



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:21 am BST

PDB ID : 3HOX  
Title : Complete RNA polymerase II elongation complex V  
Authors : Sydow, J.F.; Brueckner, F.; Cheung, A.C.M.; Damsma, G.E.; Dengl, S.;  
Lehmann, E.; Vassylyev, D.; Cramer, P.  
Deposited on : 2009-06-03  
Resolution : 3.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

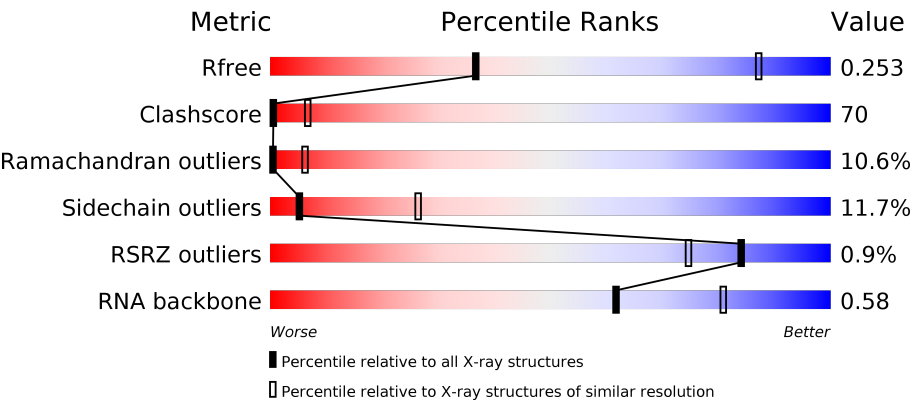
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.65 Å.

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



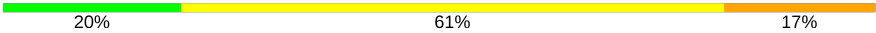
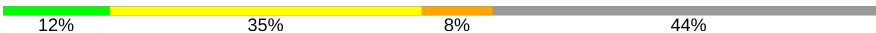

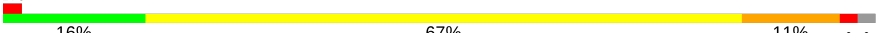
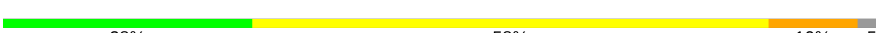

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)
RNA backbone	3102	1024 (4.30-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1733	<div><div>21%49%11%•18%</div><div>%</div></div>
2	B	1224	<div><div>20%55%15%•9%</div><div>%</div></div>
3	C	347	<div><div>13%48%15%•23%</div><div>%</div></div>
4	D	221	<div><div>19%46%15%•19%</div><div>%</div></div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	12	
14	T	26	
15	P	18	

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31918 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1417	Total	C	N	O	S	0	0	0
			11151	7027	1950	2112	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1113	Total	C	N	O	S	0	0	0
			8847	5600	1552	1640	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-28	MET	-	EXPRESSION TAG	UNP P16370
C	-27	GLY	-	EXPRESSION TAG	UNP P16370
C	-26	SER	-	EXPRESSION TAG	UNP P16370
C	-25	HIS	-	EXPRESSION TAG	UNP P16370
C	-24	HIS	-	EXPRESSION TAG	UNP P16370
C	-23	HIS	-	EXPRESSION TAG	UNP P16370
C	-22	HIS	-	EXPRESSION TAG	UNP P16370
C	-21	HIS	-	EXPRESSION TAG	UNP P16370
C	-20	HIS	-	EXPRESSION TAG	UNP P16370
C	-19	SER	-	EXPRESSION TAG	UNP P16370
C	-18	ASN	-	EXPRESSION TAG	UNP P16370
C	-17	SER	-	EXPRESSION TAG	UNP P16370
C	-16	GLY	-	EXPRESSION TAG	UNP P16370
C	-15	LEU	-	EXPRESSION TAG	UNP P16370

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	ASN	-	EXPRESSION TAG	UNP P16370
C	-13	ASP	-	EXPRESSION TAG	UNP P16370
C	-12	ILE	-	EXPRESSION TAG	UNP P16370
C	-11	PHE	-	EXPRESSION TAG	UNP P16370
C	-10	GLU	-	EXPRESSION TAG	UNP P16370
C	-9	ALA	-	EXPRESSION TAG	UNP P16370
C	-8	GLN	-	EXPRESSION TAG	UNP P16370
C	-7	LYS	-	EXPRESSION TAG	UNP P16370
C	-6	ILE	-	EXPRESSION TAG	UNP P16370
C	-5	GLU	-	EXPRESSION TAG	UNP P16370
C	-4	TRP	-	EXPRESSION TAG	UNP P16370
C	-3	HIS	-	EXPRESSION TAG	UNP P16370
C	-2	GLU	-	EXPRESSION TAG	UNP P16370
C	-1	ASP	-	EXPRESSION TAG	UNP P16370
C	0	THR	-	EXPRESSION TAG	UNP P16370
C	1	GLY	-	EXPRESSION TAG	UNP P16370

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	135	Total	C	N	O	S	0	0	0
			1081	680	183	214	4			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a DNA chain called 5'-D(\*AP\*CP\*TP\*AP\*CP\*TP\*TP\*GP\*AP\*GP\*CP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	7	Total	C	N	O	P	0	0	0
			137	68	22	41	6			

- Molecule 14 is a DNA chain called 5'-D(\*AP\*GP\*CP\*TP\*C\*AP\*AP\*GP\*TP\*AP\*GP\*TP\*TP\*AP\*AP\*GP\*CP\*CP\*(BRU)P\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
14	T	18	Total	Br	C	N	O	P	0	0	0
			369	1	176	69	106	17			

- Molecule 15 is a RNA chain called 5'-R(\*UP\*GP\*CP\*AP\*UP\*UP\*U\*CP\*AP\*AP\*CP\*CP

\*AP\*GP\*GP\*CP\*UP\*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	11	Total	C	N	O	P	0	0	0
			213	95	39	69	10			

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

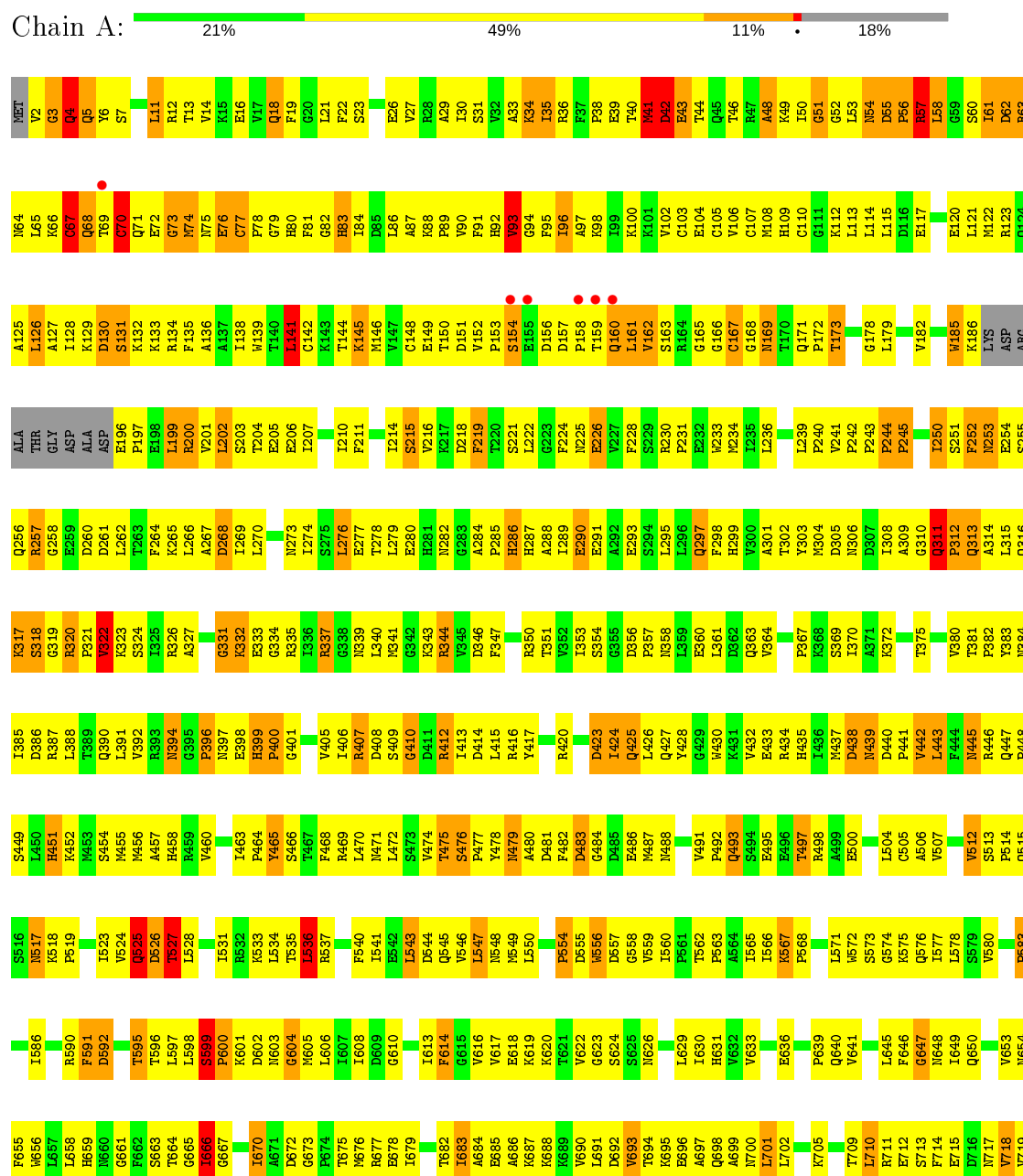
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

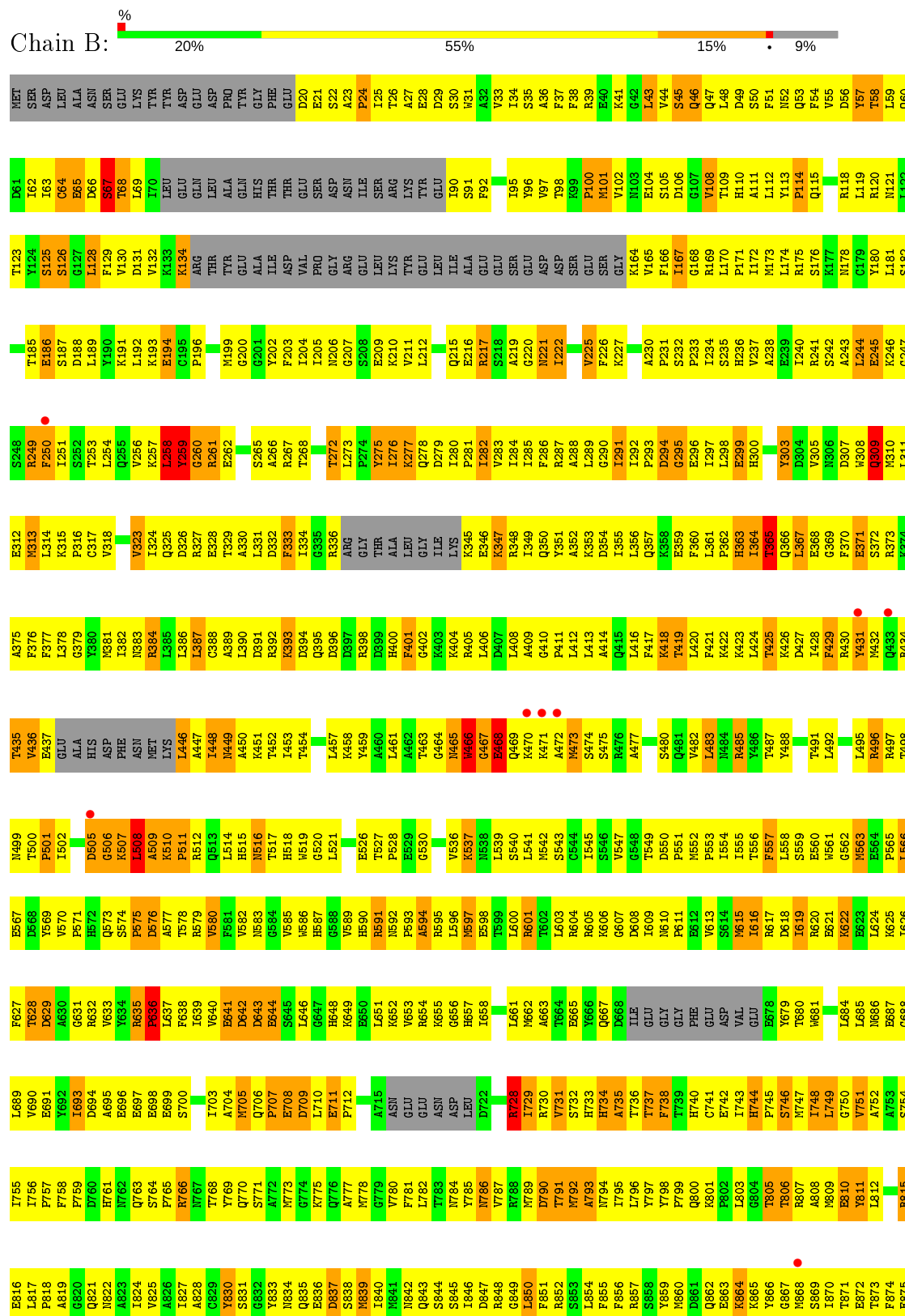


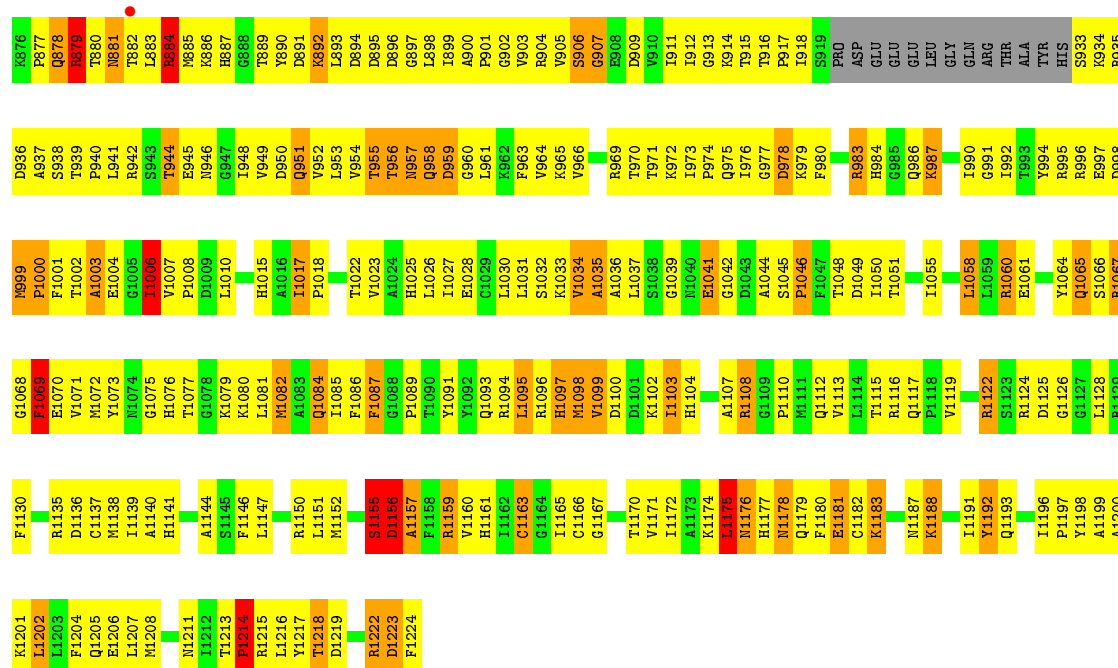




## ARG

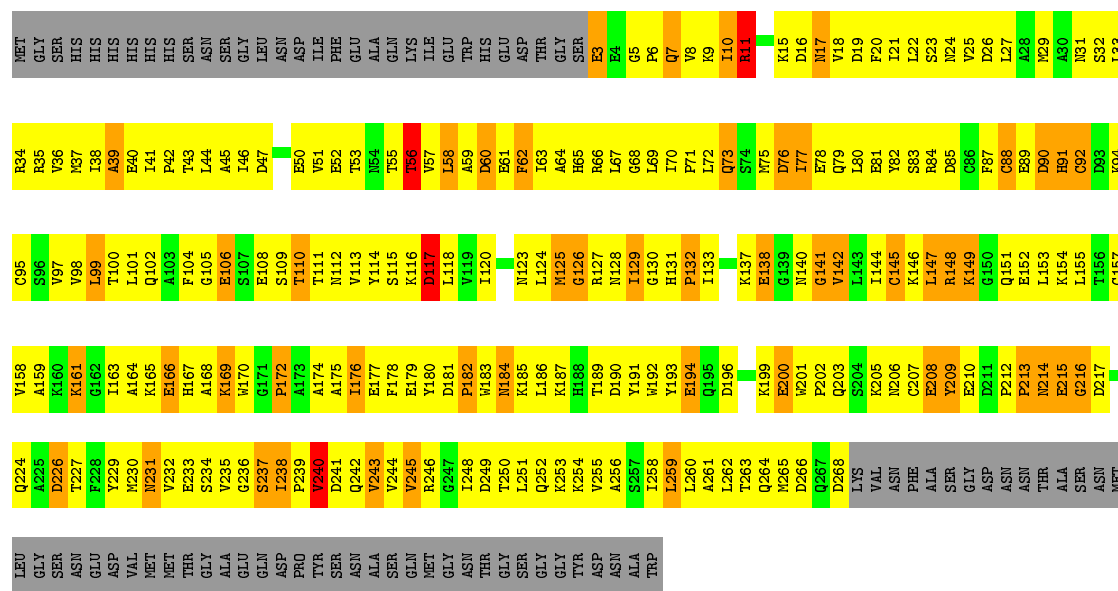
- Molecule 2: DNA-directed RNA polymerase II subunit RPB2





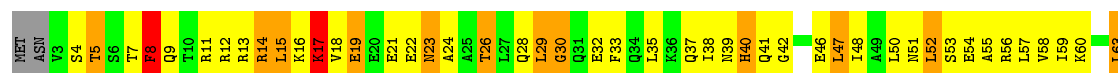
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

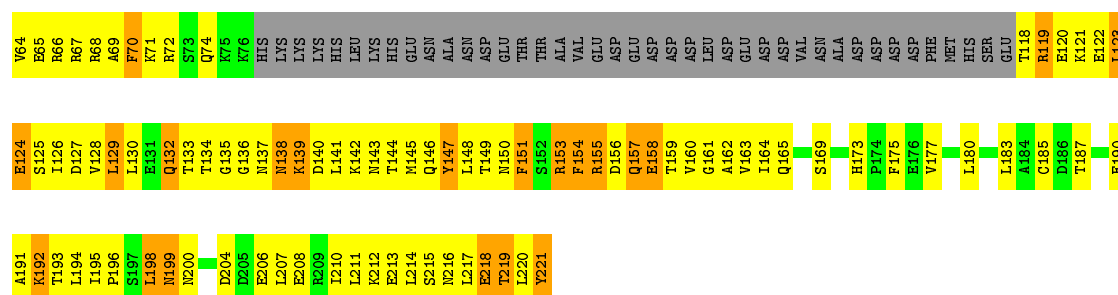
Chain C: 13% 48% 15% 23%



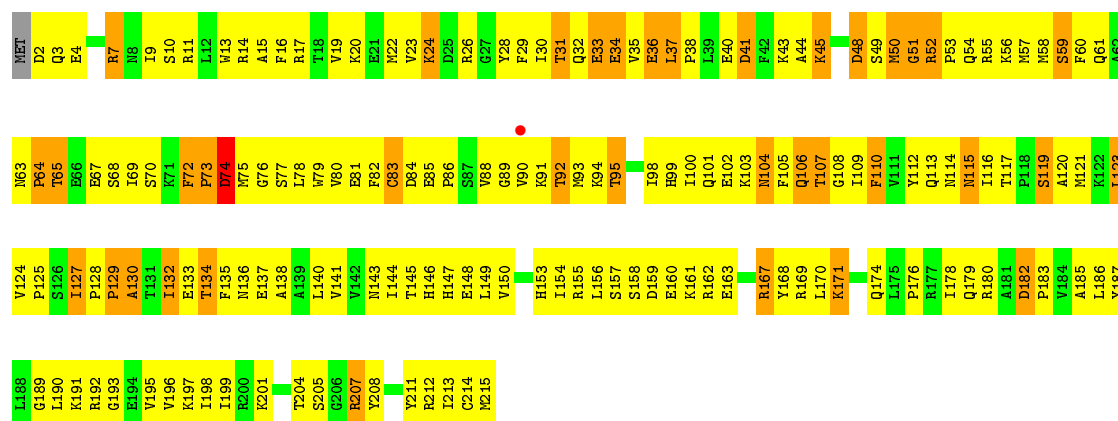
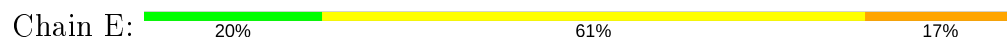
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D: 19% 46% 15% 19%

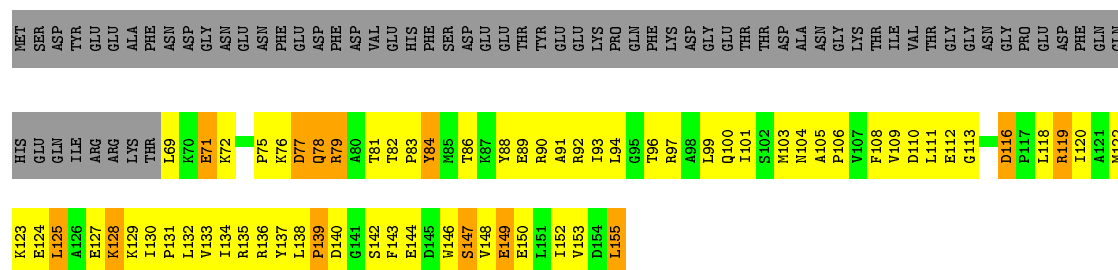




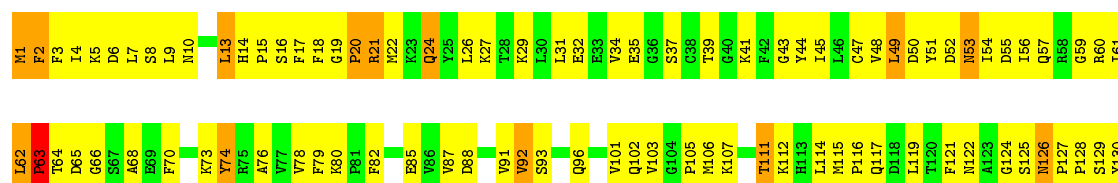
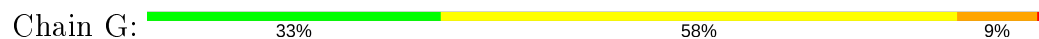
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

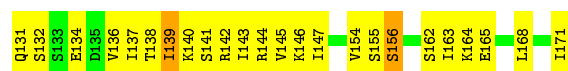


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

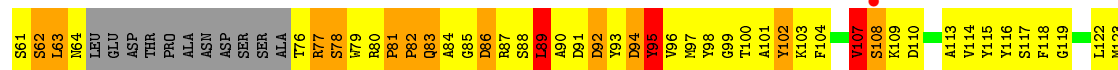
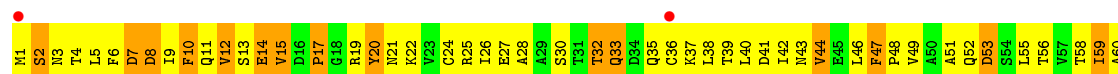
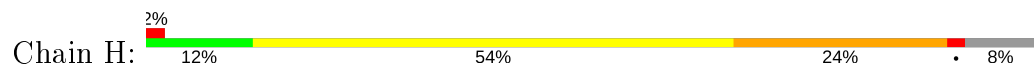


- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

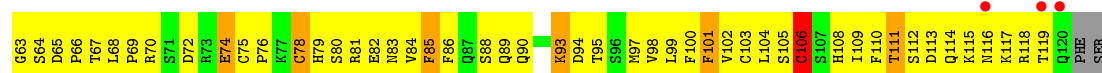
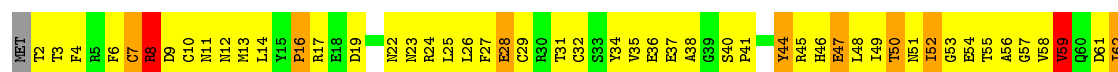




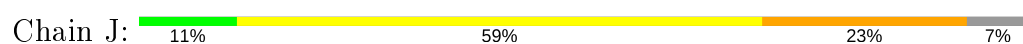
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



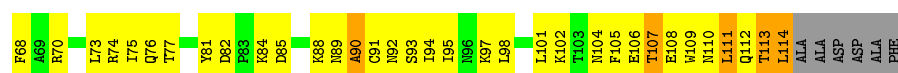
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

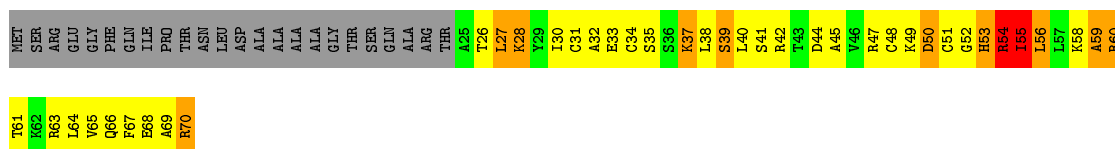


- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

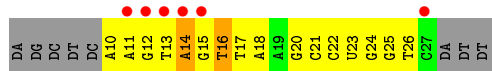




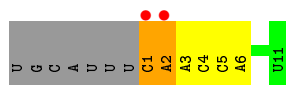
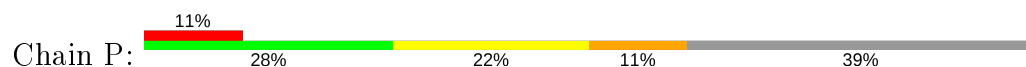
- Molecule 13: 5'-D(\*AP\*CP\*TP\*AP\*CP\*TP\*TP\*GP\*AP\*GP\*CP\*T)-3'



- Molecule 14: 5'-D(\*AP\*GP\*CP\*TP\*C\*AP\*AP\*GP\*TP\*AP\*GP\*TP\*TP\*AP\*AP\*GP\*CP\*C  
P\*(BRU)P\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'



- Molecule 15: 5'-R(\*UP\*GP\*CP\*AP\*UP\*UP\*U\*CP\*AP\*AP\*CP\*CP\*AP\*GP\*GP\*CP\*UP\*U  
) -3'



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	221.62Å 393.72Å 282.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.65 49.21 – 3.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.65) 100.0 (49.21-3.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.64 (at 3.67Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.212 , 0.250 0.214 , 0.253	Depositor DCC
$R_{free}$ test set	2686 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.1	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 106.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.015 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.021 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	31918	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.53	1/11351 (0.0%)	0.79	6/15350 (0.0%)
2	B	0.52	0/9019	0.76	1/12160 (0.0%)
3	C	0.56	2/2133 (0.1%)	0.77	1/2891 (0.0%)
4	D	0.49	0/1444	0.76	2/1935 (0.1%)
5	E	0.50	0/1788	0.73	1/2406 (0.0%)
6	F	0.59	0/717	0.84	1/967 (0.1%)
7	G	0.55	0/1368	0.77	0/1844
8	H	0.54	0/1099	0.79	0/1488
9	I	0.49	0/989	0.75	0/1331
10	J	0.53	0/541	0.87	0/727
11	K	0.49	0/937	0.72	0/1265
12	L	0.61	0/365	0.82	0/485
13	N	0.96	0/152	1.05	0/232
14	T	0.84	0/391	0.84	0/600
15	P	0.70	0/237	0.86	0/368
All	All	0.54	3/32531 (0.0%)	0.78	12/44049 (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
14	T	0	3
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	88	CYS	CB-SG	-6.13	1.71	1.82

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	CYS	CB-SG	-5.53	1.72	1.81
3	C	92	CYS	CB-SG	-5.07	1.73	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	26	THR	N-CA-C	-6.91	92.33	111.00
1	A	56	PRO	N-CA-C	-6.77	94.50	112.10
1	A	1244	ARG	N-CA-C	6.05	127.33	111.00
3	C	39	ALA	N-CA-C	5.95	127.06	111.00
1	A	311	GLN	N-CA-C	5.68	126.34	111.00
4	D	8	PHE	N-CA-C	5.58	126.08	111.00
1	A	55	ASP	N-CA-CB	5.36	120.25	110.60
5	E	171	LYS	N-CA-C	-5.33	96.59	111.00
2	B	363	HIS	N-CA-C	-5.29	96.72	111.00
1	A	4	GLN	N-CA-C	5.25	125.18	111.00
1	A	3	GLY	N-CA-C	-5.18	100.16	113.10
6	F	71	GLU	N-CA-C	-5.13	97.14	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1192	TYR	Sidechain
2	B	431	TYR	Sidechain
14	T	14	DA	Sidechain
14	T	16	DT	Sidechain
14	T	21	DC	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	11151	0	11226	1597	0
2	B	8847	0	8884	1363	0
3	C	2095	0	2051	348	0
4	D	1434	0	1460	218	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1752	0	1776	259	0
6	F	705	0	731	113	0
7	G	1340	0	1357	180	0
8	H	1081	0	1051	207	0
9	I	971	0	929	152	0
10	J	532	0	542	118	0
11	K	919	0	929	116	0
12	L	363	0	388	97	0
13	N	137	0	82	10	0
14	T	369	0	202	27	0
15	P	213	0	110	19	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
All	All	31918	0	31718	4442	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 70.

All (4442) 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)
2:B:559:SER:HA	2:B:563:MET:HB3	1.20	1.16
12:L:55:ILE:HG12	12:L:56:LEU:H	0.97	1.12
12:L:55:ILE:CG1	12:L:56:LEU:H	1.59	1.12
3:C:43:THR:HG22	3:C:44:LEU:H	1.07	1.12
1:A:53:LEU:HD23	1:A:54:ASN:N	1.65	1.10
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.12	1.10
10:J:1:MET:N	10:J:57:ILE:H	1.50	1.09
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.36	1.08
5:E:56:LYS:HE2	5:E:84:ASP:HB2	1.33	1.07
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.35	1.07
8:H:4:THR:HA	8:H:60:ALA:HB2	1.23	1.07
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.32	1.06
2:B:278:GLN:HG2	2:B:279:ASP:H	1.17	1.06
5:E:78:LEU:HD21	5:E:80:VAL:HG23	1.31	1.06
3:C:66:ARG:NH1	10:J:2:ILE:HG21	1.70	1.06

*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:HE21	1.53	1.05
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.30	1.05
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.39	1.04
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.33	1.04
2:B:642:ASP:HA	2:B:649:LYS:HA	1.39	1.04
7:G:62:LEU:HD13	7:G:63:PRO:HD2	1.40	1.04
8:H:100:THR:HG23	8:H:138:GLU:HA	1.39	1.04
2:B:615:MET:HB3	2:B:626:ILE:HG12	1.40	1.03
1:A:1364:ASN:OD1	1:A:1366:ARG:HG2	1.58	1.03
10:J:16:ASP:OD1	10:J:17:LYS:HD2	1.57	1.02
7:G:26:LEU:HD12	7:G:56:ILE:HD11	1.38	1.01
1:A:1444:MET:HG2	7:G:60:ARG:HA	1.41	1.01
12:L:55:ILE:HG12	12:L:56:LEU:N	1.75	1.01
2:B:1112:GLN:HA	15:P:1:C:H5'	1.39	1.01
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.40	1.01
5:E:40:GLU:HA	5:E:43:LYS:HE2	1.43	1.01
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.41	1.01
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.00	1.00
1:A:913:LEU:HD12	1:A:914:GLU:H	1.23	1.00
8:H:130:ARG:HH11	8:H:130:ARG:HB2	1.24	1.00
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.43	1.00
1:A:779:PHE:CE1	1:A:785:PRO:HD3	1.96	1.00
3:C:73:GLN:HE22	3:C:75:MET:HB2	1.27	0.99
2:B:806:THR:HG22	2:B:809:MET:HG2	1.41	0.99
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.01	0.99
6:F:77:ASP:O	6:F:78:GLN:HB2	1.58	0.99
2:B:652:LYS:HB3	2:B:689:LEU:HD23	1.43	0.99
1:A:901:LEU:H	1:A:926:GLN:NE2	1.59	0.99
1:A:40:THR:HG22	1:A:41:MET:HG3	1.44	0.98
7:G:15:PRO:HA	7:G:18:PHE:CD1	1.96	0.98
2:B:261:ARG:HH11	2:B:261:ARG:HB3	1.27	0.98
9:I:93:LYS:H	9:I:93:LYS:HD3	1.25	0.98
1:A:337:ARG:HE	1:A:839:ARG:NH2	1.62	0.98
1:A:225:ASN:HD22	1:A:228:PHE:H	1.01	0.97
5:E:30:ILE:HG23	5:E:34:GLU:HG2	1.44	0.97
1:A:145:LYS:HA	1:A:145:LYS:HE3	1.46	0.97
1:A:858:ASN:ND2	1:A:860:LEU:H	1.63	0.97
10:J:64:ASN:HB3	10:J:65:PRO:CD	1.94	0.97
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.04	0.97
2:B:744:HIS:HD2	2:B:745:PRO:HD2	1.30	0.96
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.07	0.96

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:36:LEU:HB2	10:J:47:ARG:HH12	1.30	0.96
2:B:168:GLY:H	2:B:450:ALA:HB1	1.28	0.96
2:B:292:ILE:HD11	2:B:327:ARG:H	1.29	0.96
10:J:1:MET:H2	10:J:57:ILE:N	1.62	0.96
1:A:43:GLU:HG3	1:A:46:THR:HB	1.47	0.96
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.29	0.96
1:A:1223:ASP:HA	1:A:1243:VAL:HG22	1.47	0.96
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.65	0.96
3:C:43:THR:HG22	3:C:44:LEU:N	1.80	0.96
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.48	0.95
4:D:154:PHE:CD1	4:D:163:VAL:HG21	2.00	0.95
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.46	0.95
1:A:754:SER:H	1:A:757:ASN:ND2	1.64	0.95
1:A:53:LEU:HD23	1:A:54:ASN:H	1.29	0.95
6:F:128:LYS:HG2	6:F:149:GLU:HA	1.49	0.95
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.01	0.95
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.31	0.95
1:A:639:PRO:HG2	1:A:640:GLN:NE2	1.82	0.94
2:B:885:MET:HA	2:B:936:ASP:HB3	1.48	0.94
1:A:855:THR:HG21	1:A:857:ARG:HE	1.30	0.94
2:B:62:ILE:HG23	2:B:418:LYS:HG2	1.45	0.94
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.32	0.94
5:E:207:ARG:HH11	5:E:207:ARG:HB3	1.29	0.94
15:P:1:C:H4'	15:P:2:A:H5''	1.48	0.94
2:B:515:HIS:HD2	2:B:516:ASN:H	1.07	0.94
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.48	0.94
1:A:107:CYS:HA	1:A:171:GLN:NE2	1.82	0.93
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.47	0.93
5:E:117:THR:HG22	5:E:119:SER:H	1.31	0.93
1:A:41:MET:CB	1:A:49:LYS:HA	1.96	0.93
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.48	0.93
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.51	0.93
1:A:741:ASN:HD22	1:A:744:LYS:H	1.09	0.93
14:T:15:DG:C8	14:T:16:DT:H72	2.04	0.93
9:I:105:SER:O	9:I:106:CYS:HB3	1.68	0.93
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.50	0.92
3:C:69:LEU:H	3:C:69:LEU:HD12	1.34	0.92
9:I:6:PHE:HB3	9:I:12:ASN:O	1.70	0.92
1:A:536:LEU:H	1:A:536:LEU:HD23	1.35	0.92
2:B:1113:VAL:H	15:P:1:C:H5''	1.33	0.92
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.51	0.92

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1445:ILE:H	1:A:1445:ILE:HD12	1.32	0.92
8:H:130:ARG:HD3	8:H:130:ARG:N	1.83	0.92
1:A:831:THR:HG23	1:A:832:ALA:H	1.34	0.92
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.52	0.92
1:A:682:THR:HG23	1:A:728:LYS:HE3	1.48	0.91
2:B:542:MET:HG2	2:B:747:MET:HE3	1.52	0.91
3:C:177:GLU:HG3	3:C:231:ASN:HD22	1.34	0.91
2:B:806:THR:HG23	2:B:808:ALA:H	1.33	0.91
1:A:108:MET:HA	1:A:210:ILE:HD13	1.51	0.91
2:B:882:THR:HG21	2:B:935:ARG:HA	1.52	0.91
2:B:842:ASN:HD22	2:B:845:SER:H	1.17	0.91
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.33	0.91
2:B:516:ASN:N	2:B:516:ASN:HD22	1.69	0.91
1:A:41:MET:HB3	1:A:49:LYS:HA	1.51	0.90
1:A:754:SER:H	1:A:757:ASN:HD22	0.93	0.90
2:B:278:GLN:CG	2:B:279:ASP:H	1.82	0.90
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.50	0.90
1:A:535:THR:HG21	1:A:616:VAL:HA	1.52	0.90
12:L:60:ARG:HG2	12:L:61:THR:H	1.36	0.90
5:E:22:MET:HE3	5:E:26:ARG:HE	1.35	0.90
2:B:515:HIS:CD2	2:B:516:ASN:H	1.89	0.90
3:C:66:ARG:HH12	10:J:2:ILE:HG21	1.32	0.90
1:A:1261:LYS:O	1:A:1264:GLU:HB3	1.72	0.90
1:A:1116:LEU:N	1:A:1308:THR:HG22	1.87	0.90
2:B:995:ARG:HH12	3:C:165:LYS:HG2	1.35	0.90
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.51	0.89
4:D:71:LYS:HA	4:D:74:GLN:HB2	1.54	0.89
10:J:12:LYS:O	10:J:14:VAL:HG23	1.71	0.89
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.12	0.89
2:B:732:SER:HB2	2:B:734:HIS:CE1	2.07	0.89
3:C:43:THR:CG2	3:C:44:LEU:H	1.85	0.89
8:H:130:ARG:NH1	8:H:130:ARG:HB2	1.88	0.89
2:B:653:VAL:HG23	2:B:689:LEU:HB3	1.55	0.89
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	1.51	0.89
7:G:62:LEU:HD13	7:G:63:PRO:CD	2.02	0.89
8:H:59:ILE:HG22	8:H:60:ALA:H	1.37	0.89
1:A:830:LYS:HE2	1:A:1081:LEU:HD12	1.55	0.88
1:A:666:ILE:HD12	1:A:667:GLY:H	1.38	0.88
3:C:186:LEU:HD21	3:C:224:GLN:O	1.73	0.88
3:C:238:ILE:HD11	3:C:246:ARG:CZ	2.03	0.88
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.54	0.88

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1418:LEU:HD23	2:B:1222:ARG:HD3	1.56	0.88
1:A:316:GLN:HG2	1:A:317:LYS:HD2	1.56	0.88
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.55	0.88
8:H:59:ILE:HG22	8:H:60:ALA:N	1.88	0.88
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.54	0.88
2:B:172:ILE:HD13	2:B:178:ASN:HD22	1.38	0.88
5:E:2:ASP:O	5:E:3:GLN:HG2	1.74	0.88
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.53	0.87
2:B:707:PRO:HG2	2:B:708:GLU:H	1.37	0.87
1:A:11:LEU:O	1:A:11:LEU:HD23	1.74	0.87
1:A:741:ASN:ND2	1:A:744:LYS:H	1.72	0.87
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.72	0.87
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.10	0.87
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.09	0.87
3:C:175:ALA:CB	10:J:43:ARG:HH22	1.87	0.87
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.57	0.87
1:A:961:ARG:HG2	1:A:965:GLN:NE2	1.90	0.87
1:A:225:ASN:ND2	1:A:228:PHE:H	1.72	0.87
2:B:37:PHE:HE1	2:B:41:LYS:HG3	1.40	0.87
6:F:109:VAL:HG11	6:F:123:LYS:HE3	1.56	0.86
2:B:59:LEU:HD12	2:B:417:PHE:CE2	2.10	0.86
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.57	0.86
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.39	0.86
1:A:1161:THR:HG21	1:A:1163:ILE:HD12	1.56	0.86
1:A:903:ASN:HD22	1:A:904:THR:N	1.73	0.86
2:B:64:CYS:HA	2:B:67:SER:OG	1.74	0.86
1:A:684:ALA:O	1:A:687:LYS:HB2	1.75	0.86
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.40	0.86
1:A:1169:ILE:HD12	1:A:1169:ILE:H	1.41	0.86
6:F:69:LEU:HB3	6:F:71:GLU:OE1	1.76	0.86
2:B:559:SER:CA	2:B:563:MET:HB3	2.04	0.86
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.56	0.86
1:A:62:ASP:O	1:A:64:ASN:HB2	1.76	0.86
1:A:55:ASP:N	1:A:56:PRO:HD3	1.89	0.85
2:B:824:ILE:HG12	10:J:48:ARG:HH12	1.38	0.85
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.58	0.85
2:B:579:ARG:HB2	2:B:586:TRP:NE1	1.91	0.85
14:T:10:DA:H2"	14:T:11:DA:C8	2.12	0.85
3:C:128:ASN:O	3:C:129:ILE:HG13	1.77	0.85
1:A:66:LYS:HZ3	1:A:68:GLN:H	1.21	0.85
9:I:8:ARG:HG3	9:I:34:TYR:HE1	1.41	0.85

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.58	0.85
4:D:220:LEU:HG	4:D:221:TYR:H	1.42	0.85
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.06	0.85
7:G:88:ASP:HB3	7:G:144:ARG:HA	1.58	0.85
1:A:55:ASP:C	1:A:57:ARG:H	1.78	0.85
2:B:613:VAL:HG13	2:B:627:PHE:O	1.77	0.85
1:A:310:GLY:O	1:A:312:PRO:HD2	1.76	0.84
3:C:17:ASN:N	3:C:240:VAL:HG11	1.91	0.84
8:H:81:PRO:HB2	8:H:82:PRO:HD2	1.59	0.84
2:B:193:LYS:NZ	12:L:32:ALA:HB1	1.92	0.84
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.39	0.84
1:A:710:LEU:HD12	1:A:710:LEU:H	1.41	0.84
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	1.77	0.84
1:A:900:ASP:HA	1:A:926:GLN:NE2	1.93	0.84
1:A:665:GLY:HA2	2:B:1026:LEU:HD22	1.60	0.84
2:B:731:VAL:HG12	2:B:732:SER:H	1.41	0.84
2:B:914:LYS:HE2	2:B:937:ALA:HB1	1.59	0.84
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.12	0.84
5:E:31:THR:HG23	5:E:34:GLU:HB2	1.60	0.84
8:H:82:PRO:C	8:H:84:ALA:H	1.76	0.84
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.43	0.84
2:B:277:LYS:HD2	2:B:277:LYS:H	1.42	0.84
7:G:14:HIS:CD2	7:G:16:SER:H	1.96	0.84
1:A:1308:THR:HG23	1:A:1309:ASP:N	1.92	0.83
9:I:85:PHE:HD2	9:I:85:PHE:H	1.25	0.83
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.07	0.83
2:B:165:VAL:HG11	2:B:448:ILE:HD13	1.61	0.83
2:B:863:GLU:OE2	2:B:873:THR:HA	1.78	0.83
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.58	0.83
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.61	0.83
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.60	0.83
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.43	0.83
8:H:130:ARG:HH11	8:H:130:ARG:CB	1.91	0.83
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.76	0.83
1:A:34:LYS:NZ	1:A:57:ARG:NH2	2.26	0.83
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.08	0.83
1:A:438:ASP:O	1:A:439:ASN:HB2	1.76	0.83
2:B:549:THR:HG22	2:B:550:ASP:H	1.41	0.83
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.43	0.83
1:A:1006:ILE:HD12	5:E:167:ARG:HB2	1.61	0.83
1:A:446:ARG:HB3	1:A:478:TYR:HB3	1.60	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.04	0.83
1:A:913:LEU:HD12	1:A:914:GLU:N	1.92	0.83
10:J:1:MET:H1	10:J:56:LEU:N	1.75	0.83
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.14	0.83
1:A:600:PRO:HG2	1:A:601:LYS:H	1.42	0.82
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.60	0.82
1:A:381:THR:HG22	1:A:383:TYR:H	1.42	0.82
2:B:806:THR:HG22	2:B:809:MET:H	1.44	0.82
3:C:177:GLU:HG3	3:C:231:ASN:HB3	1.61	0.82
6:F:103:MET:CE	7:G:66:GLY:H	1.91	0.82
1:A:567:LYS:CB	8:H:95:TYR:HA	2.08	0.82
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.62	0.82
2:B:842:ASN:ND2	2:B:845:SER:H	1.77	0.82
4:D:66:ARG:HD2	4:D:133:THR:HB	1.59	0.82
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.10	0.82
2:B:737:THR:HG21	9:I:66:PRO:HA	1.60	0.82
7:G:26:LEU:HD12	7:G:56:ILE:CD1	2.09	0.82
2:B:351:TYR:O	2:B:355:ILE:HG13	1.80	0.82
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.14	0.82
12:L:38:LEU:HG	12:L:39:SER:H	1.42	0.82
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.09	0.82
2:B:278:GLN:HG2	2:B:279:ASP:N	1.95	0.82
2:B:345:LYS:HA	2:B:348:ARG:HE	1.45	0.82
2:B:345:LYS:HG2	2:B:346:GLU:H	1.44	0.82
2:B:616:ILE:HD12	2:B:616:ILE:N	1.94	0.82
13:N:4:DA:H2"	13:N:5:DC:C6	2.15	0.82
6:F:109:VAL:CG1	6:F:123:LYS:HE3	2.10	0.81
2:B:120:ARG:NH1	12:L:54:ARG:HD3	1.95	0.81
3:C:244:VAL:O	3:C:248:ILE:HG13	1.80	0.81
5:E:19:VAL:O	5:E:23:VAL:HG23	1.79	0.81
2:B:1099:VAL:HG13	2:B:1100:ASP:N	1.96	0.81
2:B:1180:PHE:HB3	2:B:1191:ILE:HD12	1.63	0.81
12:L:32:ALA:CB	12:L:55:ILE:HG13	2.11	0.81
5:E:117:THR:HB	5:E:120:ALA:CB	2.10	0.81
2:B:345:LYS:O	2:B:347:LYS:HG2	1.79	0.81
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.59	0.81
3:C:7:GLN:HE21	3:C:7:GLN:N	1.78	0.81
1:A:665:GLY:O	1:A:667:GLY:N	2.13	0.81
1:A:534:LEU:O	1:A:574:GLY:HA3	1.81	0.81
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.61	0.81
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.61	0.81

