:GLN:OE1	2.18	0.62
1:A:858:ASN:C	1:A:858:ASN:ND2	2.53	0.62
5:E:192:ARG:HG3	5:E:192:ARG:HH11	1.64	0.62
1:A:818:MET:HG2	2:B:514:LEU:HG	1.81	0.62
2:B:1099:VAL:HG22	2:B:1103:ILE:HD13	1.80	0.62
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.88	0.62
3:C:143:LEU:HD12	3:C:145:CYS:H	1.64	0.62
3:C:63:ILE:CA	3:C:66:ARG:HG3	2.26	0.62
2:B:604:ARG:HH22	2:B:614:SER:HA	1.62	0.62
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.26	0.62
2:B:835:GLN:HA	2:B:1013:ASN:ND2	2.10	0.62
1:A:21:LEU:HG	1:A:1413:GLY:O	2.00	0.62
1:A:590:ARG:HG3	1:A:590:ARG:NH1	2.15	0.62
2:B:189:LEU:HA	2:B:192:LEU:HD12	1.82	0.62
2:B:65:GLU:HG3	2:B:66:ASP:N	2.07	0.62
1:A:289:ILE:O	1:A:291:GLU:N	2.33	0.62
1:A:998:LEU:HD12	1:A:998:LEU:H	1.65	0.62
7:G:108:VAL:HG22	7:G:159:ALA:HB3	1.81	0.62
7:G:6:ASP:HB3	7:G:73:LYS:HZ1	1.64	0.62
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.80	0.62
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.35	0.62
1:A:1279:ILE:HD11	1:A:1316:VAL:CG2	2.29	0.62
1:A:1402:PHE:O	1:A:1404:GLU:N	2.32	0.62
1:A:535:THR:HG21	1:A:617:VAL:H	1.63	0.62
11:K:91:CYS:O	11:K:94:ILE:HB	1.99	0.62
2:B:510:LYS:CG	2:B:512:ARG:H	2.11	0.62
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.80	0.62
1:A:1206:ASP:O	1:A:1207:LEU:HG	2.00	0.62
2:B:780:VAL:HG12	2:B:782:LEU:O	1.99	0.62
1:A:1029:ARG:HH11	1:A:1029:ARG:CG	2.09	0.62
2:B:1149:GLU:O	2:B:1151:LEU:N	2.32	0.62
8:H:23:VAL:HG13	8:H:42:ILE:O	2.00	0.62
8:H:102:TYR:N	8:H:102:TYR:HD2	1.96	0.62
2:B:510:LYS:HG2	2:B:512:ARG:CB	2.30	0.61
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.34	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:ILE:HG13	1:A:943:LEU:CD1	2.30	0.61
1:A:515:GLN:OE1	1:A:1071:SER:HA	1.99	0.61
11:K:12:LEU:HD21	11:K:18:LYS:HG2	1.80	0.61
1:A:605:MET:SD	1:A:621:THR:HG21	2.40	0.61
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.35	0.61
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.35	0.61
6:F:79:ARG:HG3	6:F:144:GLU:OE1	2.00	0.61
2:B:549:THR:HG22	2:B:550:ASP:N	2.12	0.61
1:A:1081:LEU:CD1	1:A:1098:VAL:HB	2.30	0.61
1:A:1164:PRO:HG2	1:A:1165:GLU:HG3	1.82	0.61
8:H:123:MET:HE3	8:H:142:LEU:CD2	2.30	0.61
4:D:170:THR:HG22	4:D:172:LEU:HG	1.82	0.61
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.64	0.61
3:C:107:SER:C	3:C:109:SER:H	2.04	0.61
2:B:880:THR:HG21	2:B:934:LYS:HE3	1.82	0.61
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	2.00	0.61
2:B:1033:LYS:HD2	2:B:1087:PHE:O	2.00	0.61
2:B:797:TYR:C	2:B:798:TYR:HD2	2.04	0.61
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.30	0.61
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.30	0.61
1:A:963:ILE:CD1	1:A:1049:ILE:HG13	2.30	0.61
1:A:708:MET:O	1:A:709:THR:O	2.17	0.61
2:B:37:PHE:CD1	2:B:41:LYS:HG3	2.35	0.61
6:F:97:ARG:NH2	6:F:108:PHE:CE1	2.68	0.61
1:A:50:ILE:C	1:A:52:GLY:H	2.03	0.61
3:C:67:LEU:HA	3:C:70:ILE:CD1	2.30	0.61
2:B:824:ILE:CG1	10:J:48:ARG:HH12	2.11	0.61
2:B:1183:LYS:CE	2:B:1183:LYS:N	2.62	0.61
12:L:31:CYS:HB3	12:L:34:CYS:C	2.21	0.61
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.36	0.61
2:B:129:PHE:HE2	2:B:166:PHE:HD1	1.49	0.61
2:B:1051:THR:HB	2:B:1054:GLY:H	1.64	0.61
2:B:292:ILE:HD11	2:B:327:ARG:H	1.64	0.61
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.81	0.61
1:A:528:LEU:O	1:A:531:ILE:HG22	2.01	0.61
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.63	0.61
1:A:133:LYS:C	1:A:135:PHE:H	2.02	0.61
4:D:40:HIS:CE1	4:D:41:GLN:HG3	2.35	0.61
7:G:114:LEU:HD23	7:G:161:GLY:O	2.00	0.61
1:A:442:VAL:O	1:A:457:ALA:HA	2.00	0.61
2:B:487:THR:HG22	2:B:488:TYR:N	2.15	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.00	0.61
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.65	0.61
2:B:975:GLN:NE2	2:B:1100:ASP:OD2	2.30	0.61
8:H:59:ILE:HG22	8:H:60:ALA:H	1.64	0.61
2:B:705:MET:N	2:B:710:LEU:HD12	2.16	0.61
8:H:81:PRO:CB	8:H:82:PRO:CD	2.77	0.61
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.31	0.61
1:A:852:TYR:CE1	6:F:136:ARG:HG2	2.36	0.61
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.83	0.61
1:A:254:GLU:CB	2:B:935:ARG:HH22	2.14	0.61
1:A:556:TRP:C	1:A:558:GLY:H	2.05	0.61
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.35	0.61
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.31	0.61
1:A:694:THR:O	1:A:698:GLN:HG3	1.99	0.61
3:C:58:LEU:CD2	3:C:58:LEU:H	2.14	0.61
1:A:857:ARG:HD3	1:A:861:GLY:O	2.00	0.61
1:A:761:MET:HA	1:A:804:TYR:HB2	1.82	0.61
4:D:51:ASN:O	4:D:54:GLU:HB3	2.01	0.61
2:B:545:ILE:HG22	2:B:546:SER:O	2.01	0.61
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.33	0.60
1:A:866:PHE:C	1:A:867:ILE:HD12	2.21	0.60
2:B:952:VAL:HG12	2:B:953:LEU:H	1.65	0.60
1:A:134:ARG:O	1:A:138:ILE:HG13	2.01	0.60
2:B:69:LEU:HD22	2:B:429:PHE:CE1	2.35	0.60
5:E:86:PRO:O	5:E:114:ASN:HB2	1.99	0.60
1:A:869:GLY:O	5:E:204:THR:HG21	2.01	0.60
3:C:169:LYS:NZ	12:L:69:ALA:HB3	2.16	0.60
1:A:332:LYS:H	1:A:337:ARG:HB3	1.66	0.60
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.30	0.60
4:D:210:ILE:O	4:D:214:LEU:HG	2.01	0.60
1:A:804:TYR:OH	2:B:763:GLN:HA	2.00	0.60
1:A:1001:ARG:O	1:A:1002:GLY:O	2.18	0.60
10:J:57:ILE:HG23	10:J:58:GLU:H	1.66	0.60
10:J:57:ILE:HG23	10:J:58:GLU:N	2.16	0.60
3:C:248:ILE:HD13	11:K:101:LEU:HD22	1.82	0.60
1:A:44:THR:O	1:A:45:GLN:HB2	1.99	0.60
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.32	0.60
3:C:212:PRO:CB	3:C:213:PRO:HD2	2.31	0.60
5:E:157:SER:C	5:E:159:ASP:H	2.04	0.60
5:E:60:PHE:CE2	5:E:80:VAL:HB	2.36	0.60
2:B:563:MET:HE1	2:B:580:VAL:HB	1.83	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:807:ARG:HH11	2:B:807:ARG:HB3	1.66	0.60
1:A:91:PHE:HD2	1:A:96:ILE:HG12	1.66	0.60
2:B:310:MET:O	2:B:313:MET:HB2	2.02	0.60
9:I:106:CYS:O	9:I:107:SER:HB2	1.99	0.60
1:A:821:ARG:O	1:A:825:ILE:HG13	2.01	0.60
2:B:113:TYR:HB3	2:B:114:PRO:CD	2.29	0.60
1:A:902:LEU:O	1:A:903:ASN:HB2	2.01	0.60
1:A:901:LEU:N	1:A:926:GLN:HE21	1.98	0.60
2:B:1072:MET:HE2	2:B:1085:ILE:HB	1.84	0.60
1:A:489:LEU:HD12	1:A:489:LEU:C	2.21	0.60
8:H:40:LEU:CD1	8:H:123:MET:HB2	2.27	0.60
8:H:91:ASP:C	8:H:93:TYR:H	2.05	0.60
1:A:606:LEU:HB2	1:A:614:PHE:CE2	2.37	0.60
1:A:412:ARG:NH2	2:B:1108:ARG:NH1	2.47	0.60
9:I:58:VAL:HA	9:I:62:ILE:CD1	2.32	0.60
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.30	0.60
7:G:145:VAL:CG1	7:G:146:LYS:N	2.64	0.60
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.84	0.60
2:B:750:GLY:O	2:B:751:VAL:C	2.39	0.60
2:B:216:GLU:HA	2:B:406:LEU:HD23	1.84	0.60
1:A:144:THR:O	1:A:146:MET:HG3	2.01	0.60
3:C:46:ILE:HD13	3:C:157:CYS:SG	2.41	0.60
1:A:225:ASN:ND2	1:A:227:VAL:H	1.98	0.60
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.32	0.60
1:A:47:ARG:HH22	1:A:254:GLU:HA	1.65	0.60
1:A:469:ARG:HG2	1:A:469:ARG:HH11	1.67	0.60
3:C:142:VAL:H	10:J:16:ASP:HB3	1.66	0.60
8:H:113:ALA:HB2	8:H:126:GLU:HG3	1.84	0.60
2:B:605:ARG:CZ	2:B:639:ILE:HD13	2.31	0.60
7:G:9:LEU:HD12	7:G:10:ASN:N	2.16	0.60
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.37	0.60
4:D:19:GLU:O	4:D:21:GLU:N	2.35	0.60
1:A:49:LYS:HE2	1:A:61:ILE:CD1	2.29	0.60
2:B:1166:CYS:HB2	2:B:1168:LEU:HD12	1.84	0.60
1:A:475:THR:HG23	1:A:476:SER:N	2.17	0.60
12:L:31:CYS:HB3	12:L:35:SER:HA	1.84	0.60
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.84	0.60
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.37	0.60
1:A:629:LEU:O	1:A:633:VAL:HG23	2.01	0.60
1:A:863:VAL:HG12	1:A:864:ILE:N	2.17	0.60
1:A:863:VAL:O	1:A:864:ILE:HG12	2.02	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.83	0.60
1:A:40:THR:HG23	1:A:54:ASN:HD21	1.67	0.60
2:B:841:MET:O	2:B:993:THR:HG22	2.02	0.60
8:H:56:THR:O	8:H:144:ILE:HA	2.01	0.60
2:B:954:VAL:O	12:L:55:ILE:O	2.20	0.60
1:A:391:LEU:O	1:A:394:ASN:N	2.35	0.60
5:E:23:VAL:HG13	5:E:78:LEU:HD13	1.84	0.60
5:E:46:TYR:CE2	5:E:58:MET:HA	2.37	0.60
9:I:8:ARG:O	9:I:10:CYS:N	2.33	0.60
6:F:72:LYS:O	6:F:73:ALA:HB3	2.02	0.60
1:A:1116:LEU:HB3	1:A:1311:VAL:HG22	1.83	0.59
1:A:786:HIS:CD2	1:A:786:HIS:N	2.69	0.59
2:B:1159:ARG:HE	2:B:1193:GLN:NE2	2.00	0.59
1:A:343:LYS:HE2	2:B:1156:ASP:OD2	2.02	0.59
1:A:1161:THR:C	1:A:1163:ILE:H	2.04	0.59
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.66	0.59
8:H:56:THR:HB	8:H:145:ARG:HG2	1.84	0.59
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.83	0.59
9:I:55:THR:HG23	9:I:100:PHE:CD2	2.33	0.59
7:G:146:LYS:HB2	7:G:168:LEU:HD11	1.82	0.59
1:A:782:ARG:NH2	2:B:699:GLU:O	2.34	0.59
2:B:533:CYS:O	2:B:535:LEU:N	2.34	0.59
1:A:1397:LEU:HA	1:A:1400:CYS:CB	2.32	0.59
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.31	0.59
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.66	0.59
5:E:198:ILE:CD1	5:E:212:ARG:HH11	2.14	0.59
1:A:1423:GLY:O	1:A:1424:VAL:C	2.40	0.59
2:B:1160:VAL:CG1	2:B:1161:HIS:N	2.66	0.59
1:A:896:ARG:HB3	1:A:897:TYR:CD1	2.37	0.59
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.31	0.59
1:A:820:GLY:C	1:A:822:GLU:H	2.05	0.59
4:D:134:THR:HG22	4:D:135:GLY:N	2.16	0.59
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.17	0.59
8:H:42:ILE:HG23	8:H:95:TYR:HE1	1.67	0.59
1:A:1237:ILE:CG2	1:A:1238:ILE:H	2.15	0.59
2:B:899:ILE:HG22	2:B:900:ALA:N	2.17	0.59
2:B:496:ARG:NH1	2:B:539:LEU:HB2	2.16	0.59
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.83	0.59
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.32	0.59
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.36	0.59
1:A:567:LYS:HD3	8:H:95:TYR:CD2	2.37	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:855:PHE:CD1	2:B:855:PHE:C	2.75	0.59
3:C:58:LEU:N	3:C:58:LEU:CD2	2.65	0.59
5:E:55:ARG:C	5:E:57:MET:H	2.04	0.59
1:A:687:LYS:O	1:A:690:VAL:HB	2.03	0.59
1:A:1372:VAL:CG1	1:A:1373:ASP:N	2.65	0.59
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.37	0.59
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.85	0.59
4:D:48:ILE:HG21	7:G:4:ILE:HB	1.85	0.59
1:A:1261:LYS:O	1:A:1264:GLU:HB3	2.01	0.59
1:A:1334:ASP:C	1:A:1336:MET:N	2.55	0.59
1:A:25:GLU:CD	1:A:25:GLU:H	2.06	0.59
2:B:815:ARG:HD3	2:B:1041:GLU:OE2	2.03	0.59
1:A:848:ILE:HB	1:A:1065:GLY:HA3	1.85	0.59
2:B:879:ARG:O	2:B:880:THR:HB	2.02	0.59
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.03	0.59
1:A:1127:ASP:O	1:A:1130:GLN:HB3	2.03	0.59
8:H:84:ALA:C	8:H:86:ASP:H	2.06	0.59
1:A:590:ARG:HH21	1:A:620:LYS:CB	2.08	0.59
1:A:446:ARG:HB2	1:A:487:MET:SD	2.43	0.59
2:B:992:ILE:HD13	2:B:994:TYR:CE1	2.38	0.59
10:J:14:VAL:HG13	10:J:50:ILE:HD11	1.85	0.59
1:A:1422:ARG:HH22	2:B:1224:PHE:C	2.06	0.59
1:A:321:PRO:O	1:A:322:VAL:HG23	2.03	0.59
5:E:164:LEU:HD22	5:E:211:TYR:CD2	2.37	0.59
2:B:483:LEU:HD12	2:B:484:ASN:H	1.67	0.59
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.03	0.59
3:C:17:ASN:OD1	3:C:233:GLU:HG3	2.02	0.59
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.33	0.59
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.32	0.59
1:A:1342:GLU:CG	5:E:198:ILE:HD13	2.33	0.59
8:H:40:LEU:HD12	8:H:122:LEU:O	2.03	0.59
9:I:6:PHE:HA	9:I:14:LEU:HG	1.85	0.59
4:D:35:LEU:H	4:D:35:LEU:CD1	2.14	0.59
11:K:31:VAL:HG12	11:K:32:VAL:N	2.18	0.59
1:A:1151:GLU:HB3	1:A:1153:TYR:HE1	1.68	0.59
1:A:1095:THR:OG1	1:A:1112:LYS:HB2	2.03	0.59
2:B:461:LEU:HD12	2:B:461:LEU:H	1.68	0.59
2:B:508:LEU:HB2	2:B:510:LYS:HB3	1.83	0.59
1:A:42:ASP:C	1:A:44:THR:H	2.06	0.59
1:A:72:GLU:O	1:A:73:GLY:O	2.20	0.59
1:A:1104:ILE:O	1:A:1106:ASN:N	2.35	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:33:PHE:CE2	7:G:80:LYS:NZ	2.70	0.59
2:B:1106:ARG:HG3	2:B:1107:ALA:H	1.65	0.59
2:B:578:THR:HG23	2:B:622:LYS:HA	1.84	0.59
1:A:697:ALA:HB2	1:A:702:LEU:HD12	1.85	0.59
9:I:88:SER:C	9:I:90:GLN:H	2.07	0.59
1:A:963:ILE:HD13	1:A:1049:ILE:CG1	2.32	0.58
1:A:535:THR:CG2	1:A:616:VAL:HA	2.33	0.58
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.31	0.58
2:B:854:LEU:HB3	2:B:856:PHE:CE1	2.37	0.58
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.84	0.58
4:D:176:GLU:OE2	4:D:198:LEU:HD23	2.02	0.58
2:B:785:TYR:HE2	10:J:60:PHE:CE1	2.22	0.58
1:A:808:LEU:HD21	1:A:816:HIS:HD2	1.68	0.58
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.68	0.58
3:C:59:ALA:O	3:C:62:PHE:HB3	2.03	0.58
2:B:798:TYR:CE1	10:J:4:PRO:HB3	2.38	0.58
2:B:603:LEU:HB3	2:B:609:ILE:HD11	1.84	0.58
2:B:46:GLN:HG3	2:B:47:GLN:H	1.68	0.58
2:B:789:MET:HE2	2:B:965:LYS:HB3	1.85	0.58
1:A:984:LYS:O	1:A:988:LEU:HB2	2.03	0.58
3:C:35:ARG:HH11	11:K:41:THR:N	2.01	0.58
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.02	0.58
1:A:667:GLY:HA3	3:C:192:TRP:CH2	2.38	0.58
1:A:57:ARG:O	1:A:58:LEU:O	2.21	0.58
3:C:174:ALA:O	3:C:175:ALA:CB	2.51	0.58
10:J:41:LEU:CD1	10:J:50:ILE:HG13	2.31	0.58
10:J:8:PHE:HD1	10:J:49:MET:HE1	1.68	0.58
1:A:598:LEU:HD22	8:H:25:ARG:NH1	2.18	0.58
2:B:640:VAL:O	2:B:641:GLU:C	2.41	0.58
1:A:305:ASP:CG	1:A:326:ARG:HD2	2.24	0.58
2:B:240:ILE:O	2:B:240:ILE:HG23	2.02	0.58
5:E:114:ASN:O	5:E:115:ASN:HB3	2.03	0.58
2:B:404:LYS:HE2	2:B:404:LYS:HA	1.85	0.58
9:I:2:THR:O	9:I:3:THR:C	2.41	0.58
2:B:296:GLU:O	2:B:299:GLU:HB2	2.04	0.58
1:A:1441:PHE:HZ	6:F:89:GLU:HA	1.67	0.58
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.86	0.58
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.84	0.58
2:B:782:LEU:HD12	2:B:788:ARG:HH11	1.67	0.58
2:B:562:GLY:HA3	2:B:590:HIS:HE1	1.65	0.58
3:C:66:ARG:NH2	10:J:5:VAL:HG23	2.19	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.14	0.58
7:G:1:MET:SD	7:G:1:MET:O	2.61	0.58
8:H:24:CYS:SG	8:H:44:VAL:HG21	2.43	0.58
1:A:847:ASP:HB2	1:A:859:SER:H	1.68	0.58
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.77	0.58
2:B:563:MET:HE3	2:B:580:VAL:HB	1.84	0.58
2:B:325:GLN:HG2	9:I:31:THR:HG23	1.86	0.58
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.84	0.58
1:A:567:LYS:CB	1:A:568:PRO:CD	2.81	0.58
1:A:1134:ILE:O	1:A:1138:ILE:HG13	2.02	0.58
9:I:59:VAL:HG12	9:I:59:VAL:O	2.04	0.58
9:I:58:VAL:HG13	9:I:62:ILE:HG13	1.84	0.58
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.84	0.58
5:E:157:SER:O	5:E:159:ASP:N	2.37	0.58
5:E:162:ARG:HG2	5:E:162:ARG:HH11	1.69	0.58
1:A:1222:ASN:O	1:A:1223:ASP:HB3	2.04	0.58
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.85	0.58
2:B:830:TYR:HE2	2:B:1000:PRO:HD3	1.66	0.58
1:A:1316:VAL:O	1:A:1322:ILE:HD13	2.04	0.58
1:A:895:LYS:HG2	1:A:895:LYS:O	2.03	0.58
1:A:827:THR:O	1:A:831:THR:HB	2.04	0.58
3:C:167:HIS:CE1	12:L:70:ARG:HA	2.39	0.58
1:A:834:THR:HG23	1:A:1077:THR:HA	1.85	0.58
4:D:33:PHE:CE1	7:G:80:LYS:HE3	2.39	0.58
1:A:1090:ALA:CA	1:A:1093:LYS:HE3	2.34	0.58
8:H:100:THR:HG22	8:H:101:ALA:N	2.19	0.58
2:B:903:VAL:HG12	2:B:904:ARG:N	2.17	0.58
7:G:119:LEU:HD13	7:G:132:SER:HB2	1.86	0.58
1:A:1289:ARG:NH1	1:A:1326:ARG:NH1	2.52	0.58
5:E:153:HIS:O	5:E:154:ILE:CG1	2.49	0.58
2:B:807:ARG:NH1	2:B:807:ARG:HB3	2.19	0.58
1:A:642:CYS:O	1:A:645:LEU:HB3	2.04	0.58
1:A:361:LEU:HG	1:A:507:VAL:HG11	1.85	0.58
2:B:773:MET:O	2:B:775:LYS:N	2.37	0.58
2:B:1147:LEU:HD23	2:B:1147:LEU:C	2.24	0.58
10:J:19:GLU:O	10:J:23:ASN:HB2	2.03	0.58
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.18	0.58
1:A:785:PRO:HG2	1:A:786:HIS:HD2	1.68	0.58
2:B:1085:ILE:HG22	2:B:1086:PHE:N	2.19	0.58
2:B:762:ASN:HD21	2:B:1024:ALA:CB	2.17	0.58
5:E:144:ILE:O	5:E:146:HIS:N	2.36	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:ARG:HH22	1:A:745:GLN:HG2	1.69	0.58
1:A:798:GLY:HA2	1:A:815:PHE:CD1	2.39	0.57
2:B:1002:THR:O	2:B:1005:GLY:N	2.32	0.57
2:B:620:ARG:NH2	9:I:89:GLN:NE2	2.52	0.57
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.33	0.57
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.86	0.57
1:A:265:LYS:O	1:A:266:LEU:C	2.41	0.57
1:A:1116:LEU:HB3	1:A:1311:VAL:CG2	2.33	0.57
1:A:775:ILE:HG13	1:A:798:GLY:HA3	1.86	0.57
3:C:163:ILE:O	3:C:166:GLU:N	2.36	0.57
3:C:143:LEU:C	3:C:143:LEU:HD12	2.25	0.57
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.34	0.57
9:I:101:PHE:O	9:I:102:VAL:HG23	2.03	0.57
1:A:528:LEU:HD23	1:A:751:SER:HA	1.85	0.57
11:K:47:ARG:HD3	11:K:59:ALA:O	2.04	0.57
1:A:115:LEU:HD12	1:A:142:CYS:SG	2.44	0.57
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.03	0.57
7:G:117:GLN:C	7:G:119:LEU:H	2.07	0.57
3:C:124:LEU:O	3:C:127:ARG:HG2	2.04	0.57
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.35	0.57
1:A:808:LEU:N	1:A:808:LEU:HD12	2.20	0.57
2:B:1159:ARG:HE	2:B:1193:GLN:HE21	1.50	0.57
2:B:918:ILE:CD1	2:B:935:ARG:HD2	2.27	0.57
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.86	0.57
12:L:62:LYS:H	12:L:62:LYS:HD2	1.70	0.57
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.39	0.57
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.89	0.57
1:A:1164:PRO:O	1:A:1166:ASP:N	2.36	0.57
2:B:1186:ASP:OD1	2:B:1186:ASP:O	2.22	0.57
7:G:117:GLN:O	7:G:119:LEU:N	2.37	0.57
2:B:286:PHE:HE2	2:B:375:ALA:HB1	1.70	0.57
1:A:864:ILE:O	1:A:865:GLN:CG	2.50	0.57
2:B:1065:GLN:HG3	2:B:1068:GLY:H	1.69	0.57
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.86	0.57
9:I:111:THR:CG2	9:I:112:SER:H	2.13	0.57
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.29	0.57
2:B:708:GLU:O	2:B:710:LEU:N	2.37	0.57
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.87	0.57
2:B:694:ASP:O	2:B:698:GLU:HB2	2.05	0.57
2:B:278:GLN:HG2	2:B:279:ASP:H	1.69	0.57
2:B:558:LEU:O	2:B:560:GLU:N	2.37	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:82:TYR:CE1	3:C:161:LYS:HD3	2.39	0.57
1:A:666:ILE:H	2:B:1026:LEU:HD22	1.70	0.57
1:A:1030:ARG:HG3	1:A:1034:GLU:OE2	2.03	0.57
2:B:235:SER:HB3	2:B:258:LEU:HG	1.86	0.57
10:J:8:PHE:CD1	10:J:49:MET:SD	2.98	0.57
2:B:325:GLN:HG2	9:I:31:THR:CG2	2.34	0.57
3:C:196:ASP:OD1	3:C:198:ALA:HB3	2.05	0.57
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.05	0.57
1:A:903:ASN:ND2	1:A:905:ASP:H	2.02	0.57