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:111:THR:CG2	7:G:114:LEU:HD13	2.10	0.81
1:A:858:ASN:C	1:A:858:ASN:HD22	1.82	0.81
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.61	0.81
3:C:35:ARG:HH12	11:K:41:THR:H	1.25	0.81
1:A:567:LYS:HB2	8:H:95:TYR:HA	1.61	0.81
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.61	0.81
14:T:10:DA:H2"	14:T:11:DA:N7	1.95	0.81
1:A:1101:LEU:O	1:A:1105:LEU:HD12	1.81	0.80
1:A:1259:MET:HA	1:A:1262:LYS:CD	2.11	0.80
1:A:49:LYS:HZ1	1:A:61:ILE:N	1.78	0.80
1:A:591:PHE:HD2	1:A:595:THR:HB	1.45	0.80
8:H:82:PRO:HG2	8:H:83:GLN:H	1.44	0.80
8:H:42:ILE:HG23	8:H:95:TYR:HE1	1.44	0.80
1:A:317:LYS:HA	2:B:471:LYS:HZ1	1.46	0.80
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.80	0.80
4:D:69:ALA:HB2	4:D:72:ARG:NH1	1.96	0.80
7:G:139:ILE:HG23	7:G:140:LYS:H	1.45	0.80
1:A:98:LYS:O	1:A:102:VAL:HG23	1.81	0.80
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.63	0.80
1:A:110:CYS:HB3	1:A:167:CYS:SG	2.22	0.80
2:B:906:SER:O	2:B:941:LEU:HD23	1.81	0.80
1:A:244:PRO:HB2	1:A:245:PRO:CD	2.12	0.80
1:A:315:LEU:HD12	2:B:471:LYS:HB3	1.64	0.80
1:A:709:THR:HG22	1:A:710:LEU:H	1.46	0.80
2:B:221:ASN:OD1	2:B:242:SER:HA	1.81	0.80
3:C:32:SER:O	3:C:36:VAL:HG23	1.82	0.80
1:A:839:ARG:HH11	1:A:839:ARG:HG2	1.45	0.80
2:B:289:LEU:HD13	2:B:375:ALA:HB2	1.62	0.80
3:C:167:HIS:CD2	12:L:70:ARG:HB3	2.17	0.80
1:A:1167:GLU:O	1:A:1170:ILE:HD12	1.81	0.79
1:A:1341:ILE:HG23	1:A:1342:GLU:N	1.96	0.79
2:B:277:LYS:HD3	2:B:336:ARG:C	2.01	0.79
2:B:39:ARG:HH21	2:B:665:GLU:HG2	1.46	0.79
8:H:95:TYR:HE2	8:H:97:MET:HG3	1.46	0.79
1:A:66:LYS:NZ	1:A:68:GLN:H	1.79	0.79
1:A:701:LEU:HD21	9:I:114:GLN:HB2	1.65	0.79
1:A:925:LEU:HD13	1:A:983:ILE:HG21	1.62	0.79
5:E:127:ILE:O	5:E:127:ILE:HG13	1.81	0.79
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.64	0.79
1:A:754:SER:N	1:A:757:ASN:HD22	1.76	0.79
2:B:360:PHE:CE2	2:B:361:LEU:HD13	2.16	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:498:THR:HG22	2:B:537:LYS:O	1.83	0.79
1:A:629:LEU:O	1:A:633:VAL:HG23	1.82	0.79
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.63	0.79
8:H:58:THR:HB	8:H:143:LEU:HD13	1.63	0.79
1:A:34:LYS:HG2	1:A:36:ARG:HH21	1.48	0.79
6:F:90:ARG:HG3	6:F:91:ALA:N	1.96	0.79
12:L:55:ILE:CG1	12:L:56:LEU:N	2.35	0.79
1:A:35:ILE:HA	1:A:52:GLY:O	1.83	0.79
2:B:957:ASN:HD22	2:B:961:LEU:HB2	1.45	0.79
3:C:189:THR:HG22	3:C:190:ASP:N	1.98	0.79
1:A:1205:LYS:O	1:A:1207:LEU:HG	1.83	0.79
1:A:288:ALA:HA	1:A:291:GLU:CD	2.02	0.79
2:B:805:THR:HG22	2:B:806:THR:H	1.48	0.79
3:C:208:GLU:O	3:C:210:GLU:N	2.15	0.79
8:H:89:LEU:C	8:H:91:ASP:H	1.86	0.79
1:A:150:THR:HG23	1:A:166:GLY:HA2	1.63	0.79
1:A:982:THR:HB	1:A:985:ASP:H	1.48	0.79
5:E:22:MET:HE1	5:E:26:ARG:HH21	1.48	0.79
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.65	0.78
1:A:388:LEU:O	1:A:392:VAL:HG23	1.82	0.78
1:A:317:LYS:HA	2:B:471:LYS:NZ	1.97	0.78
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.48	0.78
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.19	0.78
15:P:1:C:H4'	15:P:2:A:C5'	2.13	0.78
1:A:1107:VAL:HG12	1:A:1107:VAL:O	1.81	0.78
1:A:834:THR:HG21	1:A:1077:THR:HG23	1.66	0.78
1:A:2:VAL:HG11	2:B:1157:ALA:O	1.82	0.78
2:B:293:PRO:HD2	2:B:296:GLU:OE1	1.83	0.78
1:A:288:ALA:HA	1:A:291:GLU:OE1	1.82	0.78
1:A:1081:LEU:HD11	1:A:1098:VAL:H	1.48	0.78
3:C:124:LEU:O	3:C:127:ARG:HG2	1.82	0.78
5:E:14:ARG:HH21	5:E:141:VAL:HG12	1.47	0.78
8:H:12:VAL:HA	8:H:28:ALA:HB2	1.64	0.78
1:A:323:LYS:H	1:A:323:LYS:HD2	1.49	0.78
2:B:1113:VAL:H	15:P:1:C:C5'	1.95	0.78
4:D:56:ARG:HD3	4:D:149:THR:HA	1.66	0.78
5:E:120:ALA:O	5:E:123:LEU:HG	1.84	0.78
1:A:1279:ILE:HD11	1:A:1316:VAL:HG21	1.66	0.78
1:A:591:PHE:HA	1:A:595:THR:HG21	1.66	0.78
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.64	0.78
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.65	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1187:ASN:O	2:B:1188:LYS:HB2	1.83	0.78
2:B:637:LEU:HD22	2:B:741:CYS:O	1.83	0.78
4:D:155:ARG:HD3	4:D:221:TYR:CE1	2.19	0.78
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.19	0.78
8:H:15:VAL:HG13	8:H:26:ILE:HB	1.66	0.78
1:A:372:LYS:HA	1:A:435:HIS:ND1	1.99	0.78
2:B:284:ILE:HD13	2:B:333:PHE:CE2	2.18	0.78
3:C:11:ARG:HH12	3:C:205:LYS:NZ	1.81	0.78
3:C:57:VAL:HG23	3:C:58:LEU:HD23	1.64	0.78
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.14	0.78
3:C:73:GLN:NE2	3:C:75:MET:HB2	1.98	0.78
4:D:68:ARG:HG2	4:D:72:ARG:NH2	1.99	0.77
1:A:567:LYS:HB3	8:H:96:VAL:H	1.46	0.77
10:J:1:MET:H2	10:J:57:ILE:H	0.80	0.77
2:B:90:ILE:HD12	2:B:432:MET:SD	2.24	0.77
5:E:169:ARG:HD3	6:F:140:ASP:OD2	1.84	0.77
5:E:98:ILE:HA	5:E:101:GLN:HB3	1.64	0.77
6:F:99:LEU:O	6:F:103:MET:HG2	1.84	0.77
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.65	0.77
2:B:1112:GLN:CA	15:P:1:C:H5'	2.14	0.77
1:A:567:LYS:HZ2	8:H:46:LEU:HB2	1.49	0.77
2:B:654:ARG:H	2:B:657:HIS:HD2	1.28	0.77
2:B:1112:GLN:HG3	15:P:1:C:C5'	2.15	0.77
2:B:654:ARG:HG3	2:B:654:ARG:HH11	1.48	0.77
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.67	0.77
2:B:597:MET:HA	2:B:597:MET:CE	2.15	0.77
1:A:1444:MET:HG2	7:G:60:ARG:CA	2.15	0.77
8:H:84:ALA:HB2	8:H:87:ARG:HD2	1.65	0.77
9:I:93:LYS:H	9:I:93:LYS:CD	1.95	0.77
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.64	0.77
1:A:390:GLN:HE21	1:A:394:ASN:HD22	1.30	0.77
1:A:715:GLU:OE1	1:A:774:ARG:HD3	1.85	0.77
2:B:193:LYS:HZ2	12:L:32:ALA:HB1	1.49	0.77
3:C:137:LYS:HB3	3:C:138:GLU:OE1	1.85	0.77
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.20	0.77
2:B:865:LYS:NZ	2:B:869:SER:HA	2.00	0.77
8:H:38:LEU:HD12	8:H:124:ARG:O	1.85	0.77
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.67	0.77
2:B:309:GLN:HE21	2:B:309:GLN:HA	1.49	0.76
2:B:39:ARG:HH21	2:B:665:GLU:CG	1.96	0.76
7:G:1:MET:SD	7:G:2:PHE:N	2.58	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:LEU:HD11	1:A:1017:LEU:HD11	1.65	0.76
1:A:122:MET:HA	1:A:141:LEU:HD11	1.66	0.76
1:A:763:ALA:O	1:A:803:SER:HB3	1.86	0.76
1:A:903:ASN:HD22	1:A:904:THR:H	1.29	0.76
9:I:50:THR:HG23	9:I:52:ILE:H	1.49	0.76
2:B:505:ASP:HA	13:N:1:DA:C8	2.21	0.76
1:A:843:LYS:HD3	1:A:846:GLU:OE2	1.84	0.76
2:B:914:LYS:HE2	2:B:937:ALA:CB	2.15	0.76
4:D:159:THR:O	4:D:163:VAL:HG23	1.83	0.76
10:J:7:CYS:HA	10:J:49:MET:HE3	1.67	0.76
2:B:882:THR:HG23	2:B:884:ARG:HB2	1.67	0.76
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.66	0.76
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.67	0.76
2:B:708:GLU:O	2:B:710:LEU:N	2.19	0.76
5:E:23:VAL:O	5:E:28:TYR:HB2	1.86	0.76
8:H:62:SER:O	8:H:63:LEU:HG	1.86	0.76
1:A:90:VAL:HG12	1:A:297:GLN:NE2	2.01	0.76
2:B:114:PRO:HG2	2:B:115:GLN:H	1.51	0.76
2:B:216:GLU:OE1	2:B:537:LYS:HE2	1.86	0.76
2:B:558:LEU:HD21	2:B:600:LEU:HD11	1.68	0.76
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.01	0.75
1:A:698:GLN:HA	9:I:97:MET:O	1.86	0.75
1:A:1027:ALA:O	1:A:1031:VAL:HG23	1.84	0.75
1:A:1437:GLY:O	1:A:1439:GLY:N	2.20	0.75
1:A:694:THR:O	1:A:698:GLN:HG3	1.86	0.75
1:A:69:THR:O	1:A:71:GLN:HG2	1.85	0.75
1:A:960:ILE:HA	1:A:963:ILE:HG22	1.66	0.75
2:B:744:HIS:HD2	2:B:745:PRO:CD	1.98	0.75
10:J:35:ALA:O	10:J:38:ARG:HB3	1.86	0.75
1:A:66:LYS:HZ3	1:A:68:GLN:N	1.84	0.75
2:B:172:ILE:HD13	2:B:178:ASN:ND2	2.01	0.75
3:C:175:ALA:O	3:C:176:ILE:HG13	1.85	0.75
1:A:1141:THR:CG2	1:A:1205:LYS:HD3	2.15	0.75
2:B:766:ARG:HH11	2:B:766:ARG:HA	1.52	0.75
10:J:44:TYR:HD2	10:J:44:TYR:H	1.35	0.75
1:A:41:MET:HB2	1:A:49:LYS:HA	1.69	0.75
2:B:613:VAL:HG22	2:B:628:THR:HA	1.68	0.75
2:B:744:HIS:CD2	2:B:745:PRO:HD2	2.18	0.75
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.67	0.75
9:I:74:GLU:HB3	9:I:81:ARG:NE	2.02	0.75
3:C:50:GLU:HG2	12:L:64:LEU:HD22	1.68	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LYS:HD3	1:A:67:CYS:N	2.00	0.75
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.81	0.75
5:E:117:THR:HB	5:E:120:ALA:HB2	1.68	0.75
8:H:40:LEU:HD13	8:H:123:MET:HE3	1.68	0.75
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.26	0.75
1:A:1208:THR:HB	1:A:1211:GLN:CG	2.15	0.75
5:E:22:MET:HE3	5:E:26:ARG:NE	2.00	0.75
5:E:94:LYS:CE	5:E:98:ILE:HD11	2.12	0.75
7:G:91:VAL:HG23	7:G:141:SER:O	1.87	0.75
8:H:30:SER:HB2	8:H:36:CYS:HB3	1.67	0.75
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.69	0.75
2:B:101:MET:HA	2:B:112:LEU:H	1.52	0.75
1:A:1418:LEU:HB3	2:B:1222:ARG:NH1	2.00	0.75
1:A:963:ILE:HD11	1:A:1048:ASN:HB2	1.68	0.75
1:A:146:MET:HA	1:A:171:GLN:HB2	1.68	0.75
1:A:831:THR:HG23	1:A:832:ALA:N	2.01	0.75
3:C:11:ARG:HH12	3:C:205:LYS:HZ3	1.35	0.75
3:C:69:LEU:HD12	3:C:69:LEU:N	2.02	0.75
1:A:1243:VAL:O	1:A:1245:PRO:HD3	1.87	0.74
1:A:205:GLU:CD	1:A:205:GLU:H	1.88	0.74
1:A:886:ILE:HG23	1:A:887:GLY:N	2.02	0.74
1:A:1325:THR:O	5:E:148:GLU:HB2	1.85	0.74
9:I:80:SER:OG	9:I:105:SER:HB2	1.87	0.74
1:A:806:ARG:HH12	2:B:729:ILE:HD12	1.52	0.74
5:E:138:ALA:HA	5:E:141:VAL:HG23	1.70	0.74
1:A:1030:ARG:HG3	1:A:1034:GLU:OE2	1.85	0.74
1:A:70:CYS:O	1:A:72:GLU:HG2	1.86	0.74
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.70	0.74
1:A:524:VAL:HG12	1:A:525:GLN:H	1.52	0.74
7:G:131:GLN:HG2	7:G:136:VAL:HG13	1.68	0.74
1:A:1313:LEU:HB3	1:A:1338:VAL:HG21	1.68	0.74
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.68	0.74
2:B:37:PHE:HE2	2:B:542:MET:HA	1.52	0.74
1:A:1148:ILE:HG12	1:A:1198:ASP:HB2	1.70	0.74
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.23	0.74
1:A:866:PHE:C	1:A:867:ILE:HD12	2.08	0.74
3:C:196:ASP:HB3	3:C:199:LYS:HB2	1.68	0.74
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.70	0.74
1:A:898:ARG:HD2	1:A:899:VAL:H	1.52	0.74
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.03	0.74
7:G:142:ARG:HB3	7:G:171:ILE:HD12	1.68	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:111:THR:HG22	9:I:112:SER:H	1.51	0.74
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.49	0.74
1:A:960:ILE:HA	1:A:963:ILE:CG2	2.18	0.74
1:A:567:LYS:HZ1	8:H:43:ASN:HB3	1.51	0.74
3:C:189:THR:HG22	3:C:190:ASP:H	1.52	0.74
2:B:549:THR:HB	2:B:628:THR:OG1	1.88	0.74
12:L:40:LEU:HD13	12:L:44:ASP:HB3	1.70	0.74
2:B:1183:LYS:HE3	2:B:1183:LYS:N	2.02	0.73
1:A:821:ARG:HB2	1:A:821:ARG:NH1	2.03	0.73
2:B:637:LEU:HB2	2:B:693:ILE:HD11	1.68	0.73
1:A:1187:GLN:O	1:A:1244:ARG:HB2	1.87	0.73
1:A:335:ARG:O	1:A:339:ASN:HB2	1.89	0.73
1:A:568:PRO:HG2	8:H:46:LEU:HD22	1.69	0.73
1:A:718:VAL:HG12	1:A:722:LEU:HD11	1.70	0.73
2:B:36:ALA:HA	2:B:39:ARG:HD2	1.70	0.73
8:H:77:ARG:CZ	8:H:77:ARG:HB2	2.17	0.73
1:A:89:PRO:HG2	1:A:204:THR:HB	1.70	0.73
2:B:806:THR:HG23	2:B:808:ALA:N	2.03	0.73
12:L:34:CYS:HB3	12:L:51:CYS:SG	2.29	0.73
1:A:1254:ALA:O	1:A:1255:GLU:HB2	1.88	0.73
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.70	0.73
2:B:805:THR:HG22	2:B:809:MET:HG3	1.68	0.73
5:E:69:ILE:HD12	5:E:69:ILE:N	2.04	0.73
6:F:103:MET:O	6:F:104:ASN:HB2	1.87	0.73
8:H:139:ASN:O	8:H:140:ALA:HB2	1.88	0.73
9:I:93:LYS:HD3	9:I:93:LYS:N	2.02	0.73
1:A:19:PHE:O	1:A:1416:ALA:HA	1.89	0.73
2:B:359:GLU:O	2:B:362:PRO:HD3	1.88	0.73
5:E:84:ASP:O	5:E:86:PRO:HD3	1.88	0.73
1:A:39:GLU:N	1:A:39:GLU:OE2	2.22	0.73
1:A:565:ILE:HD13	1:A:567:LYS:HE2	1.68	0.73
4:D:14:ARG:HB3	4:D:14:ARG:HH11	1.53	0.73
2:B:261:ARG:NH1	2:B:261:ARG:HB3	2.02	0.73
2:B:347:LYS:HG3	2:B:348:ARG:H	1.53	0.73
2:B:282:ILE:CD1	2:B:382:ILE:HD13	2.19	0.73
2:B:811:TYR:N	2:B:811:TYR:CD1	2.53	0.73
7:G:49:LEU:HG	7:G:76:ALA:HA	1.71	0.73
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.24	0.73
9:I:7:CYS:SG	9:I:8:ARG:O	2.46	0.73
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.69	0.73
1:A:7:SER:HB3	2:B:1193:GLN:HE22	1.54	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:ILE:H	2:B:240:ILE:HD12	1.53	0.73
1:A:51:GLY:O	1:A:56:PRO:HB3	1.89	0.72
9:I:65:ASP:HB3	9:I:68:LEU:HD13	1.70	0.72
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.19	0.72
1:A:666:ILE:CD1	1:A:667:GLY:H	2.01	0.72
5:E:22:MET:HE1	5:E:26:ARG:NH2	2.03	0.72
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.19	0.72
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.03	0.72
2:B:890:TYR:O	2:B:893:LEU:HB2	1.90	0.72
1:A:416:ARG:NH1	1:A:417:TYR:HE2	1.88	0.72
1:A:425:GLN:N	1:A:425:GLN:CD	2.42	0.72
1:A:590:ARG:O	1:A:591:PHE:HB2	1.89	0.72
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.20	0.72
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.71	0.72
2:B:996:ARG:HH12	3:C:174:ALA:HA	1.54	0.72
2:B:376:PHE:CZ	2:B:569:TYR:HB3	2.25	0.72
3:C:6:PRO:HG2	11:K:101:LEU:HB2	1.70	0.72
1:A:898:ARG:HD2	1:A:899:VAL:N	2.04	0.72
2:B:418:LYS:HD3	2:B:422:LYS:NZ	2.04	0.72
6:F:82:THR:HG22	6:F:84:TYR:H	1.54	0.72
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.72	0.72
2:B:880:THR:HB	2:B:934:LYS:HG3	1.71	0.72
5:E:207:ARG:CB	5:E:207:ARG:HH11	2.03	0.72
10:J:36:LEU:CB	10:J:47:ARG:HH12	2.01	0.72
11:K:23:PRO:HA	11:K:31:VAL:HG13	1.72	0.72
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.69	0.72
2:B:873:THR:O	2:B:914:LYS:HA	1.89	0.72
3:C:56:THR:HG21	3:C:145:CYS:SG	2.30	0.72
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.04	0.72
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.24	0.72
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.18	0.72
1:A:547:LEU:HD13	11:K:58:PHE:CD1	2.24	0.72
1:A:145:LYS:CE	1:A:145:LYS:HA	2.19	0.72
3:C:108:GLU:OE1	3:C:108:GLU:HA	1.87	0.72
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.71	0.72
1:A:1438:THR:HG23	6:F:92:ARG:HB2	1.70	0.72
1:A:69:THR:O	1:A:71:GLN:N	2.23	0.72
1:A:903:ASN:ND2	1:A:904:THR:N	2.36	0.72
7:G:111:THR:HG21	7:G:114:LEU:HD13	1.70	0.72
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.25	0.71
2:B:461:LEU:HD12	2:B:461:LEU:H	1.54	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:4:SER:O	4:D:5:THR:HB	1.89	0.71
7:G:21:ARG:HD2	7:G:24:GLN:CB	2.20	0.71
3:C:167:HIS:HA	11:K:6:ARG:HH12	1.55	0.71
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.16	0.71
1:A:1211:GLN:O	1:A:1214:GLU:HB2	1.90	0.71
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.73	0.71
1:A:803:SER:OG	1:A:806:ARG:HG3	1.90	0.71
2:B:254:LEU:HD11	2:B:273:LEU:HD23	1.72	0.71
2:B:291:ILE:HG12	2:B:300:HIS:NE2	2.05	0.71
2:B:294:ASP:O	2:B:296:GLU:N	2.22	0.71
2:B:357:GLN:O	2:B:366:GLN:HA	1.90	0.71
2:B:47:GLN:HB3	2:B:173:MET:HE2	1.72	0.71
7:G:111:THR:HG23	7:G:114:LEU:HB2	1.72	0.71
7:G:139:ILE:HG23	7:G:140:LYS:N	2.04	0.71
1:A:265:LYS:CE	1:A:302:THR:HG23	2.20	0.71
2:B:852:ARG:HH22	12:L:70:ARG:C	1.94	0.71
7:G:115:MET:HB3	7:G:116:PRO:HD2	1.72	0.71
9:I:55:THR:HG23	9:I:86:PHE:HZ	1.56	0.71
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.91	0.71
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.26	0.71
1:A:946:VAL:HG12	1:A:947:PHE:CD2	2.26	0.71
2:B:865:LYS:HZ2	2:B:869:SER:HA	1.56	0.71
5:E:99:HIS:CE1	5:E:103:LYS:HD2	2.25	0.71
9:I:34:TYR:CD2	9:I:35:VAL:N	2.58	0.71
1:A:1095:THR:HG21	1:A:1112:LYS:CB	2.20	0.71
2:B:553:PRO:O	2:B:557:PHE:HB2	1.91	0.71
1:A:1444:MET:CG	7:G:60:ARG:HA	2.18	0.71
12:L:34:CYS:SG	12:L:34:CYS:O	2.49	0.71
12:L:42:ARG:HG3	12:L:42:ARG:HH11	1.53	0.71
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.53	0.71
1:A:1420:ASP:O	1:A:1421:CYS:HB2	1.90	0.71
1:A:203:SER:OG	1:A:206:GLU:HB2	1.89	0.71
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.73	0.71
2:B:333:PHE:HE1	2:B:336:ARG:NH1	1.88	0.71
3:C:251:LEU:O	3:C:255:VAL:HG23	1.90	0.71
12:L:49:LYS:O	12:L:50:ASP:HB2	1.91	0.71
1:A:34:LYS:HZ1	1:A:57:ARG:NH2	1.88	0.71
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.73	0.71
1:A:722:LEU:H	1:A:722:LEU:HD12	1.56	0.71
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.25	0.71
4:D:119:ARG:HB3	4:D:119:ARG:NH1	2.06	0.71

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:8:PHE:CD2	7:G:6:ASP:HB2	2.25	0.71
11:K:63:VAL:O	11:K:63:VAL:HG23	1.90	0.71
1:A:416:ARG:HH11	1:A:417:TYR:HE2	1.39	0.70
2:B:390:LEU:O	2:B:392:ARG:N	2.24	0.70
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.72	0.70
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.20	0.70
1:A:478:TYR:O	1:A:479:ASN:HB2	1.91	0.70
2:B:603:LEU:HD13	2:B:608:ASP:HB2	1.71	0.70
3:C:236:GLY:O	3:C:238:ILE:N	2.25	0.70
3:C:253:LYS:O	3:C:256:ALA:HB3	1.91	0.70
4:D:154:PHE:HE1	4:D:163:VAL:HG11	1.55	0.70
12:L:30:ILE:O	12:L:56:LEU:HA	1.91	0.70
1:A:302:THR:HA	1:A:305:ASP:O	1.91	0.70
1:A:921:GLY:O	1:A:923:LEU:HD12	1.91	0.70
2:B:333:PHE:CE1	2:B:336:ARG:NH1	2.59	0.70
7:G:59:GLY:HA3	7:G:70:PHE:CD2	2.26	0.70
1:A:1445:ILE:HD12	1:A:1445:ILE:N	2.04	0.70
1:A:91:PHE:H	1:A:297:GLN:HE22	1.37	0.70
1:A:886:ILE:HG23	1:A:887:GLY:H	1.56	0.70
2:B:857:ARG:HH21	2:B:942:ARG:CZ	2.03	0.70
3:C:242:GLN:HA	3:C:245:VAL:CG2	2.21	0.70
4:D:18:VAL:O	4:D:19:GLU:HB2	1.89	0.70
1:A:866:PHE:O	1:A:867:ILE:HD12	1.90	0.70
2:B:582:VAL:HB	2:B:587:HIS:CD2	2.27	0.70
4:D:51:ASN:O	4:D:52:LEU:O	2.10	0.70
1:A:1116:LEU:HB3	1:A:1308:THR:HG21	1.72	0.70
1:A:535:THR:CG2	1:A:616:VAL:HA	2.20	0.70
2:B:465:ASN:HD22	2:B:465:ASN:N	1.89	0.70
4:D:118:THR:HB	4:D:121:LYS:HB2	1.73	0.70
7:G:34:VAL:HG11	7:G:74:TYR:CE1	2.24	0.70
15:P:3:A:H2'	15:P:4:C:C6	2.26	0.70
1:A:1438:THR:HG22	6:F:92:ARG:HD3	1.73	0.70
1:A:961:ARG:HG2	1:A:965:GLN:HE21	1.54	0.70
2:B:189:LEU:O	2:B:192:LEU:N	2.25	0.70
2:B:241:ARG:HG2	2:B:253:THR:CG2	2.22	0.70
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.27	0.70
2:B:583:ASN:HD21	2:B:628:THR:CG2	2.05	0.70
10:J:63:TYR:O	10:J:64:ASN:HB2	1.92	0.70
12:L:55:ILE:CD1	12:L:56:LEU:H	2.04	0.70
1:A:2:VAL:HG11	2:B:1157:ALA:C	2.11	0.70
2:B:745:PRO:O	2:B:748:ILE:HG12	1.91	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:897:GLY:O	2:B:898:LEU:HD23	1.91	0.70
2:B:955:THR:CG2	2:B:956:THR:N	2.55	0.70
2:B:995:ARG:HH11	3:C:165:LYS:HA	1.57	0.70
4:D:139:LYS:HD3	4:D:143:ASN:HD22	1.55	0.70
5:E:90:VAL:HG23	5:E:123:LEU:HD11	1.73	0.70
8:H:127:GLY:O	8:H:128:ASN:HB2	1.91	0.70
2:B:300:HIS:O	2:B:303:TYR:HE2	1.75	0.70
5:E:157:SER:C	5:E:159:ASP:H	1.95	0.70
5:E:93:MET:CG	5:E:123:LEU:HD12	2.21	0.70
10:J:64:ASN:HB3	10:J:65:PRO:HD2	1.73	0.70
11:K:48:ALA:O	11:K:51:LEU:HB2	1.92	0.70
1:A:533:LYS:NZ	1:A:745:GLN:HE22	1.89	0.70
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.73	0.70
2:B:429:PHE:HA	2:B:432:MET:HE2	1.73	0.70
3:C:46:ILE:HD12	3:C:67:LEU:HB3	1.74	0.70
6:F:90:ARG:HD2	6:F:155:LEU:HD13	1.73	0.70
2:B:294:ASP:H	9:I:12:ASN:ND2	1.89	0.70
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.22	0.69
1:A:381:THR:CG2	1:A:382:PRO:HD2	2.22	0.69
1:A:42:ASP:O	1:A:44:THR:N	2.25	0.69
7:G:1:MET:HA	7:G:1:MET:HE2	1.74	0.69
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.57	0.69
2:B:291:ILE:HD12	2:B:291:ILE:H	1.57	0.69
2:B:728:ARG:O	2:B:729:ILE:HG13	1.92	0.69
1:A:106:VAL:HG21	1:A:214:ILE:HD13	1.75	0.69
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.07	0.69
10:J:23:ASN:C	10:J:25:LEU:H	1.96	0.69
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.20	0.69
15:P:1:C:C4'	15:P:2:A:H5"	2.22	0.69
1:A:1110:ASN:HD22	1:A:1110:ASN:N	1.90	0.69
1:A:350:ARG:HB3	2:B:1128:LEU:HD11	1.74	0.69
1:A:337:ARG:NE	1:A:839:ARG:NH2	2.39	0.69
1:A:959:ASN:HD22	1:A:962:ARG:NH2	1.89	0.69
1:A:964:ILE:O	1:A:967:ALA:HB3	1.92	0.69
2:B:291:ILE:HD12	2:B:291:ILE:N	2.07	0.69
2:B:435:THR:C	2:B:437:GLU:H	1.93	0.69
3:C:35:ARG:NH1	11:K:41:THR:H	1.91	0.69
1:A:122:MET:HA	1:A:141:LEU:CD1	2.22	0.69
1:A:696:GLU:OE2	1:A:702:LEU:HD21	1.93	0.69
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.26	0.69
2:B:618:ASP:OD1	2:B:621:GLU:HB3	1.93	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:30:ILE:HG22	12:L:31:CYS:H	1.57	0.69
1:A:347:PHE:HE2	1:A:375:THR:HG23	1.57	0.69
1:A:567:LYS:CB	1:A:568:PRO:CD	2.69	0.69
1:A:1418:LEU:HB3	2:B:1222:ARG:HH11	1.56	0.69
2:B:497:ARG:NH2	2:B:775:LYS:NZ	2.40	0.69
3:C:18:VAL:O	3:C:18:VAL:HG12	1.90	0.69
4:D:13:ARG:C	4:D:15:LEU:H	1.94	0.69
7:G:85:GLU:HB3	7:G:147:ILE:HD12	1.73	0.69
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.72	0.69
1:A:639:PRO:HG2	1:A:640:GLN:HE21	1.55	0.69
1:A:853:ASP:OD1	1:A:855:THR:HG22	1.92	0.69
2:B:773:MET:SD	2:B:987:LYS:HD2	2.32	0.69
6:F:103:MET:HE2	7:G:66:GLY:H	1.56	0.69
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.74	0.69
2:B:288:ALA:O	2:B:331:LEU:HD11	1.91	0.69
2:B:999:MET:HA	2:B:999:MET:CE	2.23	0.69
6:F:109:VAL:HG12	6:F:110:ASP:N	2.08	0.69
8:H:58:THR:HG22	8:H:59:ILE:H	1.58	0.69
12:L:61:THR:CG2	12:L:63:ARG:HG3	2.22	0.69
2:B:483:LEU:HD11	2:B:491:THR:CG2	2.16	0.69
2:B:577:ALA:CB	2:B:589:VAL:HG11	2.20	0.69
2:B:26:THR:HB	2:B:708:GLU:OE1	1.92	0.69
1:A:1148:ILE:HD11	1:A:1198:ASP:HA	1.75	0.69
5:E:134:THR:C	5:E:135:PHE:HD1	1.97	0.69
7:G:21:ARG:HD2	7:G:24:GLN:HB2	1.74	0.69
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.22	0.69
2:B:731:VAL:HG12	2:B:732:SER:N	2.08	0.69
2:B:810:GLU:HB3	2:B:811:TYR:CE1	2.28	0.69
8:H:130:ARG:H	8:H:130:ARG:HD3	1.56	0.69
8:H:12:VAL:CG1	8:H:26:ILE:HD11	2.23	0.69
8:H:95:TYR:HE2	8:H:97:MET:CG	2.06	0.69
12:L:32:ALA:HB2	12:L:55:ILE:HG13	1.74	0.69
1:A:390:GLN:O	1:A:394:ASN:HB2	1.92	0.68
1:A:62:ASP:O	1:A:63:ARG:C	2.31	0.68
2:B:516:ASN:ND2	2:B:516:ASN:N	2.39	0.68
2:B:751:VAL:HG13	2:B:812:LEU:HD22	1.75	0.68
4:D:208:GLU:HA	4:D:211:LEU:HD12	1.75	0.68
5:E:114:ASN:O	5:E:115:ASN:HB3	1.92	0.68
5:E:78:LEU:HD11	5:E:109:ILE:HD12	1.75	0.68
11:K:67:PHE:C	11:K:68:PHE:HD2	1.97	0.68
1:A:1223:ASP:HA	1:A:1243:VAL:CG2	2.21	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:LEU:O	2:B:249:ARG:HG3	1.93	0.68
2:B:642:ASP:CA	2:B:649:LYS:HA	2.19	0.68
4:D:17:LYS:HD2	4:D:18:VAL:HG13	1.75	0.68
5:E:92:THR:O	5:E:95:THR:HB	1.94	0.68
8:H:12:VAL:HG13	8:H:26:ILE:HD11	1.74	0.68
9:I:85:PHE:CD1	9:I:99:LEU:HD13	2.28	0.68
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.75	0.68
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.28	0.68
9:I:74:GLU:HB3	9:I:81:ARG:HE	1.56	0.68
1:A:1223:ASP:CA	1:A:1243:VAL:HG22	2.23	0.68
1:A:427:GLN:HB2	1:A:430:TRP:CD1	2.29	0.68
1:A:284:ALA:O	1:A:286:HIS:N	2.25	0.68
1:A:899:VAL:CB	1:A:929:LEU:HD11	2.08	0.68
2:B:819:ALA:O	2:B:1093:GLN:HG2	1.94	0.68
2:B:975:GLN:O	2:B:990:ILE:HD12	1.94	0.68
9:I:44:TYR:HD1	9:I:45:ARG:N	1.91	0.68
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.74	0.68
1:A:1385:THR:HG22	1:A:1386:ARG:H	1.59	0.68
1:A:34:LYS:HZ2	1:A:57:ARG:NH2	1.92	0.68
2:B:101:MET:HB2	2:B:109:THR:HG22	1.75	0.68
1:A:718:VAL:O	1:A:722:LEU:HD12	1.94	0.68
2:B:705:MET:H	2:B:710:LEU:HD12	1.59	0.68
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.76	0.68
3:C:69:LEU:HB3	10:J:6:ARG:CD	2.24	0.68
1:A:134:ARG:HD2	1:A:221:SER:O	1.94	0.68
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.75	0.68
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.29	0.68
6:F:119:ARG:HH11	6:F:119:ARG:CG	2.07	0.68
1:A:709:THR:HG23	9:I:94:ASP:HA	1.75	0.68
11:K:60:ALA:O	11:K:73:LEU:HD12	1.92	0.68
12:L:31:CYS:HA	12:L:55:ILE:HD11	1.76	0.68
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.76	0.68
1:A:57:ARG:O	1:A:68:GLN:HG2	1.94	0.68
1:A:709:THR:HB	1:A:712:GLU:H	1.59	0.68
2:B:307:ASP:OD2	2:B:310:MET:HB2	1.92	0.68
5:E:98:ILE:HG22	5:E:102:GLU:HG3	1.76	0.68
1:A:447:GLN:NE2	14:T:20:DG:H4'	2.09	0.68
1:A:1120:LEU:HD13	1:A:1124:HIS:O	1.94	0.67
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.09	0.67
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.29	0.67
1:A:857:ARG:HD3	1:A:861:GLY:O	1.95	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:737:THR:CG2	9:I:66:PRO:HA	2.22	0.67
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.28	0.67
2:B:868:MET:O	2:B:870:ILE:HG13	1.93	0.67
3:C:138:GLU:OE1	3:C:138:GLU:N	2.26	0.67
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.27	0.67
1:A:923:LEU:O	1:A:927:VAL:HG23	1.94	0.67
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.23	0.67
2:B:918:ILE:HD12	2:B:935:ARG:NH1	2.08	0.67
5:E:117:THR:HG22	5:E:119:SER:N	2.08	0.67
8:H:42:ILE:HG23	8:H:95:TYR:CE1	2.26	0.67
1:A:1037:LEU:HD13	1:A:1041:ALA:HB1	1.76	0.67
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.24	0.67
2:B:811:TYR:H	2:B:811:TYR:HD1	1.43	0.67
6:F:76:LYS:HA	6:F:79:ARG:HD2	1.75	0.67
1:A:1147:THR:HB	9:I:48:LEU:HD12	1.75	0.67
11:K:107:THR:HG22	11:K:108:GLU:N	2.09	0.67
1:A:1076:ALA:HA	1:A:1079:MET:CE	2.24	0.67
1:A:1258:HIS:O	1:A:1262:LYS:HG3	1.95	0.67
2:B:131:ASP:HA	2:B:164:LYS:HB3	1.76	0.67
2:B:273:LEU:O	2:B:276:ILE:HG13	1.95	0.67
2:B:705:MET:N	2:B:710:LEU:HD12	2.08	0.67
1:A:1329:THR:HG22	1:A:1331:SER:N	2.08	0.67
1:A:153:PRO:HD3	1:A:161:LEU:HD13	1.74	0.67
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.76	0.67
1:A:442:VAL:HG12	1:A:491:VAL:HA	1.77	0.67
1:A:67:CYS:C	1:A:68:GLN:HG3	2.14	0.67
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.10	0.67
1:A:196:GLU:HG2	1:A:197:PRO:HD2	1.77	0.67
2:B:308:TRP:CH2	9:I:45:ARG:HG2	2.30	0.67
2:B:1099:VAL:HG13	2:B:1100:ASP:H	1.59	0.67
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.59	0.67
2:B:305:VAL:HG12	2:B:305:VAL:O	1.95	0.67
2:B:383:ASN:ND2	2:B:387:LEU:HD12	2.09	0.67
2:B:732:SER:HB2	2:B:734:HIS:NE2	2.10	0.67
7:G:112:LYS:HA	7:G:115:MET:HE3	1.77	0.67
2:B:992:ILE:HD11	11:K:66:PRO:HB2	1.76	0.67
2:B:193:LYS:HD3	2:B:787:VAL:HG11	1.77	0.67
2:B:515:HIS:CD2	2:B:516:ASN:N	2.61	0.67
2:B:953:LEU:O	2:B:964:VAL:HG23	1.95	0.67
1:A:12:ARG:HG2	1:A:13:THR:H	1.60	0.67
2:B:1002:THR:OG1	2:B:1006:ILE:HG13	1.94	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:ARG:NH1	11:K:41:THR:N	2.43	0.67
11:K:45:LEU:HG	11:K:94:ILE:CD1	2.25	0.67
12:L:30:ILE:HG22	12:L:31:CYS:N	2.09	0.67
1:A:134:ARG:HH11	1:A:221:SER:HA	1.59	0.66
3:C:18:VAL:O	3:C:20:PHE:HD2	1.78	0.66
3:C:238:ILE:HD11	3:C:246:ARG:NE	2.09	0.66
3:C:50:GLU:OE1	12:L:64:LEU:HD13	1.95	0.66
4:D:24:ALA:HB3	4:D:26:THR:HG23	1.76	0.66
5:E:103:LYS:HD3	5:E:105:PHE:CZ	2.30	0.66
1:A:524:VAL:HG12	1:A:525:GLN:N	2.10	0.66
1:A:62:ASP:O	1:A:64:ASN:N	2.27	0.66
2:B:281:PRO:O	2:B:283:VAL:N	2.28	0.66
2:B:289:LEU:HD13	2:B:375:ALA:CB	2.25	0.66
2:B:434:ARG:O	2:B:436:VAL:HG23	1.94	0.66
2:B:883:LEU:O	2:B:885:MET:N	2.28	0.66
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.30	0.66
9:I:26:LEU:HD22	9:I:35:VAL:HG12	1.76	0.66
1:A:1029:ARG:HG3	1:A:1029:ARG:HH11	1.58	0.66
1:A:1141:THR:HA	1:A:1205:LYS:HZ3	1.60	0.66
2:B:803:LEU:HD12	2:B:1032:SER:HB3	1.77	0.66
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.76	0.66
6:F:89:GLU:OE2	6:F:134:ILE:HG21	1.96	0.66
2:B:978:ASP:OD2	2:B:1098:MET:HG2	1.96	0.66
2:B:575:PRO:HG2	2:B:576:ASP:H	1.60	0.66
3:C:184:ASN:OD1	3:C:187:LYS:HA	1.95	0.66
6:F:105:ALA:HB1	6:F:106:PRO:HD2	1.77	0.66
2:B:1017:ILE:H	2:B:1018:PRO:CD	2.08	0.66
2:B:203:PHE:HB3	2:B:205:ILE:CD1	2.25	0.66
2:B:505:ASP:OD2	13:N:1:DA:H5"	1.96	0.66
2:B:995:ARG:NH1	3:C:165:LYS:HG2	2.10	0.66
12:L:58:LYS:O	12:L:59:ALA:O	2.14	0.66
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	1.96	0.66
1:A:265:LYS:HE3	1:A:302:THR:HG23	1.76	0.66
1:A:320:ARG:HH11	1:A:320:ARG:HB3	1.60	0.66
2:B:600:LEU:O	2:B:609:ILE:HD11	1.96	0.66
4:D:124:GLU:O	4:D:128:VAL:HG23	1.94	0.66
1:A:567:LYS:NZ	8:H:43:ASN:HB3	2.09	0.66
8:H:26:ILE:HD12	8:H:49:VAL:HG11	1.76	0.66
1:A:146:MET:CA	1:A:171:GLN:HB2	2.26	0.66
3:C:101:LEU:HD13	3:C:118:LEU:CD2	2.26	0.66
3:C:133:ILE:HD12	3:C:237:SER:N	2.10	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:71:LYS:HA	4:D:74:GLN:CB	2.24	0.66
1:A:447:GLN:HE22	14:T:20:DG:H4'	1.60	0.66
1:A:12:ARG:NH2	2:B:1192:TYR:HE2	1.94	0.66
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.31	0.66
2:B:589:VAL:HG12	2:B:590:HIS:N	2.11	0.66
2:B:611:PRO:HG2	2:B:685:LEU:HD21	1.76	0.66
5:E:14:ARG:HH21	5:E:141:VAL:CG1	2.08	0.66
8:H:82:PRO:O	8:H:84:ALA:N	2.25	0.66
1:A:900:ASP:HA	1:A:926:GLN:HE22	1.61	0.66
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.78	0.66
3:C:177:GLU:CG	3:C:231:ASN:HD22	2.09	0.66
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.59	0.66
2:B:1182:CYS:SG	2:B:1182:CYS:O	2.54	0.66
2:B:417:PHE:HE1	2:B:453:ILE:HD13	1.62	0.66
2:B:597:MET:SD	2:B:624:LEU:HD11	2.36	0.66
2:B:654:ARG:H	2:B:657:HIS:CD2	2.12	0.66
5:E:112:TYR:OH	5:E:136:ASN:HB2	1.95	0.66
5:E:48:ASP:HB3	5:E:54:GLN:NE2	2.11	0.66
1:A:1105:LEU:HD23	1:A:1384:VAL:HG21	1.77	0.65
1:A:299:HIS:HA	1:A:302:THR:CG2	2.26	0.65
1:A:682:THR:HG23	1:A:728:LYS:CE	2.25	0.65
4:D:155:ARG:CZ	4:D:155:ARG:HB2	2.26	0.65
1:A:471:ASN:OD1	1:A:472:LEU:N	2.28	0.65
1:A:493:GLN:H	1:A:497:THR:HG21	1.62	0.65
1:A:567:LYS:HB3	8:H:96:VAL:N	2.10	0.65
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.77	0.65
1:A:682:THR:CG2	1:A:728:LYS:HE3	2.22	0.65
2:B:244:LEU:HD12	2:B:247:GLY:O	1.95	0.65
2:B:259:TYR:HD1	2:B:259:TYR:H	1.44	0.65
2:B:291:ILE:CD1	2:B:291:ILE:H	2.09	0.65
2:B:956:THR:HG22	2:B:960:GLY:HA2	1.77	0.65
3:C:184:ASN:HD21	3:C:189:THR:H	1.44	0.65
4:D:12:ARG:HH12	4:D:14:ARG:HA	1.62	0.65
4:D:156:ASP:O	4:D:158:GLU:N	2.30	0.65
4:D:210:ILE:O	4:D:214:LEU:HD23	1.96	0.65
5:E:98:ILE:HA	5:E:101:GLN:CB	2.25	0.65
12:L:48:CYS:HB3	12:L:51:CYS:O	1.95	0.65
1:A:464:PRO:HG2	1:A:465:TYR:CD1	2.31	0.65
1:A:34:LYS:HZ2	1:A:57:ARG:HH22	1.43	0.65
8:H:139:ASN:O	8:H:140:ALA:CB	2.44	0.65
8:H:76:THR:HG21	8:H:141:TYR:OH	1.95	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:67:THR:OG1	9:I:68:LEU:HD12	1.96	0.65
1:A:320:ARG:NH1	1:A:320:ARG:HB3	2.11	0.65
2:B:824:ILE:HG22	2:B:1087:PHE:CE2	2.31	0.65
2:B:810:GLU:HB3	2:B:811:TYR:CD1	2.30	0.65
4:D:185:CYS:O	4:D:211:LEU:HD22	1.96	0.65
9:I:82:GLU:O	9:I:104:LEU:HG	1.96	0.65
1:A:687:LYS:O	1:A:690:VAL:HB	1.97	0.65
2:B:205:ILE:N	2:B:205:ILE:HD12	2.11	0.65
2:B:589:VAL:HG12	2:B:590:HIS:H	1.62	0.65
4:D:12:ARG:HH11	4:D:12:ARG:HG2	1.61	0.65
4:D:69:ALA:HB2	4:D:72:ARG:HH12	1.59	0.65
8:H:30:SER:CB	8:H:36:CYS:HB3	2.26	0.65
9:I:111:THR:HG21	9:I:113:ASP:HB2	1.77	0.65
9:I:44:TYR:CD1	9:I:45:ARG:N	2.65	0.65
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.27	0.65
1:A:105:CYS:SG	1:A:139:TRP:HA	2.37	0.65
1:A:688:LYS:HG3	1:A:691:LEU:HD23	1.77	0.65
1:A:12:ARG:NH2	2:B:1192:TYR:CE2	2.64	0.65
2:B:1202:LEU:O	2:B:1206:GLU:HG3	1.96	0.65
2:B:866:TYR:CB	2:B:870:ILE:HB	2.25	0.65
4:D:118:THR:HG22	4:D:118:THR:O	1.97	0.65
7:G:119:LEU:HD13	7:G:132:SER:HB2	1.77	0.65
1:A:1041:ALA:O	1:A:1045:VAL:HG23	1.97	0.65
1:A:332:LYS:O	1:A:333:GLU:HB2	1.96	0.65
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.61	0.65
2:B:846:ILE:CG2	2:B:974:PRO:HG2	2.27	0.65
1:A:537:ARG:HD2	8:H:20:TYR:CE1	2.30	0.65
8:H:93:TYR:HB3	8:H:144:ILE:O	1.97	0.65
8:H:8:ASP:CG	8:H:9:ILE:H	2.00	0.65
9:I:116:ASN:C	9:I:117:LYS:HD2	2.16	0.65
1:A:298:PHE:O	1:A:302:THR:HG22	1.97	0.65
2:B:254:LEU:HD23	2:B:381:MET:CE	2.26	0.65
2:B:277:LYS:CD	2:B:277:LYS:H	2.10	0.65
2:B:520:GLY:H	2:B:748:ILE:HG22	1.62	0.65
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.79	0.65
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.77	0.65
8:H:38:LEU:HD13	8:H:125:LEU:HD12	1.77	0.65
9:I:68:LEU:N	9:I:68:LEU:HD12	2.12	0.65
12:L:38:LEU:CG	12:L:39:SER:H	2.05	0.65
1:A:1094:VAL:HG13	1:A:1113:THR:HB	1.79	0.65
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.58	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ALA:HA	1:A:291:GLU:CG	2.27	0.65
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.77	0.65
2:B:165:VAL:CG1	2:B:448:ILE:HD13	2.27	0.65
2:B:785:TYR:CD1	2:B:786:ASN:N	2.65	0.65
2:B:872:GLU:CD	2:B:914:LYS:HE3	2.17	0.65
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.13	0.64
2:B:1034:VAL:O	2:B:1037:LEU:N	2.30	0.64
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.36	0.64
2:B:855:PHE:CD2	2:B:972:LYS:HE3	2.32	0.64
2:B:878:GLN:HB3	2:B:879:ARG:NH1	2.11	0.64
3:C:196:ASP:CB	3:C:199:LYS:HD3	2.27	0.64
4:D:29:LEU:HD22	4:D:29:LEU:N	2.12	0.64
7:G:125:SER:OG	7:G:128:PRO:HA	1.98	0.64
1:A:568:PRO:CG	8:H:46:LEU:HD22	2.27	0.64
8:H:82:PRO:C	8:H:84:ALA:N	2.50	0.64
10:J:14:VAL:HG12	10:J:14:VAL:O	1.97	0.64
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.08	0.64
3:C:50:GLU:CG	12:L:64:LEU:HD22	2.27	0.64
5:E:15:ALA:O	5:E:19:VAL:HG23	1.97	0.64
2:B:20:ASP:O	2:B:22:SER:N	2.28	0.64
2:B:622:LYS:NZ	9:I:59:VAL:HG13	2.13	0.64
3:C:69:LEU:HB3	10:J:6:ARG:HD3	1.79	0.64
11:K:47:ARG:O	11:K:47:ARG:HD2	1.97	0.64
14:T:22:DC:H2"	14:T:23:BRU:OP2	1.97	0.64
1:A:107:CYS:HA	1:A:171:GLN:HE22	1.63	0.64
1:A:697:ALA:HB2	1:A:702:LEU:HD12	1.79	0.64
2:B:653:VAL:HA	2:B:657:HIS:CD2	2.32	0.64
10:J:24:LEU:CD1	10:J:38:ARG:HG2	2.28	0.64
12:L:28:LYS:HB3	12:L:39:SER:HB2	1.80	0.64
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.33	0.64
1:A:839:ARG:NH1	1:A:839:ARG:HG2	2.10	0.64
1:A:898:ARG:HD3	1:A:933:TYR:CD1	2.33	0.64
2:B:464:GLY:O	2:B:477:ALA:HA	1.98	0.64
3:C:242:GLN:HA	3:C:245:VAL:HG23	1.79	0.64
4:D:50:LEU:HD21	7:G:4:ILE:HD11	1.78	0.64
1:A:1168:GLU:OE2	1:A:1172:LEU:HD11	1.98	0.64
1:A:228:PHE:HE2	4:D:15:LEU:HD23	1.63	0.64
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.78	0.64
2:B:126:SER:OG	2:B:172:ILE:HD11	1.98	0.64
4:D:195:ILE:CG2	4:D:198:LEU:HG	2.27	0.64
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.80	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:HB3	1:A:344:ARG:HH11	1.62	0.64
1:A:73:GLY:O	1:A:75:ASN:N	2.31	0.64
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.80	0.64
4:D:12:ARG:NH1	4:D:12:ARG:HG2	2.13	0.64
4:D:15:LEU:O	4:D:15:LEU:HD12	1.97	0.64
5:E:212:ARG:HH11	5:E:212:ARG:HG3	1.63	0.64
1:A:35:ILE:HG22	1:A:35:ILE:O	1.96	0.64
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.80	0.64
2:B:365:THR:HG23	2:B:367:LEU:H	1.62	0.64
3:C:172:PRO:O	3:C:235:VAL:HG23	1.96	0.64
3:C:252:GLN:HG3	11:K:95:ILE:HG23	1.80	0.64
5:E:32:GLN:HG3	5:E:36:GLU:OE2	1.98	0.64
11:K:47:ARG:NH1	11:K:47:ARG:HB3	2.09	0.64
1:A:896:ARG:NH2	1:A:1030:ARG:NH2	2.46	0.64
2:B:1071:VAL:HG22	2:B:1084:GLN:HG3	1.79	0.64
2:B:92:PHE:HB3	2:B:130:VAL:HG11	1.79	0.64
3:C:112:ASN:HB3	3:C:114:TYR:CE1	2.33	0.64
5:E:135:PHE:HB3	5:E:140:LEU:HD21	1.78	0.64
6:F:109:VAL:HG12	6:F:110:ASP:H	1.63	0.64
11:K:21:ILE:HG23	11:K:33:ILE:HG12	1.80	0.64
14:T:16:DT:H1'	14:T:17:DT:H5'	1.78	0.64
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.97	0.63
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.28	0.63
2:B:879:ARG:HH22	2:B:885:MET:HE1	1.63	0.63
4:D:146:GLN:O	4:D:149:THR:HG22	1.98	0.63
4:D:69:ALA:HA	4:D:72:ARG:HG3	1.80	0.63
8:H:32:THR:HG22	8:H:33:GLN:OE1	1.98	0.63
8:H:4:THR:HA	8:H:60:ALA:CB	2.16	0.63
10:J:43:ARG:CD	10:J:43:ARG:H	2.11	0.63
11:K:32:VAL:HG22	11:K:74:ARG:HG3	1.80	0.63
1:A:280:GLU:HG2	1:A:289:ILE:HD11	1.79	0.63
1:A:677:ARG:HD2	1:A:678:GLU:N	2.12	0.63
1:A:829:VAL:C	1:A:831:THR:H	2.01	0.63
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.33	0.63
2:B:221:ASN:O	2:B:222:ILE:HG13	1.98	0.63
2:B:882:THR:HG22	2:B:883:LEU:N	2.12	0.63
4:D:134:THR:HG22	4:D:136:GLY:H	1.62	0.63
5:E:153:HIS:O	5:E:154:ILE:HG13	1.98	0.63
1:A:1037:LEU:HD13	1:A:1041:ALA:CB	2.29	0.63
1:A:825:ILE:HD11	2:B:512:ARG:O	1.99	0.63
2:B:880:THR:CG2	2:B:934:LYS:HG3	2.29	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:24:ALA:CB	4:D:26:THR:HG23	2.28	0.63
7:G:155:SER:O	7:G:156:SER:HB3	1.97	0.63
8:H:56:THR:HB	8:H:145:ARG:HG2	1.80	0.63
9:I:99:LEU:C	9:I:100:PHE:HD1	2.02	0.63
11:K:12:LEU:HD21	11:K:18:LYS:N	2.12	0.63
1:A:973:ILE:HD11	1:A:1038:THR:HG23	1.80	0.63
1:A:380:VAL:HG12	1:A:428:TYR:HA	1.80	0.63
1:A:61:ILE:HG22	1:A:62:ASP:H	1.64	0.63
2:B:57:TYR:CD1	2:B:57:TYR:N	2.67	0.63
3:C:80:LEU:HD12	3:C:81:GLU:H	1.63	0.63
3:C:89:GLU:O	3:C:90:ASP:HB3	1.98	0.63
4:D:213:GLU:HA	4:D:213:GLU:OE1	1.97	0.63
8:H:81:PRO:CB	8:H:82:PRO:CD	2.77	0.63
1:A:305:ASP:OD2	1:A:326:ARG:HD3	1.98	0.63
1:A:774:ARG:NH1	1:A:797:LYS:HG3	2.13	0.63
1:A:934:LYS:O	1:A:937:VAL:HG12	1.98	0.63
2:B:1103:ILE:O	2:B:1103:ILE:HG23	1.98	0.63
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.81	0.63
4:D:54:GLU:O	4:D:58:VAL:HG23	1.99	0.63
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.63	0.63
1:A:172:PRO:HD3	1:A:185:TRP:NE1	2.14	0.63
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.81	0.63
3:C:232:VAL:HG21	3:C:244:VAL:HG22	1.79	0.63
3:C:175:ALA:HB2	10:J:43:ARG:HH22	1.62	0.63
1:A:100:LYS:HE2	1:A:104:GLU:OE2	1.99	0.63
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	1.80	0.63
1:A:207:ILE:HG22	1:A:211:PHE:CE2	2.33	0.63
1:A:57:ARG:O	1:A:58:LEU:O	2.15	0.63
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.79	0.63
5:E:77:SER:O	5:E:105:PHE:HB3	1.99	0.63
5:E:23:VAL:HG13	5:E:78:LEU:HD13	1.79	0.63
4:D:32:GLU:HG3	7:G:5:LYS:HE2	1.81	0.63
1:A:1115:SER:H	1:A:1330:ASN:HD21	1.47	0.63
1:A:709:THR:HG22	1:A:710:LEU:N	2.14	0.63
2:B:579:ARG:HH11	2:B:579:ARG:HG2	1.63	0.63
2:B:831:SER:HB3	2:B:994:TYR:OH	1.99	0.63
5:E:22:MET:CE	5:E:26:ARG:HH21	2.12	0.63
6:F:90:ARG:CD	6:F:155:LEU:HD13	2.29	0.63
8:H:130:ARG:HB3	8:H:134:ASN:H	1.62	0.63
1:A:251:SER:HA	1:A:257:ARG:O	1.98	0.63
1:A:56:PRO:O	1:A:57:ARG:HG3	1.98	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:GLY:O	5:E:204:THR:HG21	1.99	0.63
2:B:850:LEU:HD12	2:B:851:PHE:N	2.14	0.63
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.33	0.63
6:F:94:LEU:HD22	6:F:122:MET:HG2	1.80	0.63
1:A:1079:MET:HG2	1:A:1359:ASP:OD1	1.98	0.62
1:A:858:ASN:ND2	1:A:858:ASN:C	2.51	0.62
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.79	0.62
6:F:111:LEU:HD12	6:F:111:LEU:H	1.64	0.62
12:L:38:LEU:CD2	12:L:48:CYS:HA	2.29	0.62
14:T:14:DA:H2"	14:T:15:DG:C8	2.33	0.62
1:A:596:THR:C	1:A:598:LEU:H	2.02	0.62
2:B:582:VAL:HB	2:B:587:HIS:HD2	1.62	0.62
7:G:44:TYR:CD2	7:G:105:PRO:HB2	2.35	0.62
9:I:58:VAL:HG12	9:I:58:VAL:O	1.98	0.62
1:A:1147:THR:HB	9:I:48:LEU:CD1	2.29	0.62
1:A:1329:THR:HG22	1:A:1331:SER:H	1.64	0.62
1:A:1385:THR:HG21	1:A:1387:HIS:CD2	2.33	0.62
1:A:809:THR:OG1	1:A:812:GLU:HG3	1.97	0.62
6:F:111:LEU:O	6:F:113:GLY:N	2.29	0.62
1:A:145:LYS:HD2	1:A:149:GLU:OE1	1.98	0.62
2:B:333:PHE:HE1	2:B:336:ARG:HH11	1.46	0.62
2:B:806:THR:H	2:B:809:MET:HG3	1.63	0.62
2:B:848:ARG:HH22	2:B:996:ARG:HD3	1.64	0.62
4:D:5:THR:O	4:D:5:THR:HG23	2.00	0.62
6:F:76:LYS:HE3	6:F:150:GLU:OE2	2.00	0.62
6:F:76:LYS:O	6:F:79:ARG:HD3	1.99	0.62
7:G:14:HIS:HD2	7:G:16:SER:H	1.43	0.62
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.29	0.62
2:B:1007:VAL:HG23	2:B:1008:PRO:HD2	1.82	0.62
2:B:1069:PHE:HD1	2:B:1069:PHE:H	1.47	0.62
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.81	0.62
2:B:284:ILE:HD13	2:B:333:PHE:CD2	2.33	0.62
2:B:990:ILE:HG22	2:B:991:GLY:N	2.14	0.62
3:C:76:ASP:C	3:C:129:ILE:HD11	2.20	0.62
5:E:78:LEU:HD23	5:E:78:LEU:C	2.19	0.62
8:H:89:LEU:HD12	8:H:91:ASP:OD1	2.00	0.62
8:H:94:ASP:O	8:H:95:TYR:HB2	1.99	0.62
1:A:1135:ARG:HG2	1:A:1136:SER:N	2.13	0.62
1:A:1436:ILE:O	1:A:1437:GLY:C	2.36	0.62
1:A:567:LYS:HZ2	8:H:46:LEU:CB	2.12	0.62
1:A:916:GLY:O	1:A:919:ILE:HG22	1.99	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1058:LEU:O	2:B:1061:GLU:HB2	1.99	0.62
2:B:425:THR:HA	2:B:428:ILE:HD12	1.82	0.62
6:F:69:LEU:O	6:F:71:GLU:HG3	1.99	0.62
1:A:504:LEU:HD11	6:F:91:ALA:CB	2.30	0.62
7:G:112:LYS:HA	7:G:115:MET:CE	2.29	0.62
7:G:52:ASP:C	7:G:53:ASN:HD22	2.03	0.62
8:H:11:GLN:HA	8:H:53:ASP:O	2.00	0.62
9:I:61:ASP:C	9:I:63:GLY:H	2.03	0.62
3:C:165:LYS:O	11:K:6:ARG:NH1	2.33	0.62
1:A:1006:ILE:HD12	5:E:167:ARG:CB	2.30	0.62
1:A:216:VAL:O	1:A:219:PHE:HB2	1.99	0.62
1:A:230:ARG:H	1:A:233:TRP:HE3	1.47	0.62
1:A:809:THR:H	1:A:812:GLU:HB2	1.63	0.62
2:B:805:THR:HA	2:B:809:MET:HE2	1.81	0.62
2:B:839:MET:CE	2:B:980:PHE:HB2	2.29	0.62
2:B:955:THR:HG23	2:B:956:THR:H	1.64	0.62
3:C:189:THR:CG2	3:C:190:ASP:H	2.12	0.62
6:F:111:LEU:HD12	6:F:111:LEU:N	2.15	0.62
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.82	0.62
1:A:66:LYS:NZ	1:A:68:GLN:N	2.46	0.62
2:B:365:THR:HG23	2:B:367:LEU:N	2.14	0.62
2:B:769:TYR:HB3	2:B:773:MET:HE3	1.81	0.62
2:B:859:TYR:OH	2:B:941:LEU:HD12	1.99	0.62
3:C:177:GLU:HG3	3:C:231:ASN:ND2	2.09	0.62
3:C:183:TRP:O	3:C:185:LYS:N	2.33	0.62
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.81	0.62
8:H:26:ILE:HG22	8:H:40:LEU:O	2.00	0.62
9:I:61:ASP:O	9:I:64:SER:N	2.32	0.62
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.30	0.62
1:A:63:ARG:HA	1:A:74:MET:HE2	1.82	0.62
2:B:125:SER:HA	2:B:171:PRO:HA	1.81	0.62
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.32	0.62
2:B:996:ARG:NH2	3:C:38:ILE:HG23	2.15	0.62
7:G:87:VAL:CG2	7:G:103:VAL:HG21	2.30	0.62
8:H:103:LYS:HB3	8:H:115:TYR:CD1	2.35	0.62
9:I:10:CYS:SG	9:I:32:CYS:HB3	2.38	0.62
1:A:946:VAL:CG2	5:E:201:LYS:HD2	2.30	0.62
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.00	0.62
2:B:948:ILE:HG22	2:B:949:VAL:O	2.00	0.62
4:D:130:LEU:HD13	4:D:142:LYS:HG2	1.81	0.62
5:E:195:VAL:HG22	5:E:213:ILE:HG13	1.82	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:204:THR:HG23	5:E:205:SER:H	1.64	0.62
10:J:30:LEU:HD23	10:J:31:ASP:H	1.65	0.62
1:A:157:ASP:OD2	1:A:160:GLN:HG3	2.00	0.61
1:A:399:HIS:O	1:A:401:GLY:N	2.33	0.61
2:B:100:PRO:O	2:B:180:TYR:OH	2.17	0.61
2:B:1102:LYS:O	2:B:1103:ILE:C	2.38	0.61
2:B:619:ILE:HG22	2:B:620:ARG:N	2.15	0.61
3:C:179:GLU:HG2	3:C:180:TYR:N	2.15	0.61
4:D:50:LEU:HD13	4:D:55:ALA:HA	1.81	0.61
8:H:40:LEU:HD22	8:H:123:MET:HE3	1.80	0.61
12:L:32:ALA:HB3	12:L:33:GLU:OE2	1.99	0.61
2:B:241:ARG:HG2	2:B:253:THR:HG22	1.81	0.61
2:B:57:TYR:N	2:B:57:TYR:HD1	1.98	0.61
2:B:815:ARG:HD3	2:B:1041:GLU:OE2	1.99	0.61
2:B:885:MET:HA	2:B:936:ASP:CB	2.26	0.61
3:C:101:LEU:C	3:C:102:GLN:HG3	2.21	0.61
5:E:93:MET:HG2	5:E:123:LEU:HD12	1.80	0.61
7:G:9:LEU:HD12	7:G:10:ASN:H	1.64	0.61
10:J:1:MET:N	10:J:56:LEU:N	2.48	0.61
12:L:38:LEU:O	12:L:39:SER:HB3	2.00	0.61
1:A:1171:GLN:OE1	1:A:1172:LEU:HG	2.01	0.61
3:C:186:LEU:N	3:C:186:LEU:HD12	2.15	0.61
4:D:122:GLU:HA	4:D:125:SER:HB3	1.81	0.61
6:F:90:ARG:HH21	6:F:94:LEU:HD11	1.64	0.61
8:H:25:ARG:HA	8:H:41:ASP:HA	1.81	0.61
1:A:322:VAL:O	1:A:322:VAL:HG13	1.99	0.61
1:A:718:VAL:O	1:A:721:PHE:HB2	2.00	0.61
1:A:855:THR:HA	1:A:866:PHE:O	2.00	0.61
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.81	0.61
1:A:782:ARG:NH2	2:B:699:GLU:O	2.32	0.61
10:J:64:ASN:CB	10:J:65:PRO:CD	2.76	0.61
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.82	0.61
1:A:743:VAL:O	1:A:747:VAL:HG23	2.01	0.61
2:B:345:LYS:HG2	2:B:349:ILE:HD11	1.82	0.61
3:C:235:VAL:HG11	10:J:6:ARG:NH2	2.15	0.61
5:E:108:GLY:HA3	5:E:132:ILE:HG23	1.81	0.61
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.83	0.61
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.82	0.61
1:A:297:GLN:O	1:A:297:GLN:HG3	1.99	0.61
1:A:311:GLN:O	1:A:313:GLN:N	2.33	0.61
1:A:332:LYS:C	1:A:334:GLY:H	2.02	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:25:VAL:HG12	3:C:26:ASP:H	1.66	0.61
3:C:52:GLU:OE2	3:C:154:LYS:HD2	2.01	0.61
3:C:88:CYS:SG	3:C:91:HIS:CA	2.88	0.61
6:F:152:ILE:HG22	6:F:153:VAL:N	2.15	0.61
8:H:43:ASN:ND2	8:H:46:LEU:HB2	2.15	0.61
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.82	0.61
14:T:14:DA:H2"	14:T:15:DG:H8	1.66	0.61
2:B:326:ASP:OD2	2:B:328:GLU:HB3	2.01	0.61
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.30	0.61
3:C:189:THR:CG2	3:C:190:ASP:N	2.64	0.61
7:G:1:MET:SD	7:G:79:PHE:CD1	2.94	0.61
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.36	0.61
1:A:34:LYS:CG	1:A:36:ARG:HH21	2.14	0.61
5:E:128:PRO:HA	5:E:129:PRO:C	2.20	0.61
9:I:53:GLY:O	9:I:89:GLN:HB2	2.00	0.61
2:B:186:GLU:HG2	10:J:62:ARG:NH2	2.16	0.61
12:L:61:THR:HG22	12:L:63:ARG:HG3	1.82	0.61
1:A:1438:THR:O	6:F:92:ARG:NH1	2.34	0.61
2:B:129:PHE:CE2	2:B:166:PHE:HB2	2.36	0.61
2:B:466:TRP:O	2:B:468:GLU:N	2.34	0.61
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.82	0.61
4:D:220:LEU:HG	4:D:221:TYR:N	2.15	0.61
4:D:7:THR:O	4:D:9:GLN:N	2.32	0.61
6:F:128:LYS:HD3	6:F:149:GLU:O	2.00	0.61
7:G:114:LEU:HD23	7:G:162:SER:HB3	1.82	0.61
2:B:230:ALA:HB3	2:B:231:PRO:HD3	1.83	0.61
2:B:378:LEU:HD12	2:B:378:LEU:O	1.99	0.61
2:B:41:LYS:HA	2:B:41:LYS:HE2	1.83	0.61
2:B:734:HIS:O	2:B:735:ALA:HB2	2.00	0.61
3:C:112:ASN:CB	3:C:114:TYR:HE1	2.13	0.61
3:C:124:LEU:H	3:C:124:LEU:HD12	1.66	0.61
8:H:11:GLN:O	8:H:28:ALA:HB1	2.01	0.61
10:J:1:MET:N	10:J:57:ILE:N	2.34	0.61
12:L:38:LEU:HD11	12:L:49:LYS:HE2	1.82	0.61
1:A:1215:ARG:NH1	1:A:1272:THR:O	2.34	0.60
1:A:129:LYS:O	1:A:130:ASP:HB2	2.00	0.60
1:A:157:ASP:OD2	1:A:159:THR:HB	2.01	0.60
1:A:23:SER:HA	1:A:233:TRP:CD1	2.36	0.60
1:A:316:GLN:HE21	1:A:317:LYS:HZ2	1.48	0.60
1:A:590:ARG:HG2	1:A:604:GLY:HA2	1.82	0.60
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.66	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1031:LEU:HB2	2:B:1055:ILE:HD13	1.82	0.60
2:B:1084:GLN:NE2	2:B:1084:GLN:N	2.49	0.60
2:B:101:MET:CE	2:B:126:SER:HA	2.31	0.60
2:B:29:ASP:OD1	2:B:658:ILE:HD13	2.01	0.60
2:B:582:VAL:HG22	2:B:626:ILE:CB	2.29	0.60
4:D:192:LYS:HD2	4:D:199:ASN:HA	1.82	0.60
4:D:219:THR:HG22	4:D:220:LEU:O	2.01	0.60
8:H:89:LEU:O	8:H:91:ASP:N	2.34	0.60
1:A:332:LYS:HB2	1:A:337:ARG:HH12	1.64	0.60
1:A:786:HIS:CD2	1:A:786:HIS:N	2.69	0.60
2:B:1099:VAL:CG1	2:B:1100:ASP:N	2.64	0.60
2:B:424:LEU:O	2:B:427:ASP:HB3	2.01	0.60
2:B:497:ARG:HH21	2:B:775:LYS:HZ1	1.49	0.60
2:B:39:ARG:HE	2:B:665:GLU:HG2	1.65	0.60
3:C:31:ASN:O	3:C:34:ARG:HB3	2.01	0.60
5:E:69:ILE:HD12	5:E:69:ILE:H	1.66	0.60
11:K:17:SER:O	11:K:18:LYS:C	2.38	0.60
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.66	0.60
1:A:167:CYS:HB2	1:A:169:ASN:HD21	1.67	0.60
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.31	0.60
2:B:56:ASP:HB3	2:B:57:TYR:CD1	2.36	0.60
2:B:957:ASN:O	2:B:960:GLY:N	2.34	0.60
4:D:207:LEU:O	4:D:211:LEU:HD12	2.01	0.60
11:K:88:LYS:O	11:K:91:CYS:HB2	2.01	0.60
1:A:1168:GLU:O	1:A:1171:GLN:OE1	2.19	0.60
1:A:1206:ASP:O	1:A:1207:LEU:HD23	2.00	0.60
1:A:321:PRO:O	1:A:322:VAL:HB	2.01	0.60
1:A:63:ARG:HA	1:A:74:MET:CE	2.31	0.60
1:A:929:LEU:HD13	1:A:929:LEU:O	2.02	0.60
2:B:770:GLN:OE1	2:B:983:ARG:CA	2.47	0.60
5:E:80:VAL:HG12	5:E:82:PHE:HE1	1.66	0.60
7:G:26:LEU:HD11	7:G:70:PHE:CD1	2.36	0.60
1:A:1153:TYR:CD2	1:A:1163:ILE:HD11	2.37	0.60
1:A:616:VAL:HG12	1:A:617:VAL:N	2.16	0.60
1:A:67:CYS:O	1:A:68:GLN:HG3	2.02	0.60
1:A:719:VAL:HA	1:A:722:LEU:HD13	1.83	0.60
2:B:102:VAL:CG2	2:B:112:LEU:HD22	2.32	0.60
2:B:361:LEU:O	2:B:363:HIS:O	2.19	0.60
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.13	0.60
2:B:644:GLU:HB2	2:B:648:HIS:O	2.02	0.60
5:E:204:THR:HG23	5:E:205:SER:N	2.17	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:90:ARG:HH21	6:F:94:LEU:CD1	2.14	0.60
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.34	0.60
1:A:125:ALA:C	1:A:127:ALA:H	2.03	0.60
1:A:596:THR:O	1:A:598:LEU:N	2.34	0.60
2:B:639:ILE:HG22	2:B:641:GLU:HG2	1.84	0.60
2:B:831:SER:CB	2:B:994:TYR:OH	2.48	0.60
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.84	0.60
8:H:15:VAL:HG13	8:H:26:ILE:CB	2.31	0.60
3:C:175:ALA:HB2	10:J:43:ARG:NH2	2.17	0.60
1:A:1035:TYR:HB3	1:A:1037:LEU:HD23	1.83	0.60
1:A:1341:ILE:CG2	1:A:1342:GLU:H	2.14	0.60
2:B:105:SER:O	2:B:106:ASP:HB2	2.00	0.60
2:B:64:CYS:HA	2:B:67:SER:HG	1.66	0.60
4:D:220:LEU:CG	4:D:221:TYR:H	2.14	0.60
4:D:56:ARG:NH2	4:D:155:ARG:HB3	2.16	0.60
5:E:40:GLU:H	5:E:40:GLU:CD	2.05	0.60
14:T:18:DA:OP1	14:T:18:DA:H3'	2.00	0.60
1:A:148:CYS:HB3	1:A:167:CYS:O	2.02	0.60
3:C:79:GLN:HE21	3:C:127:ARG:HD3	1.67	0.60
5:E:186:LEU:O	5:E:189:GLY:N	2.27	0.60
7:G:115:MET:HG2	7:G:163:ILE:HD11	1.84	0.60
9:I:82:GLU:C	9:I:104:LEU:HG	2.22	0.60
1:A:1293:SER:OG	1:A:1295:THR:HG23	2.02	0.60
2:B:233:PRO:HG2	2:B:234:ILE:HD13	1.83	0.60
2:B:430:ARG:HB3	2:B:434:ARG:NH2	2.16	0.60
2:B:210:LYS:HD3	2:B:482:VAL:HG22	1.84	0.60
2:B:810:GLU:HA	2:B:815:ARG:HH22	1.67	0.60
2:B:880:THR:CB	2:B:934:LYS:HG3	2.31	0.60
2:B:999:MET:HB3	2:B:1007:VAL:HG21	1.84	0.60
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.37	0.60
7:G:106:MET:HG2	7:G:107:LYS:N	2.16	0.60
7:G:55:ASP:OD1	7:G:57:GLN:HG3	2.02	0.60
1:A:332:LYS:HA	1:A:337:ARG:NH1	2.17	0.60
1:A:347:PHE:CE2	1:A:375:THR:HG23	2.37	0.60
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.37	0.60
1:A:728:LYS:HA	1:A:731:ARG:NH1	2.17	0.60
2:B:1023:VAL:HA	2:B:1026:LEU:HD12	1.84	0.60
2:B:758:PHE:HE1	2:B:1027:ILE:HG22	1.66	0.60
2:B:176:SER:O	2:B:182:SER:HB3	2.01	0.60
2:B:426:LYS:O	2:B:426:LYS:HG3	2.02	0.60
2:B:654:ARG:N	2:B:657:HIS:HD2	1.98	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.02	0.60
3:C:76:ASP:OD2	3:C:128:ASN:N	2.35	0.60
5:E:14:ARG:NH2	5:E:141:VAL:HG12	2.17	0.60
1:A:1109:LYS:HG3	1:A:1110:ASN:HD22	1.66	0.59
1:A:332:LYS:H	1:A:337:ARG:CB	2.15	0.59
1:A:897:TYR:HB3	1:A:936:LEU:CD1	2.32	0.59
2:B:20:ASP:C	2:B:22:SER:H	2.05	0.59
2:B:604:ARG:HB2	2:B:609:ILE:HG13	1.83	0.59
2:B:906:SER:HA	2:B:946:ASN:HB2	1.83	0.59
2:B:912:ILE:O	2:B:938:SER:HB3	2.02	0.59
2:B:984:HIS:HD2	2:B:1025:HIS:CD2	2.20	0.59
2:B:995:ARG:NH1	3:C:165:LYS:HA	2.16	0.59
3:C:88:CYS:SG	3:C:91:HIS:HA	2.42	0.59
7:G:87:VAL:HG23	7:G:103:VAL:HG21	1.82	0.59
1:A:1341:ILE:HG23	1:A:1342:GLU:H	1.66	0.59
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.84	0.59
1:A:90:VAL:HG11	1:A:297:GLN:HA	1.83	0.59
1:A:524:VAL:HG12	1:A:525:GLN:HG2	1.84	0.59
1:A:720:ARG:O	1:A:724:GLU:HB2	2.01	0.59
4:D:12:ARG:NH1	4:D:14:ARG:HA	2.18	0.59
5:E:13:TRP:O	5:E:16:PHE:HB3	2.02	0.59
7:G:129:SER:HB3	7:G:138:THR:HB	1.84	0.59
8:H:102:TYR:OH	8:H:122:LEU:HD22	2.02	0.59
8:H:135:LEU:HB2	8:H:137:GLN:HG2	1.83	0.59
9:I:26:LEU:HD22	9:I:35:VAL:CG1	2.31	0.59
12:L:38:LEU:CG	12:L:39:SER:N	2.65	0.59
15:P:5:C:H2'	15:P:6:A:O4'	2.01	0.59
1:A:868:TYR:HE1	1:A:1064:VAL:CG1	2.16	0.59
1:A:211:PHE:HA	1:A:214:ILE:HG13	1.84	0.59
1:A:289:ILE:CG2	1:A:290:GLU:N	2.65	0.59
1:A:55:ASP:C	1:A:57:ARG:N	2.50	0.59
1:A:770:VAL:HG12	1:A:771:GLU:HG3	1.84	0.59
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.36	0.59
2:B:506:GLY:O	2:B:507:LYS:HB2	2.02	0.59
2:B:637:LEU:CD2	2:B:742:GLU:HA	2.32	0.59
2:B:874:PHE:HA	2:B:913:GLY:O	2.01	0.59
4:D:118:THR:O	4:D:120:GLU:N	2.35	0.59
7:G:146:LYS:HB2	7:G:168:LEU:HD11	1.83	0.59
9:I:101:PHE:N	9:I:101:PHE:CD1	2.70	0.59
12:L:32:ALA:H	12:L:55:ILE:HD11	1.67	0.59
1:A:850:VAL:HG21	1:A:1058:VAL:HG11	1.84	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:ASP:O	1:A:854:ASN:HB2	2.01	0.59
2:B:401:PHE:HB2	2:B:517:THR:OG1	2.02	0.59
2:B:710:LEU:CA	2:B:733:HIS:HB3	2.31	0.59
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.83	0.59
5:E:120:ALA:HA	5:E:123:LEU:HD11	1.85	0.59
5:E:17:ARG:O	5:E:20:LYS:HB2	2.01	0.59
5:E:35:VAL:O	5:E:37:LEU:N	2.36	0.59
5:E:99:HIS:O	5:E:103:LYS:HB2	2.02	0.59
12:L:27:LEU:N	12:L:27:LEU:HD23	2.18	0.59
1:A:1208:THR:HG22	1:A:1210:GLY:N	2.17	0.59
1:A:23:SER:HA	1:A:233:TRP:NE1	2.18	0.59
1:A:326:ARG:HG2	1:A:326:ARG:HH11	1.67	0.59
1:A:590:ARG:NH1	1:A:592:ASP:OD2	2.35	0.59
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.36	0.59
2:B:778:MET:HE1	2:B:1094:ARG:CD	2.32	0.59
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.85	0.59
3:C:31:ASN:OD1	3:C:34:ARG:HD3	2.03	0.59
4:D:124:GLU:HA	4:D:127:ASP:HB2	1.85	0.59
4:D:153:ARG:HB3	4:D:154:PHE:CE2	2.37	0.59
1:A:228:PHE:CE2	4:D:15:LEU:HD23	2.37	0.59
4:D:39:ASN:HD22	4:D:41:GLN:HB2	1.67	0.59
5:E:120:ALA:C	5:E:123:LEU:HG	2.23	0.59
5:E:94:LYS:HE2	5:E:98:ILE:CD1	2.21	0.59
6:F:88:TYR:O	6:F:89:GLU:C	2.41	0.59
7:G:13:LEU:CD2	7:G:17:PHE:HB2	2.32	0.59
9:I:78:CYS:SG	9:I:106:CYS:HB3	2.42	0.59
2:B:1050:ILE:HG22	2:B:1051:THR:N	2.17	0.59
2:B:1065:GLN:NE2	2:B:1066:SER:N	2.50	0.59
2:B:225:VAL:HG21	2:B:384:ARG:HH21	1.67	0.59
2:B:622:LYS:HE2	9:I:59:VAL:CG2	2.33	0.59
2:B:882:THR:HG22	2:B:884:ARG:N	2.16	0.59
3:C:147:LEU:HD23	3:C:147:LEU:N	2.16	0.59
3:C:213:PRO:O	3:C:214:ASN:HB3	2.02	0.59
5:E:144:ILE:HG13	5:E:145:THR:N	2.18	0.59
6:F:82:THR:HG22	6:F:84:TYR:N	2.17	0.59
10:J:43:ARG:H	10:J:43:ARG:HD2	1.67	0.59
1:A:356:ASP:HB2	1:A:469:ARG:NH1	2.18	0.59
1:A:335:ARG:NH1	2:B:1206:GLU:OE1	2.35	0.59
2:B:1204:PHE:CE1	2:B:1216:LEU:HD11	2.37	0.59
2:B:785:TYR:CD2	2:B:795:ILE:HG12	2.37	0.59
2:B:798:TYR:HE2	3:C:62:PHE:CZ	2.20	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:249:ASP:O	3:C:252:GLN:N	2.31	0.59
6:F:84:TYR:CD1	6:F:84:TYR:N	2.69	0.59
7:G:37:SER:OG	7:G:45:ILE:HG13	2.03	0.59
1:A:108:MET:O	1:A:109:HIS:HB3	2.03	0.59
1:A:1200:ALA:HA	1:A:1203:ASN:ND2	2.17	0.59
1:A:1353:TYR:CE2	1:A:1357:ALA:HB2	2.38	0.59
1:A:665:GLY:HA2	2:B:1026:LEU:CD2	2.31	0.59
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.38	0.59
2:B:505:ASP:O	2:B:508:LEU:HD22	2.03	0.59
2:B:542:MET:CE	2:B:747:MET:HG3	2.33	0.59
3:C:82:TYR:O	3:C:83:SER:C	2.42	0.59
9:I:84:VAL:O	9:I:84:VAL:HG13	2.02	0.59
1:A:1148:ILE:CG1	1:A:1198:ASP:HB2	2.33	0.59
1:A:399:HIS:CB	1:A:400:PRO:CD	2.80	0.59
2:B:108:VAL:HG12	2:B:109:THR:N	2.18	0.59
2:B:294:ASP:HB2	9:I:12:ASN:HA	1.85	0.59
2:B:291:ILE:HG22	2:B:297:ILE:HG12	1.85	0.59
2:B:621:GLU:HG3	2:B:621:GLU:O	2.01	0.59
2:B:654:ARG:NH1	2:B:654:ARG:HG3	2.17	0.59
2:B:773:MET:CE	2:B:987:LYS:HD2	2.32	0.59
6:F:118:LEU:O	6:F:122:MET:HG3	2.03	0.59
1:A:518:LYS:HE2	1:A:624:SER:O	2.03	0.59
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.38	0.59
2:B:29:ASP:CG	2:B:658:ILE:HD13	2.22	0.59
2:B:582:VAL:CG2	2:B:626:ILE:HB	2.33	0.59
3:C:183:TRP:CZ2	3:C:212:PRO:HG3	2.38	0.59
2:B:798:TYR:HE2	3:C:62:PHE:CE2	2.21	0.59
5:E:78:LEU:HA	5:E:107:THR:HB	1.83	0.59
5:E:40:GLU:HA	5:E:43:LYS:CE	2.27	0.59
7:G:1:MET:HG2	7:G:85:GLU:OE2	2.03	0.59
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.84	0.59
11:K:108:GLU:O	11:K:112:GLN:HG2	2.03	0.59
11:K:12:LEU:HD21	11:K:17:SER:HA	1.85	0.59
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	2.91	0.58
1:A:2:VAL:HG22	1:A:3:GLY:H	1.68	0.58
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.17	0.58
2:B:245:GLU:O	2:B:246:LYS:HG3	2.03	0.58
2:B:992:ILE:HD11	11:K:66:PRO:CB	2.32	0.58
8:H:143:LEU:N	8:H:143:LEU:HD12	2.17	0.58
1:A:1111:MET:HG3	1:A:1114:PRO:HB3	1.85	0.58
1:A:598:LEU:HD23	8:H:25:ARG:NH1	2.18	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:SER:N	1:A:757:ASN:ND2	2.45	0.58
1:A:883:LEU:O	1:A:886:ILE:HG22	2.03	0.58
2:B:1112:GLN:HG3	15:P:1:C:O5'	2.03	0.58
1:A:443:LEU:HD12	2:B:1146:PHE:CE2	2.39	0.58
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.38	0.58
2:B:58:THR:O	2:B:62:ILE:HG13	2.04	0.58
2:B:952:VAL:HG12	2:B:953:LEU:N	2.18	0.58
3:C:208:GLU:C	3:C:210:GLU:H	2.06	0.58
3:C:88:CYS:SG	3:C:91:HIS:C	2.82	0.58
5:E:136:ASN:OD1	5:E:138:ALA:N	2.36	0.58
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.38	0.58
10:J:24:LEU:HD13	10:J:38:ARG:HG2	1.84	0.58
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.84	0.58
12:L:42:ARG:HG3	12:L:42:ARG:NH1	2.18	0.58
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.02	0.58
1:A:90:VAL:HG12	1:A:297:GLN:HE21	1.67	0.58
1:A:43:GLU:CG	1:A:46:THR:HB	2.27	0.58
1:A:711:ARG:HA	9:I:97:MET:HE1	1.85	0.58
1:A:925:LEU:HD13	1:A:983:ILE:CG2	2.31	0.58
2:B:294:ASP:H	9:I:12:ASN:HD22	1.48	0.58
2:B:365:THR:HG21	2:B:370:PHE:CD1	2.38	0.58
2:B:37:PHE:CD1	2:B:41:LYS:HG3	2.38	0.58
2:B:603:LEU:HD12	2:B:609:ILE:HG12	1.85	0.58
3:C:99:LEU:CD2	3:C:99:LEU:N	2.66	0.58
5:E:213:ILE:HG12	5:E:214:CYS:H	1.67	0.58
8:H:4:THR:O	8:H:5:LEU:HD23	2.04	0.58
1:A:1161:THR:CG2	1:A:1163:ILE:HD12	2.31	0.58
1:A:108:MET:CA	1:A:210:ILE:HD13	2.30	0.58
1:A:321:PRO:O	1:A:322:VAL:CB	2.51	0.58
1:A:322:VAL:CG1	1:A:322:VAL:O	2.50	0.58
1:A:675:THR:O	1:A:679:ILE:HG13	2.02	0.58
2:B:507:LYS:C	2:B:508:LEU:HD23	2.24	0.58
2:B:601:ARG:O	2:B:605:ARG:HG3	2.04	0.58
2:B:955:THR:HG23	2:B:956:THR:N	2.17	0.58
3:C:161:LYS:O	3:C:170:TRP:NE1	2.37	0.58
3:C:33:LEU:O	3:C:33:LEU:HD12	2.04	0.58
4:D:4:SER:O	4:D:5:THR:CB	2.52	0.58
5:E:56:LYS:CE	5:E:84:ASP:H	2.16	0.58
6:F:69:LEU:HB3	6:F:71:GLU:CD	2.24	0.58
8:H:136:LYS:HD2	8:H:136:LYS:N	2.17	0.58
11:K:40:HIS:ND1	11:K:61:TYR:OH	2.22	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1279:ILE:CD1	1:A:1316:VAL:HG21	2.32	0.58
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.86	0.58
1:A:1352:VAL:O	1:A:1355:VAL:HG12	2.04	0.58
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.39	0.58
1:A:831:THR:CG2	1:A:832:ALA:H	2.12	0.58
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.86	0.58
2:B:90:ILE:CD1	2:B:432:MET:SD	2.91	0.58
2:B:705:MET:H	2:B:710:LEU:CD1	2.15	0.58
9:I:34:TYR:CE2	9:I:36:GLU:HB3	2.39	0.58
1:A:1066:VAL:O	1:A:1070:GLN:HG3	2.03	0.58
1:A:1209:MET:CE	1:A:1236:LEU:HB3	2.32	0.58
1:A:517:ASN:HD22	1:A:1364:ASN:HD22	1.50	0.58
1:A:61:ILE:HG22	1:A:62:ASP:N	2.19	0.58
2:B:315:LYS:N	2:B:316:PRO:HD2	2.17	0.58
4:D:69:ALA:C	4:D:71:LYS:H	2.05	0.58
7:G:53:ASN:HD22	7:G:53:ASN:N	2.02	0.58
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.34	0.58
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.33	0.58
2:B:309:GLN:OE1	9:I:52:ILE:HD11	2.04	0.58
1:A:167:CYS:HB2	1:A:169:ASN:ND2	2.18	0.58
1:A:369:SER:HB3	11:K:2:ASN:OD1	2.03	0.58
1:A:91:PHE:N	1:A:297:GLN:HE22	2.01	0.58
2:B:1187:ASN:O	2:B:1188:LYS:CB	2.49	0.58
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.33	0.58
4:D:13:ARG:C	4:D:15:LEU:N	2.57	0.58
4:D:59:ILE:HG21	4:D:145:MET:SD	2.43	0.58
7:G:106:MET:CG	7:G:107:LYS:N	2.66	0.58
4:D:183:LEU:HD22	7:G:144:ARG:NH2	2.18	0.58
8:H:36:CYS:HA	8:H:126:GLU:HB3	1.86	0.58
8:H:11:GLN:C	8:H:28:ALA:HB1	2.24	0.58
10:J:43:ARG:CD	10:J:43:ARG:N	2.67	0.58
11:K:85:ASP:O	11:K:88:LYS:HB2	2.03	0.58
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.69	0.58
1:A:1353:TYR:CD2	1:A:1353:TYR:C	2.77	0.58
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.86	0.58
1:A:260:ASP:OD1	1:A:261:ASP:N	2.36	0.58
1:A:299:HIS:HA	1:A:302:THR:HG22	1.84	0.58
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.38	0.58
2:B:402:GLY:HA2	2:B:695:ALA:HB3	1.85	0.58
2:B:769:TYR:HB3	2:B:773:MET:CE	2.33	0.58
2:B:898:LEU:HD13	2:B:952:VAL:HG11	1.85	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:258:ILE:N	3:C:258:ILE:HD12	2.19	0.58
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.32	0.58
10:J:44:TYR:N	10:J:44:TYR:CD2	2.71	0.58
15:P:1:C:O2'	15:P:2:A:H5'	2.04	0.58
1:A:1130:GLN:O	1:A:1134:ILE:HG13	2.03	0.58
1:A:7:SER:HB3	2:B:1193:GLN:NE2	2.18	0.58
2:B:242:SER:O	2:B:251:ILE:HA	2.04	0.58
2:B:880:THR:O	2:B:881:ASN:HB2	2.04	0.58
2:B:882:THR:CG2	2:B:884:ARG:H	2.17	0.58
2:B:916:THR:CG2	2:B:935:ARG:HD2	2.33	0.58
3:C:6:PRO:HB2	3:C:25:VAL:HG22	1.86	0.58
5:E:156:LEU:HA	5:E:160:GLU:OE1	2.03	0.58
3:C:114:TYR:OH	10:J:19:GLU:OE1	2.18	0.58
1:A:50:ILE:C	1:A:52:GLY:H	2.06	0.58
1:A:767:GLN:HA	1:A:799:PHE:HA	1.86	0.58
1:A:794:PRO:C	1:A:796:SER:H	2.06	0.58
2:B:1119:VAL:O	2:B:1126:GLY:HA3	2.04	0.58
2:B:211:VAL:CG2	2:B:483:LEU:HB2	2.34	0.58
3:C:239:PRO:HB2	3:C:241:ASP:OD1	2.04	0.58
5:E:56:LYS:HE2	5:E:84:ASP:CB	2.22	0.58
6:F:119:ARG:CG	6:F:119:ARG:NH1	2.67	0.58
9:I:50:THR:HG23	9:I:51:ASN:N	2.19	0.58
2:B:1113:VAL:HG23	15:P:1:C:O4'	2.04	0.58
1:A:1100:ARG:O	1:A:1103:GLU:HB3	2.03	0.57
1:A:1241:ARG:O	1:A:1242:VAL:CB	2.52	0.57
1:A:1152:ILE:HG12	1:A:1260:LEU:HD23	1.87	0.57
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.39	0.57
1:A:523:ILE:CG1	1:A:622:VAL:HG22	2.34	0.57
1:A:962:ARG:O	1:A:964:ILE:N	2.37	0.57
2:B:364:ILE:HG13	2:B:585:VAL:HG13	1.85	0.57
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.04	0.57
2:B:637:LEU:HD21	2:B:742:GLU:HA	1.86	0.57
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.33	0.57
2:B:881:ASN:HB2	2:B:933:SER:N	2.19	0.57
3:C:242:GLN:OE1	3:C:245:VAL:HG21	2.04	0.57
4:D:147:TYR:OH	7:G:103:VAL:HG13	2.03	0.57
4:D:47:LEU:HD11	7:G:3:PHE:HD2	1.68	0.57
1:A:1200:ALA:HA	1:A:1203:ASN:HD22	1.69	0.57
1:A:1264:GLU:HG3	1:A:1265:ASN:N	2.19	0.57
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.19	0.57