2:B:766:ARG:NH2	2:B:1020:ARG:CG	2.67	0.57
2:B:522:VAL:HG12	2:B:523:CYS:N	2.19	0.57
1:A:42:ASP:HB3	1:A:45:GLN:H	1.70	0.57
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.05	0.57
1:A:560:ILE:HD12	8:H:79:TRP:O	2.05	0.57
5:E:13:TRP:O	5:E:16:PHE:HB3	2.03	0.57
1:A:996:ASN:O	1:A:998:LEU:HD12	2.04	0.57
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.19	0.57
1:A:1044:TRP:O	1:A:1047:SER:N	2.38	0.57
3:C:82:TYR:O	3:C:84:ARG:N	2.38	0.57
2:B:1182:CYS:C	2:B:1183:LYS:HE3	2.25	0.57
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.86	0.57
3:C:90:ASP:O	3:C:90:ASP:CG	2.43	0.57
8:H:83:GLN:C	8:H:85:GLY:H	2.08	0.57
4:D:51:ASN:ND2	4:D:54:GLU:OE2	2.38	0.57
2:B:57:TYR:CD1	2:B:57:TYR:N	2.72	0.57
9:I:64:SER:O	9:I:66:PRO:HD3	2.05	0.57
2:B:1145:SER:C	2:B:1147:LEU:N	2.55	0.57
3:C:114:TYR:HB3	3:C:140:ASN:O	2.04	0.57
1:A:168:GLY:O	1:A:169:ASN:C	2.43	0.57
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.04	0.57
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.05	0.57
2:B:557:PHE:C	2:B:557:PHE:CD2	2.77	0.57
1:A:18:GLN:HG3	1:A:228:PHE:CE1	2.40	0.57
7:G:13:LEU:HD23	7:G:14:HIS:H	1.70	0.57
1:A:503:GLN:C	1:A:504:LEU:HD12	2.25	0.57
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.40	0.57
5:E:84:ASP:O	5:E:86:PRO:HD3	2.05	0.57
3:C:27:LEU:HD12	3:C:228:PHE:HE2	1.70	0.57
1:A:1353:TYR:CD2	1:A:1353:TYR:C	2.77	0.57
5:E:204:THR:CG2	5:E:205:SER:N	2.67	0.56
2:B:519:TRP:C	2:B:519:TRP:CD1	2.77	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:133:ILE:CD1	3:C:237:SER:CA	2.82	0.56
3:C:242:GLN:O	3:C:246:ARG:N	2.37	0.56
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.26	0.56
1:A:1341:ILE:HD12	1:A:1379:GLY:O	2.05	0.56
6:F:75:PRO:O	6:F:77:ASP:O	2.23	0.56
1:A:744:LYS:HE2	1:A:748:MET:HE2	1.87	0.56
1:A:1453:TYR:CZ	6:F:129:LYS:HA	2.40	0.56
3:C:181:ASP:OD1	3:C:186:LEU:HD13	2.05	0.56
1:A:899:VAL:CG2	1:A:908:LEU:HD21	2.35	0.56
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.34	0.56
11:K:67:PHE:C	11:K:68:PHE:CD2	2.78	0.56
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.35	0.56
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.04	0.56
7:G:80:LYS:CE	7:G:82:PHE:HZ	2.17	0.56
1:A:289:ILE:C	1:A:291:GLU:N	2.58	0.56
6:F:111:LEU:N	6:F:111:LEU:HD12	2.18	0.56
2:B:1177:HIS:C	2:B:1179:GLN:H	2.08	0.56
2:B:394:ASP:OD1	9:I:91:ARG:HB3	2.04	0.56
12:L:43:THR:O	12:L:43:THR:HG22	2.04	0.56
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.70	0.56
2:B:1000:PRO:O	2:B:1007:VAL:HG23	2.05	0.56
1:A:668:ASP:CB	1:A:743:VAL:HG23	2.36	0.56
9:I:58:VAL:HA	9:I:62:ILE:HD11	1.87	0.56
1:A:98:LYS:O	1:A:102:VAL:HG23	2.05	0.56
1:A:306:ASN:ND2	1:A:322:VAL:HB	2.21	0.56
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.25	0.56
2:B:247:GLY:H	2:B:418:LYS:HZ3	1.53	0.56
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.40	0.56
7:G:109:PHE:CD1	7:G:110:VAL:N	2.71	0.56
2:B:570:VAL:HG23	2:B:573:GLN:HB3	1.85	0.56
1:A:730:GLY:C	1:A:732:LEU:N	2.59	0.56
1:A:47:ARG:NH1	1:A:254:GLU:HB3	2.06	0.56
1:A:78:PRO:CB	2:B:1201:LYS:HE3	2.36	0.56
1:A:896:ARG:HB3	1:A:897:TYR:HD1	1.70	0.56
1:A:1080:THR:HG22	1:A:1081:LEU:N	2.20	0.56
7:G:1:MET:CE	7:G:80:LYS:H	2.18	0.56
3:C:104:PHE:CD2	3:C:105:GLY:N	2.71	0.56
1:A:730:GLY:O	1:A:732:LEU:N	2.38	0.56
1:A:986:ILE:HD11	1:A:1032:LEU:HD11	1.87	0.56
1:A:403:LYS:O	1:A:404:TYR:CG	2.58	0.56
1:A:861:GLY:HA3	5:E:174:GLN:NE2	2.21	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:LEU:O	1:A:930:ASP:N	2.39	0.56
2:B:192:LEU:O	2:B:193:LYS:HB2	2.04	0.56
5:E:176:PRO:O	5:E:212:ARG:HA	2.06	0.56
7:G:1:MET:CE	7:G:1:MET:O	2.54	0.56
2:B:582:VAL:HA	2:B:626:ILE:O	2.06	0.56
1:A:306:ASN:HB2	1:A:324:SER:HB3	1.87	0.56
12:L:49:LYS:O	12:L:50:ASP:HB2	2.05	0.56
1:A:34:LYS:CB	1:A:36:ARG:HH21	2.18	0.56
2:B:533:CYS:C	2:B:535:LEU:H	2.09	0.56
10:J:21:TYR:HA	10:J:39:LEU:HD11	1.87	0.56
2:B:1017:ILE:HG22	2:B:1018:PRO:N	2.21	0.56
3:C:69:LEU:H	3:C:69:LEU:HD12	1.69	0.56
2:B:1172:ILE:O	2:B:1172:ILE:HG22	2.05	0.56
1:A:353:ILE:HG21	1:A:487:MET:CG	2.21	0.56
1:A:823:GLY:C	1:A:825:ILE:H	2.08	0.56
2:B:999:MET:HB3	2:B:1007:VAL:HG21	1.88	0.56
2:B:798:TYR:HE1	10:J:4:PRO:HB3	1.71	0.56
2:B:996:ARG:NH2	3:C:175:ALA:HA	2.20	0.56
11:K:53:ASP:HB3	11:K:56:VAL:HG23	1.86	0.56
2:B:860:MET:HB2	2:B:965:LYS:HG2	1.87	0.56
1:A:874:ASP:CA	1:A:1058:VAL:HG23	2.36	0.56
1:A:84:ILE:HG23	1:A:239:LEU:HB3	1.86	0.56
5:E:19:VAL:O	5:E:23:VAL:HG23	2.06	0.56
5:E:35:VAL:C	5:E:37:LEU:H	2.08	0.56
6:F:84:TYR:N	6:F:84:TYR:CD1	2.73	0.56
1:A:1335:ILE:O	1:A:1335:ILE:HG22	2.05	0.56
2:B:242:SER:OG	2:B:252:SER:O	2.23	0.56
2:B:377:PHE:O	2:B:380:TYR:N	2.39	0.56
1:A:1373:ASP:O	1:A:1376:THR:HG23	2.06	0.56
1:A:965:GLN:O	1:A:968:GLN:HB2	2.06	0.56
1:A:92:HIS:O	1:A:95:PHE:N	2.37	0.56
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.88	0.56
3:C:58:LEU:HD23	3:C:58:LEU:H	1.71	0.56
2:B:498:THR:O	2:B:536:VAL:HG13	2.05	0.56
8:H:7:ASP:O	8:H:8:ASP:HB2	2.06	0.56
1:A:130:ASP:O	1:A:132:LYS:N	2.39	0.56
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.41	0.56
1:A:936:LEU:N	1:A:936:LEU:HD23	2.21	0.56
2:B:603:LEU:HB3	2:B:609:ILE:CD1	2.35	0.56
6:F:77:ASP:C	6:F:79:ARG:H	2.07	0.56
1:A:1203:ASN:O	1:A:1204:ASP:C	2.44	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:13:VAL:HG12	10:J:14:VAL:N	2.21	0.56
1:A:1081:LEU:HD21	1:A:1098:VAL:CG2	2.35	0.56
1:A:567:LYS:CB	8:H:95:TYR:HA	2.36	0.56
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.41	0.56
3:C:89:GLU:O	3:C:90:ASP:HB3	2.05	0.56
2:B:60:GLN:O	2:B:63:ILE:HG22	2.06	0.56
10:J:23:ASN:C	10:J:25:LEU:H	2.09	0.56
1:A:597:LEU:HD12	1:A:597:LEU:N	2.21	0.56
2:B:555:ILE:HG22	2:B:556:THR:N	2.21	0.56
1:A:71:GLN:O	1:A:73:GLY:N	2.39	0.56
1:A:1421:CYS:HA	1:A:1426:GLU:HB3	1.86	0.56
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.35	0.56
1:A:1051:ALA:O	1:A:1053:PHE:N	2.39	0.56
5:E:47:CYS:HA	5:E:52:ARG:O	2.06	0.56
1:A:491:VAL:HG12	1:A:492:PRO:O	2.04	0.56
2:B:945:GLU:O	2:B:946:ASN:HB3	2.07	0.56
1:A:469:ARG:NH2	2:B:991:GLY:O	2.37	0.55
2:B:805:THR:HA	2:B:809:MET:HE1	1.88	0.55
3:C:31:ASN:O	3:C:32:SER:C	2.45	0.55
1:A:390:GLN:HE21	1:A:394:ASN:HD21	1.53	0.55
2:B:254:LEU:HD23	2:B:381:MET:CE	2.36	0.55
2:B:528:PRO:HG2	2:B:533:CYS:HA	1.87	0.55
2:B:25:ILE:HG23	2:B:29:ASP:HB3	1.88	0.55
1:A:492:PRO:O	1:A:493:GLN:NE2	2.38	0.55
1:A:455:MET:HE3	2:B:1134:GLU:HG3	1.89	0.55
2:B:784:ASN:O	2:B:788:ARG:HG3	2.06	0.55
1:A:1313:LEU:O	1:A:1315:GLU:N	2.39	0.55
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.40	0.55
10:J:64:ASN:HB3	10:J:65:PRO:HD2	1.84	0.55
1:A:49:LYS:HZ1	1:A:61:ILE:N	2.04	0.55
1:A:49:LYS:HZ2	1:A:60:SER:HA	1.70	0.55
12:L:30:ILE:O	12:L:56:LEU:HA	2.06	0.55
2:B:521:LEU:HB3	2:B:633:VAL:CG1	2.36	0.55
1:A:820:GLY:C	1:A:822:GLU:N	2.60	0.55
5:E:178:ILE:HG22	5:E:213:ILE:O	2.06	0.55
2:B:857:ARG:HH21	2:B:942:ARG:NH1	2.04	0.55
5:E:211:TYR:CD1	5:E:211:TYR:N	2.74	0.55
7:G:114:LEU:HG	7:G:162:SER:CB	2.36	0.55
9:I:90:GLN:NE2	9:I:92:ARG:HD2	2.21	0.55
3:C:9:LYS:O	3:C:10:ILE:C	2.44	0.55
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.42	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.07	0.55
8:H:5:LEU:HB2	8:H:60:ALA:H	1.71	0.55
12:L:31:CYS:HB3	12:L:35:SER:N	2.21	0.55
1:A:495:GLU:O	1:A:498:ARG:HG3	2.04	0.55
2:B:1189:ILE:HG22	2:B:1190:ASP:N	2.22	0.55
1:A:715:GLU:O	1:A:717:ASN:N	2.39	0.55
11:K:21:ILE:HG23	11:K:31:VAL:HG11	1.88	0.55
1:A:730:GLY:C	1:A:732:LEU:H	2.09	0.55
1:A:685:GLU:HG3	1:A:686:ALA:N	2.20	0.55
3:C:183:TRP:O	3:C:185:LYS:HG3	2.06	0.55
2:B:511:PRO:C	2:B:513:GLN:H	2.08	0.55
1:A:818:MET:HA	2:B:514:LEU:HB3	1.87	0.55
1:A:666:ILE:CD1	1:A:667:GLY:N	2.66	0.55
1:A:1438:THR:HB	2:B:1144:ALA:CB	2.36	0.55
2:B:37:PHE:CD2	2:B:542:MET:SD	2.99	0.55
2:B:744:HIS:CG	2:B:745:PRO:HD2	2.41	0.55
1:A:414:ASP:OD1	1:A:416:ARG:CG	2.54	0.55
4:D:27:LEU:HD11	4:D:197:SER:HB2	1.89	0.55
3:C:82:TYR:CD1	3:C:161:LYS:HD3	2.41	0.55
1:A:18:GLN:HG3	1:A:228:PHE:HE1	1.72	0.55
10:J:57:ILE:O	10:J:60:PHE:N	2.39	0.55
3:C:250:THR:O	3:C:254:LYS:HG3	2.07	0.55
1:A:69:THR:C	1:A:71:GLN:N	2.57	0.55
3:C:70:ILE:HD13	3:C:144:ILE:HD11	1.88	0.55
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.72	0.55
2:B:502:ILE:CG2	2:B:502:ILE:O	2.52	0.55
1:A:679:ILE:O	1:A:683:ILE:HG13	2.07	0.55
3:C:123:ASN:ND2	3:C:125:MET:SD	2.79	0.55
4:D:39:ASN:ND2	4:D:41:GLN:HB2	2.21	0.55
10:J:1:MET:H2	10:J:56:LEU:N	2.03	0.55
1:A:1394:THR:O	1:A:1399:ARG:NE	2.38	0.55
3:C:90:ASP:O	3:C:91:HIS:CG	2.60	0.55
1:A:744:LYS:HG2	1:A:748:MET:HE3	1.88	0.55
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.42	0.55
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.88	0.55
5:E:56:LYS:HE3	5:E:84:ASP:HB2	1.87	0.55
11:K:58:PHE:HB3	11:K:76:GLN:HE21	1.72	0.55
2:B:658:ILE:O	2:B:661:LEU:HB2	2.07	0.55
2:B:970:THR:HG22	2:B:971:THR:N	2.22	0.55
1:A:1265:ASN:C	1:A:1267:MET:H	2.09	0.55
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.06	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:GLY:O	1:A:605:MET:HB2	2.07	0.55
7:G:18:PHE:HZ	7:G:68:ALA:HB2	1.71	0.55
1:A:69:THR:C	1:A:71:GLN:H	2.10	0.55
1:A:1102:LYS:HG2	1:A:1106:ASN:ND2	2.22	0.55
1:A:1127:ASP:HB3	1:A:1130:GLN:HB2	1.88	0.55
1:A:335:ARG:HH11	2:B:1206:GLU:CD	2.10	0.55
8:H:127:GLY:HA3	8:H:130:ARG:NH2	2.22	0.55
7:G:146:LYS:NZ	7:G:165:GLU:OE2	2.38	0.55
1:A:1397:LEU:O	1:A:1400:CYS:HB3	2.06	0.55
1:A:1265:ASN:C	1:A:1267:MET:N	2.60	0.55
8:H:14:GLU:HG2	8:H:15:VAL:N	2.22	0.55
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.70	0.55
1:A:853:ASP:CG	1:A:855:THR:HB	2.26	0.55
3:C:166:GLU:O	3:C:167:HIS:HB2	2.07	0.55
2:B:789:MET:HE2	2:B:965:LYS:O	2.07	0.55
2:B:431:TYR:CE2	2:B:447:ALA:HB2	2.42	0.55
9:I:84:VAL:O	9:I:84:VAL:HG22	2.07	0.55
1:A:848:ILE:HB	1:A:1065:GLY:CA	2.37	0.55
10:J:64:ASN:CB	10:J:65:PRO:CD	2.74	0.55
1:A:356:ASP:HB3	1:A:359:LEU:HG	1.88	0.55
2:B:597:MET:SD	2:B:624:LEU:HD11	2.47	0.55
2:B:363:HIS:CD2	2:B:364:ILE:HG13	2.42	0.55
1:A:15:LYS:HG3	2:B:1218:THR:O	2.06	0.55
1:A:1334:ASP:O	1:A:1337:GLU:N	2.40	0.55
6:F:100:GLN:O	6:F:103:MET:HB2	2.07	0.55
2:B:546:SER:HG	2:B:631:GLY:H	1.53	0.55
1:A:877:HIS:CD2	1:A:1056:SER:HA	2.42	0.55
7:G:88:ASP:HA	7:G:144:ARG:HA	1.88	0.55
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.42	0.55
2:B:1095:LEU:CD1	2:B:1095:LEU:N	2.59	0.55
1:A:1116:LEU:CD2	1:A:1311:VAL:HG22	2.36	0.55
1:A:808:LEU:CD1	1:A:808:LEU:H	2.19	0.55
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	1.88	0.55
11:K:65:HIS:CD2	11:K:66:PRO:CD	2.90	0.55
2:B:873:THR:HG22	2:B:874:PHE:N	2.22	0.55
2:B:806:THR:HG22	2:B:808:ALA:N	2.22	0.55
9:I:62:ILE:CG2	9:I:62:ILE:O	2.55	0.55
2:B:363:HIS:CD2	2:B:585:VAL:HG22	2.42	0.55
2:B:711:GLU:H	2:B:712:PRO:HD2	1.72	0.55
2:B:546:SER:HG	2:B:630:ALA:HA	1.72	0.55
1:A:919:ILE:O	1:A:921:GLY:N	2.40	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:ARG:O	2:B:331:LEU:HD13	2.06	0.54
8:H:95:TYR:HE2	8:H:97:MET:HG2	1.72	0.54
2:B:217:ARG:HE	2:B:405:ARG:CB	2.15	0.54
12:L:30:ILE:HG22	12:L:31:CYS:N	2.20	0.54
1:A:135:PHE:C	1:A:137:ALA:N	2.60	0.54
8:H:130:ARG:HA	8:H:133:ASN:HB2	1.89	0.54
9:I:105:SER:O	9:I:106:CYS:HB3	2.06	0.54
1:A:4:GLN:O	1:A:5:GLN:HB2	2.06	0.54
1:A:775:ILE:CG1	1:A:798:GLY:HA3	2.37	0.54
1:A:75:ASN:O	1:A:76:GLU:CB	2.55	0.54
1:A:1029:ARG:NH1	1:A:1029:ARG:CG	2.70	0.54
5:E:124:VAL:CA	5:E:132:ILE:HD12	2.37	0.54
2:B:642:ASP:O	2:B:644:GLU:N	2.30	0.54
5:E:144:ILE:HG13	5:E:145:THR:H	1.71	0.54
1:A:308:ILE:HG22	1:A:309:ALA:H	1.73	0.54
4:D:14:ARG:O	4:D:16:LYS:N	2.41	0.54
1:A:68:GLN:C	1:A:70:CYS:H	2.09	0.54
1:A:897:TYR:HB3	1:A:936:LEU:HD12	1.89	0.54
2:B:382:ILE:O	2:B:385:LEU:HB3	2.08	0.54
2:B:1135:ARG:O	2:B:1139:ILE:HG13	2.06	0.54
2:B:693:ILE:HD11	2:B:740:HIS:CD2	2.43	0.54
1:A:381:THR:HG23	1:A:382:PRO:CD	2.36	0.54
1:A:982:THR:HG22	1:A:984:LYS:H	1.72	0.54
9:I:88:SER:O	9:I:90:GLN:N	2.41	0.54
9:I:25:LEU:HB3	9:I:38:ALA:HB2	1.89	0.54
1:A:1305:VAL:CG1	1:A:1306:LEU:N	2.71	0.54
3:C:239:PRO:O	3:C:240:VAL:C	2.45	0.54
2:B:378:LEU:O	2:B:382:ILE:HG13	2.07	0.54
3:C:67:LEU:HD23	3:C:70:ILE:HD11	1.89	0.54
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.07	0.54
7:G:81:PRO:HG3	7:G:106:MET:SD	2.47	0.54
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.89	0.54
11:K:47:ARG:HH11	11:K:48:ALA:N	2.06	0.54
9:I:34:TYR:HD2	9:I:35:VAL:N	2.06	0.54
1:A:1017:LEU:O	1:A:1017:LEU:HD12	2.07	0.54
1:A:1017:LEU:HD23	5:E:204:THR:C	2.27	0.54
1:A:896:ARG:O	1:A:1029:ARG:HB3	2.07	0.54
1:A:1125:ALA:C	1:A:1127:ASP:H	2.10	0.54
12:L:47:ARG:HH11	12:L:47:ARG:HG3	1.72	0.54
2:B:901:PRO:O	2:B:903:VAL:N	2.41	0.54
1:A:265:LYS:HE2	1:A:322:VAL:HG11	1.88	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:124:VAL:HG13	5:E:132:ILE:CD1	2.36	0.54
2:B:705:MET:HA	2:B:705:MET:HE2	1.90	0.54
9:I:7:CYS:SG	9:I:8:ARG:O	2.66	0.54
1:A:688:LYS:C	1:A:690:VAL:N	2.61	0.54
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.88	0.54
1:A:1313:LEU:CD1	1:A:1327:ILE:HD13	2.38	0.54
1:A:663:SER:OG	2:B:1085:ILE:HG23	2.06	0.54
1:A:78:PRO:HB3	2:B:1201:LYS:HE3	1.88	0.54
1:A:468:PHE:CE2	1:A:489:LEU:HD23	2.43	0.54
1:A:1396:ALA:O	1:A:1398:MET:N	2.41	0.54
1:A:867:ILE:CG2	1:A:872:GLY:N	2.71	0.54
11:K:83:PRO:O	11:K:86:ALA:N	2.41	0.54
3:C:92:CYS:H	3:C:95:CYS:HG	1.56	0.54
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.88	0.54
2:B:1187:ASN:O	2:B:1188:LYS:CB	2.56	0.54
2:B:847:ASP:C	2:B:849:GLY:H	2.09	0.54
1:A:905:ASP:C	1:A:906:HIS:HD1	2.10	0.54
1:A:72:GLU:HB3	1:A:76:GLU:HG3	1.88	0.54
2:B:356:LEU:HA	2:B:360:PHE:HB2	1.90	0.54
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.43	0.54
1:A:1436:ILE:O	1:A:1437:GLY:C	2.46	0.54
1:A:476:SER:OG	1:A:477:PRO:HD3	2.08	0.54
1:A:523:ILE:HG22	1:A:528:LEU:HB2	1.88	0.54
2:B:861:ASP:OD1	2:B:862:GLN:N	2.41	0.54
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.72	0.54
2:B:203:PHE:HB3	2:B:205:ILE:CD1	2.37	0.54
11:K:31:VAL:CG1	11:K:32:VAL:N	2.70	0.54
2:B:210:LYS:HA	2:B:481:GLN:O	2.07	0.54
2:B:1219:ASP:O	2:B:1219:ASP:OD1	2.25	0.54
1:A:1329:THR:HG22	1:A:1331:SER:N	2.15	0.54
1:A:470:LEU:CD2	1:A:487:MET:CE	2.86	0.54
7:G:14:HIS:HD2	7:G:16:SER:CB	2.03	0.54
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.37	0.54
9:I:55:THR:CG2	9:I:100:PHE:HD2	2.17	0.54
2:B:635:ARG:HB2	2:B:636:PRO:CD	2.36	0.54
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.89	0.54
3:C:33:LEU:HG	3:C:37:MET:CE	2.38	0.54
1:A:825:ILE:C	1:A:827:THR:N	2.61	0.54
1:A:41:MET:O	1:A:42:ASP:C	2.46	0.54
1:A:35:ILE:HA	1:A:52:GLY:O	2.07	0.54
1:A:1396:ALA:O	1:A:1399:ARG:N	2.41	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:GLY:N	2:B:450:ALA:HB1	2.14	0.54
1:A:534:LEU:HD13	1:A:656:TRP:CG	2.43	0.54
1:A:626:ASN:O	1:A:631:HIS:HB2	2.07	0.54
2:B:94:LYS:HG2	2:B:95:ILE:N	2.22	0.54
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.43	0.54
2:B:54:PHE:HA	2:B:58:THR:HB	1.88	0.54
2:B:488:TYR:CE2	2:B:813:LYS:HB2	2.42	0.54
1:A:695:LYS:C	1:A:697:ALA:H	2.11	0.54
2:B:230:ALA:N	2:B:231:PRO:HD2	2.23	0.54
4:D:213:GLU:O	4:D:217:LEU:HG	2.07	0.54
10:J:1:MET:HE2	10:J:60:PHE:CE2	2.43	0.54
2:B:1032:SER:C	2:B:1034:VAL:H	2.12	0.54
10:J:48:ARG:HE	10:J:49:MET:HE2	1.73	0.54
1:A:886:ILE:HG13	1:A:943:LEU:HD12	1.90	0.54
1:A:1063:MET:CE	1:A:1436:ILE:HG12	2.38	0.54
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.90	0.54
1:A:703:THR:O	1:A:705:LYS:HG2	2.07	0.54
1:A:708:MET:SD	1:A:1091:SER:OG	2.66	0.54
8:H:84:ALA:C	8:H:86:ASP:N	2.60	0.54
1:A:339:ASN:CB	2:B:1117:GLN:HE22	2.19	0.54
2:B:54:PHE:CE1	2:B:414:ALA:HA	2.43	0.54
3:C:27:LEU:O	3:C:28:ALA:C	2.46	0.54
8:H:139:ASN:O	8:H:140:ALA:HB2	2.08	0.54
1:A:1305:VAL:HG12	1:A:1306:LEU:N	2.22	0.53
2:B:879:ARG:O	2:B:934:LYS:HD2	2.08	0.53
2:B:1165:ILE:CG2	2:B:1185:CYS:HB3	2.38	0.53
1:A:472:LEU:CD1	2:B:835:GLN:NE2	2.69	0.53
2:B:1115:THR:HG22	2:B:1117:GLN:HG3	1.90	0.53
1:A:303:TYR:CE1	1:A:325:ILE:HD11	2.43	0.53
2:B:46:GLN:CG	2:B:47:GLN:H	2.22	0.53
2:B:125:SER:HA	2:B:171:PRO:HA	1.89	0.53
8:H:102:TYR:HD2	8:H:102:TYR:H	1.51	0.53
5:E:60:PHE:HE2	5:E:80:VAL:HB	1.73	0.53
9:I:103:CYS:HB3	9:I:106:CYS:SG	2.48	0.53
2:B:265:SER:O	2:B:266:ALA:HB3	2.07	0.53
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.42	0.53
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.72	0.53
10:J:1:MET:HE2	10:J:60:PHE:HE2	1.72	0.53
2:B:225:VAL:HA	2:B:237:VAL:O	2.08	0.53
3:C:144:ILE:O	3:C:145:CYS:HB2	2.08	0.53
3:C:143:LEU:HD12	3:C:145:CYS:N	2.22	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1165:ILE:CG2	2:B:1166:CYS:N	2.70	0.53
2:B:1182:CYS:SG	2:B:1182:CYS:O	2.66	0.53
6:F:77:ASP:C	6:F:79:ARG:N	2.61	0.53
5:E:90:VAL:O	5:E:90:VAL:HG22	2.07	0.53
1:A:1406:VAL:CG1	1:A:1410:PHE:CE1	2.90	0.53
5:E:124:VAL:CG1	5:E:132:ILE:HD12	2.37	0.53
1:A:381:THR:HG22	1:A:383:TYR:H	1.73	0.53
2:B:857:ARG:HG2	2:B:858:SER:N	2.24	0.53
2:B:203:PHE:HB3	2:B:205:ILE:HD11	1.91	0.53
9:I:61:ASP:C	9:I:63:GLY:H	2.12	0.53
1:A:348:SER:HB2	2:B:1128:LEU:HB2	1.90	0.53
2:B:1010:LEU:HD12	2:B:1011:ILE:N	2.22	0.53
1:A:1376:THR:O	1:A:1377:THR:C	2.46	0.53
8:H:58:THR:HG22	8:H:59:ILE:H	1.73	0.53
2:B:31:TRP:O	2:B:34:ILE:N	2.42	0.53
3:C:97:VAL:HG12	3:C:98:VAL:N	2.23	0.53
5:E:213:ILE:HG12	5:E:214:CYS:N	2.21	0.53
1:A:84:ILE:HG22	1:A:239:LEU:O	2.08	0.53
5:E:55:ARG:O	5:E:57:MET:N	2.41	0.53
3:C:183:TRP:O	3:C:185:LYS:N	2.41	0.53
9:I:43:VAL:HG12	9:I:43:VAL:O	2.09	0.53
6:F:84:TYR:HD1	6:F:84:TYR:N	2.06	0.53
2:B:817:LEU:O	2:B:818:PRO:O	2.26	0.53
1:A:786:HIS:HE1	2:B:519:TRP:CZ2	2.25	0.53
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.48	0.53
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.38	0.53
2:B:542:MET:HG2	2:B:747:MET:HB3	1.89	0.53
3:C:88:CYS:SG	3:C:91:HIS:C	2.87	0.53
1:A:133:LYS:C	1:A:135:PHE:N	2.60	0.53
4:D:123:LEU:HD23	4:D:149:THR:HG21	1.90	0.53
2:B:205:ILE:N	2:B:205:ILE:CD1	2.72	0.53
1:A:996:ASN:HA	1:A:998:LEU:CD1	2.38	0.53
2:B:487:THR:HG22	2:B:488:TYR:H	1.73	0.53
2:B:498:THR:HB	2:B:537:LYS:O	2.08	0.53
3:C:9:LYS:O	3:C:10:ILE:O	2.26	0.53
1:A:1086:PHE:O	1:A:1087:ALA:C	2.47	0.53
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.74	0.53
1:A:855:THR:HG23	1:A:856:THR:N	2.23	0.53
1:A:823:GLY:O	1:A:825:ILE:N	2.42	0.53
2:B:273:LEU:HD21	2:B:360:PHE:CE1	2.44	0.53
2:B:865:LYS:NZ	2:B:869:SER:HA	2.22	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1079:MET:HE2	1:A:1101:LEU:CD2	2.36	0.53
7:G:78:VAL:HG12	7:G:79:PHE:H	1.74	0.53
1:A:708:MET:HE2	1:A:1089:VAL:CG1	2.36	0.53
2:B:47:GLN:O	2:B:173:MET:HE1	2.08	0.53
2:B:57:TYR:N	2:B:57:TYR:HD1	2.06	0.53
9:I:106:CYS:SG	9:I:107:SER:N	2.82	0.53
2:B:214:ALA:HB3	2:B:498:THR:HA	1.90	0.53
4:D:49:ALA:HB1	4:D:178:ALA:HB2	1.91	0.53
7:G:25:TYR:O	7:G:28:THR:HB	2.09	0.53
1:A:1454:MET:HG3	1:A:1454:MET:O	2.08	0.53
1:A:867:ILE:HG22	1:A:871:ASP:N	2.24	0.53
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.43	0.53
8:H:89:LEU:C	8:H:91:ASP:H	2.12	0.53
1:A:1123:GLY:O	1:A:1125:ALA:N	2.41	0.53
1:A:1385:THR:O	1:A:1387:HIS:N	2.42	0.53
5:E:161:LYS:C	5:E:163:GLU:N	2.61	0.53
2:B:205:ILE:O	2:B:206:ASN:C	2.47	0.53
3:C:35:ARG:HH11	11:K:41:THR:CA	2.22	0.53
1:A:1397:LEU:HA	1:A:1400:CYS:HB3	1.90	0.53
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.48	0.53
7:G:128:PRO:O	7:G:138:THR:HG23	2.09	0.53
1:A:1310:GLY:O	1:A:1311:VAL:HG23	2.08	0.53
1:A:78:PRO:HA	2:B:1201:LYS:HZ2	1.71	0.53
2:B:380:TYR:OH	2:B:623:GLU:OE2	2.21	0.53
2:B:1045:SER:O	2:B:1046:PRO:O	2.27	0.53
1:A:129:LYS:O	1:A:130:ASP:HB2	2.08	0.53
1:A:423:ASP:OD1	1:A:424:ILE:N	2.42	0.53
1:A:1021:LEU:O	1:A:1025:ARG:HG2	2.08	0.53
1:A:901:LEU:HD22	1:A:919:ILE:HG21	1.91	0.53
2:B:551:PRO:C	2:B:553:PRO:HD2	2.29	0.53
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.09	0.53
3:C:174:ALA:HB2	3:C:235:VAL:HG22	1.90	0.53
2:B:955:THR:CG2	2:B:956:THR:N	2.71	0.53
3:C:99:LEU:HD12	3:C:118:LEU:HD13	1.91	0.53
3:C:99:LEU:HD23	3:C:99:LEU:N	2.23	0.53
7:G:123:ALA:C	7:G:125:SER:N	2.63	0.53
1:A:997:LEU:HD13	1:A:1018:PHE:CE2	2.42	0.53
2:B:69:LEU:HD22	2:B:429:PHE:HE1	1.74	0.53
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.91	0.53
5:E:39:LEU:O	5:E:42:PHE:HB3	2.08	0.53
6:F:116:ASP:O	6:F:120:ILE:HG13	2.09	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:57:ILE:O	10:J:60:PHE:HB2	2.09	0.53
1:A:41:MET:HB3	1:A:48:ALA:O	2.08	0.53
7:G:1:MET:HE3	7:G:80:LYS:H	1.74	0.53
1:A:516:SER:O	1:A:517:ASN:C	2.47	0.53
2:B:763:GLN:HG2	2:B:765:PRO:CD	2.39	0.53
5:E:7:ARG:O	5:E:9:ILE:N	2.42	0.53
4:D:129:LEU:O	4:D:132:GLN:HB2	2.08	0.53
2:B:856:PHE:N	2:B:856:PHE:HD1	2.06	0.53
5:E:78:LEU:HD23	5:E:78:LEU:C	2.30	0.53
11:K:46:ILE:O	11:K:50:LEU:HB2	2.07	0.53
1:A:1299:VAL:HG12	1:A:1300:LYS:H	1.74	0.53
3:C:112:ASN:HB3	3:C:114:TYR:CE1	2.44	0.53
1:A:1073:GLY:HA2	1:A:1076:ALA:HB3	1.91	0.53
2:B:347:LYS:HG3	2:B:348:ARG:H	1.74	0.53
2:B:334:ILE:HG22	2:B:334:ILE:O	2.09	0.53
2:B:257:LYS:O	2:B:385:LEU:HD21	2.08	0.53
4:D:196:PRO:C	4:D:198:LEU:H	2.11	0.53
1:A:1343:ALA:O	1:A:1346:ALA:HB3	2.09	0.53
1:A:720:ARG:O	1:A:724:GLU:HB2	2.09	0.53
2:B:984:HIS:NE2	2:B:1025:HIS:HA	2.24	0.53
2:B:189:LEU:O	2:B:192:LEU:N	2.31	0.52
2:B:563:MET:HE2	2:B:587:HIS:C	2.29	0.52
2:B:827:ILE:CD1	2:B:1086:PHE:HD2	2.21	0.52
1:A:78:PRO:O	1:A:79:GLY:O	2.25	0.52
1:A:1097:GLY:O	1:A:1100:ARG:HB3	2.09	0.52
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.91	0.52
8:H:126:GLU:C	8:H:130:ARG:HH22	2.11	0.52
5:E:48:ASP:CG	5:E:49:SER:H	2.11	0.52
1:A:151:ASP:OD1	1:A:163:SER:HB3	2.09	0.52
3:C:44:LEU:HD23	3:C:72:LEU:HB2	1.90	0.52
1:A:853:ASP:O	1:A:854:ASN:HB2	2.09	0.52
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.92	0.52
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.28	0.52
1:A:53:LEU:HD23	1:A:54:ASN:HB3	1.91	0.52
1:A:71:GLN:C	1:A:73:GLY:N	2.60	0.52
1:A:1161:THR:C	1:A:1163:ILE:N	2.61	0.52
5:E:154:ILE:O	5:E:196:VAL:HA	2.09	0.52
1:A:511:ILE:O	1:A:519:PRO:HA	2.08	0.52
3:C:31:ASN:O	3:C:34:ARG:N	2.43	0.52
4:D:130:LEU:C	4:D:132:GLN:N	2.61	0.52
11:K:58:PHE:HE2	11:K:74:ARG:HE	1.54	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:PRO:O	1:A:610:GLY:HA3	2.10	0.52
1:A:316:GLN:O	1:A:317:LYS:C	2.47	0.52
11:K:68:PHE:N	11:K:68:PHE:CD2	2.77	0.52
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.73	0.52
1:A:412:ARG:NH2	2:B:1108:ARG:HH12	2.06	0.52
1:A:262:LEU:HD22	1:A:303:TYR:HE1	1.73	0.52
4:D:47:LEU:HD11	7:G:3:PHE:HD2	1.72	0.52
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.89	0.52
12:L:36:SER:O	12:L:37:LYS:C	2.48	0.52
2:B:224:GLN:O	2:B:238:ALA:HA	2.08	0.52
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.92	0.52
1:A:1114:PRO:O	1:A:1311:VAL:CG2	2.58	0.52
7:G:18:PHE:CZ	7:G:68:ALA:HB2	2.44	0.52
1:A:808:LEU:HD21	1:A:816:HIS:CD2	2.44	0.52
2:B:225:VAL:HG22	2:B:396:ASP:OD2	2.10	0.52
2:B:298:LEU:CD2	2:B:298:LEU:N	2.72	0.52
1:A:898:ARG:HD3	1:A:933:TYR:CD1	2.44	0.52
2:B:94:LYS:HG2	2:B:95:ILE:H	1.73	0.52
1:A:688:LYS:C	1:A:690:VAL:H	2.12	0.52
2:B:558:LEU:C	2:B:560:GLU:H	2.12	0.52
7:G:109:PHE:CG	7:G:110:VAL:N	2.78	0.52
1:A:725:ALA:O	1:A:729:ALA:N	2.42	0.52
11:K:87:LEU:O	11:K:87:LEU:HD12	2.09	0.52
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.91	0.52
1:A:785:PRO:HG2	2:B:703:ILE:HD12	1.91	0.52
2:B:360:PHE:O	2:B:361:LEU:C	2.47	0.52
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.39	0.52
3:C:61:GLU:HA	3:C:64:ALA:HB3	1.91	0.52
1:A:1079:MET:HE3	1:A:1098:VAL:HG22	1.92	0.52
1:A:751:SER:O	1:A:752:LYS:HG2	2.09	0.52
2:B:857:ARG:NH2	2:B:942:ARG:NH1	2.57	0.52
1:A:1148:ILE:O	1:A:1149:ALA:HB2	2.09	0.52
1:A:1213:GLY:O	1:A:1216:ILE:N	2.42	0.52
11:K:31:VAL:O	11:K:74:ARG:HA	2.10	0.52
2:B:210:LYS:HD2	2:B:481:GLN:O	2.09	0.52
7:G:6:ASP:HB3	7:G:73:LYS:NZ	2.25	0.52
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.45	0.52
2:B:575:PRO:C	2:B:577:ALA:H	2.13	0.52
2:B:1099:VAL:O	2:B:1102:LYS:N	2.36	0.52
1:A:1377:THR:O	1:A:1379:GLY:N	2.42	0.52
8:H:6:PHE:O	8:H:58:THR:HA	2.09	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:PRO:CG	1:A:521:MET:HG2	2.39	0.52
1:A:705:LYS:C	1:A:707:GLY:N	2.62	0.52
2:B:758:PHE:CE2	2:B:1044:ALA:CA	2.92	0.52
2:B:488:TYR:HE2	2:B:813:LYS:HB2	1.75	0.52
2:B:522:VAL:CG1	2:B:523:CYS:N	2.71	0.52
1:A:986:ILE:CD1	1:A:1032:LEU:HD11	2.40	0.52
3:C:33:LEU:HG	3:C:37:MET:HE2	1.89	0.52
1:A:808:LEU:H	1:A:808:LEU:HD12	1.74	0.52
1:A:1372:VAL:HG12	1:A:1373:ASP:N	2.25	0.52
1:A:1088:GLY:O	1:A:1089:VAL:HG23	2.09	0.52
2:B:640:VAL:HG23	2:B:740:HIS:HA	1.92	0.52
2:B:1020:ARG:NH1	2:B:1020:ARG:HG2	2.20	0.52
4:D:185:CYS:HB3	4:D:211:LEU:CD1	2.39	0.52
2:B:223:VAL:CG1	2:B:381:MET:HG2	2.40	0.52
2:B:431:TYR:CZ	2:B:447:ALA:HB2	2.44	0.52
2:B:1147:LEU:O	2:B:1148:LYS:C	2.45	0.52
12:L:25:ALA:O	12:L:26:THR:HB	2.10	0.52
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.24	0.52
2:B:583:ASN:HD21	2:B:628:THR:CB	2.13	0.52
3:C:215:GLU:O	3:C:217:ASP:N	2.43	0.52
11:K:53:ASP:HB3	11:K:56:VAL:CG2	2.39	0.52
1:A:474:VAL:HG22	1:A:474:VAL:O	2.10	0.52
1:A:106:VAL:HA	1:A:114:LEU:HD21	1.91	0.52
4:D:47:LEU:HD13	4:D:48:ILE:N	2.25	0.52
7:G:143:ILE:CG2	7:G:144:ARG:N	2.73	0.52
1:A:1208:THR:O	1:A:1209:MET:C	2.48	0.52
11:K:49:GLU:OE2	11:K:97:LYS:HE3	2.09	0.52
2:B:781:PHE:O	2:B:782:LEU:CG	2.54	0.52
2:B:197:PHE:HZ	2:B:816:GLU:HG2	1.74	0.52
2:B:1065:GLN:NE2	2:B:1067:ARG:HG2	2.25	0.52
8:H:143:LEU:N	8:H:143:LEU:HD12	2.25	0.52
9:I:54:GLU:O	9:I:100:PHE:CE2	2.63	0.52
2:B:212:LEU:HD21	2:B:466:TRP:HH2	1.74	0.52
1:A:964:ILE:O	1:A:968:GLN:HG2	2.09	0.52
2:B:906:SER:O	2:B:941:LEU:HD23	2.10	0.52
1:A:996:ASN:HA	1:A:998:LEU:HD12	1.92	0.52
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.91	0.52
4:D:198:LEU:O	4:D:200:ASN:N	2.42	0.52
2:B:870:ILE:CG2	2:B:917:PRO:HG2	2.40	0.52
5:E:92:THR:O	5:E:95:THR:HB	2.10	0.52
5:E:147:HIS:CD2	5:E:149:LEU:H	2.27	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:508:LEU:O	2:B:510:LYS:N	2.42	0.52
2:B:298:LEU:N	2:B:298:LEU:HD22	2.24	0.52
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.68	0.52
1:A:321:PRO:O	1:A:322:VAL:CB	2.58	0.52
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.75	0.52
2:B:708:GLU:HG3	2:B:709:ASP:H	1.75	0.52
3:C:58:LEU:N	3:C:58:LEU:HD22	2.25	0.52
1:A:514:PRO:O	1:A:875:ALA:HB1	2.09	0.52
2:B:1082:MET:O	3:C:189:THR:HG23	2.10	0.52
2:B:1032:SER:C	2:B:1034:VAL:N	2.64	0.51
2:B:1034:VAL:HG23	2:B:1059:LEU:CD1	2.40	0.51
1:A:42:ASP:C	1:A:44:THR:N	2.64	0.51
1:A:50:ILE:C	1:A:52:GLY:N	2.62	0.51
2:B:798:TYR:CD1	10:J:4:PRO:HG3	2.45	0.51
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.25	0.51
2:B:800:GLN:CB	10:J:52:THR:HG21	2.33	0.51
3:C:80:LEU:CD1	3:C:95:CYS:HA	2.40	0.51
12:L:28:LYS:HB2	12:L:39:SER:HA	1.91	0.51
2:B:1084:GLN:HE21	2:B:1084:GLN:H	1.55	0.51
1:A:35:ILE:O	1:A:35:ILE:HG22	2.11	0.51
11:K:65:HIS:CD2	11:K:66:PRO:HD2	2.46	0.51
2:B:1149:GLU:O	2:B:1150:ARG:C	2.47	0.51
10:J:7:CYS:CA	10:J:49:MET:HE3	2.40	0.51
1:A:92:HIS:O	1:A:93:VAL:C	2.48	0.51
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.92	0.51
5:E:55:ARG:C	5:E:57:MET:N	2.63	0.51
2:B:457:LEU:O	2:B:461:LEU:HD12	2.10	0.51
9:I:68:LEU:HB3	9:I:84:VAL:HG23	1.91	0.51
1:A:317:LYS:O	1:A:318:SER:CB	2.57	0.51
2:B:323:VAL:HG12	2:B:323:VAL:O	2.09	0.51
3:C:43:THR:CG2	3:C:44:LEU:N	2.74	0.51
2:B:839:MET:HE2	2:B:1010:LEU:HD21	1.92	0.51
1:A:50:ILE:O	1:A:52:GLY:N	2.39	0.51
2:B:865:LYS:HE2	2:B:871:THR:OG1	2.10	0.51
2:B:843:GLN:O	2:B:846:ILE:HB	2.11	0.51
2:B:936:ASP:OD1	2:B:938:SER:N	2.42	0.51
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.76	0.51
2:B:546:SER:HA	2:B:612:GLU:OE2	2.11	0.51
2:B:57:TYR:O	2:B:59:LEU:N	2.42	0.51
2:B:429:PHE:HA	2:B:432:MET:CE	2.40	0.51
5:E:100:ILE:CG2	5:E:105:PHE:HB2	2.40	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1308:THR:HG23	1:A:1309:ASP:N	2.26	0.51
1:A:470:LEU:CD2	1:A:487:MET:HE3	2.40	0.51
2:B:508:LEU:HB2	2:B:510:LYS:CB	2.40	0.51
1:A:55:ASP:N	1:A:56:PRO:CD	2.73	0.51
2:B:242:SER:HB2	2:B:362:PRO:HG2	1.93	0.51
8:H:59:ILE:O	8:H:60:ALA:HB3	2.10	0.51
2:B:38:PHE:CD1	2:B:811:TYR:CD2	2.98	0.51
9:I:100:PHE:N	9:I:100:PHE:HD1	2.07	0.51
9:I:58:VAL:HG12	9:I:60:GLN:N	2.20	0.51
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.49	0.51
12:L:38:LEU:HG	12:L:39:SER:N	2.26	0.51
1:A:392:VAL:HG21	1:A:426:LEU:HD11	1.91	0.51
1:A:877:HIS:O	1:A:878:ILE:HG12	2.10	0.51
2:B:424:LEU:HD22	2:B:453:ILE:HD11	1.92	0.51
2:B:49:ASP:HA	2:B:52:ASN:HD22	1.75	0.51
1:A:18:GLN:HB3	2:B:1215:ARG:HG3	1.92	0.51
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.75	0.51
1:A:866:PHE:CD2	5:E:168:TYR:CE1	2.98	0.51
3:C:60:ASP:OD2	12:L:60:ARG:NH2	2.44	0.51
5:E:124:VAL:HG13	5:E:132:ILE:CB	2.39	0.51
2:B:401:PHE:HB2	2:B:517:THR:OG1	2.10	0.51
2:B:758:PHE:CE1	2:B:1027:ILE:CG2	2.94	0.51
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.45	0.51
1:A:675:THR:O	1:A:679:ILE:HG13	2.11	0.51
7:G:49:LEU:N	7:G:49:LEU:HD23	2.25	0.51
1:A:547:LEU:HD22	11:K:58:PHE:CE1	2.46	0.51
2:B:1177:HIS:O	2:B:1179:GLN:N	2.44	0.51
1:A:1349:TYR:CD2	1:A:1349:TYR:C	2.83	0.51
2:B:562:GLY:HA3	2:B:590:HIS:ND1	2.25	0.51
2:B:996:ARG:HH22	3:C:175:ALA:HA	1.75	0.51
10:J:5:VAL:O	10:J:6:ARG:O	2.28	0.51
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.75	0.51
2:B:1202:LEU:O	2:B:1203:LEU:C	2.49	0.51
2:B:97:VAL:HG12	2:B:178:ASN:HD21	1.74	0.51
1:A:416:ARG:O	1:A:417:TYR:HD2	1.94	0.51
1:A:34:LYS:HG2	1:A:36:ARG:NH2	2.26	0.51
2:B:446:LEU:HD23	2:B:446:LEU:N	2.26	0.51
2:B:210:LYS:HE2	2:B:462:ALA:O	2.11	0.51
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.46	0.51
8:H:62:SER:O	8:H:63:LEU:C	2.48	0.51
1:A:406:ILE:HG22	1:A:411:ASP:O	2.11	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:510:LYS:HG2	2:B:512:ARG:N	2.19	0.51
2:B:879:ARG:O	2:B:880:THR:CB	2.58	0.51
11:K:67:PHE:O	11:K:68:PHE:HD2	1.93	0.51
5:E:212:ARG:HH11	5:E:212:ARG:HG3	1.75	0.51
1:A:1364:ASN:O	1:A:1365:TYR:C	2.49	0.51
2:B:809:MET:O	2:B:812:LEU:N	2.37	0.51
9:I:100:PHE:CD1	9:I:100:PHE:N	2.78	0.51
1:A:1134:ILE:O	1:A:1135:ARG:C	2.49	0.51
2:B:44:VAL:O	2:B:45:SER:C	2.49	0.51
5:E:10:SER:O	5:E:13:TRP:HB3	2.10	0.51
1:A:898:ARG:HB2	1:A:933:TYR:HE1	1.75	0.51
2:B:644:GLU:C	2:B:646:LEU:H	2.13	0.51
2:B:209:GLU:CD	2:B:485:ARG:HE	2.14	0.51
10:J:55:ASP:OD2	10:J:58:GLU:HG2	2.10	0.51
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.93	0.51
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.27	0.51
1:A:785:PRO:CG	2:B:703:ILE:HD12	2.40	0.51
1:A:1030:ARG:CG	1:A:1034:GLU:OE2	2.59	0.51
1:A:1424:VAL:CG2	1:A:1436:ILE:HD11	2.32	0.51
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.46	0.51
8:H:40:LEU:HG	8:H:41:ASP:O	2.11	0.51
1:A:472:LEU:CD1	2:B:835:GLN:CD	2.79	0.51
1:A:525:GLN:HB3	2:B:1015:HIS:HD2	1.75	0.51
2:B:766:ARG:HH21	2:B:1020:ARG:HG2	1.70	0.51
2:B:261:ARG:HH11	2:B:261:ARG:HB3	1.76	0.51
1:A:1261:LYS:CA	1:A:1264:GLU:HB3	2.38	0.51
5:E:161:LYS:C	5:E:163:GLU:H	2.14	0.51
2:B:62:ILE:HG23	2:B:418:LYS:HG2	1.92	0.51
5:E:79:TRP:HE1	5:E:81:GLU:HB2	1.76	0.51
11:K:50:LEU:HD11	11:K:75:ILE:HD13	1.92	0.51
3:C:53:THR:O	3:C:153:LEU:HA	2.10	0.51
4:D:26:THR:O	4:D:28:GLN:HG3	2.11	0.51
1:A:856:THR:HB	1:A:865:GLN:HB2	1.93	0.51
1:A:864:ILE:HG22	1:A:864:ILE:O	2.10	0.51
1:A:841:LEU:O	1:A:845:LEU:HG	2.10	0.51
3:C:236:GLY:C	3:C:238:ILE:H	2.13	0.51
3:C:31:ASN:O	3:C:34:ARG:HB3	2.10	0.51
5:E:192:ARG:NH1	5:E:192:ARG:HG3	2.26	0.51
4:D:134:THR:HG22	4:D:136:GLY:H	1.76	0.51
2:B:91:SER:OG	2:B:133:LYS:HB2	2.11	0.51
4:D:40:HIS:CB	7:G:73:LYS:NZ	2.58	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:863:VAL:HG12	1:A:865:GLN:H	1.76	0.51
3:C:133:ILE:HD11	3:C:237:SER:CA	2.24	0.51
2:B:1102:LYS:O	2:B:1103:ILE:O	2.29	0.51
3:C:235:VAL:HG13	10:J:13:VAL:CG2	2.40	0.51
1:A:648:ASN:O	1:A:649:ILE:C	2.47	0.51
2:B:899:ILE:HG22	2:B:900:ALA:H	1.75	0.51
7:G:123:ALA:O	7:G:125:SER:N	2.43	0.51
1:A:898:ARG:HD3	1:A:933:TYR:CE1	2.45	0.51
1:A:1148:ILE:O	1:A:1148:ILE:CG2	2.59	0.51
2:B:525:ALA:O	2:B:768:THR:HG23	2.11	0.51
1:A:989:GLY:O	1:A:992:ASP:N	2.44	0.51
9:I:95:THR:HG22	9:I:96:SER:N	2.25	0.51
2:B:782:LEU:CD1	2:B:788:ARG:HH11	2.23	0.50
2:B:882:THR:HB	2:B:934:LYS:O	2.11	0.50
1:A:63:ARG:CA	1:A:74:MET:SD	2.89	0.50
2:B:843:GLN:O	2:B:846:ILE:N	2.44	0.50
1:A:709:THR:CG2	1:A:712:GLU:H	2.23	0.50
2:B:681:TRP:C	2:B:683:SER:H	2.15	0.50
1:A:1443:VAL:C	1:A:1444:MET:HG3	2.30	0.50
6:F:111:LEU:C	6:F:113:GLY:N	2.62	0.50
1:A:877:HIS:CG	1:A:1056:SER:HA	2.46	0.50
1:A:770:VAL:O	1:A:771:GLU:HB2	2.11	0.50
2:B:877:PRO:C	2:B:878:GLN:HG3	2.31	0.50
2:B:1029:CYS:SG	2:B:1086:PHE:CE2	3.05	0.50
1:A:1011:GLN:NE2	1:A:1015:VAL:CG2	2.65	0.50
10:J:46:CYS:O	10:J:49:MET:N	2.44	0.50
1:A:1161:THR:O	1:A:1163:ILE:N	2.45	0.50
1:A:1398:MET:HB2	1:A:1426:GLU:OE2	2.11	0.50
1:A:1398:MET:O	1:A:1401:SER:OG	2.22	0.50
2:B:851:PHE:CD2	2:B:1094:ARG:HB2	2.46	0.50
3:C:104:PHE:HD2	3:C:105:GLY:H	1.56	0.50
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.25	0.50
5:E:164:LEU:CD2	5:E:211:TYR:CD2	2.95	0.50
3:C:263:THR:C	3:C:265:MET:N	2.63	0.50
7:G:30:LEU:O	7:G:34:VAL:HG23	2.12	0.50
2:B:218:SER:O	2:B:219:ALA:O	2.29	0.50
2:B:459:TYR:CD2	2:B:459:TYR:C	2.85	0.50
1:A:1323:ASP:C	1:A:1325:THR:H	2.14	0.50
1:A:254:GLU:HB2	2:B:935:ARG:NH2	2.25	0.50
2:B:293:PRO:C	2:B:294:ASP:O	2.47	0.50
1:A:1167:GLU:O	1:A:1169:ILE:N	2.44	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:52:THR:O	10:J:53:HIS:O	2.30	0.50
1:A:335:ARG:HA	1:A:339:ASN:ND2	2.26	0.50
12:L:30:ILE:HG22	12:L:31:CYS:O	2.10	0.50
4:D:147:TYR:CZ	7:G:103:VAL:HG13	2.47	0.50
2:B:758:PHE:HE2	2:B:1044:ALA:HA	1.73	0.50
1:A:519:PRO:HG3	1:A:625:SER:O	2.12	0.50
4:D:52:LEU:C	4:D:54:GLU:H	2.14	0.50
3:C:35:ARG:HD3	11:K:41:THR:HA	1.93	0.50
1:A:1230:GLU:C	1:A:1232:ASN:H	2.14	0.50
9:I:27:PHE:O	9:I:28:GLU:HB3	2.11	0.50
6:F:93:ILE:O	6:F:94:LEU:C	2.49	0.50
3:C:84:ARG:NH2	11:K:11:LEU:HD21	2.27	0.50
1:A:1283:VAL:CG1	1:A:1284:MET:H	2.24	0.50
3:C:167:HIS:HD2	3:C:169:LYS:N	1.97	0.50
2:B:1059:LEU:HD23	2:B:1065:GLN:O	2.12	0.50
1:A:351:THR:HG21	2:B:1103:ILE:HG13	1.91	0.50
11:K:65:HIS:CD2	11:K:67:PHE:N	2.60	0.50
2:B:23:ALA:CB	2:B:24:PRO:HD2	2.31	0.50
1:A:556:TRP:O	1:A:558:GLY:N	2.44	0.50
1:A:1444:MET:O	6:F:132:LEU:HA	2.10	0.50
1:A:335:ARG:NE	1:A:339:ASN:HD22	2.10	0.50
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.93	0.50
1:A:326:ARG:HG2	1:A:327:ALA:N	2.24	0.50
3:C:31:ASN:OD1	3:C:34:ARG:HD3	2.10	0.50
1:A:90:VAL:CG1	1:A:91:PHE:H	2.23	0.50
1:A:1005:GLU:O	1:A:1006:ILE:C	2.49	0.50
2:B:984:HIS:CD2	2:B:1025:HIS:HB2	2.47	0.50
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.93	0.50
10:J:1:MET:HA	10:J:57:ILE:H	1.76	0.50
7:G:17:PHE:N	7:G:17:PHE:CD2	2.76	0.50
2:B:510:LYS:O	2:B:513:GLN:HB2	2.11	0.50
1:A:1341:ILE:O	1:A:1344:GLY:N	2.45	0.50
2:B:1131:GLY:O	2:B:1132:GLU:C	2.50	0.50
1:A:1444:MET:HG2	7:G:60:ARG:CA	2.40	0.50
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.40	0.50
7:G:96:GLN:HG3	7:G:97:HIS:HD2	1.76	0.50
12:L:49:LYS:O	12:L:50:ASP:CB	2.59	0.50
2:B:1145:SER:C	2:B:1147:LEU:H	2.14	0.50
10:J:21:TYR:C	10:J:23:ASN:H	2.15	0.50
10:J:21:TYR:O	10:J:23:ASN:N	2.44	0.50
1:A:1041:ALA:O	1:A:1044:TRP:HB3	2.12	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:70:PHE:N	7:G:70:PHE:CD1	2.79	0.50
1:A:590:ARG:O	1:A:591:PHE:HB2	2.12	0.50
3:C:51:VAL:HG22	3:C:155:LEU:HD21	1.93	0.50
3:C:88:CYS:O	3:C:88:CYS:SG	2.70	0.50
1:A:744:LYS:HG2	1:A:748:MET:CE	2.41	0.50
1:A:115:LEU:HB2	1:A:122:MET:CE	2.40	0.50
1:A:311:GLN:O	1:A:312:PRO:C	2.49	0.50
6:F:103:MET:O	6:F:104:ASN:HB2	2.11	0.50