2:B:172:ILE:CD1	2:B:178:ASN:HD22	2.13	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:69:LEU:HB2	6:F:72:LYS:HD2	1.86	0.57
9:I:16:PRO:HD3	9:I:27:PHE:CD2	2.39	0.57
9:I:8:ARG:CG	9:I:34:TYR:HE1	2.14	0.57
1:A:873:MET:C	1:A:1058:VAL:HG23	2.24	0.57
1:A:1313:LEU:O	1:A:1315:GLU:N	2.38	0.57
1:A:598:LEU:O	1:A:598:LEU:HD23	2.04	0.57
2:B:405:ARG:NE	2:B:629:ASP:OD2	2.29	0.57
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.30	0.57
2:B:975:GLN:HG2	2:B:976:ILE:H	1.68	0.57
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.39	0.57
8:H:84:ALA:CB	8:H:87:ARG:HD2	2.35	0.57
1:A:1236:LEU:O	1:A:1237:ILE:HG13	2.05	0.57
1:A:1253:GLU:O	1:A:1254:ALA:HB3	2.04	0.57
1:A:93:VAL:HG21	1:A:301:ALA:O	2.03	0.57
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.40	0.57
1:A:683:ILE:HG21	1:A:801:GLU:CG	2.34	0.57
2:B:241:ARG:HH11	2:B:241:ARG:HG3	1.70	0.57
2:B:597:MET:HA	2:B:597:MET:HE3	1.86	0.57
4:D:220:LEU:CG	4:D:221:TYR:N	2.68	0.57
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.85	0.57
7:G:64:THR:CG2	7:G:65:ASP:N	2.67	0.57
2:B:505:ASP:CG	13:N:1:DA:H8	2.08	0.57
14:T:15:DG:N9	14:T:16:DT:H72	2.19	0.57
1:A:512:VAL:HA	1:A:519:PRO:HA	1.85	0.57
1:A:774:ARG:HG3	1:A:797:LYS:HE3	1.87	0.57
2:B:108:VAL:HG12	2:B:109:THR:H	1.67	0.57
4:D:215:SER:HA	4:D:218:GLU:OE2	2.04	0.57
5:E:176:PRO:O	5:E:212:ARG:HA	2.05	0.57
7:G:27:LYS:O	7:G:31:LEU:HG	2.05	0.57
1:A:1124:HIS:HB2	1:A:1130:GLN:HG2	1.86	0.57
1:A:1315:GLU:O	1:A:1317:MET:N	2.37	0.57
1:A:341:MET:HE2	1:A:843:LYS:HZ1	1.69	0.57
1:A:915:SER:O	1:A:919:ILE:HB	2.04	0.57
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.87	0.57
2:B:1192:TYR:CD2	2:B:1218:THR:HG21	2.39	0.57
2:B:209:GLU:OE2	2:B:485:ARG:NE	2.37	0.57
2:B:69:LEU:CD1	2:B:432:MET:HE1	2.35	0.57
2:B:805:THR:HG23	2:B:809:MET:HE3	1.86	0.57
3:C:11:ARG:NH2	3:C:206:ASN:OD1	2.38	0.57
3:C:124:LEU:O	3:C:125:MET:C	2.42	0.57
4:D:29:LEU:HD12	7:G:82:PHE:CZ	2.39	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.33	0.57
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.69	0.57
1:A:265:LYS:HG2	1:A:303:TYR:HB2	1.85	0.57
1:A:925:LEU:O	1:A:927:VAL:N	2.38	0.57
2:B:345:LYS:HA	2:B:348:ARG:NE	2.16	0.57
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.70	0.57
7:G:21:ARG:HD2	7:G:24:GLN:HB3	1.85	0.57
1:A:452:LYS:HB3	2:B:1141:HIS:CE1	2.39	0.57
1:A:351:THR:HG21	2:B:1103:ILE:HG13	1.85	0.57
2:B:203:PHE:HB3	2:B:205:ILE:HD11	1.87	0.57
2:B:254:LEU:HD22	2:B:361:LEU:CD1	2.34	0.57
2:B:916:THR:O	2:B:935:ARG:HG2	2.04	0.57
5:E:157:SER:O	5:E:159:ASP:N	2.38	0.57
9:I:65:ASP:HB3	9:I:68:LEU:CD1	2.33	0.57
1:A:901:LEU:H	1:A:926:GLN:HE21	0.73	0.57
2:B:39:ARG:NE	2:B:665:GLU:HG2	2.19	0.57
2:B:461:LEU:N	2:B:461:LEU:HD12	2.20	0.57
2:B:510:LYS:HB3	2:B:511:PRO:HD3	1.86	0.57
2:B:695:ALA:O	2:B:698:GLU:HB3	2.05	0.57
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.87	0.57
2:B:953:LEU:CD2	2:B:965:LYS:HB2	2.30	0.57
9:I:50:THR:CG2	9:I:51:ASN:N	2.66	0.57
9:I:55:THR:O	9:I:55:THR:HG22	2.05	0.57
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.40	0.57
1:A:1076:ALA:HA	1:A:1079:MET:HE3	1.85	0.57
1:A:256:GLN:O	1:A:257:ARG:HB2	2.04	0.57
1:A:341:MET:HE2	1:A:843:LYS:NZ	2.20	0.57
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.38	0.57
2:B:222:ILE:N	2:B:240:ILE:HD12	2.19	0.57
2:B:755:ILE:HG22	2:B:755:ILE:O	2.05	0.57
3:C:71:PRO:O	3:C:72:LEU:HD23	2.05	0.57
3:C:92:CYS:SG	3:C:94:LYS:HB3	2.45	0.57
4:D:16:LYS:O	4:D:18:VAL:N	2.37	0.57
4:D:35:LEU:HD11	4:D:173:HIS:CD2	2.39	0.57
11:K:82:ASP:OD1	11:K:84:LYS:HB2	2.04	0.57
12:L:40:LEU:HD11	12:L:49:LYS:NZ	2.20	0.57
1:A:1127:ASP:CG	1:A:1130:GLN:HB2	2.25	0.56
1:A:113:LEU:HD12	1:A:218:ASP:OD1	2.05	0.56
1:A:1159:ARG:HD2	1:A:1159:ARG:N	2.20	0.56
1:A:1258:HIS:O	1:A:1262:LYS:HE3	2.04	0.56
1:A:1285:MET:O	1:A:1304:TRP:HA	2.05	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1287:TYR:CD1	1:A:1305:VAL:HG21	2.40	0.56
1:A:993:LEU:HD11	1:A:997:LEU:HD21	1.86	0.56
2:B:225:VAL:HA	2:B:237:VAL:O	2.05	0.56
3:C:106:GLU:OE2	3:C:106:GLU:HA	2.03	0.56
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.87	0.56
7:G:37:SER:OG	7:G:45:ILE:HB	2.05	0.56
1:A:838:GLN:HG2	1:A:1073:GLY:HA3	1.86	0.56
1:A:1312:ASN:HD21	1:A:1315:GLU:HG3	1.69	0.56
1:A:527:THR:CG2	1:A:650:GLN:HA	2.35	0.56
2:B:416:LEU:HD23	2:B:420:LEU:HG	1.86	0.56
2:B:169:ARG:HD2	2:B:454:THR:HG21	1.87	0.56
2:B:570:VAL:HG21	2:B:573:GLN:CD	2.25	0.56
2:B:59:LEU:HD12	2:B:417:PHE:HE2	1.66	0.56
3:C:148:ARG:CG	3:C:149:LYS:H	2.18	0.56
7:G:1:MET:SD	7:G:1:MET:C	2.82	0.56
6:F:103:MET:HE3	7:G:66:GLY:H	1.71	0.56
1:A:1048:ASN:O	1:A:1049:ILE:C	2.43	0.56
1:A:1241:ARG:O	1:A:1242:VAL:HB	2.06	0.56
1:A:595:THR:O	1:A:596:THR:HG23	2.05	0.56
1:A:665:GLY:C	1:A:666:ILE:HD12	2.25	0.56
2:B:1172:ILE:O	2:B:1172:ILE:HG22	2.04	0.56
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.87	0.56
2:B:25:ILE:HD11	2:B:653:VAL:HG12	1.85	0.56
3:C:124:LEU:HD12	3:C:124:LEU:N	2.20	0.56
5:E:9:ILE:HD11	5:E:53:PRO:HD3	1.86	0.56
7:G:79:PHE:CE2	7:G:106:MET:HE2	2.41	0.56
11:K:12:LEU:HD21	11:K:18:LYS:H	1.67	0.56
1:A:295:LEU:O	1:A:298:PHE:HB3	2.05	0.56
2:B:327:ARG:O	2:B:331:LEU:HD13	2.05	0.56
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.87	0.56
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.87	0.56
1:A:701:LEU:HA	9:I:115:LYS:HE3	1.87	0.56
11:K:82:ASP:OD1	11:K:84:LYS:N	2.38	0.56
12:L:52:GLY:O	12:L:53:HIS:C	2.43	0.56
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.21	0.56
1:A:224:PHE:HE2	1:A:234:MET:HE2	1.70	0.56
1:A:55:ASP:N	1:A:56:PRO:CD	2.65	0.56
1:A:547:LEU:HD21	1:A:560:ILE:HD13	1.87	0.56
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.88	0.56
1:A:670:ILE:HD12	2:B:1067:ARG:NH2	2.20	0.56
2:B:1122:ARG:HB3	14:T:22:DC:OP1	2.06	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:756:ILE:O	2:B:759:PRO:HD3	2.05	0.56
9:I:29:CYS:SG	9:I:32:CYS:N	2.72	0.56
11:K:45:LEU:HG	11:K:94:ILE:HD11	1.88	0.56
3:C:29:MET:HE1	11:K:98:LEU:HG	1.88	0.56
1:A:49:LYS:HZ1	1:A:61:ILE:H	1.54	0.56
2:B:345:LYS:CA	2:B:348:ARG:HE	2.16	0.56
3:C:115:SER:HB3	3:C:141:GLY:O	2.05	0.56
4:D:130:LEU:HD13	4:D:142:LYS:CG	2.36	0.56
4:D:154:PHE:HD1	4:D:163:VAL:HG21	1.64	0.56
3:C:66:ARG:NH2	10:J:3:VAL:O	2.38	0.56
1:A:1353:TYR:HD2	1:A:1353:TYR:C	2.09	0.56
1:A:225:ASN:HD22	1:A:228:PHE:N	1.86	0.56
1:A:464:PRO:HG2	1:A:465:TYR:HD1	1.69	0.56
1:A:483:ASP:HB2	2:B:987:LYS:HG2	1.88	0.56
1:A:470:LEU:HD13	1:A:487:MET:HE1	1.86	0.56
1:A:535:THR:O	1:A:575:LYS:HE2	2.06	0.56
2:B:882:THR:HG21	2:B:934:LYS:O	2.05	0.56
1:A:483:ASP:O	2:B:979:LYS:HE3	2.05	0.56
3:C:34:ARG:NH1	3:C:35:ARG:HG2	2.20	0.56
5:E:157:SER:C	5:E:159:ASP:N	2.58	0.56
8:H:59:ILE:CG2	8:H:60:ALA:N	2.61	0.56
1:A:1063:MET:SD	1:A:1436:ILE:CG1	2.89	0.56
1:A:1100:ARG:NH2	1:A:1351:GLU:CG	2.69	0.56
1:A:1210:GLY:O	1:A:1214:GLU:HG2	2.05	0.56
1:A:153:PRO:HB2	1:A:158:PRO:HA	1.88	0.56
1:A:34:LYS:N	1:A:34:LYS:HD3	2.21	0.56
1:A:482:PHE:C	1:A:484:GLY:H	2.09	0.56
1:A:626:ASN:O	1:A:631:HIS:CD2	2.59	0.56
2:B:101:MET:HE2	2:B:126:SER:HA	1.87	0.56
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.24	0.56
4:D:50:LEU:HD21	7:G:4:ILE:CD1	2.34	0.56
5:E:161:LYS:HD2	5:E:195:VAL:CG2	2.35	0.56
7:G:51:TYR:O	7:G:54:ILE:HG13	2.05	0.56
9:I:68:LEU:HD12	9:I:68:LEU:H	1.70	0.56
1:A:1107:VAL:CG1	1:A:1107:VAL:O	2.54	0.56
1:A:1385:THR:HB	1:A:1388:GLY:H	1.70	0.56
1:A:182:VAL:HG22	1:A:201:VAL:HA	1.88	0.56
1:A:286:HIS:O	1:A:289:ILE:HG22	2.06	0.56
1:A:710:LEU:HD12	1:A:710:LEU:N	2.17	0.56
2:B:1159:ARG:HB3	2:B:1159:ARG:NH1	2.21	0.56
2:B:1217:TYR:CD2	4:D:13:ARG:CZ	2.89	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:448:ILE:O	2:B:450:ALA:N	2.39	0.56
4:D:138:ASN:HB3	4:D:141:LEU:HB3	1.87	0.56
4:D:24:ALA:HB3	4:D:26:THR:CG2	2.35	0.56
7:G:80:LYS:O	7:G:82:PHE:CE1	2.59	0.56
9:I:50:THR:HG23	9:I:52:ILE:N	2.21	0.56
3:C:175:ALA:HB1	10:J:43:ARG:HH22	1.70	0.56
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.88	0.56
1:A:1214:GLU:O	1:A:1218:GLN:HG2	2.06	0.56
1:A:1445:ILE:H	1:A:1445:ILE:CD1	2.00	0.56
1:A:203:SER:O	1:A:207:ILE:HG12	2.05	0.56
1:A:683:ILE:HD13	1:A:801:GLU:CG	2.35	0.56
1:A:767:GLN:NE2	1:A:774:ARG:CB	2.69	0.56
1:A:886:ILE:CG2	1:A:887:GLY:N	2.69	0.56
1:A:949:ASP:OD1	1:A:951:GLU:HB2	2.06	0.56
2:B:205:ILE:N	2:B:205:ILE:CD1	2.68	0.56
2:B:428:ILE:HG22	2:B:432:MET:HE1	1.87	0.56
2:B:508:LEU:O	2:B:509:ALA:CB	2.54	0.56
2:B:603:LEU:CD1	2:B:609:ILE:HG12	2.36	0.56
2:B:797:TYR:HE1	2:B:854:LEU:HD23	1.71	0.56
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.87	0.56
5:E:103:LYS:HD3	5:E:105:PHE:HZ	1.70	0.56
5:E:108:GLY:O	5:E:132:ILE:HG22	2.06	0.56
5:E:182:ASP:OD1	5:E:183:PRO:HD2	2.06	0.56
6:F:86:THR:HG23	6:F:89:GLU:OE1	2.06	0.56
8:H:101:ALA:HB2	8:H:116:TYR:CZ	2.41	0.56
8:H:12:VAL:CG1	8:H:51:ALA:HA	2.36	0.56
12:L:55:ILE:CD1	12:L:56:LEU:N	2.68	0.56
12:L:61:THR:HG21	12:L:63:ARG:HG3	1.86	0.56
1:A:1076:ALA:HA	1:A:1079:MET:HE2	1.86	0.56
1:A:1278:ASN:O	1:A:1310:GLY:HA3	2.06	0.56
1:A:1451:VAL:O	1:A:1454:MET:HG2	2.06	0.56
1:A:483:ASP:OD1	2:B:987:LYS:HG3	2.05	0.56
1:A:754:SER:O	1:A:757:ASN:HB2	2.06	0.56
2:B:825:VAL:HG22	2:B:1010:LEU:HB2	1.88	0.56
2:B:557:PHE:CZ	2:B:603:LEU:HD11	2.41	0.56
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.88	0.56
2:B:849:GLY:O	2:B:850:LEU:C	2.44	0.56
3:C:196:ASP:CG	3:C:199:LYS:HD3	2.26	0.56
3:C:226:ASP:O	3:C:227:THR:HB	2.06	0.56
4:D:155:ARG:CD	4:D:221:TYR:HE1	2.19	0.56
5:E:78:LEU:HD23	5:E:79:TRP:N	2.21	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:54:GLU:OE1	9:I:118:ARG:NH2	2.39	0.56
12:L:33:GLU:H	12:L:33:GLU:CD	2.09	0.56
1:A:1112:LYS:O	1:A:1114:PRO:HD3	2.06	0.55
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	2.06	0.55
1:A:317:LYS:O	1:A:318:SER:CB	2.54	0.55
1:A:38:PRO:CA	1:A:270:LEU:HD23	2.36	0.55
1:A:463:ILE:CD1	1:A:469:ARG:HG3	2.37	0.55
1:A:688:LYS:C	1:A:690:VAL:N	2.57	0.55
1:A:979:SER:OG	1:A:980:ASP:N	2.38	0.55
2:B:508:LEU:O	2:B:509:ALA:HB2	2.06	0.55
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.06	0.55
3:C:254:LYS:O	3:C:258:ILE:HD13	2.07	0.55
7:G:139:ILE:CG2	7:G:140:LYS:H	2.18	0.55
8:H:104:PHE:CE2	8:H:136:LYS:HG3	2.41	0.55
11:K:68:PHE:N	11:K:68:PHE:CD2	2.72	0.55
1:A:1312:ASN:ND2	1:A:1315:GLU:HG3	2.21	0.55
2:B:170:LEU:O	2:B:172:ILE:HG13	2.05	0.55
2:B:794:ASN:O	2:B:795:ILE:HD12	2.06	0.55
3:C:146:LYS:C	3:C:147:LEU:HD23	2.26	0.55
5:E:56:LYS:NZ	5:E:84:ASP:H	2.04	0.55
7:G:18:PHE:HA	7:G:22:MET:HE3	1.88	0.55
12:L:32:ALA:HB3	12:L:55:ILE:HG13	1.85	0.55
1:A:1163:ILE:HG22	1:A:1165:GLU:HG2	1.88	0.55
1:A:1438:THR:CG2	6:F:92:ARG:HB2	2.37	0.55
1:A:72:GLU:HB3	1:A:76:GLU:HG2	1.88	0.55
2:B:120:ARG:NH1	12:L:54:ARG:HH11	2.05	0.55
2:B:917:PRO:O	2:B:918:ILE:HG13	2.05	0.55
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.87	0.55
2:B:622:LYS:HZ1	9:I:59:VAL:HG22	1.71	0.55
1:A:280:GLU:CG	1:A:289:ILE:HD11	2.36	0.55
1:A:388:LEU:HD22	1:A:432:VAL:HB	1.88	0.55
2:B:1072:MET:O	2:B:1081:LEU:HB2	2.07	0.55
2:B:649:LYS:HD3	2:B:736:THR:O	2.07	0.55
3:C:242:GLN:C	3:C:244:VAL:H	2.10	0.55
4:D:7:THR:HG23	4:D:7:THR:O	2.07	0.55
1:A:1261:LYS:HE2	9:I:44:TYR:HD2	1.71	0.55
1:A:256:GLN:O	1:A:257:ARG:CB	2.53	0.55
1:A:26:GLU:O	1:A:29:ALA:HB3	2.07	0.55
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.87	0.55
1:A:54:ASN:HA	1:A:58:LEU:HD12	1.88	0.55
1:A:691:LEU:HD11	1:A:695:LYS:HE3	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:HIS:H	1:A:243:PRO:CB	2.19	0.55
1:A:959:ASN:HD22	1:A:962:ARG:HH21	1.54	0.55
1:A:982:THR:C	1:A:984:LYS:N	2.58	0.55
2:B:542:MET:HG2	2:B:747:MET:CE	2.32	0.55
2:B:605:ARG:CZ	2:B:639:ILE:HD13	2.37	0.55
3:C:112:ASN:N	3:C:112:ASN:HD22	2.04	0.55
4:D:39:ASN:ND2	4:D:41:GLN:HB2	2.22	0.55
12:L:60:ARG:HG2	12:L:61:THR:N	2.14	0.55
1:A:1116:LEU:HB2	1:A:1329:THR:OG1	2.06	0.55
1:A:1158:PRO:C	1:A:1159:ARG:HD2	2.27	0.55
1:A:310:GLY:C	1:A:312:PRO:HD2	2.27	0.55
1:A:317:LYS:O	1:A:318:SER:HB3	2.07	0.55
1:A:335:ARG:NH1	2:B:1206:GLU:CD	2.59	0.55
1:A:549:MET:SD	1:A:577:ILE:CD1	2.94	0.55
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.40	0.55
2:B:487:THR:CG2	2:B:488:TYR:N	2.69	0.55
2:B:554:ILE:H	2:B:554:ILE:HD12	1.72	0.55
2:B:899:ILE:HG22	2:B:900:ALA:N	2.21	0.55
5:E:117:THR:HB	5:E:120:ALA:HB3	1.87	0.55
9:I:76:PRO:HD3	9:I:110:PHE:CD2	2.41	0.55
1:A:756:ILE:O	1:A:760:GLN:HG3	2.06	0.55
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.88	0.55
2:B:101:MET:HB2	2:B:109:THR:CG2	2.36	0.55
2:B:134:LYS:H	2:B:134:LYS:HD3	1.69	0.55
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.87	0.55
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.72	0.55
2:B:604:ARG:HG3	2:B:611:PRO:HA	1.88	0.55
3:C:174:ALA:O	3:C:175:ALA:HB3	2.07	0.55
5:E:121:MET:C	5:E:123:LEU:H	2.09	0.55
5:E:113:GLN:HG2	5:E:137:GLU:OE1	2.07	0.55
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.41	0.55
5:E:22:MET:HG3	5:E:187:TYR:CD1	2.42	0.55
8:H:4:THR:HG23	8:H:58:THR:HG22	1.89	0.55
1:A:573:SER:O	1:A:576:GLN:HB2	2.07	0.55
1:A:765:VAL:HB	1:A:800:VAL:CG1	2.36	0.55
1:A:920:LEU:HD23	1:A:921:GLY:N	2.22	0.55
1:A:954:TRP:HB3	1:A:955:PRO:HD2	1.89	0.55
2:B:249:ARG:O	2:B:251:ILE:HG13	2.06	0.55
2:B:345:LYS:O	2:B:346:GLU:HB2	2.05	0.55
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.13	0.55
2:B:696:GLU:O	2:B:699:GLU:HB2	2.07	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.40	0.55
3:C:148:ARG:HD3	3:C:149:LYS:HG3	1.89	0.55
3:C:58:LEU:N	3:C:58:LEU:HD23	2.21	0.55
4:D:14:ARG:HH12	4:D:16:LYS:NZ	2.05	0.55
5:E:155:ARG:O	5:E:156:LEU:HD23	2.06	0.55
14:T:15:DG:H2'	14:T:16:DT:H72	1.88	0.55
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.89	0.55
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.22	0.55
1:A:1235:LYS:O	1:A:1237:ILE:HD12	2.07	0.55
1:A:178:GLY:C	1:A:179:LEU:HD23	2.27	0.55
1:A:767:GLN:HE21	1:A:774:ARG:HB3	1.71	0.55
1:A:341:MET:CE	1:A:843:LYS:NZ	2.69	0.55
1:A:963:ILE:HD13	1:A:1049:ILE:HG12	1.89	0.55
2:B:446:LEU:O	2:B:448:ILE:HG13	2.07	0.55
4:D:173:HIS:O	4:D:177:VAL:HG23	2.05	0.55
5:E:48:ASP:CG	5:E:49:SER:H	2.09	0.55
8:H:12:VAL:HG11	8:H:15:VAL:HG22	1.89	0.55
10:J:47:ARG:HG2	10:J:47:ARG:NH1	2.21	0.55
1:A:832:ALA:O	14:T:18:DA:H5'	2.07	0.55
1:A:1241:ARG:O	1:A:1242:VAL:HG23	2.07	0.55
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.07	0.55
1:A:135:PHE:CD1	1:A:222:LEU:HD22	2.42	0.55
1:A:331:GLY:O	1:A:332:LYS:O	2.25	0.55
1:A:722:LEU:HD23	1:A:799:PHE:CD1	2.41	0.55
1:A:886:ILE:CG2	1:A:952:ALA:HB2	2.36	0.55
2:B:100:PRO:HB2	2:B:180:TYR:HE1	1.72	0.55
2:B:189:LEU:HD13	2:B:196:PRO:HA	1.89	0.55
2:B:508:LEU:HG	2:B:509:ALA:H	1.72	0.55
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.72	0.55
3:C:215:GLU:O	3:C:217:ASP:N	2.40	0.55
3:C:6:PRO:CB	3:C:25:VAL:HG22	2.37	0.55
4:D:14:ARG:NH1	4:D:16:LYS:HD2	2.22	0.55
4:D:155:ARG:CD	4:D:221:TYR:CE1	2.90	0.55
4:D:8:PHE:HD2	7:G:6:ASP:HB2	1.70	0.55
5:E:112:TYR:CZ	5:E:136:ASN:HB2	2.42	0.55
9:I:55:THR:HG23	9:I:86:PHE:CZ	2.38	0.55
11:K:49:GLU:HB3	11:K:90:ALA:HB1	1.88	0.55
1:A:1308:THR:HG23	1:A:1309:ASP:H	1.71	0.54
1:A:446:ARG:HB2	1:A:487:MET:SD	2.46	0.54
1:A:527:THR:O	1:A:653:VAL:HG11	2.07	0.54
1:A:820:GLY:O	1:A:822:GLU: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:637:LEU:HD12	2:B:693:ILE:HD11	1.87	0.54
3:C:235:VAL:CG1	10:J:13:VAL:HG13	2.37	0.54
4:D:136:GLY:HA2	4:D:142:LYS:NZ	2.22	0.54
1:A:583:PRO:HG2	1:A:586:ILE:HG13	1.89	0.54
1:A:595:THR:O	1:A:596:THR:CG2	2.54	0.54
1:A:886:ILE:CG2	1:A:887:GLY:H	2.19	0.54
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.71	0.54
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.08	0.54
2:B:244:LEU:HD11	2:B:250:PHE:HB2	1.89	0.54
2:B:309:GLN:CA	2:B:309:GLN:HE21	2.11	0.54
2:B:364:ILE:CG1	2:B:585:VAL:HG13	2.37	0.54
2:B:48:LEU:O	2:B:51:PHE:N	2.31	0.54
2:B:805:THR:HG22	2:B:806:THR:N	2.19	0.54
3:C:34:ARG:O	3:C:38:ILE:HG13	2.07	0.54
10:J:42:LYS:HG2	10:J:43:ARG:N	2.22	0.54
12:L:32:ALA:H	12:L:55:ILE:CG1	2.21	0.54
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.17	0.54
1:A:133:LYS:O	1:A:136:ALA:HB3	2.08	0.54
1:A:153:PRO:CD	1:A:161:LEU:HD13	2.37	0.54
1:A:491:VAL:HG12	1:A:492:PRO:O	2.06	0.54
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.72	0.54
1:A:600:PRO:HG2	1:A:601:LYS:N	2.18	0.54
1:A:999:VAL:HG12	1:A:1000:LEU:N	2.23	0.54
2:B:1037:LEU:HD21	2:B:1064:TYR:HE1	1.72	0.54
1:A:12:ARG:HB3	2:B:1218:THR:CG2	2.38	0.54
2:B:412:LEU:HB3	2:B:466:TRP:NE1	2.21	0.54
3:C:193:TYR:C	3:C:193:TYR:CD1	2.80	0.54
3:C:233:GLU:CG	3:C:234:SER:H	2.20	0.54
3:C:249:ASP:O	3:C:252:GLN:HB3	2.07	0.54
3:C:7:GLN:HE21	3:C:7:GLN:CA	2.20	0.54
4:D:51:ASN:C	4:D:52:LEU:O	2.45	0.54
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.88	0.54
1:A:1402:PHE:CD1	1:A:1403:GLU:HG2	2.42	0.54
1:A:853:ASP:OD1	1:A:855:THR:N	2.39	0.54
1:A:897:TYR:CD1	1:A:897:TYR:N	2.75	0.54
2:B:758:PHE:CE1	2:B:1027:ILE:CG2	2.90	0.54
2:B:295:GLY:H	2:B:298:LEU:HD23	1.71	0.54
2:B:332:ASP:C	2:B:334:ILE:H	2.10	0.54
2:B:707:PRO:HG2	2:B:708:GLU:N	2.16	0.54
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.90	0.54
3:C:260:LEU:O	3:C:263:THR:HB	2.07	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:129:LEU:O	4:D:129:LEU:HD12	2.07	0.54
4:D:155:ARG:NH1	4:D:155:ARG:HB2	2.21	0.54
1:A:1412:ALA:HA	1:A:1417:GLU:OE2	2.08	0.54
1:A:306:ASN:ND2	1:A:322:VAL:HG12	2.22	0.54
1:A:761:MET:HA	1:A:804:TYR:HB2	1.89	0.54
2:B:1001:PHE:CE2	3:C:34:ARG:NE	2.76	0.54
2:B:363:HIS:O	2:B:364:ILE:HB	2.06	0.54
2:B:805:THR:HG23	2:B:809:MET:CE	2.37	0.54
2:B:882:THR:CG2	2:B:934:LYS:O	2.55	0.54
4:D:156:ASP:HB2	4:D:159:THR:OG1	2.06	0.54
4:D:32:GLU:OE1	7:G:41:LYS:HE2	2.08	0.54
5:E:138:ALA:HA	5:E:141:VAL:CG2	2.36	0.54
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.43	0.54
5:E:157:SER:OG	5:E:160:GLU:HG3	2.07	0.54
8:H:15:VAL:HG13	8:H:26:ILE:CG1	2.38	0.54
12:L:66:GLN:HG2	12:L:67:PHE:N	2.22	0.54
1:A:115:LEU:HD12	1:A:142:CYS:HB3	1.90	0.54
1:A:1283:VAL:O	1:A:1306:LEU:HA	2.08	0.54
1:A:91:PHE:H	1:A:297:GLN:NE2	2.04	0.54
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.72	0.54
2:B:1003:ALA:HB1	3:C:179:GLU:HB2	1.90	0.54
2:B:277:LYS:HD2	2:B:277:LYS:N	2.15	0.54
2:B:25:ILE:HD11	2:B:653:VAL:C	2.27	0.54
2:B:707:PRO:CG	2:B:708:GLU:H	2.12	0.54
2:B:768:THR:O	2:B:771:SER:HB2	2.07	0.54
2:B:986:GLN:HE22	2:B:1022:THR:HG21	1.72	0.54
3:C:137:LYS:HE2	3:C:138:GLU:OE1	2.08	0.54
4:D:12:ARG:HH12	4:D:14:ARG:CA	2.20	0.54
5:E:9:ILE:CD1	5:E:53:PRO:HD3	2.38	0.54
9:I:50:THR:HG23	9:I:52:ILE:HG12	1.89	0.54
1:A:1215:ARG:O	1:A:1219:THR:N	2.34	0.54
1:A:1293:SER:HB3	1:A:1297:GLU:OE1	2.07	0.54
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.88	0.54
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.22	0.54
1:A:567:LYS:CG	1:A:568:PRO:CD	2.85	0.54
1:A:774:ARG:CZ	1:A:797:LYS:HB2	2.38	0.54
2:B:215:GLN:OE1	2:B:499:ASN:HB3	2.08	0.54
3:C:112:ASN:CB	3:C:114:TYR:CE1	2.91	0.54
4:D:52:LEU:O	4:D:54:GLU:N	2.40	0.54
5:E:10:SER:O	5:E:14:ARG:HG3	2.07	0.54
5:E:154:ILE:HG22	5:E:155:ARG:O	2.07	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:20:PRO:CD	7:G:21:ARG:H	2.20	0.54
8:H:123:MET:CE	8:H:142:LEU:HD21	2.37	0.54
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.90	0.54
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.08	0.54
1:A:982:THR:C	1:A:984:LYS:H	2.10	0.54
3:C:17:ASN:H	3:C:240:VAL:HG11	1.68	0.54
9:I:101:PHE:H	9:I:101:PHE:HD1	1.56	0.54
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.07	0.54
1:A:1244:ARG:HG2	1:A:1244:ARG:O	2.06	0.54
1:A:1423:GLY:CA	1:A:1426:GLU:HG3	2.37	0.54
1:A:440:ASP:O	1:A:460:VAL:HG23	2.08	0.54
1:A:600:PRO:CG	1:A:601:LYS:H	2.18	0.54
1:A:934:LYS:NZ	1:A:934:LYS:HB2	2.22	0.54
2:B:95:ILE:CG1	2:B:130:VAL:HG23	2.38	0.54
2:B:192:LEU:O	2:B:193:LYS:HB2	2.08	0.54
2:B:244:LEU:HD13	2:B:366:GLN:HE22	1.72	0.54
2:B:244:LEU:HD13	2:B:366:GLN:NE2	2.23	0.54
2:B:754:SER:O	2:B:806:THR:HG21	2.08	0.54
2:B:796:LEU:HD12	2:B:852:ARG:O	2.08	0.54
3:C:229:TYR:CD1	3:C:229:TYR:N	2.76	0.54
3:C:99:LEU:HD22	3:C:99:LEU:N	2.22	0.54
5:E:56:LYS:HZ1	5:E:85:GLU:N	2.05	0.54
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.89	0.54
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.89	0.54
9:I:19:ASP:HB3	9:I:24:ARG:HG2	1.88	0.54
10:J:7:CYS:CA	10:J:49:MET:HE3	2.37	0.54
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.72	0.54
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.08	0.54
1:A:1315:GLU:C	1:A:1317:MET:H	2.11	0.54
1:A:287:HIS:HA	1:A:290:GLU:HG3	1.89	0.54
1:A:900:ASP:CA	1:A:926:GLN:NE2	2.69	0.54
2:B:260:GLY:O	2:B:267:ARG:NH1	2.40	0.54
2:B:308:TRP:HA	2:B:311:LEU:HB2	1.91	0.54
2:B:821:GLN:HE22	2:B:851:PHE:HA	1.73	0.54
2:B:953:LEU:O	2:B:953:LEU:HD23	2.08	0.54
3:C:112:ASN:HB2	3:C:114:TYR:HE1	1.72	0.54
6:F:93:ILE:CD1	6:F:134:ILE:HD11	2.29	0.54
7:G:139:ILE:HG12	7:G:140:LYS:HG3	1.89	0.54
4:D:29:LEU:HD12	7:G:82:PHE:CE2	2.42	0.54
8:H:82:PRO:HG2	8:H:83:GLN:N	2.20	0.54
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.73	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASP:HB3	1:A:299:HIS:ND1	2.24	0.53
1:A:434:ARG:NH2	1:A:440:ASP:OD1	2.41	0.53
1:A:445:ASN:HB3	1:A:455:MET:HE2	1.89	0.53
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.56	0.53
1:A:932:GLU:HG2	1:A:933:TYR:N	2.22	0.53
2:B:1031:LEU:HD11	2:B:1042:GLY:HA3	1.91	0.53
2:B:108:VAL:CG1	2:B:109:THR:H	2.21	0.53
2:B:1099:VAL:CG1	2:B:1100:ASP:H	2.19	0.53
2:B:92:PHE:CD2	2:B:132:VAL:HG22	2.42	0.53
2:B:169:ARG:N	2:B:454:THR:OG1	2.42	0.53
2:B:291:ILE:CD1	2:B:291:ILE:N	2.71	0.53
2:B:309:GLN:NE2	2:B:309:GLN:HA	2.20	0.53
2:B:412:LEU:HB3	2:B:466:TRP:HE1	1.71	0.53
2:B:465:ASN:N	2:B:465:ASN:ND2	2.55	0.53
2:B:834:ASN:O	2:B:838:SER:O	2.26	0.53
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.90	0.53
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.41	0.53
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.90	0.53
3:C:75:MET:O	3:C:246:ARG:NH2	2.37	0.53
8:H:126:GLU:HG3	8:H:127:GLY:H	1.73	0.53
11:K:93:SER:O	11:K:97:LYS:HG3	2.09	0.53
1:A:1081:LEU:HD11	1:A:1098:VAL:N	2.18	0.53
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.72	0.53
1:A:476:SER:HB2	1:A:477:PRO:HD3	1.90	0.53
1:A:829:VAL:O	1:A:831:THR:N	2.41	0.53
1:A:889:SER:HA	1:A:1297:GLU:N	2.23	0.53
1:A:909:ASP:O	1:A:911:SER:N	2.41	0.53
2:B:999:MET:HB3	2:B:1007:VAL:CG2	2.39	0.53
2:B:1197:PRO:O	2:B:1200:ALA:N	2.39	0.53
2:B:205:ILE:O	2:B:207:GLY:N	2.41	0.53
2:B:865:LYS:C	2:B:866:TYR:HD1	2.12	0.53
3:C:66:ARG:HH12	10:J:2:ILE:CG2	2.13	0.53
7:G:144:ARG:HG2	7:G:168:LEU:HD23	1.89	0.53
7:G:1:MET:HE1	7:G:80:LYS:O	2.08	0.53
12:L:28:LYS:HE3	12:L:39:SER:OG	2.07	0.53
12:L:40:LEU:HD13	12:L:44:ASP:CB	2.37	0.53
1:A:1038:THR:H	1:A:1041:ALA:HB3	1.73	0.53
1:A:1037:LEU:HD11	1:A:1045:VAL:HG21	1.89	0.53
1:A:95:PHE:O	1:A:96:ILE:C	2.46	0.53
3:C:101:LEU:O	3:C:102:GLN:HG3	2.09	0.53
3:C:46:ILE:HD13	3:C:157:CYS:SG	2.47	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:213:ILE:HG12	5:E:214:CYS:N	2.23	0.53
8:H:82:PRO:CG	8:H:83:GLN:H	2.16	0.53
10:J:57:ILE:O	10:J:60:PHE:HB2	2.09	0.53
1:A:1287:TYR:O	1:A:1302:PRO:HA	2.09	0.53
1:A:1286:LYS:HE3	1:A:1304:TRP:CZ2	2.44	0.53
1:A:1454:MET:HG3	1:A:1454:MET:O	2.08	0.53
1:A:265:LYS:HE2	1:A:302:THR:HG23	1.88	0.53
1:A:56:PRO:O	1:A:57:ARG:NH1	2.42	0.53
2:B:1104:HIS:CG	2:B:1122:ARG:HB2	2.44	0.53
2:B:351:TYR:CD1	2:B:355:ILE:HD11	2.44	0.53
2:B:526:GLU:OE1	2:B:752:ALA:HB3	2.08	0.53
2:B:846:ILE:HG23	2:B:974:PRO:CG	2.35	0.53
3:C:167:HIS:CA	11:K:6:ARG:HH12	2.20	0.53
3:C:213:PRO:HG2	3:C:214:ASN:H	1.73	0.53
3:C:242:GLN:C	3:C:244:VAL:N	2.62	0.53
3:C:252:GLN:CG	11:K:95:ILE:HG23	2.37	0.53
5:E:168:TYR:HB3	5:E:170:LEU:HG	1.90	0.53
10:J:43:ARG:N	10:J:43:ARG:HD3	2.22	0.53
10:J:47:ARG:HG2	10:J:47:ARG:HH11	1.74	0.53
1:A:1111:MET:CG	1:A:1114:PRO:HB3	2.38	0.53
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.91	0.53
1:A:224:PHE:CE2	1:A:234:MET:HE2	2.43	0.53
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.43	0.53
1:A:523:ILE:HG12	1:A:622:VAL:HG22	1.91	0.53
1:A:595:THR:C	1:A:596:THR:HG23	2.29	0.53
1:A:768:GLN:CG	1:A:816:HIS:HA	2.26	0.53
1:A:853:ASP:C	1:A:853:ASP:OD1	2.47	0.53
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.91	0.53
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.56	0.53
2:B:217:ARG:C	2:B:217:ARG:HD2	2.29	0.53
2:B:603:LEU:HB3	2:B:609:ILE:HD11	1.90	0.53
3:C:118:LEU:HB2	3:C:132:PRO:HG2	1.90	0.53
5:E:182:ASP:O	5:E:186:LEU:HG	2.09	0.53
8:H:113:ALA:HB2	8:H:126:GLU:OE2	2.08	0.53
8:H:128:ASN:ND2	8:H:131:ASN:OD1	2.41	0.53
8:H:89:LEU:CD1	8:H:91:ASP:OD1	2.56	0.53
1:A:1141:THR:HG21	1:A:1205:LYS:HD3	1.91	0.53
1:A:1376:THR:O	1:A:1377:THR:C	2.47	0.53
1:A:1437:GLY:C	1:A:1439:GLY:H	2.12	0.53
1:A:347:PHE:H	2:B:1107:ALA:HA	1.73	0.53
1:A:709:THR:HG22	1:A:710:LEU:HD12	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:PHE:CD1	1:A:781:ASP:HA	2.44	0.53
2:B:125:SER:O	2:B:126:SER:HB3	2.08	0.53
2:B:211:VAL:O	2:B:480:SER:HA	2.09	0.53
2:B:292:ILE:CD1	2:B:327:ARG:H	2.12	0.53
2:B:497:ARG:NH2	2:B:775:LYS:HZ1	2.06	0.53
2:B:622:LYS:HZ3	9:I:59:VAL:HG13	1.72	0.53
2:B:880:THR:HB	2:B:934:LYS:CG	2.37	0.53
5:E:64:PRO:HB2	5:E:69:ILE:HD11	1.89	0.53
5:E:80:VAL:HG12	5:E:82:PHE:CE1	2.42	0.53
6:F:118:LEU:HG	6:F:118:LEU:O	2.08	0.53
7:G:20:PRO:HD2	7:G:21:ARG:H	1.74	0.53
8:H:81:PRO:HD2	8:H:83:GLN:OE1	2.09	0.53
1:A:1011:GLN:NE2	1:A:1015:VAL:CG2	2.72	0.53
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.43	0.53
2:B:172:ILE:CD1	2:B:178:ASN:ND2	2.71	0.53
2:B:818:PRO:HB2	2:B:1091:TYR:OH	2.08	0.53
3:C:33:LEU:O	3:C:37:MET:HG3	2.09	0.53
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.91	0.53
4:D:154:PHE:CE1	4:D:163:VAL:HG11	2.40	0.53
5:E:154:ILE:O	5:E:196:VAL:HA	2.08	0.53
7:G:101:VAL:CG1	7:G:102:GLN:N	2.71	0.53
8:H:2:SER:HA	8:H:62:SER:HB3	1.89	0.53
10:J:37:SER:OG	10:J:47:ARG:NH2	2.41	0.53
11:K:42:LEU:O	11:K:46:ILE:HG13	2.09	0.53
11:K:65:HIS:CD2	11:K:67:PHE:H	2.27	0.53
1:A:1048:ASN:HD22	1:A:1048:ASN:N	2.07	0.53
1:A:1045:VAL:O	1:A:1049:ILE:HG13	2.08	0.53
1:A:1171:GLN:OE1	1:A:1172:LEU:N	2.41	0.53
1:A:211:PHE:HD1	1:A:214:ILE:CD1	2.22	0.53
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.43	0.53
1:A:335:ARG:HH12	2:B:1206:GLU:CD	2.11	0.53
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.91	0.53
1:A:590:ARG:HG3	1:A:591:PHE:N	2.23	0.53
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.43	0.53
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.89	0.53
2:B:219:ALA:HB2	2:B:405:ARG:NH1	2.24	0.53
2:B:54:PHE:HE1	2:B:414:ALA:HA	1.74	0.53
2:B:69:LEU:HD13	2:B:432:MET:HE1	1.90	0.53
2:B:467:GLY:CA	2:B:475:SER:HB2	2.39	0.53
2:B:515:HIS:H	2:B:518:HIS:CD2	2.27	0.53
2:B:641:GLU:C	2:B:643:ASP:H	2.12	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:71:LYS:HA	4:D:74:GLN:CG	2.39	0.53
7:G:50:ASP:O	7:G:51:TYR:C	2.47	0.53
7:G:91:VAL:HG12	7:G:92:VAL:N	2.24	0.53
9:I:103:CYS:SG	9:I:106:CYS:SG	3.06	0.53
1:A:1239:ARG:HH22	1:A:1241:ARG:HH22	1.56	0.53
1:A:456:MET:HE2	1:A:478:TYR:CZ	2.44	0.53
1:A:96:ILE:HG22	1:A:97:ALA:N	2.23	0.53
2:B:1130:PHE:HZ	2:B:1138:MET:HG2	1.74	0.53
1:A:11:LEU:HB2	2:B:1193:GLN:HG3	1.91	0.53
2:B:562:GLY:HA3	2:B:590:HIS:ND1	2.24	0.53
2:B:603:LEU:HB3	2:B:609:ILE:CD1	2.39	0.53
2:B:705:MET:HA	2:B:705:MET:CE	2.38	0.53
2:B:842:ASN:ND2	2:B:845:SER:OG	2.42	0.53
3:C:148:ARG:NH1	10:J:64:ASN:HA	2.24	0.53
3:C:148:ARG:HG2	3:C:149:LYS:H	1.72	0.53
4:D:50:LEU:HD11	7:G:4:ILE:HD11	1.90	0.53
4:D:52:LEU:HD21	4:D:147:TYR:HE2	1.72	0.53
5:E:17:ARG:HG3	5:E:35:VAL:HG13	1.90	0.53
6:F:138:LEU:O	6:F:140:ASP:N	2.38	0.53
7:G:27:LYS:HD3	7:G:51:TYR:CE2	2.44	0.53
7:G:88:ASP:HB3	7:G:144:ARG:CA	2.35	0.53
10:J:24:LEU:HA	10:J:28:ASP:HB2	1.91	0.53
2:B:822:ASN:ND2	10:J:52:THR:HG21	2.24	0.53
12:L:40:LEU:HB3	12:L:44:ASP:HB2	1.91	0.53
14:T:15:DG:H2'	14:T:16:DT:C7	2.39	0.53
1:A:504:LEU:HD11	6:F:91:ALA:HB2	1.90	0.53
1:A:599:SER:HB3	1:A:614:PHE:CE1	2.44	0.53
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.91	0.53
2:B:644:GLU:C	2:B:646:LEU:H	2.12	0.53
2:B:803:LEU:CD1	2:B:1032:SER:HB3	2.39	0.53
3:C:124:LEU:O	3:C:126:GLY:N	2.42	0.53
9:I:61:ASP:C	9:I:63:GLY:N	2.61	0.53
12:L:47:ARG:HD3	12:L:52:GLY:HA2	1.91	0.53
14:T:11:DA:H2''	14:T:12:DG:H5'	1.90	0.53
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.89	0.52
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.90	0.52
1:A:1445:ILE:HD13	7:G:70:PHE:CE2	2.44	0.52
1:A:321:PRO:O	1:A:322:VAL:HG12	2.10	0.52
1:A:323:LYS:N	1:A:323:LYS:HD2	2.22	0.52
1:A:722:LEU:HB3	1:A:799:PHE:CE1	2.44	0.52
2:B:778:MET:HE3	2:B:1094:ARG:HD3	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1198:TYR:CD2	2:B:1198:TYR:O	2.62	0.52
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.73	0.52
2:B:378:LEU:O	2:B:382:ILE:HG13	2.08	0.52
2:B:431:TYR:CD1	2:B:447:ALA:HB2	2.43	0.52
2:B:636:PRO:HG2	2:B:743:ILE:CD1	2.40	0.52
2:B:745:PRO:O	2:B:747:MET:N	2.41	0.52
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.90	0.52
1:A:41:MET:HB2	1:A:48:ALA:O	2.08	0.52
1:A:528:LEU:O	1:A:531:ILE:HG22	2.09	0.52
1:A:903:ASN:ND2	1:A:905:ASP:H	2.08	0.52
2:B:287:ARG:HD3	2:B:325:GLN:HA	1.92	0.52
2:B:604:ARG:C	2:B:606:LYS:H	2.11	0.52
2:B:583:ASN:ND2	2:B:628:THR:HG22	2.20	0.52
5:E:180:ARG:HB2	5:E:215:MET:OXT	2.09	0.52
5:E:32:GLN:O	5:E:36:GLU:HG3	2.09	0.52
5:E:50:MET:HG3	5:E:51:GLY:N	2.24	0.52
8:H:8:ASP:CG	8:H:9:ILE:N	2.62	0.52
11:K:68:PHE:N	11:K:68:PHE:HD2	2.06	0.52
2:B:120:ARG:HH12	12:L:54:ARG:NH1	2.08	0.52
1:A:1155:ASP:OD2	1:A:1161:THR:HA	2.09	0.52
1:A:156:ASP:HB2	1:A:160:GLN:HE22	1.74	0.52
1:A:264:PHE:CE1	1:A:317:LYS:NZ	2.78	0.52
1:A:705:LYS:HG3	1:A:713:SER:HB3	1.91	0.52
1:A:834:THR:HG21	1:A:1077:THR:CG2	2.36	0.52
1:A:22:PHE:CE1	2:B:1213:THR:HG22	2.44	0.52
2:B:29:ASP:OD1	2:B:658:ILE:HG21	2.10	0.52
2:B:882:THR:CG2	2:B:884:ARG:N	2.72	0.52
2:B:855:PHE:HD2	2:B:972:LYS:HE3	1.75	0.52
7:G:17:PHE:C	7:G:19:GLY:H	2.13	0.52
13:N:5:DC:H2"	13:N:6:DT:OP2	2.09	0.52
1:A:388:LEU:HD22	1:A:432:VAL:CG2	2.39	0.52
1:A:868:TYR:HE1	1:A:1064:VAL:HG13	1.74	0.52
1:A:888:GLY:O	1:A:940:ARG:NH2	2.42	0.52
2:B:95:ILE:HG13	2:B:130:VAL:HG23	1.91	0.52
4:D:162:ALA:HA	4:D:165:GLN:NE2	2.24	0.52
7:G:137:ILE:O	7:G:138:THR:HB	2.09	0.52
9:I:14:LEU:HD22	9:I:28:GLU:C	2.30	0.52
1:A:353:ILE:HD12	1:A:487:MET:HE2	1.91	0.52
1:A:563:PRO:HD3	8:H:79:TRP:CD1	2.45	0.52
1:A:567:LYS:HD3	8:H:95:TYR:CD2	2.45	0.52
1:A:549:MET:SD	1:A:577:ILE:HD12	2.50	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:GLU:OE2	1:A:962:ARG:HD2	2.10	0.52
1:A:69:THR:HG21	2:B:1174:LYS:NZ	2.25	0.52
1:A:784:LEU:HD11	1:A:815:PHE:CE2	2.44	0.52
1:A:845:LEU:O	1:A:846:GLU:C	2.48	0.52
2:B:1174:LYS:O	2:B:1176:ASN:N	2.43	0.52
2:B:259:TYR:N	2:B:259:TYR:CD1	2.78	0.52
2:B:39:ARG:CZ	2:B:665:GLU:HG2	2.38	0.52
2:B:435:THR:C	2:B:437:GLU:N	2.63	0.52
2:B:416:LEU:HD22	2:B:457:LEU:HD23	1.92	0.52
2:B:579:ARG:HG2	2:B:579:ARG:NH1	2.25	0.52
2:B:801:LYS:HA	2:B:818:PRO:HB3	1.92	0.52
7:G:35:GLU:OE2	7:G:48:VAL:HG23	2.10	0.52
7:G:55:ASP:HB3	7:G:73:LYS:HB2	1.91	0.52
8:H:89:LEU:C	8:H:91:ASP:N	2.56	0.52
10:J:16:ASP:OD1	10:J:17:LYS:N	2.39	0.52
12:L:34:CYS:SG	12:L:51:CYS:SG	3.07	0.52
2:B:1113:VAL:N	15:P:1:C:C5'	2.70	0.52
1:A:997:LEU:HD13	1:A:1018:PHE:CE2	2.45	0.52
1:A:151:ASP:OD1	1:A:163:SER:HB3	2.10	0.52
1:A:382:PRO:CA	1:A:428:TYR:HE2	2.22	0.52
1:A:68:GLN:OE1	1:A:70:CYS:HB3	2.09	0.52
1:A:767:GLN:HE21	1:A:774:ARG:CB	2.23	0.52
1:A:767:GLN:NE2	1:A:774:ARG:HB2	2.25	0.52
2:B:1177:HIS:HB3	2:B:1179:GLN:HE21	1.74	0.52
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.24	0.52
2:B:434:ARG:O	2:B:436:VAL:N	2.43	0.52
2:B:516:ASN:ND2	2:B:516:ASN:H	2.07	0.52
2:B:54:PHE:O	2:B:58:THR:HB	2.10	0.52
2:B:653:VAL:HG13	2:B:657:HIS:HB2	1.91	0.52
2:B:707:PRO:O	2:B:708:GLU:O	2.27	0.52
2:B:999:MET:HA	2:B:999:MET:HE2	1.91	0.52
3:C:111:THR:C	3:C:112:ASN:HD22	2.12	0.52
4:D:216:ASN:C	4:D:218:GLU:N	2.61	0.52
5:E:145:THR:HG21	5:E:187:TYR:CD2	2.44	0.52
1:A:1109:LYS:HG3	1:A:1110:ASN:ND2	2.25	0.52
1:A:405:VAL:HG22	1:A:432:VAL:HG13	1.92	0.52
1:A:779:PHE:O	1:A:780:VAL:C	2.47	0.52
1:A:962:ARG:C	1:A:964:ILE:H	2.13	0.52
2:B:757:PRO:HG3	2:B:1028:GLU:OE2	2.09	0.52
2:B:288:ALA:HB2	2:B:330:ALA:HB1	1.91	0.52
2:B:459:TYR:CE1	2:B:463:THR:HG21	2.45	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:644:GLU:HA	2:B:644:GLU:OE1	2.09	0.52
1:A:806:ARG:NH1	2:B:729:ILE:HD12	2.23	0.52
2:B:770:GLN:OE1	2:B:983:ARG:C	2.48	0.52
3:C:25:VAL:HG12	3:C:26:ASP:N	2.25	0.52
3:C:31:ASN:O	3:C:35:ARG:HG3	2.09	0.52
9:I:75:CYS:HB2	9:I:76:PRO:CD	2.40	0.52
11:K:59:ALA:HA	11:K:74:ARG:O	2.09	0.52
3:C:166:GLU:C	11:K:6:ARG:NH1	2.63	0.52
1:A:1116:LEU:N	1:A:1308:THR:CG2	2.68	0.52
1:A:1146:VAL:HG12	1:A:1201:ALA:HB1	1.91	0.52
1:A:53:LEU:CD2	1:A:54:ASN:N	2.56	0.52
1:A:557:ASP:OD1	1:A:559:VAL:HB	2.09	0.52
1:A:741:ASN:ND2	1:A:744:LYS:N	2.52	0.52
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.71	0.52
1:A:963:ILE:O	1:A:963:ILE:HG12	2.10	0.52
2:B:944:THR:HG21	2:B:1122:ARG:NH2	2.25	0.52
2:B:562:GLY:O	2:B:590:HIS:ND1	2.43	0.52
2:B:744:HIS:CD2	2:B:745:PRO:CD	2.87	0.52
4:D:47:LEU:HD13	4:D:48:ILE:N	2.24	0.52
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.39	0.52
8:H:26:ILE:HG12	8:H:27:GLU:N	2.24	0.52
1:A:132:LYS:HE3	1:A:1411:GLU:OE2	2.10	0.52
1:A:16:GLU:OE1	4:D:13:ARG:NH2	2.40	0.52
1:A:679:ILE:HG12	1:A:732:LEU:HD12	1.92	0.52
1:A:66:LYS:CE	1:A:68:GLN:H	2.21	0.52
1:A:714:PHE:O	1:A:718:VAL:HG23	2.10	0.52
2:B:1045:SER:O	2:B:1048:THR:HG23	2.10	0.52
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.13	0.52
2:B:235:SER:OG	2:B:236:HIS:CD2	2.62	0.52
2:B:35:SER:O	2:B:39:ARG:HG3	2.10	0.52
2:B:506:GLY:O	2:B:507:LYS:CB	2.58	0.52
2:B:557:PHE:CZ	2:B:603:LEU:HD21	2.45	0.52
2:B:891:ASP:C	2:B:893:LEU:H	2.13	0.52
3:C:242:GLN:O	3:C:244:VAL:N	2.43	0.52
4:D:154:PHE:O	4:D:160:VAL:HG22	2.10	0.52
12:L:55:ILE:O	12:L:56:LEU:HB2	2.09	0.52
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.92	0.52
1:A:34:LYS:HG2	1:A:36:ARG:NH2	2.21	0.52
1:A:470:LEU:HD23	1:A:470:LEU:H	1.75	0.52
1:A:663:SER:OG	1:A:664:THR:N	2.43	0.52
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.38	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1124:ARG:O	2:B:1125:ASP:HB3	2.10	0.52
2:B:1147:LEU:HD23	2:B:1151:LEU:HD13	1.92	0.52
2:B:431:TYR:CE1	2:B:447:ALA:HB2	2.44	0.52
2:B:842:ASN:HD21	2:B:844:SER:HB2	1.75	0.52
8:H:109:LYS:HG2	8:H:110:ASP:H	1.73	0.52
8:H:5:LEU:HD13	8:H:133:ASN:O	2.09	0.52
11:K:47:ARG:HD2	11:K:47:ARG:C	2.30	0.52
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.92	0.52
1:A:2:VAL:HG22	1:A:3:GLY:N	2.25	0.51
1:A:55:ASP:CG	1:A:55:ASP:O	2.46	0.51
1:A:730:GLY:O	1:A:731:ARG:C	2.48	0.51
2:B:1116:ARG:HG3	2:B:1198:TYR:CD1	2.45	0.51
2:B:114:PRO:HG3	2:B:181:LEU:HD21	1.90	0.51
2:B:401:PHE:HA	2:B:404:LYS:HG3	1.92	0.51
7:G:129:SER:CB	7:G:138:THR:HB	2.39	0.51
7:G:64:THR:HG23	7:G:65:ASP:N	2.25	0.51
8:H:123:MET:HE3	8:H:142:LEU:HD21	1.92	0.51
10:J:23:ASN:C	10:J:25:LEU:N	2.61	0.51
10:J:23:ASN:O	10:J:25:LEU:N	2.43	0.51
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.91	0.51
14:T:24:DG:H2"	14:T:25:DG:OP2	2.10	0.51
1:A:186:LYS:NZ	1:A:197:PRO:HD3	2.25	0.51
1:A:794:PRO:HG2	1:A:795:GLU:OE2	2.10	0.51
1:A:901:LEU:N	1:A:926:GLN:NE2	2.35	0.51
2:B:217:ARG:HG2	2:B:217:ARG:HH11	1.75	0.51
2:B:510:LYS:CB	2:B:511:PRO:HD3	2.40	0.51
2:B:642:ASP:C	2:B:644:GLU:H	2.14	0.51
2:B:694:ASP:O	2:B:698:GLU:HB2	2.10	0.51
4:D:63:LEU:O	4:D:129:LEU:HD11	2.10	0.51
3:C:66:ARG:CZ	10:J:2:ILE:HG21	2.39	0.51
1:A:1001:ARG:O	1:A:1002:GLY:O	2.28	0.51
1:A:266:LEU:HD21	1:A:303:TYR:CE1	2.45	0.51
1:A:332:LYS:C	1:A:334:GLY:N	2.63	0.51
1:A:699:ALA:HB3	1:A:701:LEU:HG	1.93	0.51
1:A:882:SER:HB3	1:A:953:ASN:OD1	2.10	0.51
2:B:1000:PRO:O	2:B:1007:VAL:HG23	2.10	0.51
2:B:303:TYR:N	2:B:303:TYR:CD2	2.78	0.51
2:B:345:LYS:HE2	2:B:349:ILE:HD11	1.92	0.51
2:B:51:PHE:O	2:B:55:VAL:HG23	2.10	0.51
2:B:578:THR:O	2:B:589:VAL:HG13	2.10	0.51
4:D:14:ARG:C	4:D:16:LYS:H	2.14	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:35:LEU:HD12	4:D:35:LEU:N	2.25	0.51
5:E:35:VAL:C	5:E:37:LEU:H	2.13	0.51
5:E:56:LYS:NZ	5:E:84:ASP:N	2.58	0.51
6:F:128:LYS:HD3	6:F:148:VAL:O	2.10	0.51
8:H:109:LYS:HG2	8:H:110:ASP:OD1	2.10	0.51
8:H:15:VAL:HG22	8:H:26:ILE:CD1	2.41	0.51
8:H:9:ILE:HA	8:H:55:LEU:O	2.10	0.51
1:A:536:LEU:HD23	1:A:536:LEU:N	2.14	0.51
1:A:804:TYR:OH	2:B:763:GLN:HA	2.11	0.51
2:B:129:PHE:HE2	2:B:166:PHE:HB2	1.74	0.51
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.75	0.51
2:B:809:MET:O	2:B:812:LEU:N	2.41	0.51
2:B:840:ILE:HD13	2:B:994:TYR:HE1	1.75	0.51
3:C:80:LEU:HD11	3:C:95:CYS:C	2.31	0.51
4:D:190:GLU:O	4:D:194:LEU:HG	2.10	0.51
5:E:61:GLN:NE2	5:E:105:PHE:CZ	2.77	0.51
8:H:17:PRO:CB	8:H:24:CYS:SG	2.89	0.51
2:B:1076:HIS:CD2	11:K:40:HIS:NE2	2.78	0.51
1:A:883:LEU:CD1	1:A:1017:LEU:HD11	2.39	0.51
1:A:1187:GLN:HB2	1:A:1244:ARG:HH21	1.74	0.51
1:A:427:GLN:HB2	1:A:430:TRP:NE1	2.24	0.51
1:A:437:MET:N	1:A:440:ASP:OD2	2.28	0.51
1:A:622:VAL:HG22	1:A:622:VAL:O	2.11	0.51
1:A:922:ASP:OD1	1:A:924:LYS:HB2	2.10	0.51
1:A:341:MET:CE	2:B:1135:ARG:NH1	2.73	0.51
3:C:241:ASP:O	3:C:245:VAL:HG22	2.10	0.51
5:E:124:VAL:N	5:E:125:PRO:HD2	2.25	0.51
5:E:143:ASN:HD22	5:E:146:HIS:CE1	2.29	0.51
7:G:59:GLY:CA	7:G:70:PHE:CD2	2.94	0.51
12:L:32:ALA:H	12:L:55:ILE:CD1	2.23	0.51
1:A:230:ARG:HD2	1:A:233:TRP:CH2	2.45	0.51
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.93	0.51
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.91	0.51
1:A:688:LYS:HA	1:A:691:LEU:HB3	1.92	0.51
1:A:774:ARG:HG3	1:A:797:LYS:HB3	1.92	0.51
1:A:913:LEU:HD13	1:A:981:LEU:O	2.10	0.51
2:B:1001:PHE:CE2	3:C:34:ARG:CZ	2.93	0.51
2:B:1077:THR:HG22	11:K:44:ASN:ND2	2.26	0.51
2:B:333:PHE:O	2:B:333:PHE:CG	2.63	0.51
2:B:52:ASN:O	2:B:56:ASP:N	2.42	0.51
2:B:794:ASN:C	2:B:795:ILE:HD12	2.31	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:987:LYS:HD3	2:B:987:LYS:H	1.75	0.51
5:E:185:ALA:O	5:E:190:LEU:HG	2.10	0.51
6:F:76:LYS:CA	6:F:79:ARG:HD2	2.39	0.51
9:I:85:PHE:HD1	9:I:99:LEU:HD13	1.72	0.51
2:B:1077:THR:HG22	11:K:44:ASN:HD21	1.75	0.51
12:L:60:ARG:HH21	12:L:65:VAL:CG2	2.24	0.51
1:A:1166:ASP:OD2	1:A:1239:ARG:CD	2.59	0.51
1:A:1369:ALA:O	1:A:1370:LEU:C	2.49	0.51
1:A:218:ASP:O	1:A:219:PHE:C	2.48	0.51
1:A:332:LYS:CA	1:A:337:ARG:NH1	2.73	0.51
1:A:555:ASP:O	1:A:556:TRP:C	2.49	0.51
2:B:1102:LYS:O	2:B:1122:ARG:NH1	2.39	0.51
2:B:235:SER:C	2:B:236:HIS:HD2	2.14	0.51
2:B:555:ILE:HG22	2:B:556:THR:N	2.26	0.51
2:B:376:PHE:HE2	2:B:569:TYR:HD2	1.58	0.51
2:B:661:LEU:HD11	2:B:684:LEU:HD21	1.93	0.51
2:B:806:THR:CG2	2:B:809:MET:H	2.19	0.51
2:B:864:LYS:HG3	2:B:872:GLU:OE1	2.11	0.51
3:C:3:GLU:HB3	11:K:104:ASN:HD21	1.75	0.51
5:E:78:LEU:HD21	5:E:80:VAL:CG2	2.21	0.51
1:A:598:LEU:HD23	8:H:25:ARG:CZ	2.41	0.51
8:H:43:ASN:ND2	8:H:46:LEU:HD12	2.25	0.51
10:J:1:MET:O	10:J:2:ILE:O	2.28	0.51
1:A:308:ILE:HG22	1:A:309:ALA:H	1.76	0.51
1:A:316:GLN:HE21	1:A:317:LYS:NZ	2.09	0.51
1:A:774:ARG:NH2	1:A:797:LYS:HB2	2.26	0.51
4:D:71:LYS:CA	4:D:74:GLN:HB2	2.32	0.51
5:E:153:HIS:O	5:E:154:ILE:CG1	2.59	0.51
6:F:109:VAL:HG13	6:F:127:GLU:OE1	2.10	0.51
7:G:62:LEU:HD13	7:G:63:PRO:N	2.25	0.51
8:H:37:LYS:H	8:H:126:GLU:HB3	1.76	0.51
2:B:902:GLY:O	12:L:65:VAL:HG11	2.11	0.51
1:A:1110:ASN:ND2	1:A:1110:ASN:N	2.58	0.51
1:A:1445:ILE:HD12	7:G:59:GLY:O	2.11	0.51
1:A:388:LEU:HD22	1:A:432:VAL:HG21	1.92	0.51
1:A:698:GLN:O	9:I:98:VAL:HG13	2.11	0.51
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.75	0.51
1:A:953:ASN:C	1:A:954:TRP:CD1	2.84	0.51
2:B:212:LEU:HD23	2:B:480:SER:HB2	1.93	0.51
2:B:687:GLU:O	2:B:689:LEU:HG	2.10	0.51
2:B:815:ARG:HH11	2:B:815:ARG:HB2	1.74	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:872:GLU:OE2	2:B:914:LYS:HE3	2.11	0.51
2:B:970:THR:HG22	2:B:971:THR:N	2.26	0.51
6:F:94:LEU:HD21	6:F:122:MET:HA	1.93	0.51
1:A:546:VAL:HG12	1:A:550:LEU:HD11	1.93	0.51
1:A:592:ASP:N	1:A:595:THR:OG1	2.43	0.51
1:A:616:VAL:HG12	1:A:617:VAL:H	1.76	0.51
1:A:590:ARG:NH2	1:A:620:LYS:HB2	2.26	0.51
2:B:110:HIS:HB2	12:L:54:ARG:NH2	2.26	0.51
2:B:1175:LEU:HD23	2:B:1175:LEU:H	1.76	0.51
2:B:324:ILE:HD13	2:B:330:ALA:HA	1.92	0.51
2:B:640:VAL:O	2:B:641:GLU:C	2.50	0.51
4:D:153:ARG:C	4:D:154:PHE:CD2	2.84	0.51
4:D:154:PHE:CE1	4:D:163:VAL:HG21	2.42	0.51
5:E:162:ARG:HG2	5:E:162:ARG:HH11	1.76	0.51
7:G:7:LEU:CB	7:G:74:TYR:CE2	2.94	0.51
10:J:1:MET:H1	10:J:56:LEU:H	1.55	0.51
1:A:1217:LYS:HE3	1:A:1217:LYS:HA	1.93	0.50
2:B:1156:ASP:O	2:B:1157:ALA:O	2.28	0.50
2:B:418:LYS:O	2:B:420:LEU:N	2.44	0.50
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.41	0.50
4:D:119:ARG:HD3	4:D:221:TYR:CE2	2.46	0.50
4:D:12:ARG:HH12	4:D:13:ARG:C	2.14	0.50
6:F:136:ARG:O	6:F:143:PHE:HA	2.12	0.50
8:H:98:TYR:C	8:H:118:PHE:HD2	2.14	0.50
9:I:26:LEU:CD2	9:I:37:GLU:HA	2.40	0.50
2:B:799:PRO:HD3	10:J:1:MET:HG2	1.93	0.50
12:L:60:ARG:CG	12:L:61:THR:H	2.16	0.50
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.25	0.50
1:A:1403:GLU:OE1	14:T:16:DT:H4'	2.12	0.50
1:A:308:ILE:HG22	1:A:309:ALA:N	2.26	0.50
1:A:512:VAL:O	1:A:512:VAL:HG12	2.10	0.50
2:B:429:PHE:HA	2:B:432:MET:CE	2.39	0.50
9:I:51:ASN:ND2	9:I:54:GLU:OE1	2.43	0.50
1:A:1277:GLU:C	1:A:1279:ILE:H	2.14	0.50
1:A:1330:ASN:O	1:A:1332:PHE:N	2.44	0.50
1:A:168:GLY:O	1:A:169:ASN:C	2.49	0.50
1:A:34:LYS:H	1:A:34:LYS:HD3	1.77	0.50
1:A:42:ASP:HA	1:A:46:THR:O	2.10	0.50
1:A:692:ASP:O	1:A:694:THR:N	2.44	0.50
1:A:973:ILE:HD13	1:A:1037:LEU:HA	1.93	0.50
2:B:1084:GLN:HE21	2:B:1084:GLN:N	2.09	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1175:LEU:O	2:B:1176:ASN:HB2	2.11	0.50
2:B:1196:ILE:HB	2:B:1197:PRO:HD2	1.94	0.50
2:B:126:SER:O	2:B:169:ARG:HA	2.10	0.50
2:B:222:ILE:N	2:B:240:ILE:CD1	2.75	0.50
2:B:311:LEU:O	2:B:314:LEU:N	2.43	0.50
2:B:59:LEU:CD1	2:B:417:PHE:CE2	2.89	0.50
2:B:424:LEU:O	2:B:428:ILE:HG13	2.10	0.50
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.93	0.50
2:B:579:ARG:NH1	2:B:622:LYS:O	2.44	0.50
2:B:882:THR:HG21	2:B:935:ARG:CA	2.35	0.50
1:A:253:ASN:HA	2:B:884:ARG:NH2	2.26	0.50
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.93	0.50
3:C:44:LEU:HD21	3:C:159:ALA:CB	2.41	0.50
7:G:88:ASP:HB2	7:G:171:ILE:HD11	1.93	0.50
8:H:4:THR:HG22	8:H:5:LEU:N	2.26	0.50
8:H:84:ALA:C	8:H:86:ASP:N	2.58	0.50
8:H:91:ASP:C	8:H:93:TYR:H	2.15	0.50
1:A:1158:PRO:HG2	1:A:1159:ARG:NE	2.26	0.50
1:A:1280:GLU:O	1:A:1281:ARG:O	2.30	0.50
1:A:90:VAL:CG1	1:A:297:GLN:NE2	2.73	0.50
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.94	0.50
1:A:492:PRO:HB2	1:A:497:THR:CG2	2.41	0.50
1:A:526:ASP:O	1:A:527:THR:C	2.49	0.50
1:A:53:LEU:CD2	1:A:54:ASN:H	2.14	0.50
1:A:659:HIS:O	2:B:1081:LEU:HD23	2.11	0.50
1:A:828:ALA:C	1:A:831:THR:HG22	2.31	0.50
1:A:91:PHE:CE1	1:A:204:THR:HG23	2.47	0.50
1:A:2:VAL:CG1	2:B:1157:ALA:O	2.57	0.50
2:B:360:PHE:O	2:B:361:LEU:C	2.49	0.50
2:B:560:GLU:O	2:B:561:TRP:CD1	2.65	0.50
2:B:806:THR:HG22	2:B:809:MET:N	2.21	0.50
2:B:769:TYR:CD1	2:B:987:LYS:NZ	2.79	0.50
2:B:1003:ALA:HA	3:C:178:PHE:O	2.12	0.50
3:C:35:ARG:HH12	11:K:41:THR:N	1.95	0.50
5:E:69:ILE:CD1	5:E:69:ILE:N	2.73	0.50
8:H:1:MET:O	8:H:3:ASN:N	2.41	0.50
11:K:101:LEU:HD23	11:K:101:LEU:O	2.12	0.50
1:A:132:LYS:HE3	1:A:1411:GLU:HG3	1.92	0.50
1:A:666:ILE:HD12	1:A:667:GLY:N	2.17	0.50
1:A:699:ALA:O	1:A:700:ASN:HB3	2.12	0.50
1:A:913:LEU:CD1	1:A:914:GLU:N	2.71	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:ARG:HB2	2:B:398:ARG:NH1	2.26	0.50
2:B:422:LYS:HA	2:B:425:THR:HB	1.93	0.50
2:B:464:GLY:C	2:B:465:ASN:HD22	2.14	0.50
2:B:44:VAL:HG11	2:B:495:LEU:HD13	1.93	0.50
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.93	0.50
4:D:144:THR:O	4:D:148:LEU:HB2	2.12	0.50
4:D:29:LEU:N	4:D:29:LEU:CD2	2.75	0.50
5:E:124:VAL:HG13	5:E:132:ILE:CG1	2.41	0.50
5:E:65:THR:O	5:E:69:ILE:CD1	2.60	0.50
9:I:44:TYR:CD1	9:I:44:TYR:C	2.85	0.50
10:J:53:HIS:CD2	10:J:54:VAL:N	2.79	0.50
14:T:16:DT:H2''	14:T:17:DT:O5'	2.12	0.50
1:A:1062:GLU:OE2	6:F:88:TYR:OH	2.29	0.50
1:A:1164:PRO:O	1:A:1167:GLU:HB2	2.12	0.50
1:A:106:VAL:HG21	1:A:214:ILE:CD1	2.40	0.50
1:A:30:ILE:HG23	2:B:1170:THR:HG23	1.94	0.50
1:A:606:LEU:HG	1:A:613:ILE:HD12	1.92	0.50
1:A:821:ARG:HD2	2:B:512:ARG:O	2.12	0.50
1:A:851:HIS:O	1:A:853:ASP:N	2.45	0.50
2:B:1167:GLY:HA3	2:B:1216:LEU:H	1.76	0.50
2:B:171:PRO:HD2	2:B:457:LEU:HD13	1.92	0.50
2:B:373:ARG:HB3	2:B:566:LEU:HD23	1.94	0.50
2:B:704:ALA:HB2	2:B:738:PHE:CD2	2.46	0.50
3:C:241:ASP:OD1	3:C:242:GLN:N	2.44	0.50
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.94	0.50
4:D:130:LEU:C	4:D:132:GLN:H	2.15	0.50
8:H:136:LYS:HD2	8:H:136:LYS:H	1.76	0.50
8:H:56:THR:O	8:H:144:ILE:HA	2.11	0.50
1:A:12:ARG:HB3	2:B:1218:THR:HG22	1.93	0.50
1:A:290:GLU:HA	1:A:293:GLU:HB2	1.93	0.50
1:A:974:ASP:OD2	1:A:976:THR:OG1	2.30	0.50
2:B:1002:THR:O	2:B:1004:GLU:N	2.45	0.50
2:B:129:PHE:HA	2:B:165:VAL:O	2.11	0.50
2:B:287:ARG:HG3	2:B:292:ILE:HA	1.94	0.50
2:B:254:LEU:HD22	2:B:361:LEU:HD11	1.93	0.50
2:B:470:LYS:C	2:B:472:ALA:H	2.15	0.50
3:C:22:LEU:HD11	11:K:101:LEU:HD11	1.93	0.50
3:C:239:PRO:O	3:C:242:GLN:N	2.44	0.50
9:I:58:VAL:O	9:I:59:VAL:C	2.50	0.50
1:A:1173:HIS:CG	1:A:1227:ILE:HG23	2.47	0.50
1:A:889:SER:HA	1:A:1297:GLU:H	1.76	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.42	0.50
1:A:1443:VAL:C	1:A:1444:MET:HG3	2.33	0.50
1:A:420:ARG:O	1:A:424:ILE:HG13	2.12	0.50
1:A:445:ASN:ND2	1:A:455:MET:HE3	2.27	0.50
1:A:458:HIS:NE2	1:A:478:TYR:OH	2.40	0.50
1:A:53:LEU:HD22	1:A:54:ASN:HD22	1.76	0.50
1:A:666:ILE:CD1	1:A:667:GLY:N	2.73	0.50
1:A:68:GLN:O	1:A:68:GLN:OE1	2.29	0.50
1:A:853:ASP:CG	1:A:855:THR:HG22	2.32	0.50
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.27	0.50
2:B:187:SER:O	2:B:191:LYS:HG3	2.11	0.50
3:C:175:ALA:CB	10:J:43:ARG:NH2	2.64	0.50
5:E:129:PRO:O	5:E:130:ALA:C	2.50	0.50
5:E:180:ARG:HH21	5:E:192:ARG:CB	2.20	0.50
5:E:82:PHE:O	5:E:83:CYS:HB2	2.12	0.50
10:J:24:LEU:O	10:J:30:LEU:HB3	2.12	0.50
12:L:38:LEU:O	12:L:39:SER:CB	2.59	0.50
1:A:1264:GLU:OE2	9:I:46:HIS:CD2	2.65	0.50
1:A:1308:THR:CG2	1:A:1309:ASP:N	2.63	0.50
1:A:1394:THR:CG2	1:A:1398:MET:SD	3.00	0.50
1:A:728:LYS:HA	1:A:731:ARG:HH12	1.77	0.50
1:A:829:VAL:C	1:A:831:THR:N	2.66	0.50
2:B:1068:GLY:O	2:B:1069:PHE:O	2.30	0.50
1:A:351:THR:CG2	2:B:1103:ILE:HG13	2.41	0.50
2:B:1183:LYS:HE3	2:B:1183:LYS:O	2.12	0.50
2:B:50:SER:OG	2:B:411:PRO:HD3	2.12	0.50
2:B:641:GLU:O	2:B:643:ASP:N	2.44	0.50
2:B:885:MET:HG2	2:B:936:ASP:HB2	1.94	0.50
4:D:204:ASP:O	4:D:208:GLU:HB2	2.12	0.50
5:E:114:ASN:O	5:E:115:ASN:CB	2.60	0.50
5:E:74:ASP:OD1	5:E:74:ASP:N	2.39	0.50
7:G:115:MET:O	7:G:164:LYS:HD3	2.12	0.50
1:A:1444:MET:HB3	7:G:59:GLY:O	2.12	0.50
10:J:36:LEU:HA	10:J:39:LEU:HD12	1.94	0.50
2:B:120:ARG:HH12	12:L:54:ARG:HD3	1.77	0.50
1:A:1269:GLU:O	1:A:1270:ASN:HB2	2.10	0.49
1:A:1206:ASP:O	1:A:1274:ARG:NH2	2.45	0.49
1:A:1316:VAL:HG12	1:A:1316:VAL:O	2.12	0.49
1:A:288:ALA:HA	1:A:291:GLU:HG3	1.93	0.49
1:A:319:GLY:HA3	2:B:471:LYS:HA	1.94	0.49
1:A:739:ASP:OD1	8:H:19:ARG:NH2	2.45	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1085:ILE:HG22	2:B:1086:PHE:N	2.25	0.49
1:A:343:LYS:HD2	2:B:1155:SER:CB	2.42	0.49
2:B:806:THR:CG2	2:B:809:MET:HG2	2.28	0.49
2:B:984:HIS:NE2	2:B:1025:HIS:HA	2.26	0.49
2:B:996:ARG:HH12	3:C:175:ALA:H	1.60	0.49
3:C:110:THR:HG22	3:C:112:ASN:HD21	1.77	0.49
3:C:79:GLN:NE2	3:C:127:ARG:HD3	2.27	0.49
4:D:23:ASN:N	4:D:23:ASN:OD1	2.45	0.49
5:E:28:TYR:C	5:E:65:THR:HG22	2.32	0.49
6:F:77:ASP:O	6:F:78:GLN:CB	2.44	0.49
8:H:20:TYR:O	8:H:22:LYS:N	2.45	0.49
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.77	0.49
9:I:19:ASP:OD2	9:I:22:ASN:HB2	2.11	0.49
11:K:94:ILE:O	11:K:98:LEU:HG	2.11	0.49
1:A:1030:ARG:NH1	1:A:1035:TYR:OH	2.45	0.49
1:A:125:ALA:C	1:A:127:ALA:N	2.65	0.49
1:A:889:SER:CB	1:A:1297:GLU:HG3	2.42	0.49
1:A:1313:LEU:CB	1:A:1338:VAL:HG21	2.42	0.49
1:A:688:LYS:CG	1:A:691:LEU:HD23	2.42	0.49
1:A:84:ILE:O	1:A:84:ILE:HG22	2.11	0.49
1:A:890:ASP:OD2	1:A:1296:GLY:HA2	2.11	0.49
2:B:102:VAL:HG21	2:B:112:LEU:HD13	1.94	0.49
2:B:323:VAL:HG12	2:B:323:VAL:O	2.12	0.49
2:B:578:THR:C	2:B:589:VAL:HG13	2.33	0.49
2:B:662:MET:HA	2:B:665:GLU:HB2	1.94	0.49
2:B:849:GLY:O	2:B:852:ARG:HG3	2.12	0.49
2:B:882:THR:O	2:B:883:LEU:HB2	2.12	0.49
3:C:233:GLU:HG2	3:C:234:SER:H	1.77	0.49
4:D:146:GLN:HA	4:D:149:THR:HG22	1.94	0.49
5:E:116:ILE:HG22	5:E:117:THR:N	2.27	0.49
5:E:178:ILE:HG22	5:E:213:ILE:O	2.12	0.49
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.93	0.49
6:F:84:TYR:HD1	6:F:84:TYR:H	1.60	0.49
6:F:90:ARG:CG	6:F:91:ALA:N	2.73	0.49
7:G:61:ILE:HG22	7:G:62:LEU:O	2.11	0.49
8:H:127:GLY:HA3	8:H:129:TYR:CZ	2.47	0.49
11:K:21:ILE:HG22	11:K:31:VAL:HG11	1.94	0.49
1:A:1402:PHE:CG	1:A:1403:GLU:HG2	2.47	0.49
1:A:285:PRO:O	1:A:287:HIS:N	2.45	0.49
1:A:315:LEU:HD13	1:A:319:GLY:O	2.12	0.49
1:A:472:LEU:O	1:A:475:THR:HB	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:MET:HE1	2:B:1135:ARG:NH1	2.28	0.49
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.48	0.49
2:B:603:LEU:HD12	2:B:609:ILE:HG23	1.92	0.49
4:D:123:LEU:HD22	4:D:149:THR:HG21	1.94	0.49
2:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.94	0.49
11:K:12:LEU:HD21	11:K:17:SER:CA	2.42	0.49
12:L:55:ILE:HD13	12:L:56:LEU:N	2.27	0.49
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.80	0.49
1:A:265:LYS:O	1:A:269:ILE:HG13	2.11	0.49
1:A:962:ARG:O	1:A:965:GLN:N	2.46	0.49
2:B:23:ALA:O	2:B:654:ARG:HB3	2.13	0.49
2:B:23:ALA:O	2:B:654:ARG:HD2	2.13	0.49
2:B:370:PHE:HD2	2:B:373:ARG:CD	2.26	0.49
2:B:400:HIS:HA	2:B:517:THR:HG21	1.93	0.49
2:B:498:THR:O	2:B:536:VAL:HA	2.13	0.49
2:B:891:ASP:C	2:B:893:LEU:N	2.65	0.49
3:C:261:ALA:HA	3:C:264:GLN:OE1	2.11	0.49
5:E:31:THR:O	5:E:34:GLU:HB3	2.12	0.49
8:H:127:GLY:O	8:H:128:ASN:CB	2.59	0.49
9:I:25:LEU:HG	9:I:38:ALA:HB2	1.94	0.49
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.94	0.49
1:A:1118:VAL:HG12	1:A:1327:ILE:HG13	1.95	0.49
1:A:623:GLY:O	1:A:630:ILE:HD12	2.11	0.49
1:A:877:HIS:O	1:A:878:ILE:HG13	2.12	0.49
1:A:896:ARG:HB3	1:A:897:TYR:CD1	2.47	0.49
2:B:1152:MET:C	2:B:1157:ALA:HB2	2.33	0.49
2:B:290:GLY:HA2	2:B:327:ARG:HD2	1.93	0.49
2:B:405:ARG:NE	2:B:632:ARG:HG2	2.27	0.49
2:B:54:PHE:CE1	2:B:414:ALA:HA	2.47	0.49
2:B:62:ILE:CG2	2:B:418:LYS:HG2	2.31	0.49
2:B:46:GLN:OE1	2:B:47:GLN:N	2.38	0.49
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.77	0.49
2:B:872:GLU:OE1	2:B:914:LYS:HE3	2.13	0.49
1:A:254:GLU:HB2	2:B:935:ARG:HH22	1.77	0.49
2:B:950:ASP:O	2:B:951:GLN:HB2	2.12	0.49
2:B:862:GLN:CG	2:B:963:PHE:HD1	2.25	0.49
3:C:3:GLU:N	3:C:7:GLN:OE1	2.45	0.49
4:D:119:ARG:HB3	4:D:119:ARG:CZ	2.41	0.49
5:E:190:LEU:C	5:E:191:LYS:HG2	2.32	0.49
5:E:38:PRO:HG2	5:E:41:ASP:CG	2.33	0.49
8:H:109:LYS:HE3	8:H:110:ASP:OD1	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:40:LEU:HB2	8:H:123:MET:HE2	1.94	0.49
12:L:30:ILE:CG2	12:L:31:CYS:H	2.25	0.49
1:A:316:GLN:NE2	1:A:317:LYS:NZ	2.60	0.49
1:A:384:ASN:CG	1:A:388:LEU:HD12	2.33	0.49
1:A:475:THR:CG2	1:A:476:SER:N	2.75	0.49
1:A:565:ILE:HG23	1:A:567:LYS:CG	2.40	0.49
1:A:709:THR:HG21	9:I:93:LYS:O	2.13	0.49
1:A:789:LYS:HE3	9:I:67:THR:HB	1.94	0.49
1:A:896:ARG:NH2	1:A:1030:ARG:CZ	2.76	0.49
1:A:925:LEU:C	1:A:927:VAL:N	2.65	0.49
2:B:806:THR:HA	2:B:1045:SER:OG	2.12	0.49
1:A:666:ILE:HD11	2:B:1086:PHE:CE1	2.47	0.49
2:B:254:LEU:HD12	2:B:272:THR:O	2.12	0.49
2:B:46:GLN:HB2	2:B:408:LEU:CD2	2.42	0.49
2:B:563:MET:O	2:B:565:PRO:HD3	2.11	0.49
2:B:56:ASP:HB3	2:B:57:TYR:HD1	1.77	0.49
2:B:25:ILE:HD11	2:B:653:VAL:O	2.12	0.49
4:D:47:LEU:HD13	4:D:48:ILE:H	1.78	0.49
5:E:128:PRO:HA	5:E:129:PRO:O	2.13	0.49
5:E:50:MET:HG2	5:E:52:ARG:CZ	2.42	0.49
1:A:289:ILE:HG23	1:A:290:GLU:N	2.27	0.49
1:A:591:PHE:HA	1:A:595:THR:CG2	2.41	0.49
2:B:1115:THR:O	2:B:1116:ARG:HB2	2.13	0.49
2:B:169:ARG:HD2	2:B:454:THR:CG2	2.42	0.49
2:B:810:GLU:CA	2:B:815:ARG:HH22	2.26	0.49
3:C:183:TRP:O	3:C:184:ASN:C	2.50	0.49
7:G:139:ILE:CG2	7:G:140:LYS:N	2.74	0.49
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	1.93	0.49
1:A:1138:ILE:HG13	1:A:1139:GLU:N	2.28	0.49
1:A:1161:THR:C	1:A:1163:ILE:H	2.15	0.49
1:A:144:THR:O	1:A:146:MET:CE	2.60	0.49
1:A:1450:LEU:HD12	1:A:1450:LEU:O	2.13	0.49
1:A:427:GLN:HB2	1:A:430:TRP:CG	2.47	0.49
1:A:540:PHE:CE2	1:A:565:ILE:HD12	2.48	0.49
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.78	0.49
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.26	0.49
2:B:629:ASP:HB3	2:B:632:ARG:HD3	1.95	0.49
2:B:801:LYS:O	10:J:52:THR:HG21	2.13	0.49
3:C:164:ALA:HA	3:C:167:HIS:O	2.13	0.49
4:D:195:ILE:HG22	4:D:195:ILE:O	2.13	0.49
6:F:130:ILE:O	6:F:148:VAL:CG2	2.61	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:78:CYS:SG	9:I:105:SER:O	2.70	0.49
9:I:16:PRO:HD3	9:I:27:PHE:CE2	2.47	0.49
12:L:41:SER:N	12:L:44:ASP:OD2	2.45	0.49
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.75	0.49
1:A:40:THR:HB	1:A:41:MET:HE3	1.94	0.49
1:A:590:ARG:NH1	1:A:590:ARG:HG2	2.27	0.49
1:A:730:GLY:O	1:A:732:LEU:N	2.46	0.49
1:A:75:ASN:O	1:A:76:GLU:CB	2.60	0.49
1:A:870:GLU:O	5:E:205:SER:HB3	2.13	0.49
2:B:345:LYS:CG	2:B:346:GLU:H	2.18	0.49
2:B:570:VAL:HG21	2:B:573:GLN:NE2	2.27	0.49
2:B:878:GLN:O	2:B:879:ARG:O	2.30	0.49
2:B:952:VAL:HG12	2:B:953:LEU:H	1.76	0.49
3:C:31:ASN:HA	3:C:34:ARG:HB3	1.95	0.49
4:D:156:ASP:O	4:D:159:THR:N	2.46	0.49
7:G:111:THR:HG23	7:G:114:LEU:HD13	1.92	0.49
1:A:117:GLU:H	1:A:117:GLU:CD	2.17	0.49
1:A:1259:MET:HA	1:A:1262:LYS:CE	2.42	0.49
1:A:1451:VAL:CG1	1:A:1452:LYS:N	2.75	0.49
1:A:153:PRO:HD3	1:A:161:LEU:CD1	2.43	0.49
1:A:447:GLN:HA	1:A:448:PRO:C	2.33	0.49
1:A:794:PRO:O	1:A:796:SER:N	2.45	0.49
2:B:1031:LEU:O	2:B:1031:LEU:HD12	2.13	0.49
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.94	0.49
2:B:29:ASP:CB	2:B:658:ILE:HD13	2.43	0.49
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.47	0.49
2:B:542:MET:SD	2:B:747:MET:HE2	2.52	0.49
2:B:801:LYS:O	10:J:52:THR:CG2	2.61	0.49
5:E:127:ILE:N	5:E:128:PRO:CD	2.76	0.49
8:H:46:LEU:O	8:H:47:PHE:HB2	2.12	0.49
9:I:44:TYR:HD1	9:I:44:TYR:C	2.16	0.49
1:A:700:ASN:HB2	9:I:98:VAL:HG21	1.94	0.49
2:B:1112:GLN:HG3	15:P:1:C:H5"	1.91	0.49
1:A:172:PRO:HD3	1:A:185:TRP:CD1	2.48	0.48
1:A:751:SER:O	1:A:752:LYS:HG2	2.13	0.48
1:A:885:THR:HG22	1:A:940:ARG:HA	1.95	0.48
1:A:946:VAL:HG22	5:E:201:LYS:CD	2.38	0.48
2:B:1030:LEU:HD13	2:B:1067:ARG:O	2.13	0.48
1:A:351:THR:CG2	2:B:1103:ILE:HA	2.34	0.48
2:B:241:ARG:CG	2:B:253:THR:HG22	2.43	0.48
2:B:368:GLU:O	2:B:370:PHE:N	2.45	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:383:ASN:HD21	2:B:387:LEU:HD12	1.75	0.48
2:B:549:THR:HG22	2:B:550:ASP:N	2.19	0.48
2:B:526:GLU:OE1	2:B:752:ALA:CB	2.61	0.48
4:D:208:GLU:O	4:D:212:LYS:HG3	2.13	0.48
4:D:52:LEU:O	4:D:53:SER:HB3	2.13	0.48
5:E:120:ALA:HA	5:E:123:LEU:CD1	2.43	0.48
5:E:67:GLU:O	5:E:70:SER:N	2.43	0.48
9:I:82:GLU:HB3	9:I:104:LEU:HB2	1.95	0.48
9:I:40:SER:OG	9:I:41:PRO:HD2	2.12	0.48
10:J:21:TYR:HB2	10:J:39:LEU:CD1	2.43	0.48
1:A:1035:TYR:O	1:A:1036:ARG:HB2	2.11	0.48
1:A:1341:ILE:HD13	1:A:1380:GLY:HA2	1.95	0.48
1:A:146:MET:C	1:A:171:GLN:HB2	2.33	0.48
1:A:562:THR:HG22	8:H:79:TRP:HD1	1.78	0.48
1:A:57:ARG:HB2	1:A:57:ARG:HH11	1.77	0.48
1:A:590:ARG:HB3	1:A:605:MET:N	2.29	0.48
1:A:720:ARG:O	1:A:724:GLU:CB	2.61	0.48
1:A:827:THR:CG2	1:A:828:ALA:N	2.77	0.48
2:B:1180:PHE:O	2:B:1181:GLU:O	2.31	0.48
2:B:240:ILE:O	2:B:240:ILE:HG23	2.12	0.48
2:B:275:TYR:CD1	2:B:275:TYR:N	2.81	0.48
2:B:293:PRO:C	2:B:294:ASP:O	2.51	0.48
2:B:418:LYS:HD3	2:B:422:LYS:HZ2	1.73	0.48
2:B:637:LEU:CB	2:B:693:ILE:HD11	2.39	0.48
2:B:785:TYR:CE2	2:B:795:ILE:HG12	2.49	0.48
2:B:983:ARG:NH1	2:B:1028:GLU:OE1	2.45	0.48
3:C:115:SER:HB2	3:C:142:VAL:HB	1.95	0.48
3:C:5:GLY:O	3:C:7:GLN:NE2	2.45	0.48
2:B:798:TYR:CE2	3:C:62:PHE:CE2	3.00	0.48
4:D:8:PHE:CZ	4:D:37:GLN:NE2	2.81	0.48
5:E:73:PRO:O	5:E:75:MET:N	2.46	0.48
1:A:1443:VAL:HG11	6:F:132:LEU:HD13	1.95	0.48
1:A:986:ILE:HG21	1:A:1028:THR:HA	1.94	0.48
1:A:1209:MET:HE1	1:A:1236:LEU:HB3	1.95	0.48
1:A:1450:LEU:CD1	6:F:108:PHE:CZ	2.97	0.48
1:A:150:THR:CG2	1:A:166:GLY:HA2	2.40	0.48
1:A:700:ASN:HD22	9:I:115:LYS:HB2	1.78	0.48
1:A:923:LEU:HD12	1:A:923:LEU:H	1.78	0.48
2:B:227:LYS:H	2:B:395:GLN:CD	2.17	0.48
2:B:469:GLN:O	2:B:472:ALA:HB3	2.13	0.48
1:A:315:LEU:CD1	2:B:471:LYS:HB3	2.40	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:520:GLY:N	2:B:748:ILE:HG22	2.27	0.48
2:B:363:HIS:CD2	2:B:585:VAL:HG22	2.48	0.48
2:B:906:SER:O	2:B:907:GLY:O	2.31	0.48
2:B:757:PRO:HG2	2:B:984:HIS:HE1	1.77	0.48
3:C:105:GLY:O	3:C:149:LYS:O	2.30	0.48
3:C:184:ASN:OD1	3:C:187:LYS:CA	2.61	0.48
5:E:19:VAL:HG22	5:E:140:LEU:HD12	1.95	0.48
7:G:1:MET:SD	7:G:79:PHE:CE1	3.06	0.48
8:H:110:ASP:O	8:H:128:ASN:HB2	2.12	0.48
8:H:84:ALA:O	8:H:85:GLY:C	2.51	0.48
9:I:55:THR:HG22	9:I:58:VAL:CG2	2.43	0.48
9:I:62:ILE:HG12	9:I:62:ILE:O	2.12	0.48
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.43	0.48
1:A:132:LYS:HE3	1:A:1411:GLU:CG	2.43	0.48
1:A:299:HIS:CA	1:A:302:THR:HG22	2.43	0.48
1:A:332:LYS:O	1:A:334:GLY:N	2.46	0.48
1:A:34:LYS:CD	1:A:34:LYS:N	2.76	0.48
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.49	0.48
1:A:655:PHE:O	1:A:658:LEU:HB3	2.13	0.48
1:A:774:ARG:O	1:A:775:ILE:C	2.50	0.48
1:A:853:ASP:OD1	1:A:855:THR:CB	2.61	0.48
2:B:48:LEU:HD23	2:B:173:MET:SD	2.54	0.48
2:B:243:ALA:CB	2:B:251:ILE:HG12	2.43	0.48
2:B:273:LEU:HD21	2:B:360:PHE:CE1	2.49	0.48
2:B:661:LEU:HD23	2:B:679:TYR:O	2.13	0.48
2:B:686:ASN:C	2:B:688:GLY:H	2.17	0.48
2:B:69:LEU:HD22	2:B:429:PHE:CE1	2.48	0.48
2:B:708:GLU:O	2:B:709:ASP:C	2.51	0.48
4:D:56:ARG:CD	4:D:149:THR:HA	2.39	0.48
6:F:135:ARG:HG2	6:F:137:TYR:CE1	2.47	0.48
4:D:33:PHE:CE1	7:G:80:LYS:HD3	2.48	0.48
8:H:24:CYS:HB2	8:H:44:VAL:CG2	2.37	0.48
8:H:77:ARG:HG2	8:H:78:SER:H	1.79	0.48
1:A:445:ASN:HB2	1:A:454:SER:O	2.13	0.48
1:A:986:ILE:HG22	1:A:987:VAL:N	2.28	0.48
2:B:1064:TYR:O	2:B:1065:GLN:C	2.51	0.48
2:B:246:LYS:HA	2:B:249:ARG:CZ	2.44	0.48
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.43	0.48
2:B:307:ASP:C	2:B:309:GLN:N	2.64	0.48
2:B:408:LEU:HD11	2:B:545:ILE:CD1	2.43	0.48
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:615:MET:CB	2:B:626:ILE:HG12	2.27	0.48
2:B:862:GLN:HG2	2:B:963:PHE:HD1	1.79	0.48
2:B:916:THR:HB	2:B:935:ARG:HG3	1.95	0.48
4:D:191:ALA:O	4:D:193:THR:N	2.46	0.48
6:F:116:ASP:OD1	6:F:118:LEU:N	2.47	0.48
7:G:1:MET:O	7:G:2:PHE:C	2.52	0.48
7:G:74:TYR:H	7:G:74:TYR:HD2	1.60	0.48
8:H:118:PHE:O	8:H:119:GLY:C	2.52	0.48
8:H:130:ARG:HA	8:H:133:ASN:HB2	1.95	0.48
9:I:88:SER:C	9:I:90:GLN:H	2.17	0.48
1:A:834:THR:CG2	1:A:1077:THR:HG23	2.39	0.48
1:A:1171:GLN:O	1:A:1174:PHE:HB2	2.13	0.48
1:A:257:ARG:HB3	1:A:258:GLY:H	1.39	0.48
1:A:324:SER:O	1:A:327:ALA:HB3	2.12	0.48
1:A:382:PRO:CB	1:A:428:TYR:HE2	2.27	0.48
1:A:614:PHE:CD1	1:A:614:PHE:C	2.86	0.48
1:A:925:LEU:C	1:A:927:VAL:H	2.17	0.48
2:B:1117:GLN:HE21	2:B:1199:ALA:HB2	1.78	0.48
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.31	0.48
2:B:266:ALA:O	2:B:268:THR:HG22	2.14	0.48
2:B:372:SER:HB3	2:B:567:GLU:OE1	2.13	0.48
2:B:891:ASP:O	2:B:893:LEU:N	2.46	0.48
8:H:129:TYR:HA	8:H:131:ASN:ND2	2.28	0.48
8:H:39:THR:O	8:H:123:MET:HG3	2.13	0.48
8:H:77:ARG:HB2	8:H:77:ARG:NH1	2.27	0.48
1:A:1387:HIS:NE2	13:N:4:DA:H5'	2.29	0.48
1:A:350:ARG:HB3	2:B:1128:LEU:CD1	2.43	0.48
1:A:783:THR:O	1:A:784:LEU:HD23	2.14	0.48
1:A:808:LEU:HD23	1:A:812:GLU:C	2.34	0.48
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	2.13	0.48
2:B:97:VAL:HG22	2:B:128:LEU:HD12	1.95	0.48
3:C:92:CYS:N	3:C:95:CYS:SG	2.72	0.48
4:D:53:SER:H	4:D:148:LEU:CD2	2.27	0.48
5:E:103:LYS:HB3	5:E:105:PHE:CE2	2.48	0.48
5:E:22:MET:CE	5:E:26:ARG:NH2	2.74	0.48
5:E:94:LYS:O	5:E:98:ILE:HG13	2.14	0.48
6:F:148:VAL:HG23	6:F:149:GLU:N	2.27	0.48
8:H:130:ARG:N	8:H:130:ARG:CD	2.65	0.48
8:H:133:ASN:O	8:H:135:LEU:N	2.47	0.48
9:I:34:TYR:HE2	9:I:36:GLU:HB3	1.79	0.48
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.27	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:PRO:HG2	1:A:397:ASN:OD1	2.14	0.48
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.95	0.48
1:A:670:ILE:HG23	1:A:805:LEU:HG	1.95	0.48
1:A:919:ILE:HG13	1:A:925:LEU:HD12	1.95	0.48
1:A:899:VAL:O	1:A:929:LEU:HD12	2.13	0.48
2:B:327:ARG:NH2	2:B:371:GLU:HG2	2.29	0.48
2:B:313:MET:CE	2:B:386:LEU:HB3	2.44	0.48
2:B:734:HIS:O	2:B:735:ALA:CB	2.61	0.48
2:B:758:PHE:CE2	2:B:1044:ALA:CA	2.96	0.48
2:B:806:THR:HG21	2:B:808:ALA:HB3	1.94	0.48
3:C:174:ALA:HA	10:J:10:CYS:O	2.13	0.48
5:E:144:ILE:HG13	5:E:145:THR:H	1.78	0.48
5:E:64:PRO:O	5:E:69:ILE:HD11	2.14	0.48
5:E:89:GLY:C	5:E:91:LYS:H	2.17	0.48
7:G:62:LEU:HD22	7:G:62:LEU:HA	1.73	0.48
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.96	0.48
10:J:12:LYS:O	10:J:13:VAL:C	2.51	0.48
12:L:34:CYS:CB	12:L:51:CYS:SG	3.00	0.48
1:A:1315:GLU:C	1:A:1317:MET:N	2.67	0.48
1:A:156:ASP:HB2	1:A:160:GLN:NE2	2.29	0.48
1:A:446:ARG:HG2	1:A:446:ARG:HH11	1.78	0.48
1:A:77:CYS:SG	1:A:77:CYS:O	2.72	0.48
1:A:886:ILE:HG21	1:A:952:ALA:HB2	1.96	0.48
1:A:961:ARG:HG2	1:A:965:GLN:HE22	1.77	0.48
2:B:1085:ILE:HD12	2:B:1085:ILE:N	2.28	0.48
2:B:167:ILE:HD12	2:B:167:ILE:N	2.28	0.48
2:B:258:LEU:HG	2:B:258:LEU:O	2.14	0.48
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.79	0.48
2:B:590:HIS:NE2	2:B:592:ASN:O	2.47	0.48
7:G:145:VAL:HG12	7:G:146:LYS:N	2.28	0.48
8:H:109:LYS:CG	8:H:110:ASP:H	2.27	0.48
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.14	0.48
1:A:122:MET:CA	1:A:141:LEU:HD11	2.42	0.48
1:A:427:GLN:HG3	1:A:430:TRP:CE2	2.47	0.48
1:A:536:LEU:CD2	1:A:536:LEU:H	2.09	0.48
1:A:600:PRO:HA	8:H:25:ARG:NH1	2.29	0.48
1:A:665:GLY:O	1:A:666:ILE:HD12	2.14	0.48
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.95	0.48
2:B:446:LEU:N	2:B:446:LEU:HD23	2.29	0.48
2:B:209:GLU:CD	2:B:485:ARG:HE	2.17	0.48
2:B:580:VAL:HG22	2:B:624:LEU:HB3	1.95	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:582:VAL:HG22	2:B:626:ILE:CG2	2.43	0.48
3:C:147:LEU:HD12	3:C:151:GLN:O	2.14	0.48
3:C:176:ILE:HG22	3:C:176:ILE:O	2.13	0.48
3:C:177:GLU:CG	3:C:231:ASN:HB3	2.39	0.48
5:E:67:GLU:O	5:E:70:SER:CB	2.62	0.48
6:F:106:PRO:HG3	7:G:18:PHE:O	2.13	0.48
6:F:69:LEU:HD13	6:F:71:GLU:OE1	2.13	0.48
8:H:10:PHE:N	8:H:10:PHE:CD1	2.81	0.48
9:I:22:ASN:O	9:I:23:ASN:HB2	2.12	0.48
10:J:60:PHE:O	10:J:63:TYR:HD1	1.97	0.48
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.14	0.47
1:A:11:LEU:CD2	1:A:11:LEU:O	2.56	0.47
1:A:173:THR:O	1:A:173:THR:HG22	2.13	0.47
1:A:284:ALA:HB1	1:A:289:ILE:HD12	1.96	0.47
1:A:276:LEU:HD13	1:A:293:GLU:HA	1.96	0.47
1:A:364:VAL:O	1:A:364:VAL:HG13	2.14	0.47
1:A:546:VAL:HG12	1:A:550:LEU:CD1	2.44	0.47
1:A:7:SER:OG	2:B:1161:HIS:CE1	2.63	0.47
2:B:1116:ARG:HG3	2:B:1198:TYR:CE1	2.49	0.47
2:B:265:SER:O	2:B:266:ALA:HB3	2.14	0.47
2:B:636:PRO:HG2	2:B:743:ILE:HD12	1.96	0.47
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.96	0.47
4:D:135:GLY:C	4:D:137:ASN:H	2.16	0.47
4:D:214:LEU:O	4:D:218:GLU:HB2	2.13	0.47
6:F:97:ARG:O	6:F:101:ILE:HG13	2.13	0.47
1:A:973:ILE:CD1	1:A:1038:THR:HG23	2.44	0.47
1:A:1423:GLY:HA3	1:A:1426:GLU:HG3	1.95	0.47
1:A:185:TRP:CZ3	1:A:200:ARG:HG2	2.49	0.47
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.44	0.47
1:A:710:LEU:CD1	1:A:710:LEU:H	2.18	0.47
1:A:710:LEU:O	1:A:714:PHE:N	2.46	0.47
1:A:91:PHE:HB2	1:A:297:GLN:HE22	1.78	0.47
1:A:982:THR:HB	1:A:985:ASP:N	2.25	0.47
2:B:1065:GLN:NE2	2:B:1066:SER:H	2.12	0.47
2:B:241:ARG:HA	2:B:253:THR:HG22	1.94	0.47
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.96	0.47
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.49	0.47
3:C:152:GLU:HG2	3:C:153:LEU:H	1.79	0.47
5:E:134:THR:O	5:E:135:PHE:HD1	1.96	0.47
6:F:96:THR:O	6:F:100:GLN:HG3	2.13	0.47
3:C:146:LYS:HB2	10:J:61:LEU:HD11	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.96	0.47
1:A:323:LYS:H	1:A:323:LYS:CD	2.23	0.47
1:A:406:ILE:HG22	1:A:412:ARG:HA	1.96	0.47
2:B:128:LEU:HD21	2:B:170:LEU:HB2	1.95	0.47
2:B:275:TYR:HD1	2:B:275:TYR:N	2.12	0.47
2:B:418:LYS:HD3	2:B:422:LYS:HZ1	1.78	0.47
2:B:996:ARG:NH1	3:C:174:ALA:HA	2.27	0.47
3:C:233:GLU:CG	3:C:234:SER:N	2.77	0.47
3:C:8:VAL:O	3:C:9:LYS:HG3	2.14	0.47
5:E:69:ILE:CD1	5:E:69:ILE:H	2.27	0.47
8:H:25:ARG:HB2	8:H:41:ASP:OD1	2.15	0.47
8:H:89:LEU:HB2	8:H:91:ASP:OD1	2.14	0.47
1:A:1039:LYS:HE3	1:A:1043:ASP:OD2	2.15	0.47
1:A:1169:ILE:O	1:A:1169:ILE:HG22	2.14	0.47
1:A:129:LYS:O	1:A:130:ASP:CB	2.62	0.47
1:A:375:THR:OG1	1:A:433:GLU:HB3	2.14	0.47
1:A:556:TRP:CH2	1:A:558:GLY:HA2	2.49	0.47
1:A:596:THR:C	1:A:598:LEU:N	2.67	0.47
1:A:960:ILE:CA	1:A:963:ILE:HG22	2.39	0.47
1:A:967:ALA:HA	1:A:1044:TRP:CZ3	2.50	0.47
2:B:113:TYR:HB3	2:B:114:PRO:HD2	1.95	0.47
2:B:97:VAL:HG22	2:B:128:LEU:CD1	2.45	0.47
2:B:244:LEU:O	2:B:246:LYS:N	2.47	0.47
2:B:461:LEU:CD1	2:B:461:LEU:H	2.25	0.47
2:B:496:ARG:NH1	2:B:539:LEU:HB2	2.29	0.47
2:B:798:TYR:CE2	3:C:62:PHE:CZ	3.01	0.47
2:B:892:LYS:HZ3	2:B:905:VAL:HA	1.79	0.47
2:B:911:ILE:HD11	2:B:941:LEU:HB2	1.96	0.47
3:C:114:TYR:HB3	3:C:140:ASN:O	2.14	0.47
4:D:154:PHE:N	4:D:154:PHE:CD2	2.82	0.47
7:G:1:MET:HE1	7:G:3:PHE:HE1	1.79	0.47
8:H:62:SER:OG	8:H:63:LEU:N	2.44	0.47
10:J:7:CYS:SG	10:J:49:MET:CE	3.02	0.47
12:L:26:THR:HG22	12:L:27:LEU:N	2.29	0.47
1:A:1017:LEU:O	1:A:1017:LEU:HD12	2.14	0.47
1:A:1264:GLU:HG3	1:A:1265:ASN:OD1	2.14	0.47
1:A:661:GLY:HA3	2:B:1081:LEU:HD22	1.96	0.47
2:B:114:PRO:CG	2:B:115:GLN:H	2.22	0.47
2:B:241:ARG:HG2	2:B:253:THR:HG21	1.95	0.47
2:B:295:GLY:N	2:B:298:LEU:HD23	2.30	0.47
2:B:311:LEU:O	2:B:312:GLU:C	2.53	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:VAL:HG21	2:B:199:MET:O	2.14	0.47
2:B:603:LEU:HD12	2:B:609:ILE:CG1	2.44	0.47
2:B:616:ILE:H	2:B:616:ILE:HD12	1.78	0.47
2:B:661:LEU:C	2:B:663:ALA:N	2.68	0.47
3:C:69:LEU:H	3:C:69:LEU:CD1	2.14	0.47
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.97	0.47
4:D:206:GLU:O	4:D:210:ILE:HG13	2.13	0.47
14:T:25:DG:H2"	14:T:26:DT:OP2	2.15	0.47
1:A:1451:VAL:C	1:A:1453:TYR:N	2.68	0.47
1:A:285:PRO:CG	1:A:288:ALA:HB3	2.40	0.47
1:A:350:ARG:CB	2:B:1128:LEU:HD11	2.43	0.47
1:A:613:ILE:O	1:A:614:PHE:HB3	2.15	0.47
1:A:858:ASN:HD21	1:A:860:LEU:H	1.58	0.47
2:B:356:LEU:HA	2:B:360:PHE:HB2	1.97	0.47
2:B:483:LEU:CD1	2:B:491:THR:HG23	2.24	0.47
1:A:786:HIS:HE1	2:B:519:TRP:CZ2	2.32	0.47
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.97	0.47
3:C:144:ILE:O	3:C:145:CYS:HB3	2.15	0.47
5:E:162:ARG:HB3	5:E:162:ARG:CZ	2.45	0.47
6:F:69:LEU:C	6:F:71:GLU:HG3	2.34	0.47
7:G:26:LEU:CD1	7:G:56:ILE:HD11	2.28	0.47
1:A:1349:TYR:O	1:A:1350:LYS:C	2.52	0.47
1:A:401:GLY:C	1:A:435:HIS:HD2	2.18	0.47
1:A:514:PRO:O	1:A:515:GLN:C	2.53	0.47
1:A:666:ILE:H	2:B:1026:LEU:HD22	1.80	0.47
1:A:666:ILE:HD11	2:B:1086:PHE:HE1	1.79	0.47
1:A:688:LYS:C	1:A:690:VAL:H	2.16	0.47
1:A:943:LEU:C	1:A:945:GLU:H	2.18	0.47
2:B:113:TYR:CB	2:B:114:PRO:HD2	2.45	0.47
2:B:1182:CYS:C	2:B:1183:LYS:HE3	2.35	0.47
2:B:245:GLU:C	2:B:246:LYS:HG3	2.35	0.47
2:B:281:PRO:C	2:B:283:VAL:N	2.67	0.47
2:B:290:GLY:O	2:B:292:ILE:HG13	2.14	0.47
2:B:293:PRO:CD	2:B:296:GLU:OE1	2.58	0.47
2:B:308:TRP:CA	2:B:311:LEU:HD12	2.44	0.47
2:B:36:ALA:O	2:B:39:ARG:HB2	2.15	0.47
2:B:60:GLN:O	2:B:63:ILE:HG22	2.15	0.47
3:C:113:VAL:HG23	3:C:147:LEU:HD21	1.96	0.47
3:C:39:ALA:O	3:C:164:ALA:HB3	2.13	0.47
4:D:17:LYS:CD	4:D:18:VAL:HG13	2.42	0.47
6:F:111:LEU:C	6:F:113:GLY:N	2.68	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:14:LEU:HB3	9:I:27:PHE:HB3	1.95	0.47
1:A:117:GLU:HA	1:A:123:ARG:HG3	1.97	0.47
1:A:1344:GLY:O	1:A:1347:ALA:N	2.48	0.47
1:A:777:PHE:HA	1:A:782:ARG:O	2.14	0.47
1:A:76:GLU:O	1:A:78:PRO:HD3	2.15	0.47
2:B:1181:GLU:H	2:B:1188:LYS:HA	1.80	0.47
2:B:1214:PRO:O	2:B:1214:PRO:HG2	2.15	0.47
2:B:98:THR:O	2:B:126:SER:HB2	2.15	0.47
2:B:121:ASN:HA	2:B:207:GLY:HA2	1.96	0.47
2:B:26:THR:O	2:B:29:ASP:HB2	2.15	0.47
2:B:168:GLY:N	2:B:450:ALA:HB1	2.12	0.47
1:A:658:LEU:HD12	2:B:830:TYR:CD1	2.50	0.47
3:C:183:TRP:O	3:C:185:LYS:HG3	2.14	0.47
3:C:6:PRO:HA	3:C:24:ASN:HD22	1.80	0.47
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.97	0.47
5:E:124:VAL:HG13	5:E:132:ILE:CB	2.43	0.47
7:G:34:VAL:O	7:G:37:SER:CB	2.63	0.47
15:P:2:A:H2'	15:P:3:A:O4'	2.14	0.47
1:A:1004:ASN:O	1:A:1008:GLN:HG2	2.15	0.47
1:A:834:THR:HG21	1:A:1077:THR:CB	2.45	0.47
1:A:250:ILE:HG22	1:A:250:ILE:O	2.15	0.47
1:A:312:PRO:O	1:A:314:ALA:N	2.47	0.47
1:A:425:GLN:CD	1:A:425:GLN:H	2.16	0.47
1:A:470:LEU:HD23	1:A:470:LEU:N	2.30	0.47
1:A:72:GLU:HB3	1:A:76:GLU:CG	2.45	0.47
1:A:774:ARG:HB2	1:A:797:LYS:O	2.15	0.47
1:A:843:LYS:CD	1:A:846:GLU:OE2	2.61	0.47
2:B:1174:LYS:O	2:B:1175:LEU:C	2.52	0.47
2:B:1198:TYR:C	2:B:1198:TYR:CD2	2.88	0.47
2:B:284:ILE:HG12	2:B:324:ILE:HD12	1.96	0.47
2:B:364:ILE:O	2:B:365:THR:HB	2.15	0.47
2:B:787:VAL:HG12	2:B:787:VAL:O	2.14	0.47
2:B:882:THR:HB	2:B:934:LYS:O	2.15	0.47
3:C:209:TYR:H	3:C:209:TYR:HD1	1.61	0.47
4:D:134:THR:HG22	4:D:135:GLY:N	2.30	0.47
4:D:207:LEU:O	4:D:207:LEU:HD12	2.15	0.47
11:K:63:VAL:O	11:K:63:VAL:CG2	2.61	0.47
2:B:954:VAL:O	12:L:55:ILE:O	2.32	0.47
12:L:61:THR:HG22	12:L:63:ARG:H	1.79	0.47
1:A:1207:LEU:HD11	1:A:1273:LEU:HD23	1.96	0.47
1:A:1342:GLU:CG	5:E:198:ILE:HD13	2.45	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1385:THR:HG21	1:A:1387:HIS:HD2	1.80	0.47
1:A:1433:MET:HE3	7:G:63:PRO:HB2	1.97	0.47
2:B:294:ASP:C	2:B:296:GLU:H	2.15	0.47
2:B:558:LEU:CD2	2:B:596:LEU:HD11	2.45	0.47
2:B:593:PRO:O	2:B:595:ARG:N	2.48	0.47
2:B:882:THR:HG23	2:B:884:ARG:H	1.79	0.47
3:C:22:LEU:HD22	3:C:230:MET:CE	2.44	0.47
5:E:106:GLN:HE22	5:E:129:PRO:HB2	1.80	0.47
5:E:134:THR:O	5:E:135:PHE:CD1	2.68	0.47
5:E:186:LEU:O	5:E:187:TYR:C	2.50	0.47
6:F:76:LYS:HA	6:F:79:ARG:CD	2.42	0.47
1:A:567:LYS:HE3	8:H:46:LEU:HD13	1.97	0.47
9:I:8:ARG:O	9:I:10:CYS:N	2.47	0.47
11:K:13:GLY:O	11:K:14:GLU:C	2.53	0.47
12:L:30:ILE:CG2	12:L:31:CYS:N	2.77	0.47
2:B:955:THR:OG1	12:L:55:ILE:HA	2.15	0.47
1:A:1397:LEU:HB2	1:A:1426:GLU:OE1	2.14	0.47
1:A:203:SER:HB2	1:A:205:GLU:OE1	2.15	0.47
1:A:34:LYS:HZ1	1:A:57:ARG:HH21	1.63	0.47
1:A:399:HIS:O	1:A:400:PRO:C	2.53	0.47
1:A:675:THR:HG21	1:A:736:ASN:CB	2.45	0.47
1:A:997:LEU:HD13	1:A:1018:PHE:HE2	1.80	0.47
2:B:1007:VAL:HG22	2:B:1008:PRO:N	2.30	0.47
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.50	0.47
2:B:280:ILE:HB	2:B:285:ILE:HD11	1.96	0.47
2:B:485:ARG:HG3	2:B:781:PHE:CD1	2.50	0.47
3:C:45:ALA:O	3:C:159:ALA:HA	2.15	0.47
7:G:51:TYR:C	7:G:51:TYR:CD2	2.89	0.47
8:H:44:VAL:CG1	8:H:48:PRO:HA	2.45	0.47
10:J:34:THR:O	10:J:35:ALA:C	2.53	0.47
1:A:202:LEU:N	1:A:202:LEU:HD23	2.30	0.46
1:A:316:GLN:O	1:A:317:LYS:C	2.53	0.46
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.97	0.46
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.50	0.46
1:A:33:ALA:HA	1:A:57:ARG:NH1	2.30	0.46
1:A:598:LEU:O	1:A:599:SER:C	2.53	0.46
1:A:65:LEU:O	1:A:66:LYS:C	2.54	0.46
1:A:752:LYS:HD3	1:A:752:LYS:HA	1.66	0.46
2:B:1079:LYS:HG2	2:B:1080:LYS:N	2.30	0.46
2:B:565:PRO:O	2:B:567:GLU:N	2.48	0.46
2:B:654:ARG:O	2:B:656:GLY:N	2.48	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:177:GLU:HG3	3:C:231:ASN:CB	2.38	0.46
4:D:69:ALA:CB	4:D:72:ARG:NH1	2.76	0.46
5:E:112:TYR:O	5:E:137:GLU:HG3	2.14	0.46
5:E:72:PHE:CD1	5:E:72:PHE:N	2.82	0.46
6:F:101:ILE:HD13	6:F:120:ILE:CG2	2.45	0.46
7:G:117:GLN:OE1	7:G:117:GLN:N	2.48	0.46
7:G:1:MET:SD	7:G:79:PHE:HD1	2.38	0.46
8:H:104:PHE:CD2	8:H:136:LYS:HG3	2.51	0.46
9:I:86:PHE:CE1	9:I:100:PHE:HB2	2.49	0.46
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.50	0.46
1:A:1451:VAL:C	1:A:1453:TYR:H	2.17	0.46
1:A:219:PHE:O	1:A:222:LEU:HB2	2.15	0.46
1:A:583:PRO:HG2	1:A:586:ILE:CG1	2.45	0.46
1:A:676:MET:O	1:A:679:ILE:HB	2.15	0.46
1:A:821:ARG:CB	1:A:821:ARG:HH11	2.24	0.46
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.50	0.46
1:A:867:ILE:HD11	1:A:1000:LEU:HD21	1.97	0.46
2:B:121:ASN:HA	2:B:207:GLY:CA	2.45	0.46
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.50	0.46
2:B:278:GLN:CG	2:B:279:ASP:N	2.53	0.46
2:B:637:LEU:HD21	2:B:742:GLU:OE2	2.15	0.46
2:B:35:SER:HA	2:B:811:TYR:HE2	1.80	0.46
2:B:865:LYS:O	2:B:866:TYR:HD1	1.97	0.46
4:D:71:LYS:HG2	4:D:74:GLN:HG3	1.97	0.46
9:I:4:PHE:CZ	9:I:14:LEU:O	2.68	0.46
12:L:27:LEU:HD13	12:L:37:LYS:HD2	1.97	0.46
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.15	0.46
1:A:1285:MET:O	1:A:1305:VAL:N	2.47	0.46
1:A:254:GLU:O	1:A:256:GLN:N	2.48	0.46
1:A:427:GLN:O	1:A:428:TYR:C	2.53	0.46
1:A:709:THR:N	1:A:712:GLU:HB2	2.30	0.46
1:A:733:ALA:O	1:A:737:LEU:HG	2.14	0.46
2:B:1095:LEU:HD12	2:B:1095:LEU:H	1.80	0.46
2:B:373:ARG:HA	2:B:566:LEU:CD2	2.45	0.46
2:B:615:MET:HA	2:B:625:LYS:O	2.16	0.46
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.97	0.46
3:C:124:LEU:C	3:C:126:GLY:N	2.69	0.46
6:F:125:LEU:C	6:F:125:LEU:HD23	2.36	0.46
7:G:18:PHE:HA	7:G:22:MET:CE	2.44	0.46
1:A:107:CYS:HB2	1:A:114:LEU:CD2	2.46	0.46
1:A:106:VAL:CG1	1:A:107:CYS:N	2.78	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1206:ASP:HB2	1:A:1274:ARG:HH22	1.81	0.46
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.44	0.46
1:A:22:PHE:CD2	1:A:27:VAL:HG22	2.49	0.46
1:A:353:ILE:CD1	1:A:487:MET:HE2	2.45	0.46
1:A:386:ASP:O	1:A:387:ARG:C	2.52	0.46
1:A:488:ASN:OD1	1:A:488:ASN:N	2.48	0.46
1:A:49:LYS:CD	1:A:55:ASP:HB3	2.46	0.46
1:A:523:ILE:HG13	1:A:622:VAL:HG22	1.96	0.46
1:A:670:ILE:HG12	1:A:805:LEU:HD21	1.96	0.46
1:A:824:LEU:O	1:A:827:THR:HG22	2.16	0.46
1:A:341:MET:CE	1:A:843:LYS:HZ3	2.27	0.46
1:A:914:GLU:HB2	1:A:979:SER:O	2.16	0.46
1:A:973:ILE:HG22	1:A:973:ILE:O	2.14	0.46
2:B:25:ILE:CD1	2:B:653:VAL:O	2.64	0.46
2:B:703:ILE:HA	2:B:740:HIS:O	2.15	0.46
3:C:89:GLU:O	3:C:90:ASP:CB	2.64	0.46
4:D:153:ARG:HB3	4:D:154:PHE:CD2	2.50	0.46
5:E:102:GLU:C	5:E:104:ASN:H	2.16	0.46
7:G:138:THR:OG1	7:G:139:ILE:N	2.48	0.46
1:A:1387:HIS:CE1	13:N:4:DA:H4'	2.51	0.46
1:A:1173:HIS:O	1:A:1174:PHE:CD2	2.68	0.46
1:A:1170:ILE:HG22	1:A:1174:PHE:CZ	2.50	0.46
1:A:1308:THR:HG23	1:A:1310:GLY:H	1.80	0.46
1:A:153:PRO:HA	1:A:161:LEU:HA	1.98	0.46
1:A:388:LEU:HD22	1:A:432:VAL:CB	2.46	0.46
1:A:504:LEU:HD12	1:A:504:LEU:N	2.29	0.46
1:A:673:GLY:O	1:A:676:MET:HB2	2.16	0.46
2:B:1070:GLU:OE1	10:J:44:TYR:OH	2.34	0.46
2:B:1097:HIS:N	2:B:1098:MET:HE2	2.30	0.46
2:B:326:ASP:OD1	2:B:329:THR:CB	2.64	0.46
2:B:570:VAL:CG2	2:B:573:GLN:HB3	2.46	0.46
2:B:707:PRO:CG	2:B:708:GLU:N	2.77	0.46
2:B:886:LYS:HE2	2:B:940:PRO:HD3	1.96	0.46
2:B:893:LEU:HD22	2:B:897:GLY:C	2.35	0.46
3:C:226:ASP:O	3:C:227:THR:CB	2.63	0.46
4:D:217:LEU:O	4:D:219:THR:N	2.48	0.46
5:E:44:ALA:O	5:E:45:LYS:HB2	2.15	0.46
6:F:90:ARG:HE	6:F:94:LEU:CD1	2.28	0.46
7:G:137:ILE:CG2	7:G:143:ILE:HD11	2.46	0.46
8:H:8:ASP:OD2	8:H:9:ILE:N	2.40	0.46
9:I:7:CYS:HB2	9:I:34:TYR:CG	2.51	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:63:TYR:O	10:J:64:ASN:CB	2.61	0.46
11:K:31:VAL:HG12	11:K:32:VAL:N	2.31	0.46
1:A:456:MET:HE2	1:A:478:TYR:OH	2.15	0.46
1:A:565:ILE:CG2	1:A:567:LYS:HE2	2.46	0.46
1:A:567:LYS:NZ	8:H:43:ASN:HD22	2.13	0.46
1:A:774:ARG:CZ	1:A:797:LYS:CB	2.93	0.46
2:B:247:GLY:C	2:B:249:ARG:H	2.19	0.46
2:B:308:TRP:N	2:B:311:LEU:HD12	2.31	0.46
2:B:398:ARG:CB	2:B:398:ARG:HH11	2.27	0.46
2:B:427:ASP:HA	2:B:430:ARG:HD2	1.97	0.46
2:B:37:PHE:CE2	2:B:542:MET:HA	2.42	0.46
4:D:17:LYS:C	4:D:17:LYS:HD2	2.35	0.46
4:D:66:ARG:C	4:D:68:ARG:N	2.68	0.46
5:E:37:LEU:C	5:E:37:LEU:HD12	2.35	0.46
5:E:55:ARG:C	5:E:57:MET:N	2.68	0.46
1:A:852:TYR:CD1	6:F:136:ARG:HB3	2.51	0.46
4:D:40:HIS:CG	7:G:73:LYS:HD3	2.51	0.46
9:I:69:PRO:HG2	9:I:85:PHE:CE2	2.51	0.46
10:J:1:MET:N	10:J:57:ILE:HG22	2.31	0.46
12:L:34:CYS:CB	12:L:51:CYS:HG	2.29	0.46
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.15	0.46
1:A:154:SER:CB	1:A:162:VAL:HG21	2.42	0.46
1:A:543:LEU:O	1:A:544:ASP:C	2.53	0.46
1:A:798:GLY:HA2	1:A:815:PHE:CD1	2.50	0.46
2:B:63:ILE:HG12	2:B:130:VAL:HG21	1.97	0.46
2:B:603:LEU:HD13	2:B:608:ASP:CB	2.41	0.46
2:B:964:VAL:HG22	2:B:965:LYS:N	2.31	0.46
3:C:116:LYS:HG3	3:C:117:ASP:N	2.30	0.46
4:D:40:HIS:CD2	7:G:73:LYS:HD3	2.50	0.46
9:I:111:THR:CG2	9:I:113:ASP:HB2	2.46	0.46
9:I:98:VAL:HG11	9:I:111:THR:HG22	1.98	0.46
1:A:1100:ARG:NH2	1:A:1351:GLU:HG3	2.31	0.46
1:A:1366:ARG:HG2	1:A:1366:ARG:HH11	1.80	0.46
1:A:482:PHE:N	1:A:482:PHE:CD2	2.81	0.46
1:A:686:ALA:O	1:A:690:VAL:HG23	2.15	0.46
1:A:69:THR:C	1:A:71:GLN:N	2.66	0.46
1:A:713:SER:O	1:A:717:ASN:ND2	2.49	0.46
1:A:851:HIS:HB2	1:A:855:THR:CG2	2.46	0.46
1:A:92:HIS:O	1:A:94:GLY:N	2.48	0.46
2:B:1096:ARG:HB2	2:B:1096:ARG:HH11	1.79	0.46
2:B:1147:LEU:O	2:B:1151:LEU:HD13	2.16	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:408:LEU:HD11	2:B:545:ILE:HD12	1.97	0.46
2:B:497:ARG:NH2	2:B:775:LYS:HZ3	2.14	0.46
2:B:844:SER:O	2:B:847:ASP:HB2	2.16	0.46
3:C:133:ILE:CD1	3:C:236:GLY:C	2.84	0.46
7:G:35:GLU:HG3	7:G:48:VAL:HG23	1.98	0.46
8:H:113:ALA:HB1	8:H:124:ARG:HE	1.81	0.46
8:H:77:ARG:O	8:H:79:TRP:N	2.49	0.46
9:I:55:THR:HG1	9:I:100:PHE:HD2	1.63	0.46
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.98	0.46
11:K:40:HIS:O	11:K:41:THR:C	2.54	0.46
1:A:1202:MET:HE1	1:A:1207:LEU:HB3	1.98	0.46
1:A:1323:ASP:CG	1:A:1325:THR:HG22	2.34	0.46
1:A:387:ARG:O	1:A:390:GLN:HB3	2.15	0.46
1:A:50:ILE:O	1:A:52:GLY:N	2.48	0.46
1:A:692:ASP:C	1:A:694:THR:N	2.68	0.46
1:A:71:GLN:C	1:A:73:GLY:H	2.20	0.46
2:B:126:SER:CB	2:B:172:ILE:HD11	2.46	0.46
2:B:288:ALA:HB1	2:B:331:LEU:HD12	1.98	0.46
2:B:398:ARG:NH1	2:B:398:ARG:CB	2.79	0.46
2:B:508:LEU:HD11	2:B:510:LYS:NZ	2.30	0.46
2:B:642:ASP:O	2:B:644:GLU:N	2.49	0.46
2:B:658:ILE:HG22	2:B:662:MET:HE2	1.97	0.46
2:B:663:ALA:O	2:B:667:GLN:HG3	2.16	0.46
2:B:792:MET:O	2:B:793:ALA:HB2	2.15	0.46
2:B:803:LEU:HB2	2:B:1032:SER:OG	2.16	0.46
2:B:810:GLU:HA	2:B:815:ARG:NH2	2.31	0.46
3:C:63:ILE:O	3:C:66:ARG:HG3	2.16	0.46
4:D:16:LYS:C	4:D:18:VAL:H	2.20	0.46
9:I:6:PHE:CB	9:I:12:ASN:O	2.54	0.46
11:K:102:LYS:O	11:K:106:GLU:HG3	2.16	0.46
1:A:108:MET:O	1:A:109:HIS:CB	2.63	0.46
1:A:1242:VAL:CG1	1:A:1243:VAL:N	2.78	0.46
1:A:1443:VAL:CG1	6:F:132:LEU:HD13	2.46	0.46
1:A:88:LYS:HD3	1:A:293:GLU:CD	2.36	0.46
1:A:447:GLN:HB3	1:A:448:PRO:HA	1.97	0.46
1:A:969:GLN:O	1:A:969:GLN:HG3	2.16	0.46
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.51	0.46
2:B:638:PHE:CD2	2:B:690:VAL:HG22	2.51	0.46
2:B:797:TYR:HE1	2:B:854:LEU:CD2	2.29	0.46
2:B:836:GLU:O	2:B:837:ASP:HB2	2.15	0.46
3:C:123:ASN:HD21	3:C:125:MET:HG2	1.81	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:LYS:NZ	3:C:194:GLU:HA	2.31	0.46
3:C:233:GLU:HG2	3:C:234:SER:N	2.31	0.46
5:E:197:LYS:NZ	5:E:199:ILE:HD11	2.31	0.46
5:E:78:LEU:CD2	5:E:80:VAL:HG23	2.23	0.46
8:H:37:LYS:H	8:H:126:GLU:CB	2.29	0.46
9:I:17:ARG:HG2	9:I:28:GLU:HG2	1.98	0.46
11:K:50:LEU:HD11	11:K:75:ILE:HD13	1.97	0.46
1:A:1077:THR:HB	1:A:1078:GLN:HE21	1.80	0.45
1:A:1280:GLU:O	1:A:1281:ARG:C	2.54	0.45
1:A:205:GLU:CD	1:A:205:GLU:N	2.63	0.45
1:A:351:THR:HG22	2:B:1103:ILE:CA	2.37	0.45
1:A:360:GLU:O	1:A:361:LEU:C	2.53	0.45
1:A:34:LYS:CB	1:A:36:ARG:HH21	2.29	0.45
1:A:381:THR:C	1:A:383:TYR:N	2.69	0.45
1:A:493:GLN:HA	1:A:493:GLN:NE2	2.31	0.45
1:A:495:GLU:O	1:A:498:ARG:HG3	2.16	0.45
1:A:500:GLU:O	1:A:504:LEU:HB2	2.16	0.45
1:A:857:ARG:NH2	6:F:139:PRO:HG3	2.30	0.45
2:B:96:TYR:N	2:B:129:PHE:O	2.33	0.45
2:B:23:ALA:HB1	2:B:24:PRO:CD	2.41	0.45
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.30	0.45
2:B:842:ASN:HD22	2:B:845:SER:N	1.98	0.45
3:C:234:SER:OG	3:C:235:VAL:N	2.49	0.45
4:D:54:GLU:OE1	4:D:164:ILE:HD11	2.16	0.45
4:D:51:ASN:O	4:D:52:LEU:C	2.54	0.45
6:F:75:PRO:HG2	6:F:77:ASP:O	2.16	0.45
8:H:27:GLU:HG2	8:H:39:THR:HA	1.97	0.45
10:J:9:SER:OG	10:J:48:ARG:NH2	2.49	0.45
11:K:67:PHE:N	11:K:67:PHE:CD2	2.85	0.45
11:K:7:PHE:C	11:K:7:PHE:CD1	2.89	0.45
1:A:151:ASP:HA	1:A:162:VAL:O	2.16	0.45
2:B:1017:ILE:N	2:B:1018:PRO:CD	2.75	0.45
2:B:123:THR:HG21	2:B:458:LYS:HE2	1.97	0.45
2:B:226:PHE:HA	2:B:395:GLN:CG	2.46	0.45
2:B:408:LEU:N	2:B:408:LEU:HD12	2.31	0.45
2:B:411:PRO:O	2:B:414:ALA:HB3	2.16	0.45
2:B:26:THR:CB	2:B:708:GLU:OE1	2.62	0.45
2:B:782:LEU:HB3	2:B:784:ASN:OD1	2.16	0.45
2:B:990:ILE:HG22	2:B:991:GLY:H	1.82	0.45
3:C:238:ILE:HD13	3:C:242:GLN:HB3	1.98	0.45
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:48:VAL:HG13	7:G:74:TYR:HD1	1.81	0.45
8:H:96:VAL:HG13	8:H:142:LEU:O	2.17	0.45
8:H:38:LEU:HD13	8:H:125:LEU:CD1	2.44	0.45
10:J:8:PHE:H	10:J:49:MET:CE	2.29	0.45
12:L:70:ARG:HG2	12:L:70:ARG:NH1	2.31	0.45
1:A:973:ILE:CD1	1:A:1037:LEU:HA	2.46	0.45
1:A:1399:ARG:HB3	1:A:1408:ILE:HD13	1.98	0.45
1:A:482:PHE:CE1	2:B:836:GLU:HB2	2.51	0.45
1:A:700:ASN:HB2	9:I:98:VAL:CG2	2.46	0.45
1:A:839:ARG:NH1	1:A:839:ARG:CG	2.77	0.45
2:B:281:PRO:C	2:B:283:VAL:H	2.20	0.45
2:B:593:PRO:C	2:B:595:ARG:N	2.69	0.45
2:B:801:LYS:N	10:J:52:THR:HG22	2.31	0.45
2:B:880:THR:HG21	2:B:934:LYS:HG3	1.97	0.45
2:B:969:ARG:HG2	2:B:970:THR:N	2.30	0.45
2:B:990:ILE:CG2	2:B:991:GLY:N	2.80	0.45
3:C:148:ARG:HG2	3:C:149:LYS:N	2.31	0.45
3:C:181:ASP:OD1	3:C:185:LYS:HB2	2.15	0.45
3:C:82:TYR:O	3:C:84:ARG:N	2.49	0.45
5:E:171:LYS:HG2	5:E:174:GLN:CD	2.36	0.45
5:E:54:GLN:O	5:E:57:MET:HB3	2.17	0.45
7:G:13:LEU:HD21	7:G:17:PHE:CB	2.46	0.45
7:G:88:ASP:CB	7:G:144:ARG:HA	2.38	0.45
9:I:98:VAL:CG1	9:I:111:THR:HG22	2.47	0.45
10:J:27:GLU:C	10:J:29:GLU:H	2.20	0.45
3:C:10:ILE:N	11:K:108:GLU:OE1	2.49	0.45
11:K:54:ARG:HH11	11:K:54:ARG:HG3	1.82	0.45
1:A:1161:THR:C	1:A:1163:ILE:N	2.69	0.45
1:A:1215:ARG:HA	1:A:1215:ARG:NE	2.31	0.45
1:A:1235:LYS:HB3	1:A:1237:ILE:HD11	1.97	0.45
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.62	0.45
1:A:1259:MET:HE2	1:A:1263:ILE:HD11	1.97	0.45
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.46	0.45
1:A:135:PHE:CE1	1:A:222:LEU:HD22	2.52	0.45
1:A:1396:ALA:O	1:A:1400:CYS:HB3	2.17	0.45
1:A:153:PRO:O	1:A:154:SER:O	2.33	0.45
1:A:202:LEU:HA	1:A:206:GLU:OE1	2.17	0.45
1:A:211:PHE:HD1	1:A:214:ILE:HD12	1.81	0.45
1:A:524:VAL:CG1	1:A:525:GLN:H	2.27	0.45
1:A:688:LYS:O	1:A:690:VAL:N	2.49	0.45
1:A:852:TYR:CD2	1:A:1060:PRO:CB	2.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:ASP:O	2:B:334:ILE:N	2.43	0.45
2:B:604:ARG:C	2:B:606:LYS:N	2.69	0.45
2:B:850:LEU:HD12	2:B:850:LEU:C	2.36	0.45
3:C:66:ARG:C	3:C:68:GLY:N	2.69	0.45
3:C:46:ILE:CD1	3:C:67:LEU:HB3	2.45	0.45
4:D:69:ALA:C	4:D:71:LYS:N	2.70	0.45
5:E:157:SER:N	5:E:160:GLU:OE1	2.47	0.45
8:H:40:LEU:HD22	8:H:123:MET:CE	2.46	0.45
9:I:61:ASP:O	9:I:63:GLY:N	2.49	0.45
1:A:107:CYS:HB2	1:A:114:LEU:HD21	1.97	0.45
1:A:1097:GLY:H	1:A:1355:VAL:HG23	1.80	0.45
1:A:1148:ILE:HD11	1:A:1198:ASP:CA	2.44	0.45
1:A:1138:ILE:HG21	1:A:1316:VAL:HG13	1.99	0.45
1:A:427:GLN:HB2	1:A:430:TRP:CD2	2.52	0.45
1:A:493:GLN:HE21	1:A:493:GLN:CA	2.27	0.45
1:A:527:THR:HG21	1:A:650:GLN:HA	1.98	0.45
1:A:826:ASP:O	1:A:830:LYS:N	2.41	0.45
2:B:291:ILE:HG22	2:B:297:ILE:CG1	2.46	0.45
2:B:418:LYS:C	2:B:420:LEU:N	2.69	0.45
2:B:519:TRP:C	2:B:519:TRP:CD1	2.89	0.45
2:B:604:ARG:O	2:B:607:GLY:N	2.49	0.45
2:B:797:TYR:C	2:B:798:TYR:HD2	2.20	0.45
2:B:834:ASN:HA	2:B:838:SER:O	2.15	0.45
2:B:866:TYR:CG	2:B:870:ILE:HB	2.51	0.45
2:B:957:ASN:O	2:B:959:ASP:N	2.49	0.45
2:B:863:GLU:O	2:B:961:LEU:HD13	2.17	0.45
2:B:840:ILE:HG21	2:B:994:TYR:HD1	1.81	0.45
3:C:212:PRO:CB	3:C:213:PRO:HD2	2.45	0.45
4:D:12:ARG:NH1	4:D:14:ARG:CA	2.79	0.45
4:D:128:VAL:O	4:D:130:LEU:N	2.49	0.45
4:D:139:LYS:HG3	4:D:140:ASP:OD1	2.16	0.45
6:F:130:ILE:O	6:F:148:VAL:HG21	2.16	0.45
6:F:138:LEU:HB2	6:F:142:SER:HB2	1.98	0.45
8:H:100:THR:OG1	8:H:138:GLU:HG2	2.17	0.45
8:H:26:ILE:O	8:H:27:GLU:HG2	2.16	0.45
10:J:20:SER:O	10:J:24:LEU:HG	2.16	0.45
2:B:1006:ILE:HD13	10:J:44:TYR:CE2	2.51	0.45
11:K:53:ASP:HB3	11:K:56:VAL:CG2	2.46	0.45
1:A:1215:ARG:HD2	1:A:1218:GLN:HE21	1.82	0.45
1:A:1229:SER:HB2	1:A:1233:ASP:OD2	2.16	0.45
1:A:1409:LEU:O	1:A:1412:ALA:HB3	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:C	1:A:52:GLY:N	2.69	0.45
1:A:993:LEU:HD22	1:A:1046:LEU:CD2	2.47	0.45
2:B:1104:HIS:HB2	2:B:1122:ARG:HD2	1.99	0.45
2:B:204:ILE:C	2:B:205:ILE:HD12	2.37	0.45
2:B:435:THR:CG2	2:B:437:GLU:HB2	2.47	0.45
2:B:604:ARG:CA	2:B:609:ILE:HG13	2.47	0.45
2:B:896:ASP:OD2	12:L:58:LYS:HE3	2.17	0.45
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.49	0.45
3:C:109:SER:O	3:C:110:THR:C	2.55	0.45
3:C:175:ALA:O	3:C:176:ILE:CG1	2.59	0.45
3:C:23:SER:O	3:C:24:ASN:HB3	2.17	0.45
5:E:86:PRO:O	5:E:114:ASN:HB2	2.16	0.45
6:F:133:VAL:HG13	6:F:146:TRP:O	2.17	0.45
6:F:75:PRO:O	6:F:77:ASP:O	2.33	0.45
7:G:34:VAL:HG13	7:G:45:ILE:HG21	1.98	0.45
8:H:109:LYS:HG2	8:H:110:ASP:N	2.32	0.45
9:I:50:THR:HG23	9:I:51:ASN:H	1.81	0.45
11:K:52:ASN:O	11:K:54:ARG:N	2.50	0.45
1:A:1150:SER:O	1:A:1151:GLU:HG3	2.17	0.45
1:A:215:SER:O	1:A:218:ASP:HB2	2.16	0.45
1:A:554:PRO:HD2	1:A:648:ASN:OD1	2.16	0.45
1:A:590:ARG:HH11	1:A:590:ARG:HG2	1.82	0.45
1:A:722:LEU:HB3	1:A:799:PHE:CD1	2.51	0.45
1:A:806:ARG:O	2:B:761:HIS:HE1	1.99	0.45
1:A:92:HIS:O	1:A:93:VAL:C	2.55	0.45
2:B:174:LEU:HD21	2:B:204:ILE:HD11	1.97	0.45
2:B:258:LEU:O	2:B:258:LEU:CG	2.64	0.45
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.50	0.45
4:D:161:GLY:O	4:D:164:ILE:HB	2.17	0.45
5:E:211:TYR:CD1	5:E:211:TYR:N	2.84	0.45
7:G:1:MET:CE	7:G:80:LYS:O	2.65	0.45
11:K:55:LYS:CB	11:K:81:TYR:CD1	2.94	0.45
1:A:1037:LEU:HD12	1:A:1042:PHE:HA	1.99	0.45
1:A:1206:ASP:HB2	1:A:1274:ARG:HH12	1.81	0.45
1:A:182:VAL:CG2	1:A:201:VAL:HG22	2.47	0.45
1:A:219:PHE:CE1	1:A:230:ARG:HG2	2.52	0.45
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.98	0.45
1:A:372:LYS:HA	1:A:435:HIS:CE1	2.51	0.45
1:A:401:GLY:CA	1:A:435:HIS:HD2	2.30	0.45
1:A:547:LEU:HD13	11:K:58:PHE:CE1	2.52	0.45
1:A:583:PRO:O	1:A:610:GLY:HA3	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:HG21	2:B:1174:LYS:HZ2	1.82	0.45
2:B:745:PRO:O	2:B:746:SER:C	2.54	0.45
2:B:875:GLU:O	2:B:877:PRO:HD3	2.16	0.45
3:C:17:ASN:CA	3:C:240:VAL:HG11	2.47	0.45
3:C:186:LEU:N	3:C:186:LEU:CD1	2.80	0.45
3:C:191:TYR:HD2	3:C:201:TRP:CD1	2.35	0.45
5:E:26:ARG:NH1	5:E:133:GLU:OE2	2.44	0.45
6:F:148:VAL:CG2	6:F:149:GLU:N	2.80	0.45
7:G:47:CYS:O	7:G:76:ALA:HB1	2.17	0.45
8:H:82:PRO:CG	8:H:83:GLN:N	2.80	0.45
8:H:92:ASP:C	8:H:93:TYR:CD1	2.90	0.45
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.35	0.45
11:K:65:HIS:HD2	11:K:67:PHE:N	2.14	0.45
12:L:32:ALA:H	12:L:55:ILE:HG13	1.81	0.45
1:A:150:THR:HA	1:A:165:GLY:O	2.17	0.45
1:A:469:ARG:NH2	2:B:991:GLY:O	2.50	0.45
1:A:648:ASN:O	1:A:649:ILE:C	2.52	0.45
2:B:288:ALA:CB	2:B:331:LEU:HD12	2.47	0.45
2:B:435:THR:HG23	2:B:437:GLU:HB2	1.99	0.45
2:B:458:LYS:O	2:B:459:TYR:C	2.55	0.45
2:B:51:PHE:O	2:B:54:PHE:HB3	2.16	0.45
2:B:37:PHE:CD2	2:B:542:MET:SD	3.10	0.45
2:B:558:LEU:O	2:B:561:TRP:N	2.50	0.45
2:B:65:GLU:HG3	2:B:66:ASP:N	2.32	0.45
2:B:769:TYR:C	2:B:771:SER:N	2.70	0.45
3:C:91:HIS:ND1	3:C:158:VAL:HG11	2.32	0.45
3:C:167:HIS:ND1	3:C:169:LYS:HG2	2.32	0.45
3:C:69:LEU:HB3	10:J:6:ARG:HD2	1.97	0.45
4:D:60:LYS:HE3	4:D:126:ILE:HD11	1.98	0.45
5:E:212:ARG:NH1	5:E:212:ARG:HG3	2.31	0.45
5:E:31:THR:HG1	5:E:34:GLU:H	1.59	0.45
5:E:79:TRP:HE1	5:E:81:GLU:HB2	1.82	0.45
7:G:138:THR:O	7:G:140:LYS:N	2.50	0.45
1:A:1033:GLN:O	1:A:1036:ARG:NH1	2.50	0.45
1:A:1140:HIS:HA	1:A:1275:GLY:HA3	1.98	0.45
1:A:1241:ARG:O	1:A:1242:VAL:CG2	2.64	0.45
1:A:517:ASN:ND2	1:A:1364:ASN:HD22	2.15	0.45
1:A:1377:THR:O	1:A:1379:GLY:N	2.50	0.45
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.17	0.45
1:A:228:PHE:HE2	4:D:15:LEU:CD2	2.29	0.45
1:A:22:PHE:HE2	1:A:30:ILE:HD12	1.82	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:942:PHE:C	1:A:942:PHE:CD2	2.90	0.45
2:B:1147:LEU:HD23	2:B:1147:LEU:O	2.17	0.45
2:B:233:PRO:HG2	2:B:234:ILE:CD1	2.47	0.45
2:B:500:THR:O	2:B:501:PRO:C	2.56	0.45
3:C:6:PRO:HB2	11:K:101:LEU:HD12	1.99	0.45
8:H:33:GLN:HG2	8:H:129:TYR:CE2	2.52	0.45
10:J:34:THR:C	10:J:36:LEU:N	2.70	0.45
3:C:147:LEU:HA	10:J:61:LEU:HD21	1.98	0.45