2:B:59:LEU:HD12	2:B:417:PHE:CE2	2.46	0.50
6:F:127:GLU:O	6:F:129:LYS:HG3	2.12	0.50
3:C:69:LEU:HD12	3:C:69:LEU:N	2.27	0.50
1:A:992:ASP:O	1:A:995:GLU:HB2	2.11	0.50
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.11	0.50
3:C:168:ALA:O	3:C:170:TRP:N	2.44	0.50
2:B:303:TYR:N	2:B:303:TYR:CD2	2.80	0.50
1:A:1344:GLY:O	1:A:1345:ARG:C	2.50	0.50
5:E:168:TYR:CB	5:E:170:LEU:HG	2.40	0.50
8:H:59:ILE:CG2	8:H:60:ALA:N	2.73	0.50
8:H:89:LEU:O	8:H:91:ASP:N	2.39	0.50
8:H:93:TYR:N	8:H:93:TYR:CD1	2.80	0.50
1:A:1125:ALA:O	1:A:1127:ASP:N	2.45	0.50
2:B:212:LEU:HD21	2:B:466:TRP:CH2	2.47	0.50
1:A:541:ILE:HD12	1:A:577:ILE:HD11	1.93	0.50
2:B:1106:ARG:CG	2:B:1107:ALA:N	2.69	0.50
1:A:553:VAL:HG22	1:A:652:VAL:HG22	1.92	0.50
2:B:496:ARG:HH12	2:B:539:LEU:HB2	1.75	0.50
1:A:391:LEU:O	1:A:392:VAL:C	2.49	0.50
2:B:54:PHE:O	2:B:59:LEU:HB2	2.12	0.50
1:A:719:VAL:O	1:A:721:PHE:N	2.45	0.50
1:A:1213:GLY:HA2	1:A:1216:ILE:CD1	2.42	0.50
11:K:35:PHE:CD1	11:K:35:PHE:N	2.79	0.50
5:E:42:PHE:O	5:E:43:LYS:C	2.50	0.50
5:E:25:ASP:C	5:E:27:GLY:N	2.63	0.50
1:A:496:GLU:OE1	7:G:64:THR:HA	2.11	0.50
7:G:91:VAL:HA	7:G:101:VAL:HA	1.94	0.50
2:B:999:MET:HA	2:B:999:MET:CE	2.42	0.50
1:A:1369:ALA:O	1:A:1372:VAL:HG12	2.11	0.50
1:A:1127:ASP:O	1:A:1128:GLN:C	2.51	0.50
2:B:97:VAL:CG1	2:B:178:ASN:ND2	2.74	0.50
1:A:602:ASP:OD2	1:A:616:VAL:HG23	2.11	0.50
2:B:526:GLU:HG2	2:B:538:ASN:HD22	1.77	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:25:TYR:HE2	7:G:29:LYS:HD2	1.77	0.50
1:A:899:VAL:HG22	1:A:908:LEU:HD21	1.93	0.50
1:A:470:LEU:HD11	1:A:482:PHE:CZ	2.46	0.50
2:B:197:PHE:CZ	2:B:816:GLU:HG2	2.46	0.50
1:A:774:ARG:O	1:A:775:ILE:C	2.49	0.50
3:C:164:ALA:O	3:C:167:HIS:N	2.43	0.50
2:B:376:PHE:HB3	2:B:586:TRP:CZ3	2.46	0.50
2:B:377:PHE:O	2:B:378:LEU:C	2.50	0.50
3:C:143:LEU:HD21	3:C:146:LYS:HE2	1.94	0.50
8:H:25:ARG:HA	8:H:41:ASP:HA	1.93	0.50
7:G:1:MET:HE3	7:G:80:LYS:N	2.26	0.50
4:D:51:ASN:O	4:D:52:LEU:C	2.48	0.50
5:E:144:ILE:HG13	5:E:145:THR:N	2.26	0.50
5:E:23:VAL:O	5:E:28:TYR:HB2	2.12	0.50
2:B:48:LEU:O	2:B:51:PHE:N	2.44	0.50
3:C:136:ASP:OD1	3:C:138:GLU:N	2.45	0.50
10:J:60:PHE:O	10:J:63:TYR:HD1	1.94	0.49
1:A:1114:PRO:O	1:A:1311:VAL:HG21	2.11	0.49
1:A:1325:THR:CG2	1:A:1326:ARG:HG3	2.41	0.49
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.94	0.49
1:A:335:ARG:NH1	2:B:1206:GLU:CD	2.65	0.49
9:I:58:VAL:HG13	9:I:62:ILE:HD12	1.94	0.49
1:A:265:LYS:NZ	1:A:322:VAL:HG22	2.26	0.49
12:L:28:LYS:HB2	12:L:39:SER:CA	2.42	0.49
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.94	0.49
2:B:526:GLU:CD	2:B:752:ALA:HB2	2.33	0.49
8:H:27:GLU:HA	8:H:38:LEU:O	2.12	0.49
1:A:167:CYS:SG	1:A:167:CYS:O	2.69	0.49
5:E:72:PHE:CD1	5:E:72:PHE:N	2.80	0.49
2:B:269:ILE:HG22	2:B:282:ILE:HG23	1.94	0.49
1:A:1019:CYS:O	1:A:1022:LEU:N	2.45	0.49
1:A:14:VAL:HG23	1:A:1432:GLN:HE22	1.75	0.49
1:A:1364:ASN:HD22	1:A:1365:TYR:N	2.10	0.49
2:B:806:THR:HG22	2:B:808:ALA:HB3	1.94	0.49
2:B:763:GLN:C	2:B:765:PRO:HD2	2.32	0.49
2:B:497:ARG:NH2	2:B:775:LYS:NZ	2.60	0.49
1:A:997:LEU:HB3	1:A:1053:PHE:CE2	2.47	0.49
2:B:247:GLY:H	2:B:418:LYS:NZ	2.10	0.49
1:A:717:ASN:O	1:A:721:PHE:CD1	2.66	0.49
1:A:1191:TRP:HD1	1:A:1256:GLU:HB2	1.76	0.49
1:A:24:PRO:HG2	1:A:25:GLU:OE2	2.11	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PHE:CE1	2:B:1213:THR:HG22	2.47	0.49
3:C:186:LEU:N	3:C:186:LEU:CD1	2.75	0.49
11:K:84:LYS:O	11:K:87:LEU:HB3	2.12	0.49
1:A:601:LYS:HB2	1:A:603:ASN:ND2	2.27	0.49
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.47	0.49
2:B:976:ILE:O	2:B:990:ILE:HB	2.12	0.49
1:A:1048:ASN:HD22	1:A:1048:ASN:N	2.10	0.49
1:A:1290:LYS:O	1:A:1291:VAL:HG23	2.11	0.49
2:B:903:VAL:CG1	2:B:904:ARG:N	2.76	0.49
1:A:384:ASN:O	1:A:385:ILE:C	2.49	0.49
1:A:939:ASP:O	1:A:940:ARG:C	2.50	0.49
1:A:877:HIS:O	1:A:878:ILE:CG1	2.61	0.49
5:E:46:TYR:CD2	5:E:58:MET:HG2	2.48	0.49
6:F:72:LYS:HB2	6:F:142:SER:HB3	1.94	0.49
1:A:208:LEU:HG	1:A:235:ILE:HG21	1.93	0.49
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.12	0.49
1:A:587:HIS:HD2	1:A:969:GLN:CG	2.19	0.49
12:L:31:CYS:HB3	12:L:35:SER:CA	2.42	0.49
5:E:7:ARG:HG3	5:E:8:ASN:H	1.73	0.49
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.26	0.49
2:B:215:GLN:OE1	2:B:215:GLN:HA	2.12	0.49
2:B:1074:ASN:O	2:B:1078:GLY:N	2.44	0.49
4:D:53:SER:O	4:D:57:LEU:HG	2.12	0.49
1:A:907:THR:CG2	1:A:908:LEU:N	2.75	0.49
2:B:508:LEU:CA	2:B:510:LYS:H	2.24	0.49
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.95	0.49
3:C:239:PRO:HB2	3:C:241:ASP:OD1	2.12	0.49
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.95	0.49
1:A:1090:ALA:O	1:A:1091:SER:OG	2.28	0.49
2:B:760:ASP:O	2:B:761:HIS:CD2	2.66	0.49
1:A:1053:PHE:O	1:A:1056:SER:N	2.44	0.49
11:K:32:VAL:HG22	11:K:74:ARG:HG3	1.95	0.49
1:A:148:CYS:O	1:A:168:GLY:HA2	2.12	0.49
4:D:53:SER:HB3	4:D:152:SER:CB	2.42	0.49
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.95	0.49
2:B:845:SER:HB3	10:J:8:PHE:O	2.13	0.49
8:H:142:LEU:C	8:H:143:LEU:HD12	2.33	0.49
6:F:85:MET:HE1	6:F:148:VAL:HG12	1.94	0.49
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.41	0.49
2:B:594:ALA:CA	2:B:617:ARG:HH12	2.25	0.49
2:B:760:ASP:OD1	2:B:1046:PRO:HA	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1022:THR:HG23	2:B:1022:THR:O	2.12	0.49
7:G:114:LEU:HG	7:G:162:SER:HB3	1.93	0.49
1:A:1199:ARG:HG3	1:A:1236:LEU:HD11	1.93	0.49
1:A:564:ALA:HB2	1:A:576:GLN:OE1	2.12	0.49
2:B:112:LEU:CD1	2:B:113:TYR:N	2.71	0.49
2:B:563:MET:HA	2:B:589:VAL:O	2.13	0.49
1:A:838:GLN:O	1:A:842:VAL:HG23	2.13	0.49
8:H:143:LEU:C	8:H:144:ILE:HG13	2.32	0.49
1:A:472:LEU:HD13	2:B:835:GLN:OE1	2.13	0.49
3:C:86:CYS:SG	3:C:95:CYS:HB3	2.52	0.49
10:J:37:SER:OG	10:J:47:ARG:NH2	2.46	0.49
3:C:22:LEU:HD13	3:C:230:MET:HE1	1.95	0.49
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.47	0.49
1:A:852:TYR:CE1	6:F:136:ARG:HB3	2.48	0.49
4:D:134:THR:CG2	4:D:135:GLY:N	2.75	0.49
4:D:127:ASP:O	4:D:131:GLU:HG3	2.13	0.49
2:B:175:ARG:HH11	2:B:175:ARG:HG2	1.77	0.49
7:G:6:ASP:C	7:G:7:LEU:HD23	2.33	0.49
7:G:101:VAL:CG1	7:G:102:GLN:N	2.76	0.49
1:A:795:GLU:CD	1:A:795:GLU:N	2.59	0.49
7:G:15:PRO:O	7:G:18:PHE:HB2	2.11	0.49
2:B:361:LEU:N	2:B:362:PRO:CD	2.75	0.49
9:I:111:THR:HG22	9:I:113:ASP:N	2.19	0.49
1:A:1090:ALA:O	1:A:1091:SER:CB	2.60	0.49
1:A:556:TRP:C	1:A:558:GLY:N	2.65	0.49
9:I:4:PHE:CE1	9:I:13:MET:HE1	2.48	0.49
9:I:58:VAL:CG2	9:I:62:ILE:HD12	2.40	0.49
12:L:30:ILE:CG2	12:L:31:CYS:N	2.75	0.49
5:E:163:GLU:O	5:E:164:LEU:C	2.51	0.49
1:A:387:ARG:O	1:A:390:GLN:HB3	2.13	0.49
1:A:877:HIS:C	1:A:878:ILE:HG13	2.33	0.49
1:A:348:SER:HB2	2:B:1128:LEU:HD12	1.93	0.49
8:H:33:GLN:C	8:H:35:GLN:H	2.16	0.49
1:A:1038:THR:O	1:A:1039:LYS:C	2.49	0.49
1:A:929:LEU:HD23	1:A:983:ILE:HG21	1.95	0.49
1:A:1308:THR:O	1:A:1309:ASP:HB2	2.12	0.49
1:A:821:ARG:O	1:A:821:ARG:HG3	2.12	0.49
1:A:903:ASN:ND2	1:A:903:ASN:C	2.65	0.49
1:A:42:ASP:O	1:A:44:THR:N	2.38	0.49
2:B:811:TYR:N	2:B:811:TYR:CD1	2.80	0.49
1:A:1059:HIS:O	1:A:1061:GLY:N	2.46	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:LEU:HD22	3:C:129:ILE:HD13	1.94	0.49
9:I:13:MET:HG3	9:I:14:LEU:N	2.27	0.49
2:B:25:ILE:HG23	2:B:29:ASP:CB	2.42	0.49
1:A:3:GLY:O	1:A:4:GLN:O	2.31	0.49
5:E:32:GLN:HG3	5:E:36:GLU:OE2	2.12	0.49
4:D:60:LYS:O	4:D:61:GLU:C	2.51	0.49
1:A:1072:ILE:C	1:A:1075:PRO:HD2	2.33	0.49
1:A:356:ASP:C	1:A:358:ASN:H	2.16	0.49
2:B:976:ILE:CD1	2:B:992:ILE:HA	2.41	0.49
1:A:14:VAL:CG2	1:A:1430:LEU:HD13	2.42	0.49
1:A:1372:VAL:HG12	1:A:1373:ASP:H	1.78	0.49
8:H:58:THR:HB	8:H:143:LEU:HD13	1.94	0.49
2:B:806:THR:O	2:B:807:ARG:C	2.50	0.49
2:B:1106:ARG:HD3	2:B:1126:GLY:O	2.12	0.49
5:E:7:ARG:C	5:E:9:ILE:N	2.65	0.49
1:A:370:ILE:HG23	2:B:1105:ALA:CB	2.41	0.49
7:G:88:ASP:HB3	7:G:144:ARG:HB2	1.95	0.49
2:B:457:LEU:O	2:B:461:LEU:CD1	2.61	0.49
3:C:8:VAL:HG12	3:C:9:LYS:N	2.28	0.49
2:B:458:LYS:O	2:B:459:TYR:C	2.50	0.49
1:A:37:PHE:N	1:A:37:PHE:CD1	2.81	0.49
1:A:863:VAL:HG12	1:A:864:ILE:H	1.77	0.48
1:A:481:ASP:O	1:A:485:ASP:HB2	2.13	0.48
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.46	0.48
2:B:846:ILE:HG23	2:B:974:PRO:CG	2.36	0.48
4:D:144:THR:OG1	7:G:105:PRO:HD3	2.12	0.48
2:B:910:VAL:CG1	2:B:911:ILE:N	2.76	0.48
1:A:315:LEU:HD22	1:A:319:GLY:O	2.13	0.48
2:B:619:ILE:C	2:B:621:GLU:H	2.17	0.48
8:H:82:PRO:O	8:H:83:GLN:HB2	2.13	0.48
8:H:83:GLN:O	8:H:85:GLY:N	2.45	0.48
3:C:111:THR:O	3:C:147:LEU:HD23	2.12	0.48
1:A:874:ASP:N	1:A:1058:VAL:HG23	2.27	0.48
5:E:3:GLN:HG3	5:E:4:GLU:N	2.27	0.48
2:B:446:LEU:O	2:B:447:ALA:CB	2.61	0.48
3:C:79:GLN:O	3:C:127:ARG:NH1	2.46	0.48
2:B:234:ILE:HD12	2:B:234:ILE:N	2.28	0.48
1:A:1285:MET:HG3	1:A:1307:GLU:OE2	2.12	0.48
2:B:189:LEU:HD13	2:B:196:PRO:HA	1.94	0.48
11:K:65:HIS:CD2	11:K:66:PRO:N	2.81	0.48
1:A:567:LYS:HZ1	8:H:46:LEU:HB2	1.79	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:113:ASP:O	9:I:114:GLN:CG	2.61	0.48
2:B:37:PHE:HE2	2:B:542:MET:CA	2.17	0.48
1:A:433:GLU:OE2	2:B:1108:ARG:NH1	2.45	0.48
2:B:314:LEU:O	2:B:317:CYS:HB3	2.12	0.48
2:B:619:ILE:O	2:B:621:GLU:N	2.47	0.48
1:A:12:ARG:CZ	2:B:1192:TYR:HE2	2.25	0.48
11:K:21:ILE:HG23	11:K:31:VAL:CG1	2.44	0.48
3:C:168:ALA:C	3:C:170:TRP:N	2.67	0.48
7:G:62:LEU:HB3	7:G:63:PRO:HD2	1.96	0.48
1:A:809:THR:H	1:A:812:GLU:HB2	1.78	0.48
1:A:418:SER:O	1:A:421:ALA:N	2.46	0.48
1:A:946:VAL:HG12	1:A:947:PHE:N	2.28	0.48
1:A:618:GLU:CD	1:A:618:GLU:C	2.71	0.48
2:B:102:VAL:CG2	2:B:112:LEU:HD22	2.43	0.48
2:B:196:PRO:HG2	2:B:197:PHE:H	1.77	0.48
1:A:42:ASP:OD1	1:A:45:GLN:HA	2.14	0.48
2:B:221:ASN:OD1	2:B:242:SER:HA	2.14	0.48
3:C:143:LEU:HD21	3:C:146:LYS:CE	2.44	0.48
2:B:583:ASN:OD1	2:B:628:THR:N	2.47	0.48
2:B:1165:ILE:HG22	2:B:1185:CYS:HB3	1.94	0.48
2:B:821:GLN:HE22	2:B:851:PHE:N	2.09	0.48
1:A:501:LEU:HD11	2:B:1146:PHE:CD2	2.48	0.48
11:K:81:TYR:OH	11:K:86:ALA:HA	2.13	0.48
1:A:231:PRO:HA	1:A:234:MET:HE2	1.95	0.48
2:B:757:PRO:O	2:B:758:PHE:HB2	2.13	0.48
2:B:498:THR:HG22	2:B:537:LYS:H	1.78	0.48
1:A:445:ASN:ND2	1:A:455:MET:HE3	2.29	0.48
2:B:371:GLU:H	2:B:371:GLU:CD	2.17	0.48
4:D:173:HIS:O	4:D:177:VAL:HG23	2.13	0.48
1:A:780:VAL:O	1:A:780:VAL:HG12	2.14	0.48
3:C:42:PRO:HA	3:C:163:ILE:CG2	2.44	0.48
2:B:1034:VAL:HG23	2:B:1059:LEU:HD12	1.95	0.48
2:B:1020:ARG:CG	2:B:1020:ARG:NH1	2.68	0.48
4:D:190:GLU:O	4:D:194:LEU:HG	2.14	0.48
1:A:1051:ALA:O	1:A:1054:LEU:N	2.47	0.48
2:B:525:ALA:O	2:B:527:THR:HG22	2.13	0.48
2:B:810:GLU:HG3	2:B:815:ARG:HH22	1.79	0.48
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.96	0.48
1:A:726:ARG:O	1:A:727:ASP:C	2.50	0.48
1:A:437:MET:O	1:A:438:ASP:C	2.50	0.48
6:F:124:GLU:HB3	6:F:130:ILE:HG12	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:10:PHE:N	8:H:10:PHE:CD1	2.81	0.48
1:A:228:PHE:CD2	1:A:228:PHE:N	2.81	0.48
10:J:3:VAL:HG12	10:J:4:PRO:N	2.28	0.48
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.44	0.48
2:B:365:THR:CG2	2:B:367:LEU:HG	2.38	0.48
2:B:693:ILE:HD11	2:B:740:HIS:NE2	2.27	0.48
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.96	0.48
12:L:39:SER:O	12:L:40:LEU:HG	2.14	0.48
6:F:103:MET:CE	7:G:65:ASP:HB2	2.44	0.48
3:C:109:SER:O	3:C:110:THR:O	2.32	0.48
5:E:44:ALA:O	5:E:45:LYS:HB2	2.13	0.48
4:D:220:LEU:O	4:D:221:TYR:HD1	1.97	0.48
6:F:109:VAL:HG12	6:F:110:ASP:N	2.29	0.48
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.96	0.48
1:A:869:GLY:O	1:A:870:GLU:HB2	2.12	0.48
1:A:618:GLU:O	1:A:621:THR:N	2.46	0.48
2:B:509:ALA:O	2:B:510:LYS:O	2.32	0.48
1:A:936:LEU:H	1:A:936:LEU:HD23	1.78	0.48
2:B:797:TYR:HB3	2:B:798:TYR:CD2	2.49	0.48
3:C:63:ILE:O	3:C:64:ALA:C	2.50	0.48
1:A:503:GLN:O	1:A:504:LEU:HD12	2.13	0.48
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.96	0.48
8:H:84:ALA:HB2	8:H:87:ARG:HD2	1.96	0.48
2:B:681:TRP:O	2:B:683:SER:N	2.46	0.48
9:I:5:ARG:O	9:I:14:LEU:HD12	2.14	0.48
11:K:113:THR:O	11:K:114:LEU:CB	2.58	0.48
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.13	0.48
1:A:853:ASP:C	1:A:853:ASP:OD1	2.51	0.48
2:B:839:MET:N	2:B:989:THR:O	2.44	0.48
2:B:992:ILE:HD11	11:K:66:PRO:HB2	1.96	0.48
2:B:1135:ARG:NH2	2:B:1136:ASP:OD1	2.38	0.48
4:D:56:ARG:NH2	4:D:155:ARG:HA	2.28	0.48
1:A:524:VAL:HG12	1:A:525:GLN:N	2.19	0.48
1:A:626:ASN:O	1:A:628:GLY:N	2.42	0.48
1:A:1410:PHE:C	1:A:1412:ALA:H	2.15	0.48
2:B:578:THR:HA	2:B:622:LYS:HB3	1.94	0.48
4:D:185:CYS:HB3	4:D:211:LEU:HD13	1.95	0.48
8:H:81:PRO:HB3	8:H:82:PRO:HD2	1.92	0.48
1:A:852:TYR:CD2	1:A:1060:PRO:CB	2.97	0.48
6:F:99:LEU:O	6:F:103:MET:HG2	2.13	0.48
1:A:1216:ILE:O	1:A:1219:THR:HB	2.14	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:LEU:O	3:C:30:ALA:N	2.47	0.48
1:A:419:LYS:HG3	1:A:420:ARG:N	2.28	0.48
1:A:88:LYS:HE3	1:A:280:GLU:OE2	2.13	0.48
1:A:755:PHE:HA	1:A:758:ILE:HG13	1.94	0.48
1:A:1329:THR:O	1:A:1330:ASN:C	2.50	0.48
1:A:56:PRO:O	1:A:57:ARG:CG	2.57	0.48
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.33	0.48
2:B:273:LEU:HD21	2:B:360:PHE:CD1	2.48	0.48
1:A:14:VAL:HG21	1:A:1430:LEU:HD13	1.96	0.48
2:B:850:LEU:HD12	2:B:851:PHE:H	1.77	0.48
1:A:472:LEU:HD13	2:B:835:GLN:CD	2.33	0.48
1:A:1090:ALA:CB	1:A:1093:LYS:HE3	2.43	0.48
2:B:1208:MET:HA	2:B:1212:ILE:O	2.13	0.48
2:B:363:HIS:NE2	2:B:364:ILE:HG13	2.28	0.48
2:B:617:ARG:NE	2:B:619:ILE:HG12	2.28	0.48
5:E:17:ARG:O	5:E:20:LYS:HB2	2.13	0.48
2:B:654:ARG:H	2:B:657:HIS:CD2	2.28	0.48
6:F:72:LYS:O	6:F:73:ALA:CB	2.61	0.48
3:C:168:ALA:C	3:C:170:TRP:H	2.17	0.48
1:A:1293:SER:OG	1:A:1295:THR:CG2	2.62	0.48
5:E:136:ASN:OD1	5:E:137:GLU:N	2.46	0.48
1:A:817:ALA:O	1:A:818:MET:C	2.51	0.48
1:A:814:PHE:CD1	2:B:519:TRP:HE3	2.31	0.48
2:B:579:ARG:HH11	2:B:579:ARG:HG2	1.79	0.48
1:A:81:PHE:CE2	1:A:242:PRO:HA	2.48	0.48
2:B:992:ILE:CG2	2:B:994:TYR:HE1	2.26	0.48
2:B:992:ILE:HG21	2:B:994:TYR:HE1	1.79	0.48
2:B:689:LEU:O	2:B:690:VAL:HG23	2.14	0.48
9:I:58:VAL:HG13	9:I:62:ILE:CD1	2.44	0.48
1:A:261:ASP:O	1:A:264:PHE:HB2	2.13	0.48
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.29	0.48
2:B:247:GLY:C	2:B:249:ARG:H	2.16	0.48
1:A:1265:ASN:O	1:A:1267:MET:N	2.47	0.48
4:D:189:ASP:O	4:D:193:THR:HB	2.14	0.48
2:B:753:ALA:O	2:B:756:ILE:N	2.46	0.48
4:D:208:GLU:O	4:D:212:LYS:HG3	2.13	0.48
1:A:794:PRO:C	1:A:796:SER:H	2.18	0.48
1:A:779:PHE:O	1:A:780:VAL:C	2.52	0.48
1:A:351:THR:HB	2:B:1103:ILE:CD1	2.43	0.48
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.44	0.48
5:E:167:ARG:O	5:E:168:TYR:HD2	1.97	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:MET:O	1:A:123:ARG:C	2.51	0.48
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.18	0.48
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.95	0.48
1:A:1129:GLU:C	1:A:1131:ALA:N	2.67	0.48
5:E:204:THR:HG23	5:E:205:SER:N	2.28	0.47
1:A:823:GLY:C	1:A:825:ILE:N	2.66	0.47
2:B:579:ARG:HA	2:B:589:VAL:HG13	1.96	0.47
3:C:173:ALA:O	3:C:174:ALA:HB3	2.13	0.47
2:B:298:LEU:CD2	2:B:298:LEU:H	2.27	0.47
1:A:525:GLN:HB3	2:B:1015:HIS:CD2	2.48	0.47
3:C:213:PRO:O	3:C:214:ASN:CB	2.55	0.47
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.73	0.47
10:J:36:LEU:HB2	10:J:47:ARG:NH1	2.28	0.47
5:E:16:PHE:CE2	5:E:20:LYS:HE2	2.48	0.47
1:A:1388:GLY:O	1:A:1391:ARG:HG2	2.14	0.47
2:B:240:ILE:HG21	2:B:381:MET:HE1	1.96	0.47
2:B:486:TYR:CG	2:B:1096:ARG:NH2	2.82	0.47
1:A:22:PHE:CD1	2:B:1213:THR:HG22	2.49	0.47
4:D:196:PRO:C	4:D:198:LEU:N	2.67	0.47
1:A:1263:ILE:O	1:A:1263:ILE:HG22	2.14	0.47
9:I:69:PRO:O	9:I:84:VAL:HA	2.14	0.47
8:H:128:ASN:CG	8:H:128:ASN:O	2.52	0.47
5:E:202:SER:HB3	5:E:205:SER:O	2.15	0.47
10:J:61:LEU:C	10:J:63:TYR:H	2.16	0.47
1:A:821:ARG:HA	1:A:824:LEU:HD12	1.95	0.47
2:B:880:THR:HB	2:B:934:LYS:CD	2.36	0.47
12:L:54:ARG:HG3	12:L:54:ARG:NH1	2.29	0.47
6:F:132:LEU:O	6:F:148:VAL:HG22	2.14	0.47
1:A:321:PRO:O	1:A:322:VAL:HB	2.13	0.47
2:B:413:LEU:O	2:B:414:ALA:C	2.52	0.47
3:C:112:ASN:CB	3:C:114:TYR:CE1	2.98	0.47
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.95	0.47
1:A:393:ARG:O	1:A:395:GLY:N	2.47	0.47
1:A:329:LEU:HD23	1:A:329:LEU:N	2.28	0.47
1:A:1116:LEU:HA	1:A:1329:THR:HA	1.96	0.47
1:A:1311:VAL:HG11	1:A:1329:THR:HG21	1.96	0.47
2:B:831:SER:HB2	2:B:833:TYR:HD1	1.79	0.47
1:A:254:GLU:O	2:B:935:ARG:NH1	2.45	0.47
2:B:1002:THR:HG22	2:B:1006:ILE:O	2.14	0.47
2:B:681:TRP:C	2:B:683:SER:N	2.66	0.47
9:I:26:LEU:CD2	9:I:37:GLU:HA	2.41	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:ALA:O	1:A:761:MET:N	2.47	0.47
2:B:764:SER:N	2:B:765:PRO:HD2	2.29	0.47
4:D:51:ASN:C	4:D:52:LEU:O	2.52	0.47
12:L:48:CYS:O	12:L:50:ASP:N	2.47	0.47
1:A:1006:ILE:HD11	5:E:163:GLU:CG	2.44	0.47
4:D:29:LEU:N	4:D:29:LEU:HD23	2.30	0.47
11:K:63:VAL:O	11:K:63:VAL:HG23	2.15	0.47
1:A:53:LEU:HD23	1:A:54:ASN:CB	2.45	0.47
6:F:77:ASP:O	6:F:79:ARG:N	2.47	0.47
1:A:962:ARG:O	1:A:964:ILE:N	2.47	0.47
2:B:314:LEU:O	2:B:315:LYS:C	2.53	0.47
6:F:111:LEU:O	6:F:113:GLY:N	2.47	0.47
4:D:51:ASN:O	4:D:52:LEU:O	2.33	0.47
2:B:202:TYR:CE1	2:B:209:GLU:HG2	2.50	0.47
5:E:207:ARG:NH1	5:E:207:ARG:HB3	2.28	0.47
2:B:1060:ARG:NH1	2:B:1060:ARG:HG2	2.26	0.47
3:C:227:THR:C	3:C:228:PHE:CD1	2.87	0.47
2:B:1017:ILE:HG22	2:B:1018:PRO:CD	2.44	0.47
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.96	0.47
3:C:206:ASN:OD1	3:C:229:TYR:CD2	2.67	0.47
1:A:696:GLU:HG2	1:A:696:GLU:O	2.15	0.47
2:B:882:THR:O	2:B:883:LEU:CB	2.63	0.47
2:B:1155:SER:OG	2:B:1156:ASP:N	2.47	0.47
1:A:894:GLU:C	1:A:896:ARG:H	2.18	0.47
2:B:999:MET:HB3	2:B:1007:VAL:CG2	2.44	0.47
10:J:18:TRP:HA	10:J:18:TRP:CE3	2.49	0.47
10:J:48:ARG:HE	10:J:49:MET:CE	2.28	0.47
1:A:650:GLN:O	1:A:654:ASN:HB2	2.14	0.47
3:C:114:TYR:CD1	3:C:114:TYR:N	2.83	0.47
1:A:1263:ILE:O	1:A:1267:MET:HG3	2.15	0.47
6:F:128:LYS:HD3	6:F:149:GLU:O	2.15	0.47
2:B:781:PHE:CD1	2:B:781:PHE:C	2.88	0.47
2:B:510:LYS:HD3	2:B:513:GLN:H	1.80	0.47
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.95	0.47
1:A:253:ASN:OD1	2:B:884:ARG:HD2	2.14	0.47
11:K:65:HIS:CD2	11:K:65:HIS:C	2.87	0.47
1:A:1437:GLY:CA	6:F:88:TYR:CD2	2.97	0.47
1:A:567:LYS:HE3	8:H:46:LEU:HD12	1.97	0.47
2:B:38:PHE:HD1	2:B:811:TYR:CD2	2.31	0.47
7:G:81:PRO:HA	7:G:85:GLU:OE1	2.15	0.47
5:E:90:VAL:HG23	5:E:120:ALA:HA	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:GLY:O	1:A:650:GLN:HB2	2.14	0.47
2:B:1210:MET:O	2:B:1212:ILE:N	2.47	0.47
2:B:1191:ILE:C	2:B:1192:TYR:CD1	2.88	0.47
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.44	0.47
1:A:24:PRO:HG2	1:A:25:GLU:CD	2.35	0.47
2:B:658:ILE:HG22	2:B:659:ALA:N	2.28	0.47
3:C:116:LYS:HD3	3:C:140:ASN:HB3	1.95	0.47
6:F:124:GLU:O	6:F:130:ILE:HG13	2.14	0.47
1:A:590:ARG:HD3	1:A:604:GLY:CA	2.41	0.47
10:J:57:ILE:CA	10:J:60:PHE:CD2	2.90	0.47
1:A:1335:ILE:O	1:A:1335:ILE:CG2	2.63	0.47
2:B:825:VAL:CG1	2:B:826:ALA:N	2.77	0.47
3:C:47:ASP:O	3:C:48:SER:HB2	2.13	0.47
3:C:191:TYR:CD2	3:C:201:TRP:CD1	2.97	0.47
1:A:356:ASP:HB2	1:A:469:ARG:HG2	1.96	0.47
10:J:14:VAL:O	10:J:16:ASP:N	2.48	0.47
10:J:7:CYS:HA	10:J:49:MET:HE3	1.95	0.47
2:B:863:GLU:O	2:B:961:LEU:HD22	2.15	0.47
1:A:1342:GLU:CG	5:E:198:ILE:HG21	2.45	0.47
2:B:850:LEU:HD12	2:B:851:PHE:N	2.30	0.47
9:I:99:LEU:C	9:I:100:PHE:HD1	2.18	0.47
1:A:375:THR:HA	1:A:434:ARG:O	2.14	0.47
1:A:95:PHE:HD1	1:A:234:MET:CG	2.25	0.47
1:A:324:SER:O	1:A:325:ILE:C	2.52	0.47
2:B:745:PRO:O	2:B:748:ILE:CG1	2.61	0.47
5:E:7:ARG:CG	5:E:8:ASN:N	2.76	0.47
3:C:22:LEU:HD13	3:C:230:MET:CE	2.44	0.47
7:G:145:VAL:CG1	7:G:146:LYS:H	2.27	0.47
1:A:1280:GLU:O	1:A:1281:ARG:C	2.52	0.47
2:B:642:ASP:HA	2:B:649:LYS:HA	1.95	0.47
3:C:263:THR:O	3:C:265:MET:N	2.47	0.47
2:B:847:ASP:OD2	11:K:6:ARG:NH2	2.48	0.47
1:A:317:LYS:O	1:A:318:SER:HB3	2.14	0.47
8:H:39:THR:HB	8:H:124:ARG:HB3	1.97	0.47
2:B:371:GLU:OE1	2:B:371:GLU:N	2.48	0.47
1:A:1272:THR:C	1:A:1273:LEU:HD12	2.34	0.47
1:A:103:CYS:SG	1:A:108:MET:HE1	2.54	0.47
1:A:1162:VAL:HG12	1:A:1162:VAL:O	2.15	0.47
8:H:31:THR:O	8:H:31:THR:HG22	2.15	0.47
2:B:465:ASN:HD22	2:B:465:ASN:N	2.12	0.47
1:A:1111:MET:H	1:A:1111:MET:HG2	1.57	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:HIS:O	2:B:1137:CYS:SG	2.73	0.47
1:A:1157:ASP:C	1:A:1159:ARG:H	2.18	0.47
1:A:447:GLN:HB3	1:A:448:PRO:HA	1.97	0.47
1:A:1311:VAL:HG21	1:A:1329:THR:HG23	1.96	0.47
7:G:56:ILE:O	7:G:57:GLN:HB2	2.15	0.47
1:A:1081:LEU:HD21	1:A:1098:VAL:CB	2.44	0.47
5:E:177:ARG:O	5:E:212:ARG:HD3	2.15	0.47
6:F:132:LEU:HD22	7:G:61:ILE:HD11	1.97	0.47
9:I:11:ASN:O	9:I:12:ASN:ND2	2.48	0.47
2:B:899:ILE:HG23	2:B:903:VAL:HG21	1.95	0.47
6:F:119:ARG:HH11	6:F:119:ARG:CG	2.25	0.47
1:A:1227:ILE:O	1:A:1228:TRP:HB3	2.14	0.47
3:C:228:PHE:N	3:C:228:PHE:CD1	2.83	0.47
8:H:76:THR:HG22	8:H:76:THR:O	2.15	0.47
2:B:170:LEU:HG	2:B:170:LEU:O	2.14	0.47
1:A:863:VAL:O	1:A:864:ILE:CG1	2.63	0.47
1:A:983:ILE:HG22	1:A:983:ILE:O	2.15	0.47
2:B:834:ASN:HA	2:B:838:SER:O	2.15	0.47
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.96	0.47
2:B:1159:ARG:CD	2:B:1193:GLN:HE21	2.26	0.47
1:A:76:GLU:O	1:A:76:GLU:CG	2.63	0.47
2:B:293:PRO:O	2:B:294:ASP:O	2.33	0.47
2:B:294:ASP:C	2:B:296:GLU:N	2.68	0.47
5:E:198:ILE:CD1	5:E:212:ARG:NH1	2.78	0.47
1:A:500:GLU:O	1:A:504:LEU:HB2	2.15	0.47
1:A:708:MET:HE3	1:A:1090:ALA:O	2.14	0.47
2:B:956:THR:CG2	2:B:960:GLY:HA2	2.45	0.47
1:A:606:LEU:CB	1:A:614:PHE:CE2	2.97	0.47
1:A:549:MET:O	1:A:550:LEU:C	2.53	0.47
1:A:626:ASN:O	1:A:631:HIS:CB	2.63	0.47
3:C:118:LEU:HB2	3:C:132:PRO:HG2	1.97	0.47
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.50	0.47
1:A:385:ILE:HG22	1:A:386:ASP:N	2.29	0.47
2:B:942:ARG:O	2:B:944:THR:N	2.48	0.47
1:A:1057:VAL:CG1	1:A:1058:VAL:N	2.76	0.47
2:B:223:VAL:HG11	2:B:381:MET:HG2	1.96	0.47
1:A:1051:ALA:C	1:A:1053:PHE:N	2.67	0.47
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.14	0.47
1:A:125:ALA:O	1:A:127:ALA:N	2.48	0.47
2:B:785:TYR:HA	2:B:788:ARG:HG3	1.97	0.47
2:B:871:THR:HG22	2:B:872:GLU:N	2.31	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:99:LEU:HB2	9:I:101:PHE:CE1	2.50	0.47
11:K:83:PRO:O	11:K:86:ALA:HB3	2.15	0.47
1:A:668:ASP:CG	1:A:742:ASN:HD22	2.19	0.47
1:A:647:GLY:O	1:A:648:ASN:C	2.54	0.47
2:B:1204:PHE:CE1	2:B:1216:LEU:HD11	2.50	0.47
1:A:222:LEU:O	1:A:224:PHE:N	2.48	0.47
1:A:711:ARG:HA	9:I:97:MET:CE	2.44	0.47
11:K:12:LEU:HD23	11:K:16:GLU:O	2.14	0.47
4:D:130:LEU:O	4:D:132:GLN:N	2.48	0.47
2:B:752:ALA:HB1	2:B:771:SER:HB3	1.96	0.47
1:A:543:LEU:O	1:A:544:ASP:C	2.52	0.47
10:J:23:ASN:C	10:J:25:LEU:N	2.68	0.47
1:A:809:THR:HG23	1:A:812:GLU:OE1	2.15	0.47
8:H:106:GLU:HG2	8:H:112:ILE:HG12	1.96	0.47
1:A:1313:LEU:O	1:A:1314:SER:C	2.52	0.46
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.96	0.46
1:A:897:TYR:HB3	1:A:936:LEU:CD1	2.45	0.46
2:B:1150:ARG:HE	2:B:1150:ARG:HA	1.80	0.46
1:A:164:ARG:CG	1:A:165:GLY:H	2.01	0.46
1:A:866:PHE:HD2	5:E:168:TYR:CE1	2.33	0.46
2:B:1182:CYS:O	2:B:1183:LYS:C	2.53	0.46
8:H:89:LEU:C	8:H:91:ASP:N	2.68	0.46
1:A:115:LEU:O	1:A:122:MET:HE2	2.14	0.46
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.98	0.46
1:A:535:THR:O	1:A:536:LEU:O	2.34	0.46
1:A:937:VAL:C	1:A:939:ASP:N	2.68	0.46
2:B:544:CYS:O	2:B:545:ILE:HG13	2.15	0.46
2:B:69:LEU:HD13	2:B:429:PHE:HD1	1.80	0.46
1:A:1129:GLU:HG3	1:A:1132:LYS:HE3	1.97	0.46
1:A:100:LYS:O	1:A:101:LYS:C	2.54	0.46
1:A:789:LYS:HE3	9:I:67:THR:HB	1.97	0.46
1:A:548:ASN:HA	11:K:60:ALA:HB1	1.97	0.46
1:A:551:TYR:CE2	11:K:62:LYS:HE2	2.50	0.46
2:B:1079:LYS:HE3	3:C:188:HIS:CE1	2.51	0.46
1:A:944:ARG:NE	1:A:1298:TYR:HE1	2.13	0.46
1:A:907:THR:HG22	1:A:908:LEU:N	2.30	0.46
1:A:1282:VAL:O	1:A:1283:VAL:HG22	2.14	0.46
1:A:80:HIS:O	1:A:243:PRO:HB3	2.16	0.46
2:B:798:TYR:CD2	2:B:798:TYR:N	2.83	0.46
1:A:560:ILE:CG1	8:H:78:SER:HB2	2.36	0.46
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:906:SER:O	2:B:907:GLY:O	2.33	0.46
1:A:1057:VAL:CG1	1:A:1058:VAL:H	2.26	0.46
2:B:546:SER:HA	2:B:612:GLU:CD	2.35	0.46
5:E:143:ASN:OD1	5:E:187:TYR:CE1	2.68	0.46
12:L:27:LEU:HD13	12:L:37:LYS:HE2	1.96	0.46
5:E:25:ASP:C	5:E:27:GLY:H	2.17	0.46
2:B:285:ILE:O	2:B:288:ALA:HB3	2.15	0.46
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.29	0.46
1:A:353:ILE:HG23	1:A:485:ASP:O	2.16	0.46
1:A:63:ARG:HA	1:A:74:MET:CE	2.45	0.46
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.48	0.46
2:B:281:PRO:O	2:B:283:VAL:N	2.48	0.46
1:A:1122:PRO:O	1:A:1123:GLY:C	2.54	0.46
2:B:540:SER:HA	2:B:749:LEU:O	2.14	0.46
1:A:285:PRO:CG	1:A:288:ALA:HB3	2.40	0.46
1:A:1451:VAL:C	1:A:1453:TYR:H	2.19	0.46
1:A:1220:PHE:CE2	1:A:1263:ILE:HG23	2.50	0.46
1:A:103:CYS:SG	1:A:108:MET:CE	3.04	0.46
4:D:154:PHE:HB2	4:D:160:VAL:HG22	1.97	0.46
11:K:70:ARG:HG3	11:K:70:ARG:O	2.16	0.46
2:B:743:ILE:H	2:B:743:ILE:HG12	1.51	0.46
1:A:928:LEU:O	1:A:931:GLU:N	2.47	0.46
1:A:1327:ILE:HG22	5:E:147:HIS:CE1	2.51	0.46
7:G:18:PHE:HA	7:G:22:MET:CE	2.45	0.46
2:B:549:THR:CG2	2:B:550:ASP:H	2.17	0.46
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.98	0.46
1:A:1080:THR:HG22	1:A:1081:LEU:H	1.81	0.46
6:F:90:ARG:CG	6:F:91:ALA:N	2.78	0.46
8:H:143:LEU:O	8:H:144:ILE:HG13	2.16	0.46
3:C:95:CYS:O	3:C:96:SER:HB3	2.15	0.46
12:L:28:LYS:HG3	12:L:39:SER:OG	2.15	0.46
1:A:1083:THR:O	1:A:1084:PHE:O	2.34	0.46
2:B:58:THR:O	2:B:62:ILE:HG13	2.15	0.46
1:A:715:GLU:O	1:A:718:VAL:N	2.48	0.46
3:C:107:SER:C	3:C:109:SER:N	2.69	0.46
1:A:695:LYS:C	1:A:697:ALA:N	2.69	0.46
5:E:24:LYS:HG3	5:E:25:ASP:N	2.31	0.46
1:A:928:LEU:O	1:A:929:LEU:C	2.53	0.46
1:A:1119:TYR:CD2	1:A:1305:VAL:HG21	2.51	0.46
2:B:189:LEU:O	2:B:192:LEU:HB2	2.15	0.46
1:A:915:SER:O	1:A:919:ILE:HG13	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLU:H	2:B:935:ARG:HH12	1.63	0.46
1:A:43:GLU:O	1:A:44:THR:HB	2.15	0.46
2:B:1033:LYS:HB2	2:B:1089:PRO:HD2	1.97	0.46
1:A:1081:LEU:CD1	1:A:1099:PRO:HD3	2.45	0.46
1:A:867:ILE:CG2	1:A:872:GLY:H	2.29	0.46
4:D:141:LEU:O	4:D:144:THR:HB	2.16	0.46
9:I:73:ARG:HD2	9:I:101:PHE:CE2	2.50	0.46
9:I:83:ASN:HA	9:I:102:VAL:O	2.16	0.46
5:E:90:VAL:HB	5:E:119:SER:HB2	1.98	0.46
2:B:615:MET:HA	2:B:625:LYS:O	2.16	0.46
2:B:1164:GLY:HA3	2:B:1190:ASP:OD2	2.16	0.46
4:D:170:THR:HG21	4:D:172:LEU:HG	1.94	0.46
2:B:1023:VAL:HG12	2:B:1027:ILE:HG13	1.97	0.46
1:A:414:ASP:O	1:A:416:ARG:N	2.48	0.46
1:A:777:PHE:CE2	1:A:782:ARG:HA	2.51	0.46
9:I:2:THR:HG22	9:I:2:THR:O	2.15	0.46
2:B:570:VAL:HG21	2:B:573:GLN:CD	2.36	0.46
2:B:51:PHE:O	2:B:52:ASN:C	2.53	0.46
1:A:33:ALA:O	1:A:83:HIS:HD2	1.99	0.46
1:A:18:GLN:CB	2:B:1215:ARG:HB2	2.45	0.46
3:C:15:LYS:O	3:C:240:VAL:HG22	2.16	0.46
10:J:8:PHE:CE1	10:J:49:MET:SD	3.08	0.46
1:A:1081:LEU:CD2	1:A:1098:VAL:HG21	2.45	0.46
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.80	0.46
1:A:707:GLY:O	1:A:708:MET:O	2.34	0.46
8:H:100:THR:HG22	8:H:101:ALA:H	1.79	0.46
6:F:135:ARG:HD3	6:F:143:PHE:CD2	2.51	0.46
12:L:30:ILE:O	12:L:56:LEU:HD23	2.15	0.46
2:B:760:ASP:O	2:B:761:HIS:CG	2.69	0.46
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.96	0.46
12:L:52:GLY:O	12:L:53:HIS:C	2.54	0.46
11:K:88:LYS:O	11:K:91:CYS:N	2.49	0.46
1:A:298:PHE:HZ	1:A:314:ALA:HB2	1.81	0.46
11:K:78:THR:O	11:K:79:GLU:C	2.53	0.46
2:B:1111:MET:O	2:B:1112:GLN:C	2.54	0.46
11:K:10:PHE:CD2	11:K:10:PHE:N	2.84	0.46
4:D:40:HIS:CE1	4:D:41:GLN:HE21	2.34	0.46
1:A:1115:SER:OG	1:A:1116:LEU:N	2.49	0.46
2:B:834:ASN:O	2:B:838:SER:O	2.34	0.46
2:B:385:LEU:O	2:B:385:LEU:HD12	2.15	0.46
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.56	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.35	0.46
5:E:197:LYS:O	5:E:199:ILE:HG13	2.16	0.46
1:A:321:PRO:O	1:A:322:VAL:CG2	2.63	0.46
2:B:520:GLY:H	2:B:748:ILE:HG22	1.81	0.46
3:C:147:LEU:HD23	3:C:147:LEU:N	2.31	0.46
2:B:770:GLN:CD	2:B:983:ARG:HA	2.36	0.46
5:E:144:ILE:C	5:E:146:HIS:H	2.19	0.46
2:B:390:LEU:O	2:B:391:ASP:C	2.54	0.46
1:A:543:LEU:HD11	1:A:547:LEU:HD11	1.96	0.46
9:I:15:TYR:O	9:I:28:GLU:HG2	2.16	0.46
1:A:809:THR:HB	1:A:810:PRO:HD2	1.97	0.46
1:A:7:SER:O	1:A:8:SER:C	2.54	0.46
1:A:1330:ASN:C	1:A:1330:ASN:OD1	2.52	0.46
2:B:613:VAL:HG22	2:B:628:THR:HA	1.98	0.46
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	2.19	0.46
3:C:80:LEU:O	3:C:80:LEU:HG	2.16	0.46
6:F:86:THR:HG1	6:F:89:GLU:HG3	1.79	0.46
2:B:901:PRO:O	2:B:902:GLY:C	2.53	0.46
1:A:302:THR:HA	1:A:305:ASP:O	2.14	0.46
1:A:993:LEU:HD11	1:A:997:LEU:HD21	1.96	0.46
2:B:95:ILE:HG13	2:B:130:VAL:CG2	2.44	0.46
1:A:1210:GLY:O	1:A:1214:GLU:HB2	2.16	0.46
5:E:93:MET:C	5:E:95:THR:N	2.68	0.46
1:A:1116:LEU:HB2	1:A:1329:THR:OG1	2.16	0.46
1:A:353:ILE:HG13	1:A:482:PHE:CD2	2.51	0.46
7:G:14:HIS:CD2	7:G:16:SER:H	2.34	0.46
2:B:816:GLU:O	2:B:817:LEU:CD2	2.59	0.46
1:A:814:PHE:O	1:A:817:ALA:HB3	2.15	0.46
3:C:242:GLN:HA	3:C:245:VAL:CG2	2.45	0.46
2:B:1034:VAL:CG1	2:B:1035:ALA:N	2.78	0.46
1:A:1104:ILE:O	1:A:1105:LEU:C	2.53	0.46
1:A:871:ASP:CG	1:A:1366:ARG:HH22	2.19	0.46
1:A:566:ILE:O	1:A:567:LYS:O	2.34	0.46
2:B:806:THR:C	2:B:808:ALA:N	2.68	0.46
12:L:58:LYS:HG2	12:L:58:LYS:O	2.15	0.46
2:B:789:MET:CE	2:B:965:LYS:HB3	2.46	0.46
1:A:1193:LEU:HD12	1:A:1193:LEU:C	2.35	0.46
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.98	0.46
1:A:1067:LEU:O	1:A:1068:ALA:C	2.54	0.46
10:J:61:LEU:O	10:J:63:TYR:N	2.48	0.46
2:B:551:PRO:HG2	2:B:552:MET:H	1.81	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:TYR:HD2	1:A:936:LEU:CD1	2.28	0.46
2:B:990:ILE:HG22	2:B:992:ILE:H	1.81	0.46
2:B:1149:GLU:C	2:B:1151:LEU:N	2.67	0.46
3:C:56:THR:HG21	3:C:145:CYS:HG	1.77	0.46
10:J:3:VAL:CG2	10:J:18:TRP:CG	2.99	0.46
1:A:1169:ILE:O	1:A:1170:ILE:C	2.54	0.46
6:F:87:LYS:HG3	6:F:88:TYR:CD1	2.51	0.46
3:C:214:ASN:HB3	3:C:217:ASP:OD2	2.16	0.46
2:B:172:ILE:CG2	2:B:173:MET:N	2.79	0.46
1:A:1173:HIS:CG	1:A:1227:ILE:HG23	2.51	0.46
2:B:1178:ASN:O	2:B:1179:GLN:C	2.55	0.46
2:B:984:HIS:CD2	2:B:1025:HIS:HA	2.51	0.46
3:C:170:TRP:O	3:C:171:GLY:C	2.54	0.46
1:A:100:LYS:O	1:A:103:CYS:N	2.49	0.46
1:A:738:LYS:HZ1	3:C:194:GLU:C	2.18	0.46
3:C:66:ARG:HH21	10:J:5:VAL:HG23	1.80	0.45
2:B:1183:LYS:CE	2:B:1183:LYS:H	2.27	0.45
1:A:1402:PHE:CD1	1:A:1403:GLU:HG3	2.50	0.45
2:B:952:VAL:CG1	2:B:953:LEU:N	2.79	0.45
2:B:964:VAL:HG12	2:B:965:LYS:N	2.32	0.45
1:A:937:VAL:HG12	1:A:938:LYS:N	2.30	0.45
5:E:157:SER:C	5:E:159:ASP:N	2.68	0.45
1:A:989:GLY:C	1:A:991:LYS:N	2.69	0.45
2:B:20:ASP:C	2:B:22:SER:H	2.19	0.45
1:A:1329:THR:O	1:A:1331:SER:N	2.49	0.45
1:A:1330:ASN:OD1	1:A:1331:SER:N	2.49	0.45
1:A:814:PHE:C	1:A:814:PHE:CD2	2.88	0.45
2:B:838:SER:HA	2:B:989:THR:O	2.16	0.45
3:C:163:ILE:O	3:C:164:ALA:C	2.54	0.45
3:C:251:LEU:O	3:C:254:LYS:N	2.49	0.45
1:A:834:THR:CG2	1:A:1077:THR:HA	2.46	0.45
2:B:994:TYR:HB2	2:B:999:MET:CE	2.46	0.45
1:A:1102:LYS:C	1:A:1106:ASN:HD22	2.18	0.45
1:A:1354:ASN:O	1:A:1355:VAL:C	2.54	0.45
2:B:284:ILE:HG12	2:B:324:ILE:HD12	1.98	0.45
2:B:1115:THR:HG22	2:B:1117:GLN:CG	2.46	0.45
8:H:24:CYS:CB	8:H:44:VAL:HG21	2.46	0.45
8:H:98:TYR:HE1	8:H:139:ASN:HA	1.80	0.45
1:A:108:MET:O	1:A:109:HIS:HB2	2.16	0.45
1:A:125:ALA:C	1:A:127:ALA:H	2.20	0.45
7:G:27:LYS:O	7:G:31:LEU:HG	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:VAL:CG1	1:A:461:LYS:N	2.79	0.45
3:C:46:ILE:HD13	3:C:157:CYS:CB	2.46	0.45
2:B:785:TYR:CE2	10:J:60:PHE:CE1	3.04	0.45
1:A:808:LEU:N	1:A:808:LEU:CD1	2.78	0.45
2:B:975:GLN:HG2	2:B:976:ILE:N	2.32	0.45
2:B:281:PRO:HG2	2:B:284:ILE:CG1	2.44	0.45
8:H:95:TYR:HE2	8:H:97:MET:CG	2.29	0.45
2:B:43:LEU:HD11	2:B:811:TYR:O	2.15	0.45
12:L:59:ALA:O	12:L:60:ARG:O	2.34	0.45
5:E:124:VAL:CG1	5:E:132:ILE:HB	2.43	0.45
4:D:48:ILE:CG2	7:G:4:ILE:HB	2.46	0.45
5:E:16:PHE:O	5:E:17:ARG:C	2.54	0.45
1:A:1016:THR:O	1:A:1018:PHE:N	2.49	0.45
2:B:313:MET:CE	2:B:390:LEU:HD21	2.46	0.45
7:G:132:SER:HB3	7:G:135:ASP:HB2	1.97	0.45
2:B:558:LEU:C	2:B:560:GLU:N	2.70	0.45
1:A:811:GLN:O	1:A:812:GLU:C	2.55	0.45
1:A:814:PHE:CD1	2:B:519:TRP:CE3	3.05	0.45
1:A:42:ASP:CG	1:A:45:GLN:HA	2.37	0.45
1:A:1170:ILE:HG23	1:A:1174:PHE:HE1	1.78	0.45
2:B:958:GLN:C	2:B:960:GLY:H	2.19	0.45
1:A:563:PRO:HB2	1:A:565:ILE:O	2.16	0.45
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.22	0.45
2:B:899:ILE:HG22	2:B:903:VAL:HG21	1.95	0.45
10:J:36:LEU:HB2	10:J:47:ARG:HH12	1.81	0.45
1:A:688:LYS:O	1:A:690:VAL:N	2.50	0.45
4:D:176:GLU:O	4:D:180:LEU:HB2	2.17	0.45
2:B:394:ASP:OD2	9:I:91:ARG:HD2	2.17	0.45
2:B:510:LYS:HD3	2:B:513:GLN:N	2.31	0.45
2:B:555:ILE:HD11	2:B:587:HIS:NE2	2.32	0.45
2:B:882:THR:O	2:B:883:LEU:HB2	2.17	0.45
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.17	0.45
2:B:386:LEU:O	2:B:388:CYS:N	2.50	0.45
2:B:287:ARG:NH1	2:B:324:ILE:O	2.50	0.45
8:H:23:VAL:HG22	8:H:43:ASN:HA	1.99	0.45
2:B:806:THR:HG22	2:B:808:ALA:CB	2.46	0.45
1:A:550:LEU:HD11	1:A:561:PRO:HD2	1.98	0.45
2:B:638:PHE:HD2	2:B:690:VAL:HG22	1.82	0.45
12:L:60:ARG:HG2	12:L:61:THR:N	2.27	0.45
1:A:760:GLN:O	1:A:804:TYR:CD1	2.70	0.45
3:C:52:GLU:HA	12:L:64:LEU:HD22	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:51:ASN:OD1	4:D:52:LEU:O	2.34	0.45
1:A:711:ARG:HA	9:I:97:MET:HE1	1.97	0.45
1:A:1191:TRP:HB3	1:A:1260:LEU:HD23	1.97	0.45
1:A:1343:ALA:HB2	5:E:150:VAL:HG22	1.99	0.45
1:A:1359:ASP:HB2	1:A:1361:SER:OG	2.16	0.45
1:A:791:ASP:C	1:A:791:ASP:OD1	2.55	0.45
3:C:21:ILE:HG22	3:C:21:ILE:O	2.17	0.45
3:C:43:THR:HG22	3:C:44:LEU:H	1.81	0.45
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.51	0.45
1:A:44:THR:HG22	1:A:44:THR:O	2.16	0.45
2:B:1184:GLY:C	2:B:1186:ASP:N	2.66	0.45
1:A:524:VAL:CG1	1:A:525:GLN:H	2.16	0.45
1:A:849:MET:O	1:A:851:HIS:HD2	1.99	0.45
9:I:34:TYR:C	9:I:34:TYR:CD2	2.90	0.45
2:B:710:LEU:O	2:B:711:GLU:HG2	2.17	0.45
2:B:855:PHE:CD1	2:B:856:PHE:N	2.85	0.45
2:B:63:ILE:HD12	2:B:421:PHE:CE2	2.51	0.45
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.98	0.45
1:A:19:PHE:O	1:A:1416:ALA:HA	2.17	0.45
1:A:881:GLN:NE2	1:A:958:VAL:O	2.42	0.45
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.17	0.45
2:B:992:ILE:HD13	2:B:994:TYR:HE1	1.81	0.45
2:B:295:GLY:H	2:B:298:LEU:CD2	2.13	0.45
2:B:280:ILE:HG23	2:B:281:PRO:HD2	1.99	0.45
2:B:217:ARG:C	2:B:217:ARG:HD2	2.37	0.45
1:A:642:CYS:O	1:A:643:ALA:C	2.55	0.45
1:A:1406:VAL:HG12	1:A:1410:PHE:CD1	2.52	0.45
2:B:758:PHE:O	2:B:760:ASP:N	2.49	0.45
3:C:22:LEU:CD2	3:C:25:VAL:HG21	2.47	0.45
12:L:40:LEU:HD22	12:L:44:ASP:CB	2.47	0.45
1:A:1261:LYS:C	1:A:1264:GLU:H	2.20	0.45
1:A:1385:THR:CG2	1:A:1386:ARG:N	2.79	0.45
1:A:1213:GLY:O	1:A:1214:GLU:C	2.54	0.45
1:A:1397:LEU:HA	1:A:1400:CYS:HB2	1.99	0.45
4:D:53:SER:HB3	4:D:153:ARG:H	1.81	0.45
2:B:753:ALA:HA	2:B:756:ILE:HG13	1.99	0.45
4:D:122:GLU:HA	4:D:125:SER:OG	2.17	0.45
2:B:372:SER:O	2:B:376:PHE:HD1	2.00	0.45
2:B:274:PRO:O	2:B:275:TYR:HB2	2.16	0.45
2:B:1181:GLU:OE1	2:B:1183:LYS:HG3	2.17	0.45
2:B:851:PHE:O	2:B:974:PRO:HD3	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ARG:NE	2:B:1192:TYR:HE2	2.15	0.45
2:B:202:TYR:N	2:B:202:TYR:CD2	2.84	0.45
1:A:1227:ILE:CG2	1:A:1228:TRP:N	2.78	0.45
1:A:847:ASP:N	1:A:847:ASP:OD1	2.48	0.45
1:A:1293:SER:OG	1:A:1295:THR:HG23	2.17	0.45
1:A:512:VAL:HG11	1:A:876:ALA:O	2.16	0.45
2:B:255:GLN:O	2:B:271:ALA:HB1	2.17	0.45
8:H:12:VAL:HA	8:H:28:ALA:HB2	1.99	0.45
1:A:1271:ILE:CG2	1:A:1271:ILE:O	2.65	0.45
10:J:1:MET:HB2	10:J:1:MET:HE2	1.86	0.45
2:B:981:ALA:CB	2:B:987:LYS:HA	2.46	0.45
1:A:901:LEU:CG	1:A:926:GLN:HE21	2.28	0.45
1:A:78:PRO:O	1:A:78:PRO:HG2	2.17	0.45
2:B:293:PRO:HG2	2:B:296:GLU:OE1	2.16	0.45
3:C:178:PHE:O	3:C:179:GLU:HB2	2.16	0.45
5:E:117:THR:O	5:E:120:ALA:N	2.45	0.45
1:A:556:TRP:CE2	1:A:558:GLY:HA2	2.51	0.45
2:B:578:THR:HG23	2:B:622:LYS:CA	2.47	0.45
3:C:50:GLU:HB3	3:C:156:THR:HB	1.98	0.45
5:E:135:PHE:CB	5:E:140:LEU:HD11	2.47	0.45
12:L:38:LEU:O	12:L:39:SER:CB	2.58	0.45