11:K:110:ASN:C	11:K:112:GLN:H	2.21	0.45
12:L:27:LEU:N	12:L:27:LEU:CD2	2.79	0.45
1:A:100:LYS:O	1:A:103:CYS:HB2	2.16	0.44
1:A:1148:ILE:O	1:A:1149:ALA:HB2	2.17	0.44
1:A:1339:LEU:CD1	5:E:147:HIS:CD2	2.99	0.44
1:A:199:LEU:N	1:A:199:LEU:HD23	2.32	0.44
1:A:600:PRO:C	1:A:602:ASP:H	2.20	0.44
1:A:939:ASP:O	1:A:942:PHE:HB3	2.17	0.44
1:A:78:PRO:HB2	2:B:1201:LYS:HE3	1.99	0.44
2:B:1219:ASP:C	2:B:1219:ASP:OD1	2.55	0.44
2:B:185:THR:O	2:B:186:GLU:C	2.55	0.44
3:C:87:PHE:CD1	3:C:87:PHE:N	2.85	0.44
1:A:1224:LEU:HG	1:A:1226:VAL:HG23	2.00	0.44
1:A:1394:THR:HG22	1:A:1398:MET:SD	2.57	0.44
1:A:1427:ASN:O	1:A:1431:GLY:N	2.47	0.44
1:A:185:TRP:CH2	1:A:200:ARG:HG2	2.52	0.44
1:A:471:ASN:O	1:A:474:VAL:HG12	2.18	0.44
1:A:566:ILE:O	1:A:567:LYS:O	2.36	0.44
1:A:546:VAL:HG13	1:A:577:ILE:HG21	1.99	0.44
1:A:841:LEU:HA	1:A:841:LEU:HD23	1.77	0.44
2:B:1022:THR:HG23	2:B:1022:THR:O	2.17	0.44
2:B:298:LEU:HD13	2:B:314:LEU:HD13	1.98	0.44
2:B:34:ILE:O	2:B:37:PHE:HB3	2.16	0.44
2:B:44:VAL:O	2:B:45:SER:C	2.56	0.44
2:B:710:LEU:O	2:B:711:GLU:HG2	2.16	0.44
2:B:871:THR:HG22	2:B:872:GLU:N	2.33	0.44
3:C:44:LEU:CD2	3:C:159:ALA:HB1	2.47	0.44
5:E:116:ILE:CG2	5:E:117:THR:N	2.80	0.44
9:I:17:ARG:HG3	9:I:28:GLU:OE1	2.17	0.44
9:I:58:VAL:HG13	9:I:62:ILE:HD13	1.98	0.44
1:A:1157:ASP:C	1:A:1159:ARG:H	2.21	0.44
1:A:120:GLU:C	1:A:122:MET:N	2.68	0.44
1:A:1383:SER:O	1:A:1388:GLY:HA3	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ALA:CA	1:A:291:GLU:HG3	2.48	0.44
1:A:463:ILE:HD11	1:A:469:ARG:HG3	1.99	0.44
1:A:545:GLN:O	1:A:546:VAL:C	2.56	0.44
1:A:722:LEU:O	1:A:725:ALA:HB3	2.17	0.44
1:A:81:PHE:CZ	2:B:1208:MET:HE2	2.52	0.44
2:B:1033:LYS:HA	2:B:1089:PRO:HD2	1.99	0.44
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.43	0.44
2:B:38:PHE:HD1	2:B:811:TYR:CD2	2.36	0.44
2:B:653:VAL:HG13	2:B:657:HIS:CB	2.47	0.44
2:B:791:THR:O	2:B:792:MET:O	2.35	0.44
2:B:877:PRO:C	2:B:878:GLN:HG3	2.38	0.44
2:B:901:PRO:HD2	12:L:59:ALA:O	2.17	0.44
2:B:904:ARG:NH1	12:L:66:GLN:O	2.51	0.44
8:H:40:LEU:HB2	8:H:123:MET:CE	2.47	0.44
11:K:107:THR:O	11:K:111:LEU:HG	2.16	0.44
12:L:38:LEU:HG	12:L:39:SER:N	2.18	0.44
1:A:1319:VAL:O	1:A:1322:ILE:HG12	2.18	0.44
1:A:49:LYS:NZ	1:A:60:SER:HA	2.32	0.44
1:A:58:LEU:HD21	1:A:82:GLY:HA3	2.00	0.44
1:A:740:LEU:HD12	1:A:741:ASN:N	2.32	0.44
1:A:81:PHE:CE1	2:B:1208:MET:HE2	2.52	0.44
2:B:20:ASP:C	2:B:22:SER:N	2.70	0.44
2:B:307:ASP:O	2:B:309:GLN:N	2.51	0.44
2:B:364:ILE:HG22	2:B:365:THR:N	2.32	0.44
2:B:30:SER:HB3	2:B:743:ILE:O	2.18	0.44
2:B:879:ARG:HH22	2:B:885:MET:CE	2.30	0.44
2:B:882:THR:C	2:B:884:ARG:H	2.20	0.44
2:B:769:TYR:HD1	2:B:987:LYS:NZ	2.15	0.44
3:C:259:LEU:CD2	11:K:91:CYS:HB3	2.47	0.44
4:D:12:ARG:HH11	4:D:12:ARG:CG	2.28	0.44
4:D:46:GLU:HG2	4:D:47:LEU:N	2.32	0.44
5:E:134:THR:C	5:E:135:PHE:CD1	2.85	0.44
6:F:127:GLU:O	6:F:128:LYS:C	2.56	0.44
7:G:111:THR:CG2	7:G:114:LEU:HB2	2.46	0.44
10:J:21:TYR:HB2	10:J:39:LEU:HD11	2.00	0.44
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.16	0.44
1:A:108:MET:H	1:A:171:GLN:HE22	1.64	0.44
1:A:1220:PHE:O	1:A:1221:LYS:CB	2.65	0.44
1:A:1387:HIS:HA	1:A:1391:ARG:HE	1.81	0.44
1:A:22:PHE:HE2	1:A:30:ILE:CD1	2.30	0.44
1:A:256:GLN:O	1:A:257:ARG:HG3	2.18	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:GLN:O	1:A:312:PRO:C	2.56	0.44
1:A:353:ILE:HD12	1:A:487:MET:CE	2.47	0.44
1:A:555:ASP:O	1:A:556:TRP:O	2.35	0.44
1:A:600:PRO:CG	1:A:601:LYS:N	2.80	0.44
2:B:242:SER:HB2	2:B:362:PRO:HG2	2.00	0.44
2:B:509:ALA:O	2:B:510:LYS:C	2.55	0.44
2:B:847:ASP:C	2:B:849:GLY:H	2.21	0.44
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.37	0.44
1:A:667:GLY:HA3	3:C:192:TRP:CH2	2.52	0.44
4:D:126:ILE:HD13	4:D:145:MET:CE	2.48	0.44
5:E:124:VAL:HB	5:E:125:PRO:CD	2.46	0.44
6:F:90:ARG:O	6:F:91:ALA:C	2.56	0.44
1:A:504:LEU:CD1	6:F:91:ALA:CB	2.96	0.44
6:F:99:LEU:O	6:F:103:MET:CG	2.59	0.44
8:H:12:VAL:HB	8:H:52:GLN:N	2.32	0.44
8:H:58:THR:HG22	8:H:59:ILE:N	2.28	0.44
9:I:85:PHE:N	9:I:85:PHE:CD2	2.74	0.44
1:A:1187:GLN:HA	1:A:1244:ARG:HB2	1.99	0.44
1:A:123:ARG:HA	1:A:126:LEU:HD12	1.98	0.44
1:A:226:GLU:HG2	1:A:226:GLU:O	2.16	0.44
1:A:219:PHE:CE2	1:A:231:PRO:HD2	2.53	0.44
1:A:316:GLN:NE2	1:A:317:LYS:HZ2	2.15	0.44
1:A:458:HIS:HE2	1:A:478:TYR:HH	1.62	0.44
1:A:723:ASN:O	1:A:724:GLU:C	2.56	0.44
1:A:916:GLY:C	1:A:919:ILE:HG22	2.37	0.44
2:B:1065:GLN:HB3	2:B:1069:PHE:O	2.18	0.44
2:B:1107:ALA:O	2:B:1108:ARG:O	2.35	0.44
2:B:1119:VAL:HB	2:B:1124:ARG:NH2	2.32	0.44
2:B:293:PRO:O	2:B:294:ASP:O	2.36	0.44
2:B:770:GLN:CD	2:B:983:ARG:HA	2.36	0.44
3:C:59:ALA:O	3:C:62:PHE:HB3	2.17	0.44
3:C:8:VAL:HG12	3:C:9:LYS:N	2.32	0.44
3:C:97:VAL:HG12	3:C:99:LEU:CD2	2.48	0.44
5:E:110:PHE:CD1	5:E:110:PHE:C	2.91	0.44
5:E:136:ASN:OD1	5:E:137:GLU:N	2.50	0.44
7:G:44:TYR:CE2	7:G:105:PRO:HB2	2.53	0.44
12:L:28:LYS:HB3	12:L:39:SER:CB	2.47	0.44
1:A:1239:ARG:HH12	1:A:1241:ARG:HH12	1.64	0.44
1:A:1313:LEU:C	1:A:1315:GLU:N	2.70	0.44
1:A:341:MET:HE1	1:A:843:LYS:HZ3	1.83	0.44
1:A:381:THR:CG2	1:A:382:PRO:CD	2.93	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:GLN:HE21	1:A:394:ASN:ND2	2.07	0.44
1:A:493:GLN:CA	1:A:493:GLN:NE2	2.80	0.44
1:A:517:ASN:ND2	1:A:1364:ASN:HB2	2.33	0.44
1:A:567:LYS:HZ1	8:H:43:ASN:HD22	1.65	0.44
1:A:722:LEU:O	1:A:723:ASN:C	2.56	0.44
1:A:994:GLN:O	1:A:996:ASN:N	2.51	0.44
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.53	0.44
2:B:542:MET:HE2	2:B:747:MET:HG3	2.00	0.44
2:B:857:ARG:HD2	2:B:945:GLU:OE1	2.17	0.44
3:C:44:LEU:HD13	3:C:129:ILE:HG23	1.99	0.44
15:P:4:C:H2'	15:P:5:C:C6	2.52	0.44
1:A:1042:PHE:CE2	1:A:1046:LEU:HD11	2.52	0.44
1:A:1167:GLU:HA	1:A:1170:ILE:HD11	1.98	0.44
1:A:1199:ARG:O	1:A:1200:ALA:C	2.57	0.44
1:A:298:PHE:CD2	1:A:299:HIS:HD2	2.36	0.44
1:A:382:PRO:HB3	1:A:428:TYR:HE2	1.82	0.44
1:A:497:THR:CG2	1:A:498:ARG:N	2.81	0.44
1:A:526:ASP:O	1:A:528:LEU:N	2.51	0.44
1:A:604:GLY:O	1:A:605:MET:HB2	2.18	0.44
1:A:650:GLN:HB3	1:A:654:ASN:ND2	2.33	0.44
1:A:912:LEU:HB2	1:A:913:LEU:H	1.66	0.44
2:B:1104:HIS:CD2	2:B:1122:ARG:HB2	2.52	0.44
2:B:31:TRP:CE3	2:B:31:TRP:HA	2.53	0.44
2:B:48:LEU:O	2:B:49:ASP:C	2.56	0.44
2:B:67:SER:HB3	2:B:92:PHE:HD1	1.83	0.44
3:C:10:ILE:HG22	3:C:11:ARG:O	2.18	0.44
3:C:215:GLU:O	3:C:216:GLY:C	2.56	0.44
4:D:120:GLU:O	4:D:120:GLU:HG2	2.17	0.44
4:D:128:VAL:C	4:D:130:LEU:N	2.71	0.44
4:D:32:GLU:HG3	7:G:5:LYS:CE	2.47	0.44
5:E:81:GLU:HG2	5:E:82:PHE:N	2.33	0.44
6:F:109:VAL:HG12	6:F:123:LYS:HE3	1.94	0.44
4:D:70:PHE:HE1	7:G:51:TYR:CE1	2.35	0.44
10:J:1:MET:H2	10:J:57:ILE:HG22	1.83	0.44
11:K:53:ASP:HB3	11:K:56:VAL:HG23	2.00	0.44
1:A:1436:ILE:O	1:A:1439:GLY:N	2.44	0.44
1:A:321:PRO:O	1:A:322:VAL:CG1	2.66	0.44
1:A:398:GLU:O	1:A:399:HIS:O	2.36	0.44
1:A:50:ILE:HG22	1:A:52:GLY:H	1.82	0.44
1:A:544:ASP:OD1	1:A:545:GLN:N	2.50	0.44
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.77	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1115:THR:HG22	2:B:1117:GLN:HB2	1.99	0.44
2:B:1182:CYS:O	2:B:1183:LYS:C	2.57	0.44
2:B:220:GLY:O	2:B:221:ASN:C	2.56	0.44
2:B:305:VAL:CG1	2:B:305:VAL:O	2.65	0.44
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.83	0.44
2:B:69:LEU:HD13	2:B:432:MET:CE	2.47	0.44
2:B:43:LEU:HD11	2:B:811:TYR:O	2.18	0.44
3:C:133:ILE:CD1	3:C:237:SER:N	2.79	0.44
3:C:18:VAL:CG2	3:C:240:VAL:HB	2.47	0.44
4:D:12:ARG:NH1	4:D:13:ARG:C	2.70	0.44
4:D:138:ASN:HD21	7:G:35:GLU:HB3	1.82	0.44
4:D:140:ASP:O	4:D:144:THR:N	2.51	0.44
4:D:38:ILE:CG2	4:D:42:GLY:HA2	2.48	0.44
5:E:68:SER:O	5:E:72:PHE:O	2.35	0.44
7:G:126:ASN:C	7:G:126:ASN:HD22	2.19	0.44
8:H:14:GLU:OE1	8:H:15:VAL:O	2.36	0.44
1:A:266:LEU:HD21	1:A:303:TYR:CZ	2.53	0.43
1:A:973:ILE:HD11	1:A:1041:ALA:CB	2.48	0.43
1:A:973:ILE:HD11	1:A:1041:ALA:HB2	2.00	0.43
1:A:95:PHE:O	1:A:98:LYS:N	2.51	0.43
2:B:1176:ASN:H	2:B:1178:ASN:H	1.65	0.43
2:B:230:ALA:HB3	2:B:231:PRO:CD	2.47	0.43
3:C:181:ASP:N	3:C:182:PRO:CD	2.81	0.43
3:C:187:LYS:HD3	8:H:22:LYS:HE2	2.00	0.43
3:C:43:THR:CG2	3:C:44:LEU:N	2.51	0.43
3:C:52:GLU:HB2	12:L:64:LEU:HD21	1.99	0.43
4:D:220:LEU:HD23	4:D:221:TYR:N	2.33	0.43
5:E:59:SER:HB3	5:E:79:TRP:CZ2	2.53	0.43
7:G:80:LYS:O	7:G:82:PHE:CD1	2.71	0.43
11:K:68:PHE:HB3	11:K:70:ARG:HH11	1.82	0.43
1:A:1143:LEU:O	1:A:1146:VAL:HG23	2.17	0.43
1:A:1402:PHE:CE1	1:A:1403:GLU:HG2	2.53	0.43
1:A:144:THR:O	1:A:146:MET:HE2	2.18	0.43
1:A:332:LYS:HB2	1:A:337:ARG:NH1	2.32	0.43
1:A:35:ILE:HD13	1:A:241:VAL:HG11	1.99	0.43
1:A:392:VAL:HG13	1:A:415:LEU:HD11	2.00	0.43
1:A:409:SER:O	1:A:410:GLY:C	2.56	0.43
1:A:443:LEU:HD23	1:A:456:MET:O	2.18	0.43
2:B:1072:MET:HB2	2:B:1085:ILE:HD13	2.01	0.43
2:B:232:SER:HA	14:T:11:DA:OP1	2.18	0.43
2:B:25:ILE:HG23	2:B:29:ASP:CB	2.48	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:94:LYS:CD	5:E:98:ILE:HD11	2.47	0.43
6:F:103:MET:HE2	7:G:66:GLY:N	2.31	0.43
7:G:91:VAL:CG1	7:G:92:VAL:N	2.81	0.43
8:H:42:ILE:O	8:H:44:VAL:HG23	2.18	0.43
12:L:40:LEU:HD11	12:L:49:LYS:HZ1	1.82	0.43
1:A:1134:ILE:O	1:A:1138:ILE:HG12	2.18	0.43
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	2.01	0.43
1:A:26:GLU:O	1:A:27:VAL:C	2.56	0.43
1:A:445:ASN:CB	1:A:455:MET:HG2	2.47	0.43
1:A:903:ASN:ND2	1:A:903:ASN:C	2.69	0.43
2:B:830:TYR:HE2	2:B:1000:PRO:HD3	1.77	0.43
2:B:1034:VAL:O	2:B:1036:ALA:N	2.51	0.43
2:B:418:LYS:O	2:B:419:THR:C	2.56	0.43
2:B:1084:GLN:OE1	3:C:189:THR:CG2	2.67	0.43
3:C:258:ILE:N	3:C:258:ILE:CD1	2.79	0.43
4:D:14:ARG:CB	4:D:14:ARG:HH11	2.27	0.43
4:D:29:LEU:CD1	7:G:82:PHE:CE2	3.01	0.43
5:E:147:HIS:CD2	5:E:149:LEU:H	2.36	0.43
5:E:79:TRP:HD1	5:E:100:ILE:HD11	1.83	0.43
5:E:82:PHE:N	5:E:82:PHE:CD1	2.87	0.43
6:F:111:LEU:H	6:F:111:LEU:CD1	2.29	0.43
7:G:59:GLY:HA3	7:G:70:PHE:CE2	2.53	0.43
8:H:12:VAL:HG11	8:H:15:VAL:CG2	2.48	0.43
8:H:129:TYR:C	8:H:131:ASN:H	2.21	0.43
8:H:4:THR:HG22	8:H:6:PHE:H	1.83	0.43
9:I:100:PHE:CD1	9:I:100:PHE:N	2.85	0.43
9:I:117:LYS:N	9:I:117:LYS:HD2	2.33	0.43
12:L:33:GLU:N	12:L:33:GLU:CD	2.72	0.43
1:A:1035:TYR:CB	1:A:1037:LEU:HD23	2.47	0.43
1:A:1042:PHE:HE2	1:A:1046:LEU:HD11	1.83	0.43
1:A:1207:LEU:CD1	1:A:1273:LEU:HD23	2.48	0.43
1:A:1334:ASP:C	1:A:1336:MET:N	2.71	0.43
1:A:534:LEU:HG	1:A:534:LEU:O	2.18	0.43
1:A:545:GLN:O	1:A:548:ASN:N	2.51	0.43
1:A:758:ILE:H	1:A:758:ILE:HG13	1.55	0.43
1:A:894:GLU:O	1:A:898:ARG:CB	2.67	0.43
2:B:828:ALA:HB2	2:B:1085:ILE:HG23	1.99	0.43
2:B:1115:THR:HG22	2:B:1117:GLN:CG	2.49	0.43
2:B:217:ARG:HG2	2:B:217:ARG:NH1	2.33	0.43
2:B:550:ASP:CG	2:B:551:PRO:HD2	2.39	0.43
3:C:40:GLU:OE1	3:C:254:LYS:HE3	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:64:PRO:CB	5:E:69:ILE:HD11	2.48	0.43
8:H:130:ARG:H	8:H:130:ARG:CD	2.29	0.43
8:H:14:GLU:OE1	8:H:15:VAL:N	2.50	0.43
11:K:12:LEU:HD12	11:K:37:LYS:HG2	1.99	0.43
14:T:13:DT:H2''	14:T:14:DA:OP2	2.18	0.43
14:T:16:DT:C1'	14:T:17:DT:H5'	2.48	0.43
1:A:1029:ARG:HG3	1:A:1029:ARG:NH1	2.28	0.43
1:A:125:ALA:O	1:A:127:ALA:N	2.52	0.43
1:A:730:GLY:O	1:A:733:ALA:N	2.51	0.43
2:B:1183:LYS:CE	2:B:1183:LYS:O	2.67	0.43
2:B:496:ARG:NH1	2:B:496:ARG:HB3	2.33	0.43
2:B:540:SER:HA	2:B:749:LEU:O	2.19	0.43
2:B:705:MET:HA	2:B:705:MET:HE2	2.01	0.43
2:B:856:PHE:N	2:B:856:PHE:CD1	2.86	0.43
2:B:886:LYS:NZ	2:B:936:ASP:OD1	2.52	0.43
2:B:957:ASN:O	2:B:958:GLN:C	2.56	0.43
3:C:166:GLU:C	11:K:6:ARG:HH11	2.22	0.43
3:C:15:LYS:O	3:C:240:VAL:HG22	2.17	0.43
2:B:1001:PHE:HE2	3:C:34:ARG:CZ	2.31	0.43
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.83	0.43
4:D:120:GLU:O	4:D:123:LEU:HB2	2.18	0.43
5:E:24:LYS:HB2	5:E:30:ILE:HB	2.00	0.43
6:F:123:LYS:O	6:F:127:GLU:HG3	2.18	0.43
4:D:147:TYR:CZ	7:G:103:VAL:HG13	2.52	0.43
3:C:6:PRO:CG	11:K:101:LEU:HB2	2.43	0.43
12:L:50:ASP:HB3	12:L:51:CYS:H	1.69	0.43
1:A:1237:ILE:HG22	1:A:1238:ILE:H	1.82	0.43
1:A:298:PHE:HD2	1:A:299:HIS:CD2	2.37	0.43
1:A:482:PHE:C	1:A:484:GLY:N	2.71	0.43
1:A:577:ILE:O	1:A:578:LEU:C	2.57	0.43
1:A:590:ARG:CG	1:A:591:PHE:N	2.79	0.43
1:A:672:ASP:HB3	1:A:736:ASN:HD21	1.83	0.43
2:B:1117:GLN:HG3	2:B:1156:ASP:OD1	2.18	0.43
1:A:22:PHE:HB2	2:B:1211:ASN:CG	2.39	0.43
2:B:29:ASP:HB3	2:B:658:ILE:HD11	2.00	0.43
2:B:363:HIS:O	2:B:364:ILE:CB	2.67	0.43
2:B:371:GLU:OE1	2:B:371:GLU:N	2.52	0.43
2:B:640:VAL:HG12	2:B:640:VAL:O	2.18	0.43
2:B:903:VAL:CG1	2:B:904:ARG:N	2.81	0.43
3:C:33:LEU:HG	3:C:37:MET:CE	2.49	0.43
3:C:77:ILE:HA	3:C:77:ILE:HD13	1.88	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:126:ILE:O	4:D:128:VAL:N	2.52	0.43
4:D:35:LEU:H	4:D:35:LEU:HD12	1.83	0.43
4:D:64:VAL:C	4:D:66:ARG:N	2.72	0.43
6:F:147:SER:O	6:F:148:VAL:C	2.55	0.43
7:G:102:GLN:HG3	7:G:106:MET:O	2.18	0.43
12:L:53:HIS:O	12:L:55:ILE:N	2.50	0.43
1:A:108:MET:HB3	1:A:210:ILE:HD11	2.01	0.43
1:A:1253:GLU:O	1:A:1254:ALA:CB	2.66	0.43
1:A:224:PHE:CE2	1:A:231:PRO:HG3	2.53	0.43
1:A:577:ILE:HG13	1:A:578:LEU:N	2.34	0.43
1:A:700:ASN:C	1:A:701:LEU:HD23	2.39	0.43
1:A:761:MET:HE3	1:A:761:MET:HB2	1.85	0.43
1:A:786:HIS:N	1:A:786:HIS:HD2	2.16	0.43
1:A:962:ARG:HA	1:A:965:GLN:NE2	2.34	0.43
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.83	0.43
1:A:343:LYS:HE2	2:B:1156:ASP:OD2	2.18	0.43
2:B:203:PHE:N	2:B:203:PHE:CD1	2.87	0.43
2:B:288:ALA:HA	2:B:331:LEU:HD12	2.01	0.43
2:B:592:ASN:OD1	2:B:595:ARG:HG2	2.18	0.43
2:B:980:PHE:CD2	2:B:1094:ARG:HA	2.53	0.43
3:C:167:HIS:HA	11:K:6:ARG:NH1	2.29	0.43
3:C:44:LEU:HD21	3:C:159:ALA:HB1	2.01	0.43
3:C:66:ARG:HA	3:C:69:LEU:HD13	2.00	0.43
4:D:29:LEU:H	4:D:29:LEU:CD2	2.32	0.43
7:G:115:MET:HB3	7:G:116:PRO:CD	2.46	0.43
8:H:88:SER:O	8:H:89:LEU:HD23	2.19	0.43
9:I:55:THR:O	9:I:58:VAL:HG23	2.19	0.43
1:A:1081:LEU:HD11	1:A:1098:VAL:HG23	2.01	0.43
1:A:11:LEU:HB2	2:B:1193:GLN:CG	2.49	0.43
1:A:1289:ARG:NH1	1:A:1326:ARG:NH1	2.66	0.43
1:A:41:MET:O	1:A:42:ASP:O	2.37	0.43
1:A:353:ILE:HD11	1:A:480:ALA:HB1	2.01	0.43
1:A:808:LEU:HD23	1:A:812:GLU:O	2.19	0.43
1:A:814:PHE:O	1:A:817:ALA:HB3	2.19	0.43
1:A:853:ASP:OD1	1:A:855:THR:HB	2.18	0.43
2:B:1115:THR:CG2	2:B:1117:GLN:HB2	2.48	0.43
2:B:249:ARG:NH2	2:B:418:LYS:NZ	2.66	0.43
2:B:758:PHE:N	2:B:759:PRO:CD	2.82	0.43
2:B:903:VAL:HG12	2:B:904:ARG:N	2.32	0.43
3:C:203:GLN:HG3	3:C:207:CYS:SG	2.58	0.43
4:D:122:GLU:CA	4:D:125:SER:HB3	2.48	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:23:ASN:HA	4:D:28:GLN:O	2.18	0.43
1:A:1001:ARG:NE	6:F:83:PRO:HD3	2.34	0.43
7:G:137:ILE:HG22	7:G:138:THR:N	2.33	0.43
7:G:34:VAL:O	7:G:37:SER:HB3	2.19	0.43
8:H:94:ASP:N	8:H:94:ASP:OD1	2.52	0.43
9:I:100:PHE:N	9:I:100:PHE:HD1	2.17	0.43
10:J:14:VAL:CG1	10:J:14:VAL:O	2.65	0.43
14:T:15:DG:C2'	14:T:16:DT:H72	2.48	0.43
1:A:114:LEU:HB2	1:A:142:CYS:HB2	2.00	0.43
1:A:423:ASP:O	1:A:424:ILE:O	2.37	0.43
2:B:114:PRO:CG	2:B:181:LEU:HD11	2.48	0.43
2:B:423:LYS:O	2:B:427:ASP:HB2	2.19	0.43
2:B:553:PRO:HG2	2:B:554:ILE:HD12	2.00	0.43
2:B:637:LEU:O	2:B:690:VAL:HG13	2.19	0.43
2:B:611:PRO:CG	2:B:685:LEU:HD21	2.45	0.43
3:C:123:ASN:CG	3:C:125:MET:H	2.22	0.43
4:D:7:THR:HG21	4:D:32:GLU:CD	2.40	0.43
1:A:1006:ILE:CD1	5:E:163:GLU:HG3	2.35	0.43
5:E:161:LYS:NZ	5:E:193:GLY:O	2.43	0.43
5:E:30:ILE:HG22	5:E:31:THR:O	2.18	0.43
5:E:59:SER:O	5:E:60:PHE:HB3	2.19	0.43
1:A:1446:ASP:HB2	6:F:133:VAL:HG23	2.01	0.43
6:F:81:THR:O	6:F:82:THR:C	2.55	0.43
1:A:598:LEU:CD1	8:H:124:ARG:HB2	2.49	0.43
10:J:31:ASP:OD1	10:J:34:THR:OG1	2.34	0.43
11:K:107:THR:CG2	11:K:108:GLU:N	2.78	0.43
11:K:89:ASN:O	11:K:91:CYS:N	2.52	0.43
1:A:1227:ILE:CG2	1:A:1228:TRP:N	2.81	0.43
1:A:315:LEU:HD23	1:A:315:LEU:N	2.32	0.43
1:A:492:PRO:O	1:A:493:GLN:NE2	2.52	0.43
1:A:49:LYS:HD2	1:A:55:ASP:HB3	2.01	0.43
1:A:779:PHE:CD1	1:A:785:PRO:HD3	2.50	0.43
1:A:831:THR:O	1:A:834:THR:HB	2.19	0.43
2:B:205:ILE:C	2:B:207:GLY:N	2.71	0.43
2:B:241:ARG:HH11	2:B:241:ARG:CG	2.31	0.43
2:B:39:ARG:HH21	2:B:665:GLU:CD	2.21	0.43
2:B:610:ASN:OD1	2:B:611:PRO:HD2	2.19	0.43
2:B:790:ASP:N	2:B:790:ASP:OD2	2.39	0.43
3:C:140:ASN:O	3:C:141:GLY:O	2.36	0.43
5:E:120:ALA:O	5:E:123:LEU:CG	2.59	0.43
6:F:127:GLU:O	6:F:129:LYS:N	2.52	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:102:VAL:HG22	9:I:109:ILE:HG12	2.00	0.43
10:J:28:ASP:O	10:J:29:GLU:C	2.56	0.43
10:J:7:CYS:SG	10:J:49:MET:HE3	2.58	0.43
1:A:1213:GLY:O	1:A:1214:GLU:C	2.57	0.42
1:A:1259:MET:SD	1:A:1262:LYS:HD2	2.58	0.42
1:A:185:TRP:H	1:A:185:TRP:HE3	1.66	0.42
1:A:224:PHE:N	1:A:224:PHE:CD1	2.85	0.42
1:A:547:LEU:HA	1:A:550:LEU:HD12	2.00	0.42
1:A:856:THR:HG22	1:A:856:THR:O	2.18	0.42
1:A:855:THR:CG2	1:A:857:ARG:HE	2.16	0.42
1:A:486:GLU:OE1	2:B:1102:LYS:HD3	2.19	0.42
2:B:1165:ILE:HG22	2:B:1166:CYS:N	2.33	0.42
2:B:457:LEU:HD23	2:B:457:LEU:HA	1.91	0.42
3:C:236:GLY:O	3:C:237:SER:C	2.57	0.42
3:C:249:ASP:O	3:C:250:THR:C	2.55	0.42
3:C:39:ALA:HA	3:C:164:ALA:HB3	2.00	0.42
3:C:80:LEU:HD12	3:C:81:GLU:N	2.31	0.42
9:I:34:TYR:C	9:I:34:TYR:CD2	2.92	0.42
1:A:1119:TYR:CE1	1:A:1326:ARG:O	2.73	0.42
1:A:1163:ILE:CG2	1:A:1164:PRO:HD2	2.49	0.42
1:A:1215:ARG:HD2	1:A:1218:GLN:NE2	2.34	0.42
1:A:1424:VAL:HG11	2:B:1139:ILE:CD1	2.46	0.42
1:A:239:LEU:HA	1:A:240:PRO:HD2	1.88	0.42
1:A:794:PRO:C	1:A:796:SER:N	2.71	0.42
1:A:984:LYS:HG2	1:A:988:LEU:HD12	2.01	0.42
2:B:1079:LYS:N	3:C:27:LEU:HD21	2.33	0.42
2:B:1110:PRO:HG2	2:B:1119:VAL:HG22	2.01	0.42
2:B:1223:ASP:HB3	2:B:1224:PHE:H	1.64	0.42
2:B:352:ALA:O	2:B:353:LYS:C	2.57	0.42
2:B:354:ASP:O	2:B:357:GLN:N	2.50	0.42
2:B:589:VAL:CG1	2:B:590:HIS:N	2.81	0.42
2:B:615:MET:HB3	2:B:626:ILE:CG1	2.30	0.42
3:C:59:ALA:O	3:C:60:ASP:C	2.57	0.42
5:E:106:GLN:NE2	5:E:130:ALA:HA	2.34	0.42
5:E:48:ASP:CG	5:E:49:SER:N	2.72	0.42
5:E:67:GLU:O	5:E:70:SER:HB3	2.19	0.42
7:G:15:PRO:O	7:G:16:SER:C	2.56	0.42
7:G:9:LEU:HD12	7:G:10:ASN:N	2.31	0.42
10:J:47:ARG:CG	10:J:47:ARG:HH11	2.30	0.42
11:K:19:LEU:HA	11:K:19:LEU:HD23	1.90	0.42
1:A:1001:ARG:O	1:A:1002:GLY:C	2.57	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:GLN:O	1:A:1041:ALA:C	2.58	0.42
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.34	0.42
1:A:1202:MET:CE	1:A:1212:VAL:HG21	2.50	0.42
1:A:304:MET:O	1:A:324:SER:HB2	2.19	0.42
1:A:414:ASP:OD1	1:A:416:ARG:CG	2.64	0.42
1:A:483:ASP:O	2:B:979:LYS:CE	2.68	0.42
1:A:549:MET:CE	1:A:656:TRP:HD1	2.32	0.42
1:A:942:PHE:HE2	1:A:946:VAL:HG21	1.85	0.42
2:B:446:LEU:N	2:B:446:LEU:CD2	2.82	0.42
2:B:593:PRO:O	2:B:594:ALA:C	2.57	0.42
2:B:657:HIS:CE1	2:B:689:LEU:HD11	2.54	0.42
2:B:750:GLY:O	2:B:751:VAL:C	2.57	0.42
2:B:996:ARG:NH1	3:C:175:ALA:H	2.16	0.42
4:D:151:PHE:N	4:D:151:PHE:CD1	2.87	0.42
4:D:180:LEU:HD23	4:D:180:LEU:HA	1.88	0.42
4:D:40:HIS:CE1	7:G:7:LEU:O	2.72	0.42
5:E:153:HIS:C	5:E:154:ILE:HG13	2.40	0.42
5:E:178:ILE:HG13	5:E:182:ASP:OD2	2.19	0.42
8:H:4:THR:HG22	8:H:5:LEU:H	1.83	0.42
9:I:70:ARG:HA	9:I:83:ASN:O	2.20	0.42
11:K:30:ALA:CB	11:K:76:GLN:HB2	2.49	0.42
11:K:92:ASN:O	11:K:93:SER:C	2.57	0.42
1:A:339:ASN:O	1:A:343:LYS:HE3	2.19	0.42
1:A:868:TYR:OH	1:A:1366:ARG:HD3	2.20	0.42
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	2.02	0.42
2:B:1107:ALA:O	2:B:1108:ARG:HB3	2.20	0.42
2:B:1165:ILE:HD12	2:B:1187:ASN:HD22	1.84	0.42
1:A:12:ARG:HH21	2:B:1192:TYR:HE2	1.64	0.42
2:B:290:GLY:O	2:B:292:ILE:N	2.52	0.42
2:B:69:LEU:HD13	2:B:429:PHE:HD1	1.83	0.42
2:B:69:LEU:HD12	2:B:432:MET:HE1	2.01	0.42
2:B:638:PHE:HD2	2:B:690:VAL:HG22	1.84	0.42
2:B:64:CYS:O	2:B:65:GLU:HB3	2.18	0.42
2:B:616:ILE:HG23	2:B:700:SER:OG	2.20	0.42
2:B:637:LEU:HD11	2:B:703:ILE:HD13	2.01	0.42
2:B:800:GLN:HB3	10:J:52:THR:HG22	1.99	0.42
2:B:805:THR:CG2	2:B:806:THR:H	2.27	0.42
3:C:61:GLU:HG2	3:C:62:PHE:N	2.34	0.42
4:D:67:ARG:N	4:D:133:THR:HG21	2.35	0.42
4:D:141:LEU:O	4:D:145:MET:HG2	2.20	0.42
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.27	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:THR:CG2	9:I:94:ASP:HA	2.44	0.42
1:A:1036:ARG:HG2	1:A:1036:ARG:NH1	2.35	0.42
1:A:1141:THR:HA	1:A:1205:LYS:NZ	2.32	0.42
1:A:1144:LYS:HD2	1:A:1269:GLU:HG3	2.01	0.42
1:A:225:ASN:ND2	1:A:228:PHE:N	2.53	0.42
1:A:236:LEU:HD11	1:A:304:MET:HE1	2.01	0.42
1:A:260:ASP:OD1	1:A:262:LEU:N	2.45	0.42
1:A:305:ASP:OD1	1:A:306:ASN:N	2.53	0.42
1:A:326:ARG:HG2	1:A:326:ARG:NH1	2.31	0.42
1:A:451:HIS:O	1:A:452:LYS:C	2.56	0.42
1:A:497:THR:HG22	1:A:498:ARG:N	2.35	0.42
1:A:66:LYS:O	1:A:67:CYS:HB2	2.19	0.42
2:B:1002:THR:HG22	2:B:1072:MET:HG2	2.01	0.42
2:B:1187:ASN:HB3	2:B:1188:LYS:H	1.61	0.42
2:B:287:ARG:NE	2:B:292:ILE:O	2.52	0.42
2:B:303:TYR:HH	2:B:586:TRP:HH2	1.63	0.42
2:B:557:PHE:HZ	2:B:603:LEU:HD21	1.80	0.42
2:B:624:LEU:HA	2:B:624:LEU:HD12	1.67	0.42
2:B:638:PHE:HB3	2:B:651:LEU:HD22	2.00	0.42
2:B:67:SER:O	2:B:68:THR:O	2.38	0.42
2:B:803:LEU:HD13	2:B:1032:SER:O	2.19	0.42
4:D:119:ARG:CB	4:D:119:ARG:NH1	2.80	0.42
4:D:155:ARG:HE	4:D:219:THR:HG21	1.85	0.42
5:E:161:LYS:C	5:E:163:GLU:N	2.73	0.42
7:G:15:PRO:O	7:G:18:PHE:HD1	2.03	0.42
10:J:41:LEU:HD11	10:J:50:ILE:HG13	2.02	0.42
10:J:5:VAL:O	10:J:6:ARG:O	2.37	0.42
11:K:23:PRO:CA	11:K:31:VAL:HG13	2.47	0.42
12:L:38:LEU:HD22	12:L:48:CYS:HA	1.99	0.42
1:A:197:PRO:HG2	1:A:199:LEU:HD21	2.01	0.42
1:A:380:VAL:CG2	1:A:426:LEU:HD13	2.50	0.42
1:A:446:ARG:HD3	1:A:480:ALA:HB2	2.02	0.42
2:B:821:GLN:O	2:B:1091:TYR:HA	2.20	0.42
2:B:129:PHE:CD2	2:B:166:PHE:HA	2.55	0.42
2:B:168:GLY:HA2	2:B:450:ALA:O	2.19	0.42
2:B:309:GLN:CA	2:B:309:GLN:NE2	2.82	0.42
3:C:152:GLU:HG2	3:C:153:LEU:N	2.34	0.42
3:C:260:LEU:HD12	3:C:260:LEU:O	2.20	0.42
3:C:64:ALA:O	3:C:65:HIS:C	2.58	0.42
3:C:66:ARG:O	3:C:68:GLY:N	2.52	0.42
4:D:191:ALA:C	4:D:193:THR:H	2.23	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:117:THR:HG22	5:E:120:ALA:H	1.83	0.42
5:E:121:MET:C	5:E:123:LEU:N	2.72	0.42
6:F:131:PRO:O	6:F:132:LEU:HD23	2.19	0.42
1:A:1445:ILE:HD11	7:G:68:ALA:HB1	2.02	0.42
9:I:79:HIS:O	9:I:81:ARG:HD2	2.19	0.42
10:J:24:LEU:HD13	10:J:38:ARG:CG	2.49	0.42
11:K:19:LEU:HD22	11:K:33:ILE:CG2	2.50	0.42
11:K:8:GLU:O	11:K:37:LYS:HD2	2.19	0.42
1:A:1095:THR:HG21	1:A:1112:LYS:HD2	2.01	0.42
1:A:1155:ASP:O	1:A:1190:PRO:O	2.38	0.42
1:A:120:GLU:HB2	1:A:123:ARG:NH2	2.35	0.42
1:A:1407:GLU:N	1:A:1407:GLU:CD	2.73	0.42
1:A:1450:LEU:CG	1:A:1450:LEU:O	2.67	0.42
1:A:18:GLN:HB3	2:B:1215:ARG:HG3	2.01	0.42
1:A:186:LYS:HZ3	1:A:197:PRO:HD3	1.84	0.42
1:A:273:ASN:O	1:A:274:ILE:C	2.57	0.42
1:A:401:GLY:C	1:A:435:HIS:CD2	2.92	0.42
1:A:40:THR:CG2	1:A:41:MET:HG3	2.33	0.42
1:A:565:ILE:HG21	1:A:567:LYS:HE2	2.01	0.42
1:A:61:ILE:O	1:A:62:ASP:C	2.57	0.42
1:A:833:GLU:O	1:A:837:ILE:HG13	2.20	0.42
2:B:616:ILE:CG2	2:B:700:SER:OG	2.68	0.42
4:D:118:THR:O	4:D:119:ARG:C	2.58	0.42
4:D:130:LEU:O	4:D:134:THR:HB	2.19	0.42
4:D:147:TYR:O	4:D:148:LEU:C	2.57	0.42
5:E:11:ARG:C	5:E:13:TRP:N	2.70	0.42
5:E:29:PHE:O	5:E:30:ILE:HG13	2.19	0.42
6:F:116:ASP:C	6:F:116:ASP:OD1	2.57	0.42
8:H:80:ARG:HB3	8:H:83:GLN:OE1	2.20	0.42
9:I:82:GLU:HB3	9:I:104:LEU:CG	2.50	0.42
1:A:1146:VAL:HG11	1:A:1207:LEU:HD12	2.02	0.42
1:A:305:ASP:C	1:A:305:ASP:OD1	2.58	0.42
1:A:356:ASP:OD1	1:A:358:ASN:HB2	2.19	0.42
1:A:608:ILE:HB	1:A:613:ILE:HD11	2.01	0.42
1:A:647:GLY:O	1:A:648:ASN:C	2.56	0.42
1:A:533:LYS:HZ1	1:A:745:GLN:HE22	1.65	0.42
2:B:102:VAL:O	2:B:109:THR:HA	2.20	0.42
2:B:303:TYR:OH	2:B:586:TRP:HH2	2.03	0.42
2:B:309:GLN:OE1	9:I:52:ILE:CD1	2.66	0.42
2:B:466:TRP:N	2:B:475:SER:OG	2.53	0.42
2:B:706:GLN:NE2	2:B:730:ARG:HD2	2.35	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:860:MET:HB2	2:B:965:LYS:HG2	2.01	0.42
3:C:236:GLY:C	3:C:238:ILE:N	2.73	0.42
4:D:122:GLU:O	4:D:125:SER:HB3	2.19	0.42
4:D:29:LEU:O	4:D:30:GLY:O	2.37	0.42
11:K:56:VAL:HG22	11:K:77:THR:HG22	2.01	0.42
12:L:33:GLU:OE1	12:L:53:HIS:CB	2.68	0.42
1:A:1029:ARG:NH1	1:A:1029:ARG:CG	2.83	0.42
1:A:1203:ASN:O	1:A:1204:ASP:C	2.57	0.42
1:A:115:LEU:CD1	1:A:142:CYS:HB3	2.50	0.42
1:A:207:ILE:HG22	1:A:211:PHE:CD2	2.54	0.42
1:A:207:ILE:CG2	1:A:211:PHE:CE2	3.02	0.42
1:A:423:ASP:HB3	1:A:424:ILE:H	1.55	0.42
1:A:875:ALA:HA	1:A:878:ILE:HD12	2.02	0.42
1:A:929:LEU:CD1	1:A:929:LEU:O	2.67	0.42
2:B:1222:ARG:O	2:B:1223:ASP:C	2.58	0.42
2:B:235:SER:C	2:B:236:HIS:CD2	2.93	0.42
2:B:283:VAL:HG21	2:B:317:CYS:O	2.20	0.42
2:B:640:VAL:HG23	2:B:740:HIS:HA	2.00	0.42
2:B:711:GLU:HB2	2:B:712:PRO:CD	2.50	0.42
2:B:866:TYR:O	2:B:867:GLY:C	2.57	0.42
2:B:120:ARG:CG	2:B:955:THR:HG21	2.46	0.42
3:C:213:PRO:O	3:C:214:ASN:CB	2.68	0.42
4:D:149:THR:HG23	4:D:150:ASN:N	2.35	0.42
5:E:197:LYS:HG3	5:E:211:TYR:CE2	2.54	0.42
6:F:82:THR:CG2	6:F:84:TYR:H	2.26	0.42
3:C:258:ILE:HG12	11:K:42:LEU:HD21	2.02	0.42
14:T:15:DG:C2'	14:T:16:DT:C7	2.97	0.42
1:A:1067:LEU:O	1:A:1068:ALA:C	2.58	0.42
1:A:1112:LYS:O	1:A:1114:PRO:CD	2.68	0.42
1:A:1127:ASP:O	1:A:1128:GLN:C	2.58	0.42
1:A:1152:ILE:HG23	1:A:1260:LEU:HD22	2.02	0.42
1:A:1299:VAL:CG1	1:A:1300:LYS:N	2.83	0.42
1:A:332:LYS:O	1:A:333:GLU:CB	2.60	0.42
1:A:504:LEU:HD21	6:F:88:TYR:CD2	2.55	0.42
1:A:53:LEU:HD23	1:A:54:ASN:CB	2.49	0.42
2:B:1031:LEU:HD11	2:B:1042:GLY:CA	2.50	0.42
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.55	0.42
2:B:235:SER:HB3	2:B:258:LEU:HG	2.01	0.42
2:B:552:MET:O	2:B:553:PRO:C	2.58	0.42
2:B:840:ILE:HG21	2:B:994:TYR:CD1	2.55	0.42
2:B:845:SER:HB3	2:B:850:LEU:HD23	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:166:GLU:O	11:K:6:ARG:NH1	2.53	0.42
5:E:90:VAL:CA	5:E:120:ALA:HB2	2.50	0.42
7:G:122:ASN:HD22	7:G:131:GLN:HE21	1.67	0.42
7:G:138:THR:HG23	7:G:139:ILE:HG22	2.01	0.42
8:H:117:SER:HB2	8:H:122:LEU:CD2	2.50	0.42
8:H:33:GLN:C	8:H:35:GLN:H	2.22	0.42
8:H:93:TYR:CD1	8:H:93:TYR:N	2.87	0.42
9:I:85:PHE:CE1	9:I:99:LEU:HD13	2.54	0.42
10:J:30:LEU:HD23	10:J:31:ASP:N	2.33	0.42
13:N:2:DC:C6	13:N:3:DT:H72	2.54	0.42
1:A:102:VAL:CG1	1:A:211:PHE:HE1	2.33	0.41
1:A:1151:GLU:HB3	1:A:1153:TYR:HE1	1.85	0.41
1:A:1121:GLU:HB2	1:A:1321:GLY:O	2.20	0.41
1:A:537:ARG:O	1:A:540:PHE:CE1	2.73	0.41
1:A:53:LEU:HD23	1:A:54:ASN:HB3	2.02	0.41
1:A:556:TRP:CE3	1:A:558:GLY:HA2	2.56	0.41
1:A:31:SER:OG	1:A:82:GLY:HA2	2.20	0.41
1:A:857:ARG:NH2	6:F:139:PRO:CG	2.83	0.41
1:A:943:LEU:C	1:A:945:GLU:N	2.73	0.41
1:A:882:SER:HA	1:A:952:ALA:O	2.20	0.41
2:B:1017:ILE:H	2:B:1018:PRO:HD3	1.83	0.41
2:B:388:CYS:C	2:B:390:LEU:N	2.74	0.41
2:B:487:THR:HG22	2:B:488:TYR:N	2.35	0.41
2:B:498:THR:HG23	2:B:537:LYS:H	1.85	0.41
2:B:405:ARG:HA	2:B:631:GLY:O	2.19	0.41
2:B:648:HIS:CG	2:B:649:LYS:N	2.86	0.41
2:B:833:TYR:C	2:B:835:GLN:H	2.24	0.41
2:B:855:PHE:HZ	2:B:857:ARG:NH1	2.18	0.41
3:C:100:THR:HG22	3:C:101:LEU:N	2.35	0.41
3:C:262:LEU:HA	3:C:262:LEU:HD23	1.91	0.41
4:D:126:ILE:C	4:D:128:VAL:N	2.71	0.41
4:D:65:GLU:O	4:D:68:ARG:HB3	2.20	0.41
6:F:120:ILE:O	6:F:124:GLU:HG3	2.19	0.41
7:G:21:ARG:CD	7:G:24:GLN:HB2	2.46	0.41
12:L:30:ILE:HD11	12:L:59:ALA:HB2	2.02	0.41
1:A:1198:ASP:OD2	1:A:1200:ALA:HB3	2.19	0.41
1:A:135:PHE:HD1	1:A:222:LEU:HD22	1.86	0.41
1:A:279:LEU:HD12	1:A:289:ILE:HA	2.01	0.41
1:A:573:SER:O	1:A:574:GLY:C	2.55	0.41
1:A:80:HIS:H	1:A:243:PRO:HB3	1.86	0.41
2:B:1007:VAL:CG2	2:B:1008:PRO:CD	2.98	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1180:PHE:CB	2:B:1191:ILE:HD12	2.40	0.41
2:B:296:GLU:O	2:B:299:GLU:HB2	2.20	0.41
2:B:579:ARG:HA	2:B:589:VAL:HG13	2.00	0.41
2:B:637:LEU:HD12	2:B:693:ILE:CD1	2.50	0.41
2:B:497:ARG:HH21	2:B:775:LYS:NZ	2.07	0.41
2:B:835:GLN:O	2:B:836:GLU:HB2	2.21	0.41
2:B:874:PHE:HB3	2:B:896:ASP:O	2.20	0.41
2:B:973:ILE:HG23	2:B:974:PRO:CD	2.49	0.41
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.55	0.41
3:C:131:HIS:HA	3:C:132:PRO:HD3	1.90	0.41
3:C:98:VAL:C	3:C:99:LEU:HD22	2.39	0.41
4:D:139:LYS:HD3	4:D:143:ASN:ND2	2.28	0.41
4:D:24:ALA:C	4:D:26:THR:H	2.24	0.41
5:E:37:LEU:CD1	5:E:41:ASP:HB2	2.50	0.41
7:G:29:LYS:HD2	7:G:32:GLU:OE1	2.20	0.41
8:H:135:LEU:CB	8:H:137:GLN:HG2	2.49	0.41
8:H:12:VAL:CG1	8:H:15:VAL:HG22	2.50	0.41
2:B:308:TRP:CZ3	9:I:45:ARG:HG2	2.54	0.41
9:I:75:CYS:HB2	9:I:76:PRO:HD2	2.02	0.41
11:K:49:GLU:CG	11:K:94:ILE:HG13	2.43	0.41
12:L:47:ARG:NH2	12:L:54:ARG:HE	2.18	0.41
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	2.02	0.41
1:A:1017:LEU:HD23	5:E:204:THR:O	2.20	0.41
1:A:1106:ASN:O	1:A:1107:VAL:HB	2.21	0.41
1:A:1120:LEU:HD12	1:A:1120:LEU:C	2.41	0.41
1:A:1377:THR:O	1:A:1378:GLN:C	2.59	0.41
1:A:154:SER:HB3	1:A:162:VAL:CG2	2.45	0.41
1:A:75:ASN:O	1:A:76:GLU:HB2	2.20	0.41
2:B:113:TYR:CE2	2:B:192:LEU:HD22	2.56	0.41
2:B:244:LEU:HG	2:B:250:PHE:H	1.84	0.41
2:B:316:PRO:HG2	2:B:317:CYS:H	1.85	0.41
2:B:387:LEU:O	2:B:392:ARG:HB2	2.20	0.41
2:B:593:PRO:HG2	2:B:617:ARG:HH21	1.80	0.41
2:B:657:HIS:ND1	2:B:679:TYR:OH	2.46	0.41
2:B:843:GLN:HB3	2:B:995:ARG:HG3	2.02	0.41
3:C:112:ASN:N	3:C:112:ASN:ND2	2.68	0.41
3:C:131:HIS:O	3:C:133:ILE:N	2.53	0.41
3:C:142:VAL:HG12	3:C:142:VAL:O	2.19	0.41
4:D:14:ARG:NH1	4:D:16:LYS:NZ	2.68	0.41
5:E:102:GLU:C	5:E:104:ASN:N	2.72	0.41
5:E:182:ASP:O	5:E:185:ALA:HB3	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:37:LEU:HG	5:E:37:LEU:O	2.20	0.41
7:G:26:LEU:O	7:G:29:LYS:N	2.53	0.41
9:I:75:CYS:SG	9:I:79:HIS:N	2.93	0.41
3:C:233:GLU:OE1	10:J:12:LYS:HG3	2.21	0.41
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.55	0.41
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.80	0.41
1:A:130:ASP:C	1:A:130:ASP:OD1	2.58	0.41
1:A:337:ARG:HE	1:A:839:ARG:HH22	1.55	0.41
1:A:399:HIS:CG	1:A:400:PRO:N	2.86	0.41
1:A:441:PRO:O	1:A:441:PRO:HG2	2.21	0.41
1:A:446:ARG:NH1	1:A:446:ARG:HG2	2.36	0.41
1:A:698:GLN:NE2	9:I:99:LEU:HD21	2.35	0.41
1:A:898:ARG:HD3	1:A:933:TYR:CE1	2.56	0.41
1:A:752:LYS:HG3	2:B:1015:HIS:O	2.20	0.41
2:B:1113:VAL:N	15:P:1:C:H5'	2.35	0.41
2:B:410:GLY:O	2:B:413:LEU:HB2	2.21	0.41
2:B:473:MET:C	2:B:475:SER:H	2.24	0.41
2:B:622:LYS:HE2	9:I:59:VAL:HG21	2.01	0.41
2:B:792:MET:HA	2:B:856:PHE:O	2.20	0.41
2:B:879:ARG:N	2:B:879:ARG:CZ	2.83	0.41
2:B:882:THR:HB	2:B:934:LYS:C	2.41	0.41
2:B:889:THR:HG23	2:B:891:ASP:H	1.85	0.41
3:C:110:THR:HG22	3:C:112:ASN:ND2	2.36	0.41
5:E:162:ARG:CG	5:E:162:ARG:HH11	2.33	0.41
7:G:56:ILE:O	7:G:57:GLN:HB2	2.19	0.41
8:H:83:GLN:C	8:H:85:GLY:H	2.22	0.41
10:J:45:CYS:O	10:J:48:ARG:HG3	2.20	0.41
10:J:64:ASN:HD22	10:J:65:PRO:HD3	1.86	0.41
11:K:91:CYS:O	11:K:94:ILE:HB	2.20	0.41
1:A:1134:ILE:HG13	1:A:1134:ILE:H	1.48	0.41
1:A:1187:GLN:HA	1:A:1244:ARG:HE	1.85	0.41
1:A:1263:ILE:O	1:A:1267:MET:HG3	2.19	0.41
1:A:319:GLY:CA	2:B:471:LYS:HA	2.50	0.41
1:A:877:HIS:O	1:A:878:ILE:CG1	2.68	0.41
1:A:947:PHE:CE1	1:A:954:TRP:CD1	3.09	0.41
1:A:962:ARG:C	1:A:964:ILE:N	2.73	0.41
2:B:1084:GLN:HE21	2:B:1084:GLN:H	1.67	0.41
1:A:335:ARG:NH1	2:B:1206:GLU:OE2	2.46	0.41
2:B:254:LEU:HD22	2:B:361:LEU:HD12	2.03	0.41
2:B:314:LEU:O	2:B:318:VAL:HG23	2.21	0.41
2:B:292:ILE:HD13	2:B:326:ASP:HA	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:405:ARG:CD	2:B:631:GLY:O	2.68	0.41
2:B:68:THR:HG22	2:B:91:SER:HB3	2.02	0.41
2:B:731:VAL:CG1	2:B:732:SER:N	2.78	0.41
2:B:809:MET:O	2:B:811:TYR:N	2.53	0.41
2:B:916:THR:HG22	2:B:935:ARG:HD2	2.03	0.41
3:C:120:ILE:HD11	3:C:130:GLY:O	2.21	0.41
3:C:200:GLU:O	3:C:202:PRO:HD3	2.20	0.41
3:C:249:ASP:O	3:C:252:GLN:CB	2.69	0.41
4:D:64:VAL:C	4:D:66:ARG:H	2.23	0.41
5:E:110:PHE:C	5:E:110:PHE:HD1	2.22	0.41
5:E:143:ASN:O	5:E:146:HIS:HB2	2.21	0.41
5:E:52:ARG:HA	5:E:53:PRO:HD2	1.85	0.41
6:F:116:ASP:O	6:F:119:ARG:HB2	2.20	0.41
7:G:14:HIS:HD2	7:G:16:SER:N	2.14	0.41
7:G:96:GLN:HA	7:G:121:PHE:CE2	2.54	0.41
8:H:19:ARG:O	8:H:20:TYR:CD2	2.74	0.41
8:H:51:ALA:O	8:H:52:GLN:HB2	2.20	0.41
10:J:30:LEU:HD11	10:J:38:ARG:NH1	2.35	0.41
11:K:7:PHE:C	11:K:9:LEU:H	2.24	0.41
15:P:2:A:O5'	15:P:2:A:H8	2.03	0.41
1:A:1187:GLN:HA	1:A:1244:ARG:NE	2.36	0.41
1:A:818:MET:HA	2:B:514:LEU:HB3	2.01	0.41
1:A:93:VAL:HG23	1:A:304:MET:HE3	2.02	0.41
2:B:1064:TYR:O	2:B:1065:GLN:O	2.39	0.41
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.84	0.41
2:B:1181:GLU:HB2	2:B:1188:LYS:HG2	2.02	0.41
2:B:449:ASN:OD1	2:B:451:LYS:HB3	2.20	0.41
2:B:123:THR:CB	2:B:458:LYS:HE2	2.50	0.41
2:B:56:ASP:C	2:B:57:TYR:HD1	2.24	0.41
2:B:640:VAL:HB	2:B:738:PHE:O	2.20	0.41
2:B:653:VAL:N	2:B:689:LEU:HD22	2.36	0.41
2:B:703:ILE:HG22	2:B:704:ALA:N	2.35	0.41
2:B:542:MET:HE3	2:B:747:MET:HG3	2.03	0.41
2:B:745:PRO:C	2:B:747:MET:N	2.73	0.41
2:B:816:GLU:O	2:B:817:LEU:HD23	2.20	0.41
3:C:101:LEU:HA	3:C:101:LEU:HD12	1.87	0.41
4:D:156:ASP:O	4:D:157:GLN:C	2.59	0.41
4:D:29:LEU:H	4:D:29:LEU:HD22	1.84	0.41
4:D:60:LYS:O	4:D:64:VAL:HG23	2.19	0.41
5:E:117:THR:C	5:E:119:SER:N	2.74	0.41
5:E:58:MET:O	5:E:59:SER:O	2.38	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:96:GLN:HA	7:G:121:PHE:CD2	2.55	0.41
8:H:138:GLU:O	8:H:139:ASN:O	2.38	0.41
3:C:10:ILE:HG13	11:K:108:GLU:HB3	2.02	0.41
12:L:55:ILE:O	12:L:56:LEU:CB	2.69	0.41
1:A:141:LEU:HD23	1:A:141:LEU:HA	1.90	0.41
1:A:178:GLY:O	1:A:179:LEU:HD23	2.21	0.41
1:A:266:LEU:O	1:A:267:ALA:C	2.57	0.41
1:A:38:PRO:HG2	1:A:39:GLU:OE2	2.19	0.41
1:A:413:ILE:HG21	1:A:424:ILE:HD11	2.01	0.41
1:A:382:PRO:CD	1:A:428:TYR:CE2	3.04	0.41
1:A:540:PHE:HE2	1:A:565:ILE:HD12	1.85	0.41
1:A:577:ILE:O	1:A:580:VAL:HG23	2.20	0.41
1:A:67:CYS:O	1:A:68:GLN:CG	2.68	0.41
1:A:69:THR:O	1:A:70:CYS:C	2.59	0.41
1:A:896:ARG:HH22	1:A:1030:ARG:NH2	2.16	0.41
1:A:898:ARG:HA	1:A:933:TYR:CD1	2.55	0.41
2:B:1082:MET:HA	3:C:189:THR:HA	2.03	0.41
2:B:364:ILE:O	2:B:365:THR:CB	2.69	0.41
2:B:398:ARG:HB3	2:B:398:ARG:HH11	1.85	0.41
2:B:420:LEU:O	2:B:423:LYS:N	2.54	0.41
2:B:485:ARG:HG3	2:B:781:PHE:HD1	1.84	0.41
2:B:571:PRO:O	2:B:574:SER:O	2.38	0.41
2:B:604:ARG:CB	2:B:609:ILE:HG13	2.48	0.41
2:B:970:THR:CG2	2:B:971:THR:N	2.84	0.41
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.56	0.41
3:C:80:LEU:HD11	3:C:95:CYS:CA	2.51	0.41
4:D:216:ASN:C	4:D:218:GLU:H	2.22	0.41
5:E:182:ASP:HB3	5:E:185:ALA:HB2	2.01	0.41
8:H:104:PHE:CD2	8:H:114:VAL:HG12	2.56	0.41
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.61	0.41
1:A:196:GLU:HG2	1:A:197:PRO:CD	2.48	0.41
1:A:541:ILE:HG22	1:A:546:VAL:CG2	2.50	0.41
1:A:557:ASP:O	1:A:559:VAL:HG23	2.21	0.41
1:A:567:LYS:HE3	8:H:46:LEU:HB3	2.02	0.41
1:A:683:ILE:HG21	1:A:801:GLU:CD	2.41	0.41
2:B:123:THR:OG1	2:B:458:LYS:HE2	2.20	0.41
2:B:258:LEU:HD12	2:B:258:LEU:C	2.41	0.41
2:B:313:MET:HE3	2:B:386:LEU:HB3	2.02	0.41
2:B:448:ILE:H	2:B:448:ILE:HG13	1.74	0.41
2:B:46:GLN:HB2	2:B:408:LEU:HD21	2.01	0.41
2:B:500:THR:HA	2:B:501:PRO:HD2	1.76	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:492:LEU:HB2	2:B:751:VAL:HG11	2.01	0.41
2:B:882:THR:CB	2:B:934:LYS:O	2.69	0.41
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.51	0.41
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.91	0.41
7:G:126:ASN:HA	7:G:127:PRO:HA	1.98	0.41
11:K:19:LEU:HD21	11:K:35:PHE:CE2	2.56	0.41
14:T:16:DT:H2''	14:T:17:DT:C5'	2.50	0.41
1:A:848:ILE:HD13	1:A:1370:LEU:HD11	2.03	0.41
1:A:252:PHE:O	1:A:256:GLN:NE2	2.53	0.41
1:A:49:LYS:NZ	1:A:61:ILE:N	2.59	0.41
1:A:719:VAL:HG13	1:A:723:ASN:HD21	1.84	0.41
1:A:757:ASN:O	1:A:761:MET:HG3	2.21	0.41
1:A:818:MET:HB3	1:A:818:MET:HE2	1.65	0.41
2:B:110:HIS:O	2:B:112:LEU:N	2.54	0.41
2:B:1137:CYS:O	2:B:1140:ALA:HB3	2.21	0.41
2:B:291:ILE:HG12	2:B:300:HIS:CD2	2.56	0.41
2:B:505:ASP:CG	13:N:1:DA:C8	2.91	0.41
2:B:594:ALA:HB2	2:B:617:ARG:HH12	1.85	0.41
4:D:12:ARG:HH12	4:D:14:ARG:N	2.19	0.41
4:D:12:ARG:NH1	4:D:14:ARG:N	2.68	0.41
4:D:218:GLU:O	4:D:219:THR:C	2.59	0.41
5:E:117:THR:C	5:E:119:SER:H	2.23	0.41
5:E:28:TYR:C	5:E:65:THR:CG2	2.89	0.41
5:E:93:MET:HG2	5:E:120:ALA:O	2.21	0.41
7:G:106:MET:HE3	7:G:106:MET:HB3	1.74	0.41
7:G:145:VAL:CG1	7:G:146:LYS:N	2.84	0.41
7:G:39:THR:O	7:G:43:GLY:HA2	2.21	0.41
8:H:13:SER:N	8:H:27:GLU:O	2.54	0.41
11:K:5:ASP:O	11:K:6:ARG:C	2.60	0.41
11:K:67:PHE:N	11:K:67:PHE:HD2	2.18	0.41
12:L:59:ALA:O	12:L:60:ARG:O	2.38	0.41
1:A:1120:LEU:HD23	1:A:1304:TRP:O	2.20	0.41
1:A:1147:THR:HA	1:A:1197:LEU:HD23	2.01	0.41
1:A:114:LEU:O	1:A:115:LEU:HG	2.21	0.41
1:A:1325:THR:CG2	1:A:1326:ARG:HG3	2.50	0.41
1:A:1341:ILE:CD1	1:A:1380:GLY:HA2	2.51	0.41
1:A:332:LYS:H	1:A:337:ARG:HB2	1.84	0.41
1:A:592:ASP:HB2	1:A:604:GLY:H	1.85	0.41
1:A:629:LEU:CD1	1:A:645:LEU:HD21	2.51	0.41
1:A:709:THR:H	1:A:712:GLU:HB2	1.86	0.41
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.56	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:943:LEU:O	1:A:945:GLU:N	2.54	0.41
2:B:1103:ILE:O	2:B:1103:ILE:CG2	2.68	0.41
2:B:379:GLY:O	2:B:382:ILE:N	2.54	0.41
2:B:428:ILE:HG22	2:B:432:MET:CE	2.49	0.41
2:B:769:TYR:HD1	2:B:987:LYS:HZ3	1.69	0.41
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.49	0.41
2:B:961:LEU:HD23	2:B:961:LEU:HA	1.89	0.41
3:C:148:ARG:CG	3:C:149:LYS:N	2.84	0.41
5:E:90:VAL:HG23	5:E:120:ALA:HA	2.01	0.41
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.81	0.41
7:G:26:LEU:HA	7:G:26:LEU:HD23	1.87	0.41
9:I:118:ARG:HB3	9:I:118:ARG:NH1	2.36	0.41
9:I:13:MET:HG2	9:I:14:LEU:N	2.35	0.41
10:J:21:TYR:CE1	10:J:36:LEU:HD21	2.56	0.41
10:J:32:GLU:O	10:J:33:GLY:C	2.58	0.41
12:L:27:LEU:O	12:L:28:LYS:HB2	2.20	0.41
1:A:1015:VAL:O	1:A:1016:THR:C	2.59	0.41
1:A:384:ASN:OD1	1:A:388:LEU:HD12	2.21	0.41
1:A:4:GLN:O	1:A:5:GLN:O	2.39	0.41
1:A:691:LEU:O	1:A:694:THR:HB	2.20	0.41
1:A:6:TYR:CG	1:A:7:SER:N	2.88	0.41
1:A:83:HIS:O	1:A:84:ILE:HG13	2.21	0.41
1:A:894:GLU:O	1:A:898:ARG:HB2	2.21	0.41
2:B:384:ARG:HB3	2:B:384:ARG:HE	1.58	0.41
2:B:653:VAL:HA	2:B:689:LEU:HD22	2.03	0.41
2:B:785:TYR:HD1	2:B:786:ASN:N	2.19	0.41
2:B:789:MET:HE2	2:B:965:LYS:HB2	2.03	0.41
4:D:35:LEU:O	4:D:46:GLU:HA	2.21	0.41
1:A:1325:THR:OG1	5:E:146:HIS:O	2.38	0.41
5:E:63:ASN:HB3	5:E:64:PRO:HD2	2.02	0.41
5:E:29:PHE:N	5:E:65:THR:HG22	2.36	0.41
8:H:107:VAL:O	8:H:108:SER:O	2.39	0.41
1:A:102:VAL:HB	1:A:211:PHE:CZ	2.56	0.40
1:A:1044:TRP:O	1:A:1045:VAL:C	2.58	0.40
1:A:350:ARG:HA	1:A:468:PHE:HE1	1.86	0.40
1:A:556:TRP:CZ2	1:A:558:GLY:HA2	2.56	0.40
1:A:645:LEU:O	1:A:646:PHE:C	2.58	0.40
1:A:666:ILE:HG23	2:B:1026:LEU:HB3	2.03	0.40
1:A:809:THR:N	1:A:812:GLU:HB2	2.35	0.40
1:A:947:PHE:CE1	1:A:954:TRP:CE2	3.10	0.40
2:B:115:GLN:HE21	2:B:119:LEU:CD1	2.35	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:THR:H	2:B:188:ASP:CG	2.24	0.40
2:B:312:GLU:O	2:B:315:LYS:HB2	2.21	0.40
2:B:350:GLN:O	2:B:353:LYS:N	2.54	0.40
2:B:365:THR:CG2	2:B:367:LEU:HB2	2.51	0.40
2:B:500:THR:O	2:B:500:THR:HG22	2.21	0.40
2:B:637:LEU:HA	2:B:637:LEU:HD23	1.83	0.40
1:A:658:LEU:CD1	2:B:830:TYR:CD1	3.04	0.40
2:B:871:THR:O	2:B:917:PRO:HG3	2.21	0.40
2:B:996:ARG:HH12	3:C:174:ALA:CA	2.29	0.40
3:C:116:LYS:O	3:C:118:LEU:N	2.54	0.40
3:C:34:ARG:HG2	3:C:35:ARG:N	2.36	0.40
5:E:179:GLN:HA	5:E:179:GLN:OE1	2.20	0.40
5:E:33:GLU:OE1	5:E:33:GLU:N	2.54	0.40
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.50	0.40
11:K:50:LEU:HD13	11:K:75:ILE:HG12	2.03	0.40
1:A:1142:THR:O	1:A:1145:SER:OG	2.32	0.40
1:A:1208:THR:O	1:A:1212:VAL:HG23	2.21	0.40
1:A:145:LYS:HE3	1:A:145:LYS:CA	2.32	0.40
1:A:524:VAL:CG1	1:A:525:GLN:N	2.80	0.40
1:A:603:ASN:O	1:A:604:GLY:C	2.59	0.40
1:A:820:GLY:O	1:A:823:GLY:N	2.54	0.40
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.52	0.40
1:A:666:ILE:HD11	2:B:1067:ARG:O	2.20	0.40
2:B:1096:ARG:NH1	2:B:1096:ARG:CB	2.84	0.40
2:B:273:LEU:HB2	2:B:276:ILE:CD1	2.46	0.40
2:B:521:LEU:HB3	2:B:633:VAL:CG1	2.51	0.40
2:B:549:THR:CG2	2:B:550:ASP:H	2.22	0.40
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.86	0.40
2:B:648:HIS:CD2	2:B:649:LYS:O	2.73	0.40
2:B:654:ARG:NH1	2:B:654:ARG:CG	2.83	0.40
2:B:736:THR:O	2:B:736:THR:HG22	2.21	0.40
3:C:16:ASP:O	3:C:17:ASN:CG	2.59	0.40
3:C:11:ARG:HD3	3:C:21:ILE:CD1	2.52	0.40
3:C:82:TYR:O	3:C:85:ASP:N	2.38	0.40
4:D:193:THR:O	4:D:196:PRO:HD3	2.21	0.40
5:E:33:GLU:N	5:E:33:GLU:CD	2.75	0.40
7:G:121:PHE:HB2	7:G:130:TYR:CE2	2.56	0.40
7:G:26:LEU:O	7:G:27:LYS:C	2.60	0.40
4:D:8:PHE:CE2	7:G:6:ASP:HB2	2.56	0.40
8:H:26:ILE:HG21	8:H:42:ILE:HD12	2.01	0.40
8:H:7:ASP:O	8:H:8:ASP:HB2	2.21	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:119:THR:O	9:I:119:THR:HG22	2.21	0.40
9:I:69:PRO:HG2	9:I:85:PHE:CD2	2.56	0.40
3:C:66:ARG:NH2	10:J:5:VAL:HG23	2.36	0.40
14:T:10:DA:C2	14:T:11:DA:C6	3.09	0.40
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.37	0.40
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.36	0.40
1:A:112:LYS:HG2	1:A:113:LEU:N	2.36	0.40
1:A:1187:GLN:C	1:A:1244:ARG:HB2	2.42	0.40
1:A:1424:VAL:HG13	1:A:1436:ILE:HD12	2.03	0.40
1:A:215:SER:HB3	1:A:218:ASP:OD2	2.22	0.40
1:A:350:ARG:NH1	1:A:488:ASN:OD1	2.44	0.40
1:A:506:ALA:O	1:A:507:VAL:C	2.59	0.40
1:A:640:GLN:O	1:A:641:VAL:C	2.60	0.40
1:A:856:THR:HG21	1:A:1370:LEU:HD21	2.03	0.40
2:B:216:GLU:HA	2:B:406:LEU:HD23	2.04	0.40
2:B:591:ARG:O	2:B:592:ASN:C	2.59	0.40
3:C:163:ILE:O	3:C:170:TRP:HB2	2.22	0.40
3:C:168:ALA:O	3:C:170:TRP:N	2.54	0.40
3:C:18:VAL:O	3:C:19:ASP:C	2.60	0.40
3:C:133:ILE:HD12	3:C:237:SER:CA	2.51	0.40
3:C:238:ILE:HG22	3:C:243:VAL:HG22	2.03	0.40
3:C:33:LEU:O	3:C:34:ARG:C	2.60	0.40
6:F:152:ILE:CG2	6:F:153:VAL:N	2.83	0.40
8:H:130:ARG:HH11	8:H:130:ARG:H	1.70	0.40
2:B:294:ASP:N	9:I:12:ASN:HD22	2.18	0.40
10:J:13:VAL:O	10:J:14:VAL:HG23	2.22	0.40
11:K:43:GLY:O	11:K:44:ASN:C	2.60	0.40
13:N:3:DT:H2"	13:N:4:DA:C8	2.57	0.40
1:A:1129:GLU:O	1:A:1130:GLN:C	2.59	0.40
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	2.03	0.40
1:A:1393:ASN:O	1:A:1394:THR:C	2.60	0.40
1:A:278:THR:O	1:A:282:ASN:HB2	2.21	0.40
1:A:41:MET:O	1:A:42:ASP:C	2.60	0.40
1:A:407:ARG:HB3	1:A:430:TRP:CE2	2.55	0.40
1:A:68:GLN:O	1:A:70:CYS:N	2.52	0.40
1:A:711:ARG:HD2	9:I:95:THR:O	2.22	0.40
1:A:341:MET:HE1	1:A:843:LYS:NZ	2.36	0.40
2:B:1197:PRO:O	2:B:1198:TYR:C	2.59	0.40
2:B:241:ARG:CB	2:B:253:THR:HG22	2.51	0.40
2:B:326:ASP:OD1	2:B:329:THR:OG1	2.35	0.40
2:B:365:THR:HG22	2:B:365:THR:O	2.22	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:798:TYR:CD2	2:B:798:TYR:N	2.89	0.40
2:B:916:THR:HB	2:B:935:ARG:CG	2.52	0.40
2:B:955:THR:HG22	2:B:956:THR:N	2.34	0.40
2:B:1079:LYS:HA	3:C:27:LEU:HD21	2.02	0.40
4:D:155:ARG:C	4:D:156:ASP:OD2	2.60	0.40
4:D:66:ARG:C	4:D:68:ARG:H	2.25	0.40
5:E:112:TYR:HB3	5:E:116:ILE:HD11	2.03	0.40
5:E:192:ARG:HG3	5:E:192:ARG:HH11	1.85	0.40
5:E:3:GLN:HG3	5:E:4:GLU:N	2.37	0.40
8:H:138:GLU:O	8:H:139:ASN:C	2.60	0.40
9:I:2:THR:O	9:I:3:THR:C	2.60	0.40
9:I:88:SER:HB3	9:I:95:THR:HG21	2.03	0.40
1:A:1035:TYR:N	1:A:1035:TYR:CD2	2.88	0.40
1:A:1189:SER:OG	1:A:1191:TRP:HB2	2.21	0.40
1:A:130:ASP:O	1:A:131:SER:C	2.59	0.40
1:A:1407:GLU:H	1:A:1407:GLU:CD	2.25	0.40
1:A:241:VAL:HA	1:A:242:PRO:HD2	1.98	0.40
1:A:606:LEU:CG	1:A:613:ILE:HD12	2.51	0.40
1:A:779:PHE:HD2	1:A:779:PHE:HA	1.77	0.40
2:B:175:ARG:HH11	2:B:175:ARG:HG2	1.85	0.40
2:B:192:LEU:C	2:B:194:GLU:H	2.25	0.40
2:B:189:LEU:CD1	2:B:196:PRO:HA	2.51	0.40
2:B:505:ASP:O	2:B:506:GLY:O	2.40	0.40
2:B:606:LYS:HD2	2:B:608:ASP:OD2	2.21	0.40
2:B:644:GLU:OE2	2:B:646:LEU:HB2	2.22	0.40
2:B:875:GLU:O	2:B:877:PRO:CD	2.69	0.40
3:C:193:TYR:HD1	3:C:193:TYR:C	2.22	0.40
3:C:238:ILE:CG2	3:C:243:VAL:HG22	2.51	0.40
3:C:91:HIS:O	3:C:91:HIS:CD2	2.75	0.40
4:D:216:ASN:O	4:D:218:GLU:N	2.55	0.40
5:E:89:GLY:C	5:E:91:LYS:N	2.74	0.40
6:F:75:PRO:C	6:F:77:ASP:N	2.75	0.40
6:F:90:ARG:HG3	6:F:91:ALA:H	1.81	0.40
7:G:48:VAL:HG13	7:G:74:TYR:CD1	2.56	0.40
7:G:9:LEU:HD22	7:G:34:VAL:HG23	2.04	0.40
8:H:83:GLN:HE22	11:K:57:LEU:HD21	1.86	0.40
8:H:99:GLY:HA3	8:H:118:PHE:CD2	2.56	0.40
3:C:235:VAL:HG13	10:J:13:VAL:HG13	2.04	0.40
11:K:113:THR:O	11:K:114:LEU:CB	2.70	0.40
11:K:49:GLU:C	11:K:51:LEU:N	2.74	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1407/1733 (81%)	977 (69%)	291 (21%)	139 (10%)	0	8
2	B	1097/1224 (90%)	736 (67%)	235 (21%)	126 (12%)	0	5
3	C	264/347 (76%)	182 (69%)	50 (19%)	32 (12%)	0	5
4	D	174/221 (79%)	116 (67%)	41 (24%)	17 (10%)	0	8
5	E	212/215 (99%)	141 (66%)	51 (24%)	20 (9%)	0	9
6	F	85/155 (55%)	66 (78%)	15 (18%)	4 (5%)	2	22
7	G	169/171 (99%)	138 (82%)	23 (14%)	8 (5%)	2	22
8	H	131/146 (90%)	84 (64%)	21 (16%)	26 (20%)	0	1
9	I	117/122 (96%)	80 (68%)	26 (22%)	11 (9%)	0	9
10	J	63/70 (90%)	39 (62%)	12 (19%)	12 (19%)	0	1
11	K	112/120 (93%)	82 (73%)	25 (22%)	5 (4%)	2	23
12	L	44/70 (63%)	25 (57%)	7 (16%)	12 (27%)	0	0
All	All	3875/4594 (84%)	2666 (69%)	797 (21%)	412 (11%)	0	6