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.50	0.45
11:K:90:ALA:O	11:K:94:ILE:HG13	2.17	0.45
9:I:88:SER:C	9:I:90:GLN:N	2.70	0.45
1:A:1143:LEU:HD12	1:A:1146:VAL:HG23	1.99	0.45
5:E:138:ALA:HA	5:E:141:VAL:CG2	2.47	0.45
2:B:489:SER:OG	2:B:490:SER:N	2.49	0.45
7:G:101:VAL:HG12	7:G:102:GLN:N	2.32	0.45
2:B:1026:LEU:HD23	2:B:1086:PHE:CE2	2.52	0.45
3:C:62:PHE:O	3:C:65:HIS:HB3	2.17	0.45
10:J:7:CYS:SG	10:J:49:MET:CE	3.01	0.45
1:A:1170:ILE:O	1:A:1174:PHE:HD1	1.99	0.45
5:E:171:LYS:O	5:E:172:GLU:C	2.55	0.45
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.52	0.45
2:B:766:ARG:HH22	2:B:1020:ARG:HG2	1.79	0.45
8:H:44:VAL:O	8:H:44:VAL:CG1	2.61	0.45
2:B:233:PRO:HG2	2:B:234:ILE:CD1	2.47	0.45
3:C:44:LEU:HG	3:C:159:ALA:HB1	1.99	0.44
3:C:46:ILE:HD13	3:C:157:CYS:HB3	1.99	0.44
10:J:1:MET:N	10:J:56:LEU:N	2.65	0.44
1:A:470:LEU:HD11	1:A:482:PHE:CE2	2.52	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:921:GLY:O	1:A:922:ASP:C	2.55	0.44
3:C:242:GLN:CA	3:C:245:VAL:HG23	2.43	0.44
5:E:153:HIS:C	5:E:154:ILE:HG13	2.34	0.44
5:E:22:MET:HE3	5:E:26:ARG:CZ	2.46	0.44
9:I:55:THR:HG22	9:I:56:ALA:N	2.32	0.44
3:C:80:LEU:HD11	3:C:95:CYS:CA	2.47	0.44
3:C:88:CYS:SG	3:C:91:HIS:N	2.90	0.44
2:B:615:MET:C	2:B:616:ILE:HD12	2.36	0.44
1:A:648:ASN:OD1	1:A:648:ASN:N	2.50	0.44
6:F:86:THR:O	6:F:89:GLU:HB2	2.18	0.44
4:D:147:TYR:CE1	7:G:103:VAL:HG13	2.52	0.44
1:A:381:THR:O	1:A:384:ASN:N	2.45	0.44
9:I:15:TYR:CD1	9:I:15:TYR:N	2.85	0.44
1:A:673:GLY:O	1:A:676:MET:HB2	2.16	0.44
3:C:158:VAL:O	3:C:158:VAL:HG12	2.17	0.44
1:A:1115:SER:O	1:A:1329:THR:HG23	2.17	0.44
1:A:1329:THR:C	1:A:1331:SER:N	2.71	0.44
1:A:52:GLY:O	1:A:56:PRO:HG2	2.17	0.44
1:A:68:GLN:NE2	1:A:80:HIS:CD2	2.79	0.44
1:A:896:ARG:NH2	1:A:1030:ARG:NH2	2.66	0.44
1:A:30:ILE:HD11	2:B:1168:LEU:HD13	1.99	0.44
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.99	0.44
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.99	0.44
2:B:460:ALA:HB1	2:B:466:TRP:CE3	2.52	0.44
1:A:563:PRO:HB3	1:A:571:LEU:O	2.17	0.44
2:B:97:VAL:CG1	2:B:178:ASN:HD21	2.28	0.44
11:K:33:ILE:HB	11:K:35:PHE:HE1	1.81	0.44
1:A:697:ALA:HB2	1:A:702:LEU:CD1	2.46	0.44
1:A:925:LEU:C	1:A:927:VAL:H	2.20	0.44
2:B:780:VAL:HG21	10:J:56:LEU:HD11	1.99	0.44
2:B:509:ALA:C	2:B:510:LYS:HD2	2.36	0.44
1:A:783:THR:HG21	1:A:815:PHE:CE2	2.53	0.44
3:C:73:GLN:HE21	3:C:74:SER:H	1.60	0.44
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.99	0.44
1:A:1104:ILE:C	1:A:1106:ASN:N	2.71	0.44
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.60	0.44
8:H:95:TYR:CE2	8:H:97:MET:CG	3.00	0.44
7:G:82:PHE:O	7:G:84:GLY:N	2.50	0.44
2:B:683:SER:O	2:B:687:GLU:HB2	2.16	0.44
5:E:7:ARG:C	5:E:9:ILE:H	2.19	0.44
2:B:642:ASP:C	2:B:644:GLU:H	2.19	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:21:TYR:C	10:J:23:ASN:N	2.70	0.44
2:B:373:ARG:HG3	2:B:566:LEU:HD23	2.00	0.44
2:B:215:GLN:OE1	2:B:499:ASN:HB3	2.18	0.44
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.83	0.44
11:K:106:GLU:O	11:K:107:THR:C	2.56	0.44
1:A:1313:LEU:HD12	1:A:1327:ILE:HD13	1.99	0.44
1:A:483:ASP:HB2	2:B:987:LYS:HG3	1.99	0.44
2:B:1085:ILE:CG2	2:B:1086:PHE:N	2.80	0.44
2:B:828:ALA:HB2	2:B:1085:ILE:HG21	2.00	0.44
2:B:1150:ARG:NE	2:B:1150:ARG:HA	2.33	0.44
1:A:1427:ASN:O	1:A:1430:LEU:N	2.43	0.44
2:B:1182:CYS:O	2:B:1183:LYS:O	2.36	0.44
2:B:542:MET:CG	2:B:747:MET:HB3	2.48	0.44
1:A:1336:MET:HE2	1:A:1381:LEU:HG	1.99	0.44
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.52	0.44
2:B:186:GLU:O	2:B:187:SER:C	2.55	0.44
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.99	0.44
1:A:43:GLU:HB2	1:A:46:THR:HB	2.00	0.44
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.16	0.44
2:B:604:ARG:O	2:B:606:LYS:N	2.50	0.44
5:E:177:ARG:HD3	5:E:215:MET:HG3	1.99	0.44
9:I:32:CYS:HB2	9:I:33:SER:H	1.39	0.44
5:E:117:THR:HG22	5:E:119:SER:N	2.20	0.44
1:A:541:ILE:HD13	1:A:549:MET:CE	2.45	0.44
1:A:1242:VAL:O	1:A:1243:VAL:HB	2.17	0.44
1:A:1206:ASP:HB2	1:A:1274:ARG:HH22	1.83	0.44
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.99	0.44
1:A:928:LEU:C	1:A:930:ASP:N	2.70	0.44
1:A:848:ILE:O	1:A:1065:GLY:N	2.39	0.44
1:A:783:THR:O	1:A:784:LEU:HD23	2.16	0.44
2:B:824:ILE:CD1	10:J:48:ARG:NH1	2.80	0.44
1:A:1101:LEU:HD12	1:A:1101:LEU:O	2.17	0.44
1:A:1121:GLU:O	1:A:1122:PRO:O	2.35	0.44
7:G:80:LYS:O	7:G:80:LYS:CG	2.62	0.44
1:A:525:GLN:O	1:A:526:ASP:C	2.56	0.44
1:A:962:ARG:O	1:A:965:GLN:N	2.51	0.44
2:B:910:VAL:HG12	2:B:911:ILE:H	1.79	0.44
7:G:96:GLN:HA	7:G:121:PHE:CD2	2.52	0.44
1:A:1007:ILE:C	1:A:1009:ASN:N	2.71	0.44
2:B:1084:GLN:OE1	3:C:191:TYR:HA	2.17	0.44
1:A:55:ASP:O	1:A:57:ARG:N	2.51	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.37	0.44
2:B:806:THR:O	2:B:808:ALA:N	2.51	0.44
3:C:91:HIS:HB2	3:C:96:SER:OG	2.18	0.44
2:B:1107:ALA:O	2:B:1108:ARG:O	2.36	0.44
1:A:668:ASP:HA	1:A:741:ASN:OD1	2.17	0.44
1:A:456:MET:HE3	1:A:507:VAL:HG22	1.99	0.44
2:B:59:LEU:CD1	2:B:417:PHE:CE2	3.01	0.44
7:G:119:LEU:HD12	7:G:131:GLN:O	2.18	0.44
1:A:727:ASP:O	1:A:731:ARG:HG3	2.18	0.44
2:B:598:GLU:HG2	2:B:598:GLU:O	2.17	0.44
1:A:1092:LYS:HD2	1:A:1092:LYS:HA	1.82	0.44
1:A:735:VAL:HG12	1:A:735:VAL:O	2.18	0.44
1:A:1115:SER:HA	1:A:1308:THR:HG23	1.99	0.44
1:A:814:PHE:CE1	2:B:519:TRP:HA	2.52	0.44
1:A:666:ILE:N	2:B:1026:LEU:HD22	2.33	0.44
2:B:360:PHE:C	2:B:360:PHE:CD2	2.91	0.44
2:B:874:PHE:HA	2:B:913:GLY:O	2.17	0.44
4:D:33:PHE:CZ	7:G:80:LYS:NZ	2.84	0.44
3:C:94:LYS:HB2	3:C:94:LYS:HE3	1.67	0.44
2:B:680:THR:HB	2:B:681:TRP:H	1.58	0.44
1:A:384:ASN:O	1:A:386:ASP:N	2.50	0.44
2:B:1031:LEU:HD13	2:B:1055:ILE:HD11	2.00	0.44
2:B:789:MET:CE	2:B:965:LYS:O	2.65	0.44
2:B:634:TYR:CE1	2:B:692:TYR:CD1	3.06	0.44
4:D:137:ASN:ND2	4:D:137:ASN:C	2.70	0.44
2:B:67:SER:O	2:B:68:THR:C	2.56	0.44
2:B:558:LEU:O	2:B:561:TRP:N	2.49	0.44
5:E:92:THR:HG22	5:E:92:THR:O	2.18	0.44
8:H:38:LEU:HD12	8:H:124:ARG:O	2.18	0.44
8:H:38:LEU:HD12	8:H:39:THR:H	1.82	0.44
1:A:789:LYS:HD2	9:I:67:THR:OG1	2.17	0.44
5:E:205:SER:O	5:E:206:GLY:C	2.55	0.44
10:J:54:VAL:HG12	10:J:56:LEU:HD23	2.00	0.44
1:A:1116:LEU:HD12	1:A:1116:LEU:C	2.38	0.44
1:A:76:GLU:O	1:A:76:GLU:HG3	2.18	0.44
2:B:378:LEU:HD12	2:B:378:LEU:C	2.35	0.44
3:C:144:ILE:O	3:C:145:CYS:CB	2.66	0.44
1:A:1101:LEU:HD11	1:A:1105:LEU:HD11	2.00	0.44
1:A:1342:GLU:HG2	5:E:198:ILE:HD13	1.99	0.44
1:A:477:PRO:HG2	1:A:521:MET:HG2	1.99	0.44
2:B:911:ILE:HG23	2:B:966:VAL:HG11	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.99	0.44
1:A:384:ASN:CG	1:A:388:LEU:HD12	2.38	0.44
5:E:185:ALA:O	5:E:190:LEU:HG	2.18	0.44
1:A:1210:GLY:O	1:A:1211:GLN:C	2.56	0.44
2:B:129:PHE:CD2	2:B:166:PHE:HA	2.53	0.44
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.18	0.44
1:A:573:SER:CB	8:H:119:GLY:O	2.65	0.44
1:A:396:PRO:HB3	1:A:402:ALA:O	2.18	0.44
1:A:1099:PRO:O	1:A:1102:LYS:HB3	2.17	0.43
2:B:287:ARG:NH2	2:B:325:GLN:HE22	2.16	0.43
1:A:567:LYS:HD3	8:H:95:TYR:HA	1.99	0.43
7:G:44:TYR:HE1	7:G:157:ILE:HB	1.83	0.43
2:B:540:SER:HB3	2:B:747:MET:O	2.18	0.43
2:B:616:ILE:N	2:B:625:LYS:O	2.37	0.43
6:F:143:PHE:C	6:F:143:PHE:CD1	2.90	0.43
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.18	0.43
1:A:645:LEU:O	1:A:646:PHE:C	2.54	0.43
12:L:60:ARG:CG	12:L:61:THR:H	2.29	0.43
2:B:758:PHE:C	2:B:760:ASP:N	2.72	0.43
1:A:536:LEU:HG	1:A:536:LEU:H	1.51	0.43
1:A:1242:VAL:CG1	1:A:1243:VAL:H	2.23	0.43
2:B:482:VAL:O	2:B:483:LEU:C	2.57	0.43
5:E:80:VAL:HG12	5:E:81:GLU:N	2.33	0.43
2:B:695:ALA:O	2:B:698:GLU:HB3	2.18	0.43
5:E:29:PHE:O	5:E:30:ILE:HG13	2.18	0.43
7:G:39:THR:C	7:G:41:LYS:N	2.70	0.43
3:C:77:ILE:HG23	3:C:161:LYS:HE3	2.00	0.43
2:B:510:LYS:HD3	2:B:510:LYS:O	2.13	0.43
3:C:237:SER:O	3:C:238:ILE:HG13	2.18	0.43
2:B:293:PRO:O	2:B:296:GLU:HB3	2.17	0.43
1:A:1437:GLY:O	1:A:1438:THR:C	2.56	0.43
7:G:1:MET:CE	7:G:80:LYS:O	2.66	0.43
2:B:912:ILE:HD11	2:B:966:VAL:HG23	1.99	0.43
4:D:47:LEU:CD1	4:D:48:ILE:N	2.81	0.43
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.47	0.43
1:A:715:GLU:C	1:A:717:ASN:N	2.71	0.43
2:B:1076:HIS:ND1	2:B:1076:HIS:N	2.66	0.43
2:B:486:TYR:CD1	2:B:1096:ARG:NH2	2.86	0.43
1:A:967:ALA:N	1:A:1044:TRP:HZ3	2.16	0.43
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.25	0.43
3:C:242:GLN:HB3	3:C:246:ARG:HG3	1.99	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.53	0.43
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.33	0.43
9:I:111:THR:HG21	9:I:113:ASP:HB2	2.00	0.43
1:A:608:ILE:CB	1:A:613:ILE:HD11	2.44	0.43
6:F:86:THR:O	6:F:89:GLU:N	2.51	0.43
2:B:901:PRO:HB2	12:L:60:ARG:HA	2.00	0.43
4:D:48:ILE:HG21	7:G:4:ILE:CD1	2.40	0.43
12:L:32:ALA:CB	12:L:55:ILE:HD12	2.48	0.43
1:A:877:HIS:C	1:A:878:ILE:CG1	2.86	0.43
1:A:1230:GLU:C	1:A:1232:ASN:N	2.71	0.43
2:B:214:ALA:HA	2:B:408:LEU:HD12	2.00	0.43
2:B:230:ALA:N	2:B:231:PRO:CD	2.81	0.43
5:E:129:PRO:O	5:E:130:ALA:C	2.57	0.43
7:G:47:CYS:O	7:G:76:ALA:HB1	2.18	0.43
2:B:787:VAL:HG12	2:B:787:VAL:O	2.19	0.43
1:A:1384:VAL:O	1:A:1384:VAL:HG12	2.19	0.43
3:C:44:LEU:HD23	3:C:72:LEU:CB	2.48	0.43
11:K:7:PHE:O	11:K:11:LEU:HB2	2.18	0.43
2:B:781:PHE:HD1	2:B:782:LEU:HG	1.83	0.43
10:J:1:MET:H2	10:J:55:ASP:HA	1.82	0.43
1:A:1313:LEU:HD11	1:A:1327:ILE:HD13	1.99	0.43
1:A:353:ILE:HD13	1:A:487:MET:HG3	2.00	0.43
2:B:114:PRO:O	2:B:115:GLN:C	2.57	0.43
2:B:830:TYR:CD2	2:B:1000:PRO:HD3	2.53	0.43
2:B:872:GLU:CD	2:B:914:LYS:HE2	2.39	0.43
1:A:1081:LEU:HA	1:A:1081:LEU:HD13	1.84	0.43
6:F:88:TYR:N	6:F:88:TYR:CD1	2.85	0.43
8:H:97:MET:SD	8:H:121:LEU:HD12	2.59	0.43
7:G:1:MET:SD	7:G:79:PHE:CD1	3.12	0.43
9:I:71:SER:O	9:I:83:ASN:ND2	2.51	0.43
11:K:53:ASP:OD1	11:K:55:LYS:HB2	2.17	0.43
12:L:47:ARG:NH2	12:L:54:ARG:HE	2.16	0.43
5:E:117:THR:C	5:E:119:SER:H	2.21	0.43
1:A:347:PHE:N	2:B:1107:ALA:HA	2.26	0.43
6:F:135:ARG:HG2	6:F:137:TYR:CE1	2.52	0.43
1:A:231:PRO:O	1:A:233:TRP:N	2.52	0.43
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.53	0.43
1:A:711:ARG:HG3	9:I:97:MET:HE2	2.00	0.43
1:A:718:VAL:O	1:A:721:PHE:HB2	2.18	0.43
11:K:35:PHE:N	11:K:35:PHE:HD1	2.15	0.43
1:A:582:ILE:O	1:A:583:PRO:O	2.36	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:21:GLU:O	5:E:24:LYS:HG2	2.19	0.43
2:B:465:ASN:N	2:B:465:ASN:ND2	2.65	0.43
1:A:64:ASN:O	1:A:65:LEU:C	2.56	0.43
1:A:47:ARG:CZ	1:A:255:SER:H	2.31	0.43
2:B:235:SER:OG	2:B:236:HIS:CD2	2.72	0.43
2:B:236:HIS:O	2:B:237:VAL:HG23	2.19	0.43
2:B:258:LEU:HG	2:B:258:LEU:O	2.19	0.43
10:J:45:CYS:SG	10:J:46:CYS:N	2.91	0.43
1:A:886:ILE:HG13	1:A:943:LEU:HD13	2.00	0.43
2:B:324:ILE:CG2	2:B:325:GLN:N	2.81	0.43
1:A:1161:THR:HG1	1:A:1170:ILE:HD11	1.84	0.43
1:A:1189:SER:OG	1:A:1190:PRO:HD2	2.18	0.43
1:A:1121:GLU:O	1:A:1122:PRO:C	2.57	0.43
1:A:646:PHE:O	1:A:647:GLY:C	2.55	0.43
8:H:81:PRO:HB3	8:H:82:PRO:CD	2.49	0.43
1:A:426:LEU:O	1:A:427:GLN:HG2	2.19	0.43
1:A:1208:THR:O	1:A:1211:GLN:N	2.52	0.43
11:K:30:ALA:HA	11:K:75:ILE:O	2.18	0.43
11:K:32:VAL:HA	11:K:73:LEU:O	2.19	0.43
2:B:1145:SER:O	2:B:1147:LEU:N	2.51	0.43
10:J:25:LEU:O	10:J:29:GLU:HA	2.19	0.43
1:A:496:GLU:OE1	7:G:63:PRO:O	2.37	0.43
1:A:576:GLN:O	1:A:579:SER:HB2	2.18	0.43
2:B:20:ASP:O	2:B:22:SER:N	2.48	0.43
1:A:1000:LEU:HD23	1:A:1000:LEU:HA	1.64	0.43
7:G:126:ASN:HA	7:G:127:PRO:C	2.37	0.43
1:A:845:LEU:HD22	1:A:1374:VAL:HG21	2.00	0.43
1:A:1282:VAL:HG22	1:A:1308:THR:HA	2.01	0.43
1:A:483:ASP:HB2	2:B:987:LYS:CG	2.48	0.43
3:C:73:GLN:NE2	3:C:75:MET:N	2.54	0.43
2:B:977:GLY:CA	2:B:1099:VAL:HB	2.44	0.43
2:B:975:GLN:HG2	2:B:976:ILE:H	1.82	0.43
2:B:798:TYR:HD2	2:B:798:TYR:N	2.16	0.43
2:B:1162:ILE:HG22	2:B:1163:CYS:O	2.19	0.43
2:B:1132:GLU:O	2:B:1135:ARG:N	2.52	0.43
8:H:145:ARG:O	8:H:146:ARG:HB2	2.18	0.43
8:H:91:ASP:C	8:H:93:TYR:N	2.70	0.43
1:A:1319:VAL:O	1:A:1322:ILE:HG12	2.19	0.43
1:A:465:TYR:N	11:K:2:ASN:HB3	2.32	0.43
1:A:108:MET:SD	1:A:210:ILE:HD13	2.59	0.43
3:C:44:LEU:HG	3:C:45:ALA:N	2.34	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:14:HIS:CG	7:G:15:PRO:HD2	2.53	0.43
1:A:814:PHE:HE1	2:B:519:TRP:HA	1.83	0.43
1:A:243:PRO:CB	1:A:244:PRO:HD2	2.46	0.43
1:A:43:GLU:O	1:A:44:THR:CB	2.66	0.43
2:B:282:ILE:HD13	2:B:382:ILE:HD13	2.01	0.43
2:B:597:MET:O	2:B:599:THR:N	2.52	0.43
1:A:1239:ARG:HB3	1:A:1239:ARG:NH1	2.33	0.43
2:B:843:GLN:O	2:B:844:SER:C	2.56	0.43
1:A:706:HIS:C	1:A:708:MET:H	2.22	0.43
1:A:135:PHE:CE1	1:A:222:LEU:HD22	2.53	0.43
1:A:98:LYS:O	1:A:99:ILE:C	2.56	0.43
2:B:591:ARG:O	2:B:592:ASN:C	2.57	0.43
4:D:146:GLN:O	4:D:150:ASN:N	2.51	0.43
2:B:1160:VAL:CG1	2:B:1161:HIS:H	2.30	0.43
5:E:140:LEU:HG	5:E:140:LEU:H	1.63	0.43
2:B:1076:HIS:CD2	11:K:40:HIS:NE2	2.86	0.43
5:E:25:ASP:O	5:E:27:GLY:N	2.52	0.43
3:C:76:ASP:HB2	3:C:128:ASN:O	2.18	0.43
1:A:929:LEU:HD13	1:A:929:LEU:O	2.19	0.43
1:A:841:LEU:HD13	1:A:1072:ILE:HB	2.00	0.43
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.83	0.43
2:B:283:VAL:O	2:B:284:ILE:C	2.57	0.43
5:E:198:ILE:HD11	5:E:212:ARG:HH11	1.84	0.43
2:B:821:GLN:NE2	2:B:851:PHE:H	2.14	0.43
5:E:154:ILE:HG22	5:E:155:ARG:O	2.19	0.43
8:H:95:TYR:HB3	8:H:144:ILE:HB	2.00	0.43
1:A:475:THR:CG2	1:A:476:SER:N	2.81	0.43
9:I:73:ARG:HH12	9:I:112:SER:HB2	1.83	0.43
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	2.00	0.43
1:A:1051:ALA:O	1:A:1052:GLN:C	2.57	0.43
1:A:1226:VAL:C	1:A:1227:ILE:HG13	2.37	0.43
1:A:996:ASN:C	1:A:998:LEU:H	2.22	0.43
2:B:390:LEU:O	2:B:392:ARG:N	2.51	0.43
3:C:69:LEU:H	3:C:69:LEU:CD1	2.32	0.43
2:B:847:ASP:C	2:B:849:GLY:N	2.72	0.43
2:B:371:GLU:N	2:B:371:GLU:CD	2.70	0.43
4:D:192:LYS:NZ	4:D:204:ASP:OD1	2.35	0.43
1:A:362:ASP:N	1:A:362:ASP:OD2	2.48	0.43
2:B:939:THR:HA	2:B:940:PRO:HD2	1.92	0.43
1:A:971:PHE:CE2	1:A:1040:GLN:HG2	2.53	0.43
1:A:1064:VAL:O	1:A:1065:GLY:C	2.55	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:147:HIS:O	5:E:148:GLU:C	2.57	0.43
2:B:987:LYS:O	2:B:987:LYS:HG2	2.18	0.43
1:A:244:PRO:CG	1:A:245:PRO:HD3	2.47	0.43
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.72	0.43
2:B:949:VAL:HG12	2:B:950:ASP:N	2.34	0.43
12:L:63:ARG:O	12:L:63:ARG:HG3	2.19	0.43
1:A:464:PRO:HG2	1:A:465:TYR:HD1	1.84	0.43
2:B:545:ILE:C	2:B:634:TYR:HE2	2.22	0.43
1:A:1209:MET:O	1:A:1210:GLY:C	2.55	0.43
1:A:1151:GLU:HB3	1:A:1153:TYR:CE1	2.50	0.43
2:B:1017:ILE:HD13	2:B:1017:ILE:HA	1.82	0.43
1:A:419:LYS:HG3	1:A:420:ARG:H	1.84	0.43
1:A:1021:LEU:O	1:A:1024:SER:HB3	2.19	0.43
1:A:722:LEU:O	1:A:725:ALA:HB3	2.19	0.43
1:A:449:SER:O	2:B:1133:MET:HB3	2.18	0.43
1:A:157:ASP:C	1:A:159:THR:H	2.22	0.43
2:B:176:SER:O	2:B:182:SER:HB3	2.19	0.43
1:A:955:PRO:HG2	1:A:955:PRO:O	2.18	0.43
1:A:117:GLU:H	1:A:117:GLU:CD	2.23	0.43
1:A:1116:LEU:O	1:A:1308:THR:HG22	2.19	0.43
1:A:353:ILE:HG13	1:A:482:PHE:HD2	1.83	0.43
2:B:508:LEU:O	2:B:509:ALA:C	2.51	0.43
1:A:784:LEU:HD11	1:A:815:PHE:CE2	2.54	0.43
3:C:41:ILE:HD11	3:C:247:GLY:CA	2.49	0.43
1:A:1164:PRO:O	1:A:1167:GLU:HG3	2.19	0.43
1:A:1169:ILE:HD11	1:A:1229:SER:HB3	2.01	0.43
1:A:525:GLN:CD	2:B:836:GLU:HG2	2.39	0.43
1:A:751:SER:OG	2:B:1015:HIS:CE1	2.72	0.43
1:A:703:THR:HB	1:A:705:LYS:HE2	2.01	0.43
1:A:1444:MET:HG2	7:G:59:GLY:O	2.19	0.43
6:F:85:MET:HE1	6:F:148:VAL:CG1	2.48	0.43
2:B:758:PHE:HB2	2:B:1024:ALA:HB1	2.00	0.43
1:A:858:ASN:O	1:A:860:LEU:N	2.52	0.43
1:A:416:ARG:C	1:A:417:TYR:CD2	2.92	0.43
12:L:50:ASP:O	12:L:52:GLY:N	2.52	0.43
2:B:485:ARG:HH11	2:B:485:ARG:HG3	1.83	0.43
2:B:543:SER:O	2:B:544:CYS:SG	2.75	0.43
2:B:166:PHE:C	2:B:167:ILE:HG13	2.39	0.43
8:H:27:GLU:HG2	8:H:39:THR:HG23	2.00	0.43
4:D:63:LEU:HD13	4:D:133:THR:OG1	2.19	0.43
2:B:1170:THR:HB	2:B:1171:VAL:H	1.68	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1283:VAL:CG1	1:A:1284:MET:N	2.78	0.42
2:B:702:LEU:C	2:B:703:ILE:HG13	2.39	0.42
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.49	0.42
3:C:175:ALA:HB3	10:J:43:ARG:NH2	2.33	0.42
2:B:616:ILE:CD1	2:B:616:ILE:N	2.81	0.42
5:E:182:ASP:O	5:E:185:ALA:HB3	2.19	0.42
8:H:38:LEU:HD13	8:H:125:LEU:HD13	2.00	0.42
11:K:62:LYS:O	11:K:62:LYS:HG3	2.19	0.42
6:F:138:LEU:O	6:F:140:ASP:N	2.52	0.42
1:A:1017:LEU:HD23	5:E:204:THR:O	2.18	0.42
1:A:1072:ILE:O	1:A:1075:PRO:CG	2.66	0.42
2:B:1085:ILE:HD12	2:B:1085:ILE:N	2.34	0.42
1:A:343:LYS:HE2	2:B:1156:ASP:HB2	2.01	0.42
9:I:55:THR:HG22	9:I:56:ALA:H	1.84	0.42
12:L:62:LYS:O	12:L:63:ARG:C	2.58	0.42
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.54	0.42
1:A:261:ASP:O	1:A:264:PHE:N	2.51	0.42
7:G:115:MET:HB2	7:G:116:PRO:CD	2.44	0.42
1:A:370:ILE:O	1:A:371:ALA:C	2.57	0.42
6:F:100:GLN:HG2	7:G:66:GLY:HA3	2.01	0.42
5:E:144:ILE:C	5:E:146:HIS:N	2.72	0.42
2:B:63:ILE:O	2:B:67:SER:HB3	2.19	0.42
11:K:88:LYS:O	11:K:89:ASN:C	2.56	0.42
1:A:185:TRP:O	1:A:197:PRO:HA	2.18	0.42
4:D:26:THR:O	4:D:28:GLN:N	2.52	0.42
1:A:1272:THR:HG22	1:A:1273:LEU:N	2.34	0.42
1:A:1067:LEU:O	1:A:1067:LEU:HD12	2.20	0.42
1:A:2:VAL:HG21	2:B:1158:PHE:N	2.34	0.42
2:B:564:GLU:O	2:B:565:PRO:C	2.58	0.42
1:A:862:ASN:HA	5:E:174:GLN:O	2.19	0.42
1:A:786:HIS:CE1	2:B:519:TRP:CZ2	3.05	0.42
3:C:247:GLY:C	3:C:249:ASP:N	2.72	0.42
1:A:49:LYS:HZ1	1:A:60:SER:C	2.22	0.42
2:B:1003:ALA:HA	3:C:178:PHE:O	2.19	0.42
1:A:566:ILE:O	1:A:567:LYS:C	2.57	0.42
1:A:600:PRO:HA	8:H:25:ARG:NH2	2.34	0.42
7:G:106:MET:HG2	7:G:107:LYS:N	2.34	0.42
1:A:962:ARG:O	1:A:963:ILE:C	2.58	0.42
3:C:80:LEU:HD11	3:C:96:SER:N	2.33	0.42
2:B:591:ARG:O	2:B:593:PRO:HD3	2.19	0.42
5:E:124:VAL:HG13	5:E:132:ILE:CG1	2.50	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:744:HIS:HD2	2:B:746:SER:CB	2.32	0.42
1:A:366:VAL:O	1:A:463:ILE:HG12	2.19	0.42
12:L:32:ALA:CB	12:L:55:ILE:HG13	2.49	0.42
9:I:65:ASP:HA	9:I:66:PRO:HD2	1.88	0.42
7:G:117:GLN:C	7:G:119:LEU:N	2.71	0.42
1:A:533:LYS:HE3	1:A:745:GLN:NE2	2.34	0.42
5:E:33:GLU:C	5:E:35:VAL:N	2.72	0.42
11:K:105:PHE:O	11:K:106:GLU:C	2.57	0.42
1:A:1152:ILE:HG13	9:I:44:TYR:HD2	1.83	0.42