All (412) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	GLN
1	A	54	ASN
1	A	58	LEU
1	A	62	ASP
1	A	63	ARG
1	A	67	CYS
1	A	70	CYS
1	A	74	MET
1	A	76	GLU
1	A	130	ASP
1	A	154	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	255	SER
1	A	257	ARG
1	A	286	HIS
1	A	311	GLN
1	A	312	PRO
1	A	318	SER
1	A	322	VAL
1	A	332	LYS
1	A	399	HIS
1	A	410	GLY
1	A	424	ILE
1	A	466	SER
1	A	526	ASP
1	A	543	LEU
1	A	556	TRP
1	A	567	LYS
1	A	666	ILE
1	A	780	VAL
1	A	821	ARG
1	A	891	ALA
1	A	963	ILE
1	A	986	ILE
1	A	1002	GLY
1	A	1120	LEU
1	A	1122	PRO
1	A	1124	HIS
1	A	1223	ASP
1	A	1233	ASP
1	A	1242	VAL
1	A	1255	GLU
1	A	1270	ASN
1	A	1281	ARG
1	A	1309	ASP
1	A	1405	THR
1	A	1438	THR
2	B	21	GLU
2	B	27	ALA
2	B	58	THR
2	B	67	SER
2	B	68	THR
2	B	108	VAL
2	B	206	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	B	259	TYR
2	B	282	ILE
2	B	291	ILE
2	B	294	ASP
2	B	367	LEU
2	B	369	GLY
2	B	391	ASP
2	B	435	THR
2	B	449	ASN
2	B	467	GLY
2	B	501	PRO
2	B	502	ILE
2	B	508	LEU
2	B	509	ALA
2	B	629	ASP
2	B	643	ASP
2	B	708	GLU
2	B	709	ASP
2	B	728	ARG
2	B	731	VAL
2	B	735	ALA
2	B	749	LEU
2	B	792	MET
2	B	810	GLU
2	B	879	ARG
2	B	906	SER
2	B	907	GLY
2	B	958	GLN
2	B	1046	PRO
2	B	1069	PHE
2	B	1103	ILE
2	B	1176	ASN
2	B	1181	GLU
2	B	1222	ARG
2	B	1223	ASP
3	C	60	ASP
3	C	141	GLY
3	C	142	VAL
3	C	149	LYS
3	C	161	LYS
3	C	172	PRO
3	C	176	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	C	209	TYR
3	C	215	GLU
3	C	216	GLY
3	C	237	SER
4	D	5	THR
4	D	8	PHE
4	D	17	LYS
4	D	19	GLU
4	D	52	LEU
4	D	119	ARG
4	D	157	GLN
4	D	198	LEU
4	D	218	GLU
5	E	36	GLU
5	E	45	LYS
5	E	74	ASP
5	E	115	ASN
5	E	129	PRO
6	F	128	LYS
7	G	139	ILE
8	H	21	ASN
8	H	47	PHE
8	H	82	PRO
8	H	95	TYR
8	H	108	SER
8	H	128	ASN
8	H	140	ALA
10	J	2	ILE
10	J	6	ARG
10	J	42	LYS
10	J	64	ASN
12	L	50	ASP
12	L	53	HIS
12	L	54	ARG
12	L	55	ILE
12	L	59	ALA
12	L	60	ARG
1	A	41	MET
1	A	43	GLU
1	A	48	ALA
1	A	57	ARG
1	A	73	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	93	VAL
1	A	96	ILE
1	A	128	ILE
1	A	167	CYS
1	A	169	ASN
1	A	219	PHE
1	A	250	ILE
1	A	400	PRO
1	A	423	ASP
1	A	439	ASN
1	A	465	TYR
1	A	517	ASN
1	A	597	LEU
1	A	604	GLY
1	A	619	LYS
1	A	683	ILE
1	A	731	ARG
1	A	753	GLY
1	A	755	PHE
1	A	795	GLU
1	A	830	LYS
1	A	846	GLU
1	A	875	ALA
1	A	885	THR
1	A	926	GLN
1	A	1064	VAL
1	A	1169	ILE
1	A	1206	ASP
1	A	1221	LYS
1	A	1254	ALA
1	A	1314	SER
1	A	1316	VAL
1	A	1377	THR
1	A	1378	GLN
2	B	24	PRO
2	B	43	LEU
2	B	45	SER
2	B	65	GLU
2	B	186	GLU
2	B	221	ASN
2	B	245	GLU
2	B	257	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	258	LEU
2	B	260	GLY
2	B	295	GLY
2	B	333	PHE
2	B	365	THR
2	B	409	ALA
2	B	466	TRP
2	B	506	GLY
2	B	507	LYS
2	B	566	LEU
2	B	591	ARG
2	B	642	ASP
2	B	655	LYS
2	B	729	ILE
2	B	734	HIS
2	B	746	SER
2	B	751	VAL
2	B	864	LYS
2	B	881	ASN
2	B	884	ARG
2	B	1003	ALA
2	B	1065	GLN
2	B	1075	GLY
2	B	1108	ARG
2	B	1171	VAL
2	B	1175	LEU
3	C	11	ARG
3	C	90	ASP
3	C	110	THR
3	C	125	MET
3	C	126	GLY
3	C	184	ASN
3	C	213	PRO
3	C	231	ASN
4	D	30	GLY
4	D	192	LYS
5	E	59	SER
5	E	76	GLY
5	E	130	ALA
5	E	158	SER
5	E	167	ARG
7	G	156	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	H	2	SER
8	H	12	VAL
8	H	17	PRO
8	H	32	THR
8	H	59	ILE
8	H	62	SER
8	H	78	SER
8	H	89	LEU
8	H	90	ALA
8	H	139	ASN
9	I	9	ASP
9	I	11	ASN
9	I	57	GLY
9	I	106	CYS
10	J	17	LYS
10	J	24	LEU
10	J	28	ASP
10	J	29	GLU
12	L	28	LYS
1	A	51	GLY
1	A	61	ILE
1	A	86	LEU
1	A	313	GLN
1	A	331	GLY
1	A	479	ASN
1	A	527	THR
1	A	583	PRO
1	A	591	PHE
1	A	852	TYR
1	A	910	PRO
1	A	995	GLU
1	A	1139	GLU
1	A	1244	ARG
1	A	1365	TYR
2	B	114	PRO
2	B	277	LYS
2	B	511	PRO
2	B	541	LEU
2	B	575	PRO
2	B	619	ILE
2	B	641	GLU
2	B	711	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	738	PHE
2	B	850	LEU
2	B	894	ASP
2	B	1017	ILE
2	B	1035	ALA
2	B	1082	MET
2	B	1097	HIS
2	B	1155	SER
2	B	1157	ALA
2	B	1214	PRO
3	C	117	ASP
3	C	132	PRO
4	D	21	GLU
4	D	129	LEU
4	D	199	ASN
4	D	219	THR
5	E	51	GLY
5	E	65	THR
5	E	73	PRO
5	E	104	ASN
6	F	78	GLN
7	G	2	PHE
8	H	77	ARG
8	H	81	PRO
8	H	134	ASN
9	I	8	ARG
9	I	16	PRO
9	I	56	ALA
9	I	78	CYS
10	J	13	VAL
10	J	14	VAL
11	K	53	ASP
12	L	35	SER
12	L	37	LYS
12	L	39	SER
1	A	42	ASP
1	A	126	LEU
1	A	131	SER
1	A	226	GLU
1	A	276	LEU
1	A	592	ASP
1	A	722	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	789	LYS
1	A	1231	ASP
1	A	1308	THR
1	A	1403	GLU
2	B	125	SER
2	B	249	ARG
2	B	347	LYS
2	B	418	LYS
2	B	419	THR
2	B	436	VAL
2	B	448	ILE
2	B	474	SER
2	B	483	LEU
2	B	594	ALA
2	B	744	HIS
2	B	1041	GLU
2	B	1099	VAL
2	B	1188	LYS
3	C	17	ASN
3	C	56	THR
3	C	148	ARG
3	C	169	LYS
3	C	214	ASN
4	D	147	TYR
4	D	169	SER
5	E	48	ASP
5	E	64	PRO
5	E	83	CYS
6	F	139	PRO
6	F	149	GLU
7	G	20	PRO
7	G	154	VAL
8	H	8	ASP
8	H	83	GLN
8	H	107	VAL
11	K	6	ARG
11	K	90	ALA
12	L	56	LEU
1	A	35	ILE
1	A	253	ASN
1	A	525	GLN
1	A	536	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	693	VAL
1	A	944	ARG
1	A	958	VAL
1	A	975	HIS
1	A	1016	THR
2	B	28	GLU
2	B	111	ALA
2	B	126	SER
2	B	309	GLN
2	B	323	VAL
2	B	468	GLU
2	B	543	SER
2	B	636	PRO
2	B	707	PRO
2	B	764	SER
2	B	793	ALA
2	B	951	GLN
2	B	1156	ASP
3	C	10	ILE
3	C	208	GLU
3	C	243	VAL
5	E	95	THR
5	E	106	GLN
7	G	63	PRO
7	G	124	GLY
8	H	44	VAL
8	H	63	LEU
9	I	47	GLU
10	J	33	GLY
11	K	12	LEU
11	K	14	GLU
1	A	77	CYS
1	A	138	ILE
1	A	141	LEU
1	A	730	GLY
1	A	763	ALA
1	A	1158	PRO
1	A	1369	ALA
2	B	421	PHE
2	B	892	LYS
3	C	129	ILE
5	E	92	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
8	H	92	ASP
12	L	45	ALA
1	A	554	PRO
1	A	987	VAL
2	B	100	PRO
3	C	240	VAL
9	I	59	VAL
10	J	57	ILE
1	A	599	SER
1	A	647	GLY
3	C	182	PRO
7	G	92	VAL
9	I	62	ILE
1	A	244	PRO
1	A	718	VAL
1	A	1114	PRO
2	B	1006	ILE
1	A	600	PRO
1	A	1212	VAL
1	A	1335	ILE
2	B	1034	VAL
1	A	1049	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1240/1520 (82%)	1114 (90%)	126 (10%)	7	31
2	B	965/1061 (91%)	839 (87%)	126 (13%)	4	22
3	C	234/299 (78%)	203 (87%)	31 (13%)	4	21
4	D	160/200 (80%)	135 (84%)	25 (16%)	2	16
5	E	196/197 (100%)	176 (90%)	20 (10%)	7	31
6	F	77/137 (56%)	68 (88%)	9 (12%)	5	26
7	G	152/152 (100%)	138 (91%)	14 (9%)	9	36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	118/128 (92%)	99 (84%)	19 (16%)	2	15
9	I	113/116 (97%)	97 (86%)	16 (14%)	3	19
10	J	60/65 (92%)	54 (90%)	6 (10%)	7	32
11	K	99/102 (97%)	91 (92%)	8 (8%)	11	41
12	L	40/57 (70%)	35 (88%)	5 (12%)	4	23
All	All	3454/4034 (86%)	3049 (88%)	405 (12%)	5	26

All (405) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	18	GLN
1	A	34	LYS
1	A	41	MET
1	A	42	ASP
1	A	57	ARG
1	A	68	GLN
1	A	70	CYS
1	A	83	HIS
1	A	93	VAL
1	A	121	LEU
1	A	141	LEU
1	A	145	LYS
1	A	160	GLN
1	A	161	LEU
1	A	162	VAL
1	A	173	THR
1	A	185	TRP
1	A	199	LEU
1	A	200	ARG
1	A	202	LEU
1	A	215	SER
1	A	245	PRO
1	A	252	PHE
1	A	268	ASP
1	A	277	GLU
1	A	290	GLU
1	A	297	GLN
1	A	317	LYS
1	A	320	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	322	VAL
1	A	337	ARG
1	A	344	ARG
1	A	354	SER
1	A	385	ILE
1	A	394	ASN
1	A	396	PRO
1	A	407	ARG
1	A	408	ASP
1	A	412	ARG
1	A	425	GLN
1	A	438	ASP
1	A	442	VAL
1	A	443	LEU
1	A	445	ASN
1	A	449	SER
1	A	451	HIS
1	A	475	THR
1	A	476	SER
1	A	481	ASP
1	A	483	ASP
1	A	493	GLN
1	A	497	THR
1	A	505	CYS
1	A	512	VAL
1	A	513	SER
1	A	525	GLN
1	A	527	THR
1	A	536	LEU
1	A	547	LEU
1	A	571	LEU
1	A	595	THR
1	A	599	SER
1	A	614	PHE
1	A	618	GLU
1	A	666	ILE
1	A	670	ILE
1	A	685	GLU
1	A	701	LEU
1	A	710	LEU
1	A	740	LEU
1	A	764	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	768	GLN
1	A	774	ARG
1	A	779	PHE
1	A	805	LEU
1	A	821	ARG
1	A	827	THR
1	A	838	GLN
1	A	839	ARG
1	A	858	ASN
1	A	903	ASN
1	A	929	LEU
1	A	941	LYS
1	A	969	GLN
1	A	1009	ASN
1	A	1029	ARG
1	A	1030	ARG
1	A	1037	LEU
1	A	1048	ASN
1	A	1067	LEU
1	A	1077	THR
1	A	1110	ASN
1	A	1116	LEU
1	A	1122	PRO
1	A	1124	HIS
1	A	1129	GLU
1	A	1134	ILE
1	A	1146	VAL
1	A	1166	ASP
1	A	1170	ILE
1	A	1171	GLN
1	A	1187	GLN
1	A	1193	LEU
1	A	1217	LYS
1	A	1230	GLU
1	A	1232	ASN
1	A	1264	GLU
1	A	1288	ASP
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1308	THR
1	A	1333	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1345	ARG
1	A	1353	TYR
1	A	1370	LEU
1	A	1394	THR
1	A	1400	CYS
1	A	1426	GLU
1	A	1436	ILE
1	A	1438	THR
1	A	1442	ASP
1	A	1445	ILE
1	A	1447	GLU
1	A	1451	VAL
2	B	46	GLN
2	B	57	TYR
2	B	64	CYS
2	B	67	SER
2	B	101	MET
2	B	104	GLU
2	B	128	LEU
2	B	134	LYS
2	B	167	ILE
2	B	194	GLU
2	B	217	ARG
2	B	222	ILE
2	B	225	VAL
2	B	244	LEU
2	B	250	PHE
2	B	258	LEU
2	B	259	TYR
2	B	261	ARG
2	B	262	GLU
2	B	272	THR
2	B	275	TYR
2	B	276	ILE
2	B	286	PHE
2	B	299	GLU
2	B	303	TYR
2	B	309	GLN
2	B	313	MET
2	B	364	ILE
2	B	365	THR
2	B	371	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	384	ARG
2	B	387	LEU
2	B	393	LYS
2	B	394	ASP
2	B	396	ASP
2	B	401	PHE
2	B	425	THR
2	B	429	PHE
2	B	446	LEU
2	B	452	THR
2	B	465	ASN
2	B	466	TRP
2	B	468	GLU
2	B	473	MET
2	B	485	ARG
2	B	496	ARG
2	B	505	ASP
2	B	508	LEU
2	B	510	LYS
2	B	516	ASN
2	B	537	LYS
2	B	557	PHE
2	B	563	MET
2	B	576	ASP
2	B	580	VAL
2	B	597	MET
2	B	598	GLU
2	B	601	ARG
2	B	615	MET
2	B	616	ILE
2	B	622	LYS
2	B	628	THR
2	B	635	ARG
2	B	636	PRO
2	B	644	GLU
2	B	680	THR
2	B	693	ILE
2	B	705	MET
2	B	728	ARG
2	B	737	THR
2	B	748	ILE
2	B	766	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	780	VAL
2	B	786	ASN
2	B	790	ASP
2	B	791	THR
2	B	805	THR
2	B	806	THR
2	B	811	TYR
2	B	815	ARG
2	B	830	TYR
2	B	837	ASP
2	B	839	MET
2	B	878	GLN
2	B	879	ARG
2	B	884	ARG
2	B	887	HIS
2	B	895	ASP
2	B	909	ASP
2	B	915	THR
2	B	939	THR
2	B	944	THR
2	B	955	THR
2	B	956	THR
2	B	957	ASN
2	B	959	ASP
2	B	978	ASP
2	B	983	ARG
2	B	987	LYS
2	B	997	GLU
2	B	999	MET
2	B	1000	PRO
2	B	1006	ILE
2	B	1046	PRO
2	B	1049	ASP
2	B	1058	LEU
2	B	1060	ARG
2	B	1067	ARG
2	B	1069	PHE
2	B	1084	GLN
2	B	1087	PHE
2	B	1095	LEU
2	B	1098	MET
2	B	1122	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	1150	ARG
2	B	1155	SER
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1163	CYS
2	B	1175	LEU
2	B	1178	ASN
2	B	1183	LYS
2	B	1202	LEU
2	B	1214	PRO
2	B	1218	THR
3	C	3	GLU
3	C	7	GLN
3	C	11	ARG
3	C	53	THR
3	C	55	THR
3	C	56	THR
3	C	58	LEU
3	C	62	PHE
3	C	73	GLN
3	C	76	ASP
3	C	77	ILE
3	C	78	GLU
3	C	91	HIS
3	C	99	LEU
3	C	104	PHE
3	C	106	GLU
3	C	117	ASP
3	C	138	GLU
3	C	145	CYS
3	C	147	LEU
3	C	166	GLU
3	C	194	GLU
3	C	200	GLU
3	C	226	ASP
3	C	238	ILE
3	C	240	VAL
3	C	245	VAL
3	C	259	LEU
3	C	265	MET
3	C	266	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	C	268	ASP
4	D	11	ARG
4	D	14	ARG
4	D	15	LEU
4	D	17	LYS
4	D	22	GLU
4	D	23	ASN
4	D	29	LEU
4	D	40	HIS
4	D	47	LEU
4	D	57	LEU
4	D	63	LEU
4	D	70	PHE
4	D	123	LEU
4	D	124	GLU
4	D	132	GLN
4	D	138	ASN
4	D	139	LYS
4	D	151	PHE
4	D	153	ARG
4	D	154	PHE
4	D	155	ARG
4	D	158	GLU
4	D	187	THR
4	D	200	ASN
4	D	221	TYR
5	E	7	ARG
5	E	24	LYS
5	E	31	THR
5	E	33	GLU
5	E	34	GLU
5	E	37	LEU
5	E	41	ASP
5	E	50	MET
5	E	52	ARG
5	E	72	PHE
5	E	74	ASP
5	E	107	THR
5	E	110	PHE
5	E	119	SER
5	E	123	LEU
5	E	127	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	E	132	ILE
5	E	134	THR
5	E	182	ASP
5	E	207	ARG
6	F	77	ASP
6	F	79	ARG
6	F	84	TYR
6	F	112	GLU
6	F	116	ASP
6	F	119	ARG
6	F	125	LEU
6	F	147	SER
6	F	155	LEU
7	G	1	MET
7	G	8	SER
7	G	13	LEU
7	G	21	ARG
7	G	24	GLN
7	G	49	LEU
7	G	53	ASN
7	G	62	LEU