1:A:693:VAL:O	1:A:693:VAL:HG12	2.18	0.42
7:G:7:LEU:O	7:G:73:LYS:HD2	2.19	0.42
7:G:126:ASN:HA	7:G:126:ASN:HD22	1.64	0.42
1:A:825:ILE:O	1:A:827:THR:N	2.52	0.42
3:C:248:ILE:H	3:C:248:ILE:HG13	1.65	0.42
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.84	0.42
2:B:575:PRO:HG2	2:B:576:ASP:H	1.84	0.42
1:A:252:PHE:HB2	1:A:256:GLN:HB3	2.01	0.42
1:A:896:ARG:CD	1:A:897:TYR:CE1	2.93	0.42
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.54	0.42
3:C:63:ILE:O	3:C:67:LEU:HG	2.19	0.42
2:B:597:MET:C	2:B:599:THR:H	2.22	0.42
2:B:292:ILE:N	2:B:293:PRO:HD2	2.34	0.42
2:B:324:ILE:HG22	2:B:325:GLN:N	2.34	0.42
10:J:52:THR:O	10:J:53:HIS:C	2.57	0.42
2:B:315:LYS:HE2	9:I:4:PHE:CD2	2.55	0.42
2:B:515:HIS:CD2	2:B:517:THR:HG23	2.54	0.42
1:A:368:LYS:O	1:A:369:SER:C	2.58	0.42
1:A:873:MET:C	1:A:1058:VAL:HG23	2.40	0.42
2:B:496:ARG:NH1	2:B:496:ARG:HB3	2.29	0.42
1:A:1450:LEU:HD11	6:F:108:PHE:CZ	2.54	0.42
2:B:174:LEU:HD11	2:B:204:ILE:CD1	2.49	0.42
2:B:62:ILE:HG23	2:B:418:LYS:CG	2.49	0.42
2:B:1090:THR:O	2:B:1091:TYR:C	2.57	0.42
2:B:431:TYR:CD2	2:B:447:ALA:HB2	2.54	0.42
11:K:35:PHE:HD1	11:K:35:PHE:H	1.67	0.42
1:A:532:ARG:HD3	1:A:749:ALA:HB2	2.00	0.42
1:A:7:SER:HB2	2:B:1175:LEU:CD2	2.50	0.42
1:A:716:ASP:O	1:A:716:ASP:OD1	2.37	0.42
3:C:258:ILE:N	3:C:258:ILE:HD12	2.35	0.42
2:B:700:SER:O	2:B:701:ILE:HG22	2.20	0.42
1:A:254:GLU:N	2:B:935:ARG:HH22	2.17	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:86:CYS:C	3:C:88:CYS:N	2.72	0.42
1:A:266:LEU:O	1:A:267:ALA:C	2.58	0.42
1:A:324:SER:O	1:A:327:ALA:HB3	2.19	0.42
1:A:304:MET:O	1:A:326:ARG:HB3	2.19	0.42
5:E:135:PHE:CD1	5:E:135:PHE:N	2.88	0.42
6:F:103:MET:CE	7:G:66:GLY:H	2.32	0.42
1:A:675:THR:O	1:A:675:THR:HG22	2.19	0.42
1:A:1453:TYR:CE2	6:F:129:LYS:HA	2.54	0.42
2:B:1017:ILE:O	2:B:1018:PRO:C	2.58	0.42
1:A:1143:LEU:HD23	1:A:1267:MET:O	2.19	0.42
1:A:1129:GLU:O	1:A:1131:ALA:N	2.52	0.42
1:A:8:SER:O	1:A:9:ALA:C	2.57	0.42
1:A:1074:GLU:N	1:A:1075:PRO:CD	2.82	0.42
1:A:1282:VAL:C	1:A:1283:VAL:CG2	2.87	0.42
1:A:49:LYS:HZ1	1:A:60:SER:CA	2.33	0.42
2:B:395:GLN:HG2	2:B:396:ASP:H	1.83	0.42
1:A:1080:THR:C	1:A:1081:LEU:HD22	2.40	0.42
1:A:1373:ASP:HA	1:A:1376:THR:CG2	2.49	0.42
6:F:88:TYR:HD1	6:F:88:TYR:H	1.67	0.42
2:B:1073:TYR:N	2:B:1073:TYR:CD1	2.87	0.42
1:A:567:LYS:HB3	8:H:95:TYR:CA	2.48	0.42
2:B:835:GLN:HE21	2:B:835:GLN:HB2	1.57	0.42
12:L:54:ARG:HH11	12:L:54:ARG:HG3	1.85	0.42
3:C:80:LEU:HD12	3:C:95:CYS:HA	2.01	0.42
1:A:231:PRO:C	1:A:233:TRP:N	2.72	0.42
1:A:299:HIS:C	1:A:301:ALA:N	2.73	0.42
1:A:325:ILE:O	1:A:328:ARG:HB2	2.20	0.42
2:B:644:GLU:C	2:B:646:LEU:N	2.71	0.42
1:A:889:SER:C	1:A:891:ALA:N	2.72	0.42
1:A:1213:GLY:O	1:A:1215:ARG:N	2.53	0.42
10:J:21:TYR:HB2	10:J:39:LEU:HD13	2.02	0.42
1:A:893:PHE:CD2	1:A:893:PHE:C	2.92	0.42
1:A:821:ARG:CB	1:A:821:ARG:HH11	2.25	0.42
3:C:169:LYS:NZ	12:L:69:ALA:CB	2.81	0.42
3:C:241:ASP:O	3:C:244:VAL:HB	2.19	0.42
1:A:253:ASN:HB2	2:B:935:ARG:NH1	2.34	0.42
1:A:68:GLN:O	1:A:70:CYS:N	2.43	0.42
1:A:469:ARG:CG	1:A:469:ARG:HH11	2.32	0.42
2:B:999:MET:HE3	2:B:999:MET:HA	2.01	0.42
2:B:599:THR:O	2:B:603:LEU:HB2	2.20	0.42
1:A:830:LYS:HB2	1:A:1081:LEU:CD2	2.43	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1377:THR:O	1:A:1378:GLN:C	2.57	0.42
1:A:1125:ALA:C	1:A:1127:ASP:N	2.72	0.42
1:A:472:LEU:O	1:A:475:THR:HG22	2.19	0.42
1:A:475:THR:O	1:A:479:ASN:N	2.53	0.42
4:D:33:PHE:CE1	7:G:80:LYS:CE	3.02	0.42
1:A:526:ASP:OD2	2:B:829:CYS:HB3	2.20	0.42
1:A:705:LYS:C	1:A:707:GLY:H	2.22	0.42
3:C:91:HIS:O	3:C:91:HIS:CD2	2.72	0.42
2:B:615:MET:HA	2:B:626:ILE:HA	2.01	0.42
4:D:149:THR:O	4:D:149:THR:HG23	2.20	0.42
2:B:222:ILE:O	2:B:240:ILE:HA	2.19	0.42
11:K:40:HIS:O	11:K:41:THR:C	2.58	0.42
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.34	0.42
1:A:24:PRO:HG2	1:A:25:GLU:OE1	2.20	0.42
1:A:1308:THR:OG1	1:A:1309:ASP:N	2.53	0.42
1:A:919:ILE:O	1:A:920:LEU:C	2.57	0.42
3:C:249:ASP:O	3:C:250:THR:C	2.58	0.42
2:B:1073:TYR:HE2	3:C:180:TYR:CE2	2.37	0.42
11:K:55:LYS:HB2	11:K:81:TYR:HE1	1.84	0.42
2:B:956:THR:HG22	2:B:960:GLY:HA2	2.02	0.42
12:L:31:CYS:SG	12:L:34:CYS:N	2.93	0.42
1:A:324:SER:O	1:A:327:ALA:N	2.53	0.42
3:C:97:VAL:HG12	3:C:98:VAL:H	1.84	0.42
2:B:45:SER:O	2:B:46:GLN:C	2.58	0.42
1:A:874:ASP:HA	1:A:1058:VAL:HG23	2.01	0.42
1:A:937:VAL:O	1:A:938:LYS:C	2.58	0.42
6:F:119:ARG:CG	6:F:119:ARG:NH1	2.81	0.42
1:A:1001:ARG:HH11	1:A:1001:ARG:HG2	1.83	0.42
1:A:695:LYS:O	1:A:697:ALA:N	2.53	0.42
2:B:1017:ILE:HG22	2:B:1018:PRO:HD3	2.01	0.42
6:F:94:LEU:HD23	6:F:94:LEU:HA	1.64	0.42
2:B:259:TYR:N	2:B:259:TYR:CD1	2.88	0.42
1:A:7:SER:HB2	2:B:1175:LEU:HD22	2.02	0.42
1:A:408:ASP:C	1:A:410:GLY:H	2.23	0.42
2:B:730:ARG:O	2:B:731:VAL:O	2.38	0.42
1:A:1050:GLU:O	1:A:1050:GLU:HG3	2.18	0.42
2:B:114:PRO:HG2	2:B:115:GLN:N	2.29	0.42
3:C:75:MET:HE2	3:C:239:PRO:HD3	2.02	0.42
2:B:1169:MET:CE	2:B:1201:LYS:CA	2.89	0.42
2:B:1201:LYS:HE2	2:B:1205:GLN:NE2	2.35	0.42
2:B:386:LEU:C	2:B:388:CYS:N	2.73	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:995:ARG:O	2:B:997:GLU:N	2.52	0.42
2:B:603:LEU:HD13	2:B:608:ASP:HB2	2.00	0.42
1:A:1348:LEU:HG	1:A:1372:VAL:CG2	2.50	0.42
1:A:526:ASP:HB3	1:A:657:LEU:HD23	2.01	0.42
1:A:550:LEU:HD22	1:A:556:TRP:CD1	2.55	0.42
2:B:635:ARG:HG3	2:B:635:ARG:NH1	2.35	0.42
2:B:1106:ARG:HD3	2:B:1126:GLY:C	2.39	0.42
4:D:47:LEU:CD1	7:G:3:PHE:HD2	2.33	0.42
1:A:757:ASN:O	1:A:761:MET:HG3	2.20	0.42
1:A:506:ALA:O	1:A:509:LEU:N	2.51	0.42
2:B:172:ILE:HG22	2:B:173:MET:N	2.35	0.42
1:A:933:TYR:C	1:A:935:GLN:N	2.72	0.42
2:B:642:ASP:HB3	2:B:649:LYS:CE	2.49	0.42
2:B:644:GLU:O	2:B:646:LEU:N	2.53	0.42
1:A:1300:LYS:HG3	1:A:1300:LYS:H	1.47	0.42
3:C:181:ASP:N	3:C:182:PRO:CD	2.83	0.42
1:A:971:PHE:N	1:A:971:PHE:CD1	2.88	0.42
1:A:282:ASN:O	1:A:284:ALA:N	2.53	0.42
1:A:960:ILE:O	1:A:960:ILE:HG22	2.20	0.42
1:A:784:LEU:C	1:A:786:HIS:H	2.23	0.42
11:K:101:LEU:O	11:K:102:LYS:C	2.58	0.42
2:B:376:PHE:HE2	2:B:569:TYR:HD2	1.65	0.42
1:A:35:ILE:HD12	1:A:241:VAL:CG2	2.50	0.42
10:J:6:ARG:HB3	10:J:11:GLY:O	2.20	0.42
1:A:1348:LEU:HG	1:A:1372:VAL:HG23	2.01	0.42
1:A:567:LYS:CE	8:H:46:LEU:HB2	2.50	0.42
2:B:34:ILE:O	2:B:35:SER:C	2.58	0.42
1:A:606:LEU:HB3	1:A:614:PHE:CD2	2.55	0.42
1:A:556:TRP:CD2	1:A:558:GLY:HA2	2.55	0.42
2:B:1202:LEU:HD22	2:B:1206:GLU:CD	2.39	0.42
1:A:231:PRO:C	1:A:233:TRP:H	2.23	0.42
1:A:95:PHE:CD1	1:A:234:MET:CG	2.96	0.42
4:D:52:LEU:O	4:D:54:GLU:N	2.46	0.42
1:A:1381:LEU:HA	1:A:1381:LEU:HD23	1.82	0.42
7:G:30:LEU:HD13	7:G:72:VAL:HG11	2.01	0.42
2:B:487:THR:CG2	2:B:488:TYR:N	2.82	0.42
3:C:197:SER:O	3:C:198:ALA:C	2.58	0.42
2:B:373:ARG:CG	2:B:566:LEU:HD23	2.50	0.42
1:A:552:TRP:O	1:A:554:PRO:HD3	2.20	0.42
3:C:245:VAL:C	3:C:247:GLY:N	2.73	0.41
1:A:254:GLU:H	2:B:935:ARG:NH1	2.18	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:824:ILE:HG22	2:B:1087:PHE:CE2	2.55	0.41
2:B:581:PHE:HB2	2:B:624:LEU:O	2.20	0.41
2:B:293:PRO:CG	2:B:296:GLU:OE1	2.68	0.41
1:A:598:LEU:CD2	8:H:25:ARG:NH1	2.83	0.41
8:H:58:THR:HG22	8:H:59:ILE:N	2.34	0.41
1:A:523:ILE:HD12	1:A:622:VAL:CG2	2.49	0.41
1:A:515:GLN:HB2	1:A:1071:SER:HB3	2.02	0.41
1:A:515:GLN:HB3	1:A:1071:SER:OG	2.20	0.41
10:J:47:ARG:HG2	10:J:47:ARG:HH11	1.85	0.41
2:B:952:VAL:CG1	2:B:953:LEU:H	2.31	0.41
9:I:90:GLN:O	9:I:92:ARG:N	2.48	0.41
7:G:27:LYS:HE2	7:G:54:ILE:HB	2.02	0.41
1:A:483:ASP:OD2	1:A:485:ASP:OD1	2.38	0.41
1:A:58:LEU:O	1:A:59:GLY:O	2.36	0.41
2:B:976:ILE:HG22	2:B:977:GLY:N	2.34	0.41
2:B:628:THR:O	2:B:629:ASP:O	2.38	0.41
2:B:31:TRP:HA	2:B:31:TRP:CE3	2.55	0.41
1:A:540:PHE:CB	1:A:571:LEU:HD23	2.39	0.41
1:A:527:THR:O	1:A:653:VAL:HG11	2.19	0.41
2:B:1115:THR:O	2:B:1116:ARG:CB	2.65	0.41
1:A:262:LEU:HD22	1:A:303:TYR:CE1	2.55	0.41
1:A:320:ARG:HH21	1:A:323:LYS:NZ	2.18	0.41
1:A:90:VAL:HG12	1:A:91:PHE:O	2.20	0.41
2:B:770:GLN:OE1	2:B:983:ARG:HA	2.20	0.41
2:B:247:GLY:N	2:B:418:LYS:HZ3	2.16	0.41
2:B:570:VAL:HA	2:B:571:PRO:HD2	1.78	0.41
8:H:115:TYR:CE2	8:H:124:ARG:HG3	2.54	0.41
12:L:66:GLN:C	12:L:67:PHE:CD1	2.94	0.41
5:E:165:LEU:O	5:E:166:LYS:C	2.58	0.41
2:B:349:ILE:HG22	2:B:349:ILE:O	2.20	0.41
2:B:508:LEU:HB3	2:B:510:LYS:N	2.25	0.41
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.35	0.41
2:B:1032:SER:O	2:B:1034:VAL:N	2.53	0.41
2:B:1098:MET:O	2:B:1101:ASP:HB2	2.19	0.41
2:B:798:TYR:HE2	3:C:62:PHE:CE2	2.37	0.41
1:A:1435:PRO:C	1:A:1436:ILE:HG13	2.40	0.41
1:A:503:GLN:HE21	6:F:90:ARG:NH2	2.02	0.41
1:A:598:LEU:O	1:A:599:SER:C	2.58	0.41
3:C:217:ASP:HA	3:C:218:PRO:HD3	1.95	0.41
2:B:637:LEU:HD21	2:B:742:GLU:OE2	2.20	0.41
4:D:146:GLN:O	4:D:147:TYR:C	2.58	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:634:TYR:HE1	2:B:692:TYR:CD1	2.38	0.41
2:B:57:TYR:HD1	2:B:57:TYR:H	1.67	0.41
2:B:90:ILE:HD11	2:B:432:MET:SD	2.60	0.41
2:B:849:GLY:O	2:B:852:ARG:HG3	2.20	0.41
8:H:104:PHE:HZ	8:H:135:LEU:O	2.04	0.41
1:A:870:GLU:HG2	5:E:208:TYR:CE2	2.55	0.41
5:E:147:HIS:HD2	5:E:149:LEU:H	1.68	0.41
1:A:900:ASP:HA	1:A:926:GLN:HE22	1.84	0.41
3:C:241:ASP:HB3	11:K:109:TRP:CH2	2.55	0.41
2:B:1098:MET:O	2:B:1099:VAL:C	2.59	0.41
11:K:65:HIS:NE2	11:K:67:PHE:CG	2.88	0.41
3:C:66:ARG:NH2	10:J:5:VAL:CG2	2.84	0.41
6:F:90:ARG:HG3	6:F:91:ALA:N	2.35	0.41
2:B:593:PRO:O	2:B:594:ALA:C	2.59	0.41
3:C:98:VAL:O	3:C:99:LEU:HD23	2.18	0.41
4:D:50:LEU:HD11	7:G:4:ILE:CG1	2.51	0.41
12:L:50:ASP:HB3	12:L:51:CYS:H	1.58	0.41
6:F:97:ARG:O	6:F:98:ALA:C	2.58	0.41
1:A:1192:LEU:CG	1:A:1193:LEU:N	2.81	0.41
2:B:1060:ARG:C	2:B:1062:HIS:H	2.22	0.41
11:K:58:PHE:CB	11:K:76:GLN:HE21	2.32	0.41
10:J:21:TYR:HB2	10:J:39:LEU:CD1	2.51	0.41
1:A:809:THR:O	1:A:810:PRO:C	2.58	0.41
2:B:121:ASN:HA	2:B:207:GLY:HA2	2.02	0.41
1:A:216:VAL:O	1:A:219:PHE:HB2	2.20	0.41
1:A:639:PRO:HG2	1:A:640:GLN:H	1.85	0.41
1:A:18:GLN:OE1	1:A:18:GLN:C	2.59	0.41
7:G:13:LEU:HD12	7:G:26:LEU:HD21	2.03	0.41
2:B:186:GLU:O	2:B:189:LEU:HB2	2.21	0.41
3:C:164:ALA:O	3:C:165:LYS:C	2.58	0.41
3:C:249:ASP:O	3:C:252:GLN:N	2.53	0.41
1:A:70:CYS:O	1:A:71:GLN:C	2.58	0.41
10:J:18:TRP:HA	10:J:18:TRP:HE3	1.85	0.41
10:J:48:ARG:C	10:J:48:ARG:HD2	2.41	0.41
2:B:295:GLY:HA2	2:B:298:LEU:HB2	2.01	0.41
1:A:399:HIS:O	1:A:400:PRO:C	2.54	0.41
2:B:809:MET:O	2:B:811:TYR:N	2.54	0.41
1:A:608:ILE:O	1:A:609:ASP:C	2.58	0.41
5:E:124:VAL:HB	5:E:125:PRO:CD	2.50	0.41
2:B:515:HIS:CG	2:B:516:ASN:N	2.88	0.41
2:B:515:HIS:HD2	2:B:517:THR:N	2.12	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:ILE:O	2:B:240:ILE:CG2	2.69	0.41
5:E:39:LEU:O	5:E:40:GLU:C	2.59	0.41
3:C:187:LYS:HG3	3:C:219:PHE:CE1	2.55	0.41
2:B:233:PRO:HG2	2:B:234:ILE:HD12	2.03	0.41
2:B:792:MET:O	2:B:793:ALA:HB2	2.20	0.41
2:B:785:TYR:HE2	10:J:60:PHE:CZ	2.38	0.41
7:G:22:MET:O	7:G:23:LYS:C	2.59	0.41
1:A:785:PRO:O	2:B:702:LEU:HD12	2.21	0.41
1:A:42:ASP:HB3	1:A:45:GLN:N	2.33	0.41
1:A:52:GLY:N	1:A:56:PRO:HG3	2.35	0.41
2:B:274:PRO:CG	2:B:359:GLU:HB3	2.51	0.41
10:J:14:VAL:CG1	10:J:50:ILE:CD1	2.90	0.41
2:B:973:ILE:CG2	2:B:974:PRO:HD2	2.51	0.41
8:H:96:VAL:HA	8:H:142:LEU:O	2.21	0.41
1:A:562:THR:HA	1:A:563:PRO:HD3	1.84	0.41
1:A:630:ILE:HG23	1:A:642:CYS:SG	2.60	0.41
2:B:1115:THR:CG2	2:B:1117:GLN:HB2	2.50	0.41
1:A:92:HIS:HB3	1:A:95:PHE:HB2	2.02	0.41
9:I:16:PRO:HA	9:I:26:LEU:O	2.21	0.41
2:B:1192:TYR:N	2:B:1192:TYR:CD1	2.89	0.41
1:A:518:LYS:HE2	1:A:624:SER:O	2.20	0.41
2:B:952:VAL:O	2:B:953:LEU:HB3	2.20	0.41
12:L:53:HIS:O	12:L:55:ILE:HG12	2.20	0.41
1:A:1006:ILE:CD1	5:E:163:GLU:HG3	2.51	0.41
5:E:114:ASN:O	5:E:115:ASN:CB	2.68	0.41
2:B:1177:HIS:C	2:B:1179:GLN:N	2.73	0.41
1:A:130:ASP:C	1:A:132:LYS:H	2.24	0.41
1:A:493:GLN:HE21	1:A:493:GLN:CA	2.33	0.41
2:B:866:TYR:O	2:B:868:MET:N	2.53	0.41
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	2.02	0.41
2:B:788:ARG:HE	2:B:788:ARG:HB3	1.52	0.41
2:B:700:SER:C	2:B:701:ILE:CG2	2.89	0.41
3:C:236:GLY:C	3:C:238:ILE:N	2.73	0.41
2:B:830:TYR:CE2	2:B:1000:PRO:CD	2.93	0.41
2:B:377:PHE:C	2:B:379:GLY:N	2.71	0.41
3:C:59:ALA:O	3:C:62:PHE:CB	2.67	0.41
1:A:1362:TYR:CE1	1:A:1364:ASN:HA	2.56	0.41
2:B:1013:ASN:OD1	2:B:1014:PRO:HD2	2.21	0.41
9:I:101:PHE:O	9:I:102:VAL:CG2	2.67	0.41
3:C:215:GLU:O	3:C:216:GLY:C	2.59	0.41
1:A:704:ALA:O	1:A:705:LYS:CB	2.66	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1291:VAL:HG13	1:A:1292:PRO:N	2.36	0.41
2:B:687:GLU:O	2:B:688:GLY:C	2.59	0.41
1:A:322:VAL:CG1	1:A:323:LYS:N	2.82	0.41
1:A:370:ILE:HG22	1:A:374:LEU:HD12	2.00	0.41
2:B:544:CYS:O	2:B:545:ILE:CG1	2.68	0.41
11:K:50:LEU:HD11	11:K:75:ILE:HD11	2.03	0.41
1:A:1451:VAL:O	1:A:1453:TYR:N	2.54	0.41
3:C:183:TRP:O	3:C:184:ASN:C	2.58	0.41
1:A:726:ARG:O	1:A:729:ALA:N	2.53	0.41
4:D:59:ILE:O	4:D:60:LYS:C	2.58	0.41
4:D:156:ASP:C	4:D:158:GLU:N	2.74	0.41
1:A:942:PHE:C	1:A:942:PHE:CD2	2.94	0.41
6:F:150:GLU:O	6:F:151:LEU:C	2.59	0.41
4:D:40:HIS:CG	4:D:41:GLN:N	2.89	0.41
1:A:899:VAL:O	1:A:929:LEU:HD12	2.21	0.41
1:A:618:GLU:O	1:A:619:LYS:C	2.59	0.41
1:A:44:THR:O	1:A:45:GLN:CB	2.65	0.41
1:A:78:PRO:O	1:A:79:GLY:C	2.58	0.41
2:B:360:PHE:CE2	2:B:361:LEU:HB2	2.55	0.41
3:C:235:VAL:HG21	10:J:6:ARG:HH21	1.85	0.41
3:C:61:GLU:HG2	3:C:62:PHE:N	2.36	0.41
1:A:1436:ILE:HD13	2:B:1139:ILE:CG2	2.45	0.41
2:B:38:PHE:O	2:B:39:ARG:C	2.59	0.41
1:A:1279:ILE:CD1	1:A:1316:VAL:HG21	2.48	0.41
2:B:401:PHE:C	2:B:403:LYS:H	2.24	0.41
1:A:107:CYS:HB2	1:A:171:GLN:HG2	2.01	0.41
4:D:34:GLN:O	4:D:47:LEU:HD23	2.21	0.41
2:B:526:GLU:HG2	2:B:538:ASN:HB2	2.01	0.41
2:B:216:GLU:HB2	2:B:406:LEU:CD2	2.51	0.41
2:B:408:LEU:HA	2:B:408:LEU:HD12	1.75	0.41
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.51	0.41
3:C:18:VAL:O	3:C:20:PHE:CD2	2.73	0.41
7:G:39:THR:HB	7:G:42:PHE:H	1.86	0.41
9:I:45:ARG:HE	9:I:47:GLU:HG3	1.85	0.41
2:B:329:THR:O	2:B:332:ASP:HB3	2.21	0.41
5:E:66:GLU:HA	5:E:69:ILE:HD12	2.02	0.41
6:F:123:LYS:C	6:F:125:LEU:N	2.73	0.41
4:D:167:LEU:C	4:D:169:SER:H	2.24	0.41
1:A:225:ASN:HD21	1:A:228:PHE:H	1.54	0.41
1:A:863:VAL:CG1	1:A:864:ILE:N	2.84	0.41
10:J:57:ILE:CG2	10:J:58:GLU:N	2.84	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:510:LYS:HE2	2:B:513:GLN:OE1	2.21	0.41
2:B:102:VAL:O	2:B:109:THR:HG23	2.21	0.41
1:A:920:LEU:CD2	1:A:920:LEU:C	2.89	0.41
2:B:878:GLN:O	2:B:879:ARG:C	2.58	0.41
3:C:191:TYR:HB3	3:C:201:TRP:CD1	2.56	0.41
2:B:1065:GLN:HG3	2:B:1068:GLY:N	2.35	0.41
1:A:41:MET:HB2	1:A:42:ASP:H	1.46	0.41
2:B:996:ARG:HH22	3:C:175:ALA:CA	2.34	0.41
2:B:824:ILE:CG1	10:J:48:ARG:NH1	2.79	0.41
2:B:995:ARG:O	2:B:996:ARG:C	2.59	0.41
10:J:43:ARG:HG2	10:J:46:CYS:SG	2.61	0.41
2:B:624:LEU:HA	2:B:624:LEU:HD12	1.79	0.41
1:A:1167:GLU:O	1:A:1168:GLU:C	2.58	0.41
1:A:1438:THR:CG2	2:B:1144:ALA:HB3	2.51	0.41
7:G:1:MET:SD	7:G:79:PHE:CE1	3.14	0.41
7:G:80:LYS:HA	7:G:81:PRO:HD2	1.74	0.41
7:G:80:LYS:CE	7:G:82:PHE:CZ	2.98	0.41
1:A:501:LEU:HD11	2:B:1146:PHE:CE2	2.56	0.41
2:B:419:THR:HG21	2:B:468:GLU:OE2	2.20	0.41
1:A:707:GLY:C	1:A:708:MET:HG3	2.41	0.41
1:A:546:VAL:HG21	1:A:572:TRP:CD2	2.55	0.41
1:A:335:ARG:NE	1:A:339:ASN:ND2	2.57	0.41
2:B:515:HIS:HD2	2:B:517:THR:OG1	2.03	0.41
4:D:50:LEU:HD11	7:G:4:ILE:HG13	2.03	0.41
7:G:97:HIS:CD2	7:G:97:HIS:N	2.88	0.41
2:B:857:ARG:O	2:B:858:SER:HB3	2.21	0.41
2:B:642:ASP:HB3	2:B:649:LYS:HG3	2.03	0.41
1:A:1037:LEU:HD23	1:A:1037:LEU:N	2.36	0.41
11:K:12:LEU:HD11	11:K:18:LYS:HE2	2.02	0.41
2:B:543:SER:C	2:B:544:CYS:SG	2.99	0.41
5:E:143:ASN:ND2	5:E:146:HIS:ND1	2.68	0.41
7:G:45:ILE:HD13	7:G:45:ILE:HA	1.99	0.41
2:B:526:GLU:CD	2:B:752:ALA:CB	2.89	0.41
2:B:535:LEU:HA	2:B:535:LEU:HD23	1.87	0.41
7:G:132:SER:O	7:G:134:GLU:N	2.54	0.41
1:A:420:ARG:O	1:A:424:ILE:HG13	2.21	0.41
5:E:112:TYR:CE1	5:E:136:ASN:HB2	2.56	0.41
1:A:393:ARG:C	1:A:395:GLY:N	2.75	0.41
4:D:29:LEU:O	4:D:30:GLY:O	2.39	0.41
6:F:138:LEU:O	6:F:139:PRO:C	2.59	0.41
9:I:40:SER:HB2	9:I:41:PRO:HD2	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.50	0.41
10:J:61:LEU:C	10:J:63:TYR:N	2.75	0.41
1:A:1327:ILE:HG22	5:E:147:HIS:HE1	1.85	0.41
1:A:1419:ASP:OD1	1:A:1426:GLU:OE1	2.39	0.41
1:A:1365:TYR:O	1:A:1367:HIS:N	2.54	0.41
2:B:1004:GLU:CB	2:B:1006:ILE:HD11	2.51	0.41
6:F:75:PRO:HG3	6:F:78:GLN:OE1	2.21	0.41
8:H:3:ASN:HB3	8:H:4:THR:H	1.61	0.41
4:D:33:PHE:CD1	7:G:80:LYS:HE3	2.55	0.41
2:B:466:TRP:O	2:B:467:GLY:C	2.58	0.41
5:E:116:ILE:HG22	5:E:117:THR:N	2.35	0.41
5:E:117:THR:C	5:E:119:SER:N	2.73	0.41
3:C:80:LEU:CD1	3:C:95:CYS:CA	2.99	0.41
2:B:1187:ASN:HD21	2:B:1190:ASP:HB3	1.86	0.41
1:A:114:LEU:O	1:A:115:LEU:HG	2.20	0.41
1:A:239:LEU:HA	1:A:240:PRO:HD2	1.88	0.41
1:A:547:LEU:HD22	11:K:58:PHE:HD1	1.85	0.41
4:D:217:LEU:O	4:D:219:THR:N	2.54	0.41
3:C:187:LYS:C	3:C:189:THR:H	2.24	0.41
4:D:151:PHE:O	4:D:152:SER:O	2.38	0.41
1:A:7:SER:CB	2:B:1175:LEU:HD22	2.51	0.41
5:E:29:PHE:N	5:E:63:ASN:O	2.47	0.41
2:B:27:ALA:O	2:B:30:SER:OG	2.29	0.41
10:J:2:ILE:HG12	10:J:57:ILE:CD1	2.46	0.40
10:J:1:MET:N	10:J:55:ASP:HA	2.36	0.40
1:A:1114:PRO:O	1:A:1115:SER:O	2.38	0.40
1:A:1120:LEU:N	1:A:1120:LEU:HD12	2.36	0.40
2:B:510:LYS:HG3	2:B:512:ARG:HD2	2.03	0.40
2:B:113:TYR:CB	2:B:114:PRO:HD2	2.38	0.40
1:A:922:ASP:OD1	1:A:922:ASP:C	2.60	0.40
1:A:40:THR:CG2	1:A:259:GLU:OE2	2.64	0.40
1:A:73:GLY:O	1:A:74:MET:C	2.59	0.40
1:A:1027:ALA:O	1:A:1030:ARG:N	2.54	0.40
2:B:1002:THR:O	2:B:1003:ALA:C	2.59	0.40
2:B:903:VAL:O	2:B:948:ILE:HG23	2.21	0.40
1:A:218:ASP:HA	1:A:221:SER:OG	2.21	0.40
1:A:935:GLN:C	1:A:937:VAL:N	2.71	0.40
12:L:32:ALA:HB3	12:L:55:ILE:CG1	2.52	0.40
1:A:391:LEU:O	1:A:394:ASN:HB2	2.21	0.40
1:A:1450:LEU:HD21	7:G:19:GLY:O	2.20	0.40
1:A:34:LYS:HD3	1:A:34:LYS:H	1.86	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:143:ILE:HG22	7:G:144:ARG:H	1.86	0.40
11:K:85:ASP:O	11:K:89:ASN:ND2	2.53	0.40
2:B:408:LEU:O	2:B:412:LEU:HG	2.21	0.40
1:A:151:ASP:OD1	1:A:163:SER:CB	2.68	0.40
6:F:134:ILE:N	6:F:146:TRP:O	2.50	0.40
4:D:173:HIS:HA	4:D:174:PRO:HD3	1.95	0.40
1:A:88:LYS:HA	1:A:89:PRO:HD2	1.72	0.40
5:E:112:TYR:HE1	5:E:136:ASN:HD22	1.69	0.40
1:A:1007:ILE:HG12	1:A:1007:ILE:H	1.73	0.40
1:A:825:ILE:O	1:A:828:ALA:N	2.49	0.40
1:A:786:HIS:N	1:A:786:HIS:HD2	2.17	0.40
2:B:1198:TYR:O	2:B:1199:ALA:C	2.59	0.40
2:B:1007:VAL:HG23	2:B:1008:PRO:HD2	1.96	0.40
2:B:873:THR:CG2	2:B:874:PHE:N	2.84	0.40
2:B:331:LEU:HD12	2:B:331:LEU:N	2.37	0.40
1:A:839:ARG:O	1:A:842:VAL:HB	2.21	0.40
2:B:1183:LYS:HA	2:B:1186:ASP:HA	2.04	0.40
2:B:843:GLN:HA	2:B:846:ILE:HG13	2.02	0.40
2:B:38:PHE:CE2	2:B:43:LEU:HD23	2.57	0.40
1:A:703:THR:O	1:A:704:ALA:C	2.59	0.40
1:A:541:ILE:CD1	1:A:577:ILE:HD11	2.51	0.40
2:B:711:GLU:N	2:B:712:PRO:HD2	2.35	0.40
1:A:506:ALA:O	1:A:507:VAL:C	2.60	0.40
1:A:933:TYR:C	1:A:935:GLN:H	2.24	0.40
6:F:103:MET:HE3	7:G:66:GLY:H	1.86	0.40
1:A:1191:TRP:HD1	1:A:1256:GLU:CB	2.35	0.40
3:C:8:VAL:CG1	3:C:9:LYS:N	2.83	0.40
2:B:847:ASP:O	2:B:849:GLY:N	2.55	0.40
4:D:173:HIS:NE2	4:D:201:LYS:NZ	2.68	0.40
1:A:1187:GLN:HG3	1:A:1188:GLN:H	1.85	0.40
2:B:530:GLY:O	2:B:532:ALA:N	2.54	0.40
11:K:20:LYS:HB2	11:K:20:LYS:HE3	1.89	0.40
7:G:51:TYR:C	7:G:51:TYR:CD2	2.94	0.40
7:G:5:LYS:CG	7:G:7:LEU:HD21	2.51	0.40
1:A:241:VAL:HA	1:A:242:PRO:HD2	1.92	0.40
1:A:932:GLU:HG3	1:A:936:LEU:HD21	2.02	0.40
1:A:351:THR:CG2	2:B:1103:ILE:HA	2.39	0.40
3:C:61:GLU:HA	3:C:64:ALA:CB	2.52	0.40
1:A:1164:PRO:CG	1:A:1165:GLU:H	2.33	0.40
1:A:1063:MET:SD	1:A:1436:ILE:HG23	2.61	0.40
2:B:842:ASN:O	2:B:846:ILE:HG13	2.21	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:79:ARG:HG2	6:F:79:ARG:NH1	2.35	0.40
1:A:477:PRO:HG3	1:A:521:MET:HG2	2.03	0.40
2:B:806:THR:N	2:B:809:MET:HE3	2.37	0.40
1:A:1138:ILE:CG2	1:A:1316:VAL:HG13	2.52	0.40
2:B:912:ILE:O	2:B:938:SER:HB3	2.22	0.40
1:A:135:PHE:O	1:A:137:ALA:N	2.54	0.40
2:B:1027:ILE:HD13	2:B:1052:VAL:CG2	2.51	0.40
1:A:289:ILE:HG22	1:A:290:GLU:N	2.37	0.40
1:A:369:SER:HB3	11:K:2:ASN:HD21	1.86	0.40
5:E:114:ASN:HD22	5:E:114:ASN:HA	1.65	0.40
1:A:1001:ARG:O	1:A:1002:GLY:C	2.59	0.40
2:B:533:CYS:C	2:B:535:LEU:N	2.72	0.40
1:A:130:ASP:C	1:A:132:LYS:N	2.75	0.40
8:H:13:SER:O	8:H:14:GLU:HB2	2.22	0.40
11:K:84:LYS:H	11:K:84:LYS:HG3	1.70	0.40
2:B:351:TYR:O	2:B:355:ILE:HG13	2.20	0.40
3:C:229:TYR:CD1	3:C:229:TYR:N	2.89	0.40
1:A:209:ASN:O	1:A:210:ILE:C	2.58	0.40
7:G:18:PHE:HA	7:G:22:MET:HE2	2.04	0.40
2:B:1064:TYR:O	2:B:1065:GLN:C	2.59	0.40
2:B:385:LEU:HD12	2:B:385:LEU:C	2.42	0.40
3:C:88:CYS:HB3	3:C:92:CYS:HB3	2.02	0.40
1:A:741:ASN:ND2	1:A:743:VAL:HB	2.36	0.40
9:I:34:TYR:HE2	9:I:36:GLU:CB	2.32	0.40
1:A:711:ARG:O	1:A:714:PHE:HB3	2.21	0.40
12:L:32:ALA:HB3	12:L:55:ILE:HG13	2.03	0.40
6:F:97:ARG:O	6:F:100:GLN:N	2.54	0.40
1:A:1211:GLN:O	1:A:1214:GLU:HB2	2.21	0.40
1:A:544:ASP:CG	1:A:545:GLN:N	2.74	0.40
3:C:102:GLN:HA	3:C:153:LEU:O	2.22	0.40
2:B:218:SER:HB3	2:B:241:ARG:HH11	1.87	0.40
10:J:35:ALA:O	10:J:38:ARG:HB3	2.21	0.40
7:G:5:LYS:HG3	7:G:7:LEU:HD21	2.03	0.40
1:A:867:ILE:HG22	1:A:871:ASP:H	1.85	0.40
2:B:1182:CYS:C	2:B:1183:LYS:O	2.60	0.40
11:K:55:LYS:O	11:K:77:THR:HG22	2.20	0.40
1:A:706:HIS:CD2	1:A:706:HIS:H	2.38	0.40
3:C:92:CYS:SG	3:C:95:CYS:N	2.95	0.40
8:H:87:ARG:HB3	8:H:88:SER:H	1.81	0.40
2:B:635:ARG:HH11	2:B:635:ARG:CG	2.33	0.40
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.86	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LEU:HD13	1:A:171:GLN:HE22	1.86	0.40
2:B:763:GLN:O	2:B:764:SER:C	2.59	0.40
8:H:83:GLN:C	8:H:85:GLY:N	2.74	0.40
1:A:1147:THR:HG22	1:A:1148:ILE:N	2.36	0.40
2:B:313:MET:HE2	2:B:390:LEU:HD21	2.02	0.40
1:A:1260:LEU:HG	1:A:1260:LEU:O	2.20	0.40
9:I:8:ARG:HB2	9:I:9:ASP:OD1	2.22	0.40
2:B:533:CYS:SG	2:B:534:GLY:N	2.95	0.40
1:A:967:ALA:HA	1:A:1044:TRP:CZ3	2.56	0.40
2:B:121:ASN:HA	2:B:207:GLY:CA	2.51	0.40
4:D:188:ALA:O	4:D:191:ALA:N	2.55	0.40
4:D:202:ILE:O	4:D:202:ILE:CG2	2.70	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	1418/1455 (98%)	914 (64%)	316 (22%)	188 (13%)	0	7
2	B	1096/1224 (90%)	725 (66%)	223 (20%)	148 (14%)	0	7
3	C	264/268 (98%)	169 (64%)	62 (24%)	33 (12%)	0	8
4	D	173/221 (78%)	129 (75%)	27 (16%)	17 (10%)	1	14
5	E	212/215 (99%)	141 (66%)	50 (24%)	21 (10%)	1	14
6	F	82/84 (98%)	60 (73%)	15 (18%)	7 (8%)	1	18
7	G	169/171 (99%)	123 (73%)	34 (20%)	12 (7%)	1	22
8	H	129/146 (88%)	93 (72%)	25 (19%)	11 (8%)	1	18
9	I	117/122 (96%)	80 (68%)	22 (19%)	15 (13%)	0	8
10	J	63/70 (90%)	36 (57%)	14 (22%)	13 (21%)	0	3

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	112/120 (93%)	82 (73%)	25 (22%)	5 (4%)	3	33
12	L	44/46 (96%)	18 (41%)	14 (32%)	12 (27%)	0	0
All	All	3879/4142 (94%)	2570 (66%)	827 (21%)	482 (12%)	1	8

All (482) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	48	ALA
1	A	55	ASP
1	A	58	LEU
1	A	62	ASP
1	A	70	CYS
1	A	73	GLY
1	A	76	GLU
1	A	93	VAL
1	A	130	ASP
1	A	286	HIS
1	A	311	GLN
1	A	322	VAL
1	A	385	ILE
1	A	399	HIS
1	A	423	ASP
1	A	516	SER
1	A	525	GLN
1	A	536	LEU
1	A	567	LYS
1	A	583	PRO
1	A	626	ASN
1	A	708	MET
1	A	709	THR
1	A	780	VAL
1	A	821	ARG
1	A	920	LEU
1	A	1002	GLY
1	A	1036	ARG
1	A	1115	SER
1	A	1122	PRO
1	A	1124	HIS
1	A	1165	GLU
1	A	1167	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1212	VAL
1	A	1223	ASP
1	A	1231	ASP
1	A	1242	VAL
1	A	1281	ARG
1	A	1308	THR
1	A	1309	ASP
1	A	1335	ILE
1	A	1341	ILE
1	A	1366	ARG
1	A	1377	THR
1	A	1378	GLN
1	A	1386	ARG
1	A	1392	SER
1	A	1396	ALA
1	A	1397	LEU
1	A	1403	GLU
1	A	1405	THR
1	A	1424	VAL
2	B	43	LEU
2	B	45	SER
2	B	58	THR
2	B	67	SER
2	B	108	VAL
2	B	124	TYR
2	B	186	GLU
2	B	219	ALA
2	B	261	ARG
2	B	367	LEU
2	B	391	ASP
2	B	466	TRP
2	B	467	GLY
2	B	468	GLU
2	B	474	SER
2	B	510	LYS
2	B	530	GLY
2	B	531	GLN
2	B	571	PRO
2	B	591	ARG
2	B	620	ARG
2	B	629	ASP
2	B	636	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	643	ASP
2	B	648	HIS
2	B	709	ASP
2	B	727	LYS
2	B	731	VAL
2	B	751	VAL
2	B	752	ALA
2	B	818	PRO
2	B	901	PRO
2	B	903	VAL
2	B	943	SER
2	B	958	GLN
2	B	992	ILE
2	B	1046	PRO
2	B	1108	ARG
2	B	1157	ALA
2	B	1167	GLY
2	B	1171	VAL
2	B	1175	LEU
2	B	1181	GLU
2	B	1188	LYS
2	B	1211	ASN
3	C	10	ILE
3	C	60	ASP
3	C	81	GLU
3	C	83	SER
3	C	87	PHE
3	C	110	THR
3	C	149	LYS
3	C	167	HIS
3	C	175	ALA
3	C	184	ASN
3	C	213	PRO
3	C	214	ASN
3	C	215	GLU
3	C	216	GLY
4	D	12	ARG
4	D	15	LEU
4	D	20	GLU
4	D	152	SER
5	E	130	ALA
5	E	158	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	F	81	THR
7	G	118	ASP
8	H	81	PRO
8	H	84	ALA
8	H	140	ALA
9	I	9	ASP
9	I	11	ASN
9	I	84	VAL
10	J	6	ARG
10	J	15	GLY
10	J	53	HIS
10	J	64	ASN
12	L	50	ASP
12	L	53	HIS
12	L	59	ALA
12	L	60	ARG
1	A	42	ASP
1	A	44	THR
1	A	45	GLN
1	A	54	ASN
1	A	57	ARG
1	A	61	ILE
1	A	74	MET
1	A	79	GLY
1	A	111	GLY
1	A	126	LEU
1	A	131	SER
1	A	154	SER
1	A	219	PHE
1	A	223	GLY
1	A	244	PRO
1	A	290	GLU
1	A	317	LYS
1	A	318	SER
1	A	331	GLY
1	A	332	LYS
1	A	335	ARG
1	A	400	PRO
1	A	415	LEU
1	A	418	SER
1	A	419	LYS
1	A	424	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	473	SER
1	A	557	ASP
1	A	594	GLY
1	A	598	LEU
1	A	619	LYS
1	A	716	ASP
1	A	720	ARG
1	A	738	LYS
1	A	760	GLN
1	A	765	VAL
1	A	775	ILE
1	A	824	LEU
1	A	846	GLU
1	A	847	ASP
1	A	859	SER
1	A	864	ILE
1	A	875	ALA
1	A	929	LEU
1	A	968	GLN
1	A	979	SER
1	A	1006	ILE
1	A	1016	THR
1	A	1052	GLN
1	A	1084	PHE
1	A	1089	VAL
1	A	1104	ILE
1	A	1105	LEU
1	A	1126	ALA
1	A	1128	GLN
1	A	1164	PRO
1	A	1168	GLU
1	A	1169	ILE
1	A	1170	ILE
1	A	1224	LEU
1	A	1314	SER
1	A	1365	TYR
1	A	1376	THR
2	B	21	GLU
2	B	46	GLN
2	B	65	GLU
2	B	68	THR
2	B	114	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	229	ALA
2	B	258	LEU
2	B	260	GLY
2	B	266	ALA
2	B	294	ASP
2	B	322	PHE
2	B	504	ARG
2	B	509	ALA
2	B	526	GLU
2	B	534	GLY
2	B	559	SER
2	B	605	ARG
2	B	613	VAL
2	B	641	GLU
2	B	810	GLU
2	B	867	GLY
2	B	869	SER
2	B	880	THR
2	B	881	ASN
2	B	891	ASP
2	B	902	GLY
2	B	907	GLY
2	B	1018	PRO
2	B	1041	GLU
2	B	1096	ARG
2	B	1099	VAL
2	B	1150	ARG
2	B	1156	ASP
2	B	1170	THR
2	B	1183	LYS
2	B	1186	ASP
2	B	1190	ASP
3	C	74	SER
3	C	141	GLY
3	C	161	LYS
4	D	6	SER
4	D	8	PHE
4	D	16	LYS
4	D	19	GLU
4	D	30	GLY
4	D	199	ASN
4	D	218	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
5	E	36	GLU
5	E	45	LYS
5	E	59	SER
5	E	106	GLN
5	E	145	THR
5	E	189	GLY
5	E	206	GLY
6	F	131	PRO
7	G	83	LYS
7	G	154	VAL
8	H	59	ILE
8	H	77	ARG
8	H	82	PRO
8	H	108	SER
8	H	128	ASN
9	I	3	THR
9	I	34	TYR
9	I	62	ILE
9	I	89	GLN
9	I	106	CYS
9	I	107	SER
10	J	2	ILE
10	J	62	ARG
11	K	37	LYS
11	K	103	THR
12	L	43	THR
12	L	51	CYS
12	L	56	LEU
1	A	59	GLY
1	A	66	LYS
1	A	89	PRO
1	A	124	GLN
1	A	167	CYS
1	A	283	GLY
1	A	394	ASN
1	A	396	PRO
1	A	517	ASN
1	A	543	LEU
1	A	592	ASP
1	A	640	GLN
1	A	647	GLY
1	A	707	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	731	ARG
1	A	774	ARG
1	A	903	ASN
1	A	1017	LEU
1	A	1060	PRO
1	A	1062	GLU
1	A	1131	ALA
1	A	1221	LYS
1	A	1229	SER
1	A	1452	LYS
2	B	115	GLN
2	B	131	ASP
2	B	176	SER
2	B	206	ASN
2	B	295	GLY
2	B	308	TRP
2	B	334	ILE
2	B	365	THR
2	B	369	GLY
2	B	469	GLN
2	B	480	SER
2	B	551	PRO
2	B	598	GLU
2	B	645	SER
2	B	688	GLY
2	B	711	GLU
2	B	712	PRO
2	B	738	PHE
2	B	761	HIS
2	B	792	MET
2	B	822	ASN
2	B	996	ARG
2	B	1017	ILE
2	B	1153	GLU
2	B	1155	SER
2	B	1189	ILE
3	C	6	PRO
3	C	28	ALA
3	C	91	HIS
3	C	169	LYS
3	C	202	PRO
3	C	212	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	C	218	PRO
3	C	264	GLN
4	D	52	LEU
5	E	8	ASN
5	E	44	ALA
5	E	56	LYS
5	E	74	ASP
7	G	17	PHE
7	G	139	ILE
7	G	147	ILE
9	I	7	CYS
9	I	113	ASP
10	J	22	LEU
12	L	35	SER
12	L	49	LYS
1	A	35	ILE
1	A	67	CYS
1	A	100	LYS
1	A	196	GLU
1	A	253	ASN
1	A	312	PRO
1	A	465	TYR
1	A	526	ASP
1	A	605	MET
1	A	986	ILE
1	A	1040	GLN
1	A	1139	GLU
1	A	1206	ASP
1	A	1266	THR
1	A	1280	GLU
2	B	387	LEU
2	B	409	ALA
2	B	430	ARG
2	B	682	SER
2	B	754	SER
2	B	848	ARG
2	B	884	ARG
2	B	946	ASN
2	B	1029	CYS
2	B	1143	ALA
2	B	1178	ASN
2	B	1202	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	C	90	ASP
3	C	198	ALA
3	C	227	THR
3	C	240	VAL
4	D	131	GLU
4	D	168	LYS
5	E	73	PRO
5	E	115	ASN
5	E	192	ARG
6	F	73	ALA
6	F	112	GLU
7	G	133	SER
8	H	92	ASP
9	I	32	CYS
9	I	73	ARG
9	I	86	PHE
9	I	95	THR
10	J	9	SER
10	J	29	GLU
10	J	51	LEU
10	J	63	TYR
11	K	64	GLU
12	L	42	ARG
1	A	84	ILE
1	A	197	PRO
1	A	696	GLU
1	A	759	ALA
1	A	789	LYS
1	A	795	GLU
1	A	808	LEU
1	A	817	ALA
1	A	958	VAL
1	A	1160	SER
1	A	1188	GLN
1	A	1302	PRO
1	A	1435	PRO
2	B	22	SER
2	B	56	ASP
2	B	368	GLU
2	B	483	LEU
2	B	490	SER
2	B	565	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	878	GLN
2	B	879	ARG
2	B	883	LEU
2	B	1019	SER
2	B	1100	ASP
3	C	148	ARG
4	D	27	LEU
4	D	142	LYS
5	E	40	GLU
5	E	172	GLU
5	E	183	PRO
6	F	108	PHE
7	G	30	LEU
7	G	124	GLY
7	G	165	GLU
8	H	52	GLN
11	K	70	ARG
1	A	599	SER
1	A	641	VAL
1	A	719	VAL
1	A	1162	VAL
1	A	1338	VAL
2	B	171	PRO
2	B	259	TYR
2	B	282	ILE
2	B	450	ALA
2	B	543	SER
2	B	694	ASP
2	B	758	PHE
2	B	906	SER
2	B	1103	ILE
2	B	1118	PRO
3	C	126	GLY
3	C	171	GLY
4	D	201	LYS
6	F	139	PRO
8	H	8	ASP
10	J	18	TRP
12	L	26	THR
12	L	46	VAL
1	A	507	VAL
1	A	1057	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	635	ARG
3	C	142	VAL
6	F	93	ILE
1	A	9	ALA
1	A	653	VAL
1	A	886	ILE
1	A	963	ILE
1	A	1158	PRO
2	B	985	GLY
5	E	37	LEU
7	G	63	PRO
1	A	392	VAL
1	A	673	GLY
1	A	1379	GLY
2	B	410	GLY
2	B	502	ILE
2	B	552	MET
2	B	974	PRO
1	A	250	ILE
1	A	649	ILE
1	A	1031	VAL
10	J	14	VAL
11	K	43	GLY
1	A	357	PRO
1	A	1061	GLY
2	B	575	PRO
7	G	157	ILE
5	E	129	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1246/1270 (98%)	1133 (91%)	113 (9%)	12	43
2	B	964/1061 (91%)	880 (91%)	84 (9%)	13	45
3	C	234/236 (99%)	205 (88%)	29 (12%)	6	30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	140/200 (70%)	126 (90%)	14 (10%)	9	38
5	E	196/197 (100%)	184 (94%)	12 (6%)	23	60
6	F	74/74 (100%)	63 (85%)	11 (15%)	4	23
7	G	152/152 (100%)	143 (94%)	9 (6%)	24	61
8	H	117/128 (91%)	110 (94%)	7 (6%)	24	60
9	I	113/116 (97%)	97 (86%)	16 (14%)	4	26
10	J	60/65 (92%)	55 (92%)	5 (8%)	14	49
11	K	99/102 (97%)	91 (92%)	8 (8%)	15	50
12	L	40/40 (100%)	33 (82%)	7 (18%)	2	16
All	All	3435/3641 (94%)	3120 (91%)	315 (9%)	16	43

All (315) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	13	THR
1	A	14	VAL
1	A	18	GLN
1	A	34	LYS
1	A	41	MET
1	A	54	ASN
1	A	62	ASP
1	A	83	HIS
1	A	93	VAL
1	A	108	MET
1	A	167	CYS
1	A	195	ASP
1	A	200	ARG
1	A	208	LEU
1	A	215	SER
1	A	220	THR
1	A	270	LEU
1	A	303	TYR
1	A	308	ILE
1	A	326	ARG
1	A	329	LEU
1	A	335	ARG
1	A	354	SER
1	A	362	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	375	THR
1	A	381	THR
1	A	406	ILE
1	A	408	ASP
1	A	425	GLN
1	A	434	ARG
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	453	MET
1	A	454	SER
1	A	466	SER
1	A	469	ARG
1	A	481	ASP
1	A	487	MET
1	A	489	LEU
1	A	493	GLN
1	A	498	ARG
1	A	501	LEU
1	A	503	GLN
1	A	523	ILE
1	A	524	VAL
1	A	560	ILE
1	A	562	THR
1	A	596	THR
1	A	618	GLU
1	A	626	ASN
1	A	629	LEU
1	A	734	GLU
1	A	739	ASP
1	A	754	SER
1	A	762	SER
1	A	774	ARG
1	A	786	HIS
1	A	791	ASP
1	A	816	HIS
1	A	821	ARG
1	A	831	THR
1	A	833	GLU
1	A	845	LEU
1	A	852	TYR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	854	ASN
1	A	858	ASN
1	A	879	GLU
1	A	890	ASP
1	A	897	TYR
1	A	903	ASN
1	A	906	HIS
1	A	920	LEU
1	A	929	LEU
1	A	936	LEU
1	A	949	ASP
1	A	969	GLN
1	A	1029	ARG
1	A	1035	TYR
1	A	1048	ASN
1	A	1050	GLU
1	A	1058	VAL
1	A	1081	LEU
1	A	1082	ASN
1	A	1110	ASN
1	A	1111	MET
1	A	1114	PRO
1	A	1116	LEU
1	A	1122	PRO
1	A	1127	ASP
1	A	1142	THR
1	A	1155	ASP
1	A	1166	ASP
1	A	1236	LEU
1	A	1264	GLU
1	A	1271	ILE
1	A	1274	ARG
1	A	1291	VAL
1	A	1295	THR
1	A	1298	TYR
1	A	1300	LYS
1	A	1325	THR
1	A	1333	ILE
1	A	1353	TYR
1	A	1358	SER
1	A	1362	TYR
1	A	1364	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1372	VAL
1	A	1376	THR
1	A	1445	ILE
1	A	1447	GLU
2	B	44	VAL
2	B	57	TYR
2	B	128	LEU
2	B	175	ARG
2	B	194	GLU
2	B	217	ARG
2	B	223	VAL
2	B	261	ARG
2	B	268	THR
2	B	286	PHE
2	B	294	ASP
2	B	298	LEU
2	B	365	THR
2	B	371	GLU
2	B	378	LEU
2	B	393	LYS
2	B	401	PHE
2	B	408	LEU
2	B	419	THR
2	B	427	ASP
2	B	429	PHE
2	B	463	THR
2	B	466	TRP
2	B	476	ARG
2	B	485	ARG
2	B	496	ARG
2	B	498	THR
2	B	510	LYS
2	B	511	PRO
2	B	582	VAL
2	B	603	LEU
2	B	615	MET
2	B	629	ASP
2	B	635	ARG
2	B	636	PRO
2	B	644	GLU
2	B	658	ILE
2	B	682	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	724	ASP
2	B	737	THR
2	B	742	GLU
2	B	743	ILE
2	B	748	ILE
2	B	751	VAL
2	B	766	ARG
2	B	815	ARG
2	B	830	TYR
2	B	835	GLN
2	B	839	MET
2	B	855	PHE
2	B	856	PHE
2	B	859	TYR
2	B	878	GLN
2	B	895	ASP
2	B	901	PRO
2	B	909	ASP
2	B	939	THR
2	B	953	LEU
2	B	986	GLN
2	B	987	LYS
2	B	993	THR
2	B	997	GLU
2	B	999	MET
2	B	1002	THR
2	B	1006	ILE
2	B	1026	LEU
2	B	1034	VAL
2	B	1047	PHE
2	B	1051	THR
2	B	1076	HIS
2	B	1084	GLN
2	B	1087	PHE
2	B	1092	TYR
2	B	1095	LEU
2	B	1096	ARG
2	B	1104	HIS
2	B	1137	CYS
2	B	1138	MET
2	B	1159	ARG
2	B	1170	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	1183	LYS
2	B	1202	LEU
2	B	1212	ILE
2	B	1224	PHE
3	C	23	SER
3	C	44	LEU
3	C	54	ASN
3	C	55	THR
3	C	56	THR
3	C	57	VAL
3	C	58	LEU
3	C	62	PHE
3	C	74	SER
3	C	77	ILE
3	C	86	CYS
3	C	88	CYS
3	C	89	GLU
3	C	91	HIS
3	C	100	THR
3	C	104	PHE
3	C	108	GLU
3	C	129	ILE
3	C	138	GLU
3	C	140	ASN
3	C	143	LEU
3	C	147	LEU
3	C	186	LEU
3	C	193	TYR
3	C	214	ASN
3	C	240	VAL
3	C	245	VAL
3	C	250	THR
3	C	266	ASP
4	D	47	LEU
4	D	63	LEU
4	D	70	PHE
4	D	137	ASN
4	D	139	LYS
4	D	148	LEU
4	D	149	THR
4	D	152	SER
4	D	177	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	D	182	SER
4	D	187	THR
4	D	193	THR
4	D	197	SER
4	D	206	GLU
5	E	60	PHE
5	E	72	PHE
5	E	83	CYS
5	E	104	ASN
5	E	114	ASN
5	E	135	PHE
5	E	153	HIS
5	E	169	ARG
5	E	183	PRO
5	E	207	ARG
5	E	211	TYR
5	E	212	ARG
6	F	77	ASP
6	F	79	ARG
6	F	81	THR
6	F	84	TYR
6	F	86	THR
6	F	90	ARG
6	F	96	THR
6	F	119	ARG
6	F	143	PHE
6	F	148	VAL
6	F	153	VAL
7	G	1	MET
7	G	38	CYS
7	G	39	THR
7	G	70	PHE
7	G	78	VAL
7	G	80	LYS
7	G	96	GLN
7	G	126	ASN
7	G	171	ILE
8	H	10	PHE
8	H	86	ASP
8	H	95	TYR
8	H	102	TYR
8	H	130	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	H	134	ASN
8	H	141	TYR
9	I	6	PHE
9	I	8	ARG
9	I	9	ASP
9	I	10	CYS
9	I	13	MET
9	I	32	CYS
9	I	34	TYR
9	I	46	HIS
9	I	75	CYS
9	I	78	CYS
9	I	85	PHE
9	I	86	PHE
9	I	100	PHE
9	I	101	PHE
9	I	106	CYS
9	I	113	ASP
10	J	2	ILE
10	J	28	ASP
10	J	46	CYS
10	J	48	ARG
10	J	55	ASP
11	K	10	PHE
11	K	25	THR
11	K	35	PHE
11	K	47	ARG
11	K	70	ARG
11	K	78	THR
11	K	81	TYR
11	K	114	LEU
12	L	33	GLU
12	L	48	CYS
12	L	51	CYS
12	L	55	ILE
12	L	63	ARG
12	L	65	VAL
12	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	80	HIS
1	A	83	HIS
1	A	92	HIS
1	A	213	HIS
1	A	225	ASN
1	A	256	GLN
1	A	299	HIS
1	A	339	ASN
1	A	394	ASN
1	A	435	HIS
1	A	445	ASN
1	A	451	HIS
1	A	493	GLN
1	A	503	GLN
1	A	587	HIS
1	A	603	ASN
1	A	611	GLN
1	A	631	HIS
1	A	654	ASN
1	A	659	HIS
1	A	706	HIS
1	A	741	ASN
1	A	757	ASN
1	A	786	HIS
1	A	851	HIS
1	A	858	ASN
1	A	877	HIS
1	A	903	ASN
1	A	926	GLN
1	A	1048	ASN
1	A	1085	HIS
1	A	1106	ASN
1	A	1432	GLN
2	B	52	ASN
2	B	60	GLN
2	B	121	ASN
2	B	178	ASN
2	B	236	HIS
2	B	325	GLN
2	B	366	GLN
2	B	465	ASN
2	B	515	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	657	HIS
2	B	744	HIS
2	B	821	GLN
2	B	835	GLN
2	B	957	ASN
2	B	984	HIS
2	B	1015	HIS
2	B	1065	GLN
2	B	1084	GLN
2	B	1117	GLN
2	B	1161	HIS
2	B	1179	GLN
2	B	1193	GLN
3	C	65	HIS
3	C	73	GLN
3	C	79	GLN
3	C	91	HIS
3	C	112	ASN
3	C	167	HIS
3	C	252	GLN
4	D	28	GLN
4	D	39	ASN
4	D	40	HIS
4	D	51	ASN
4	D	137	ASN
5	E	101	GLN
5	E	104	ASN
5	E	114	ASN
5	E	143	ASN
5	E	147	HIS
7	G	14	HIS
7	G	53	ASN
7	G	97	HIS
7	G	122	ASN
7	G	126	ASN
9	I	12	ASN
9	I	83	ASN
9	I	89	GLN
9	I	90	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
11	K	65	HIS
11	K	76	GLN
11	K	89	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 ⓘ

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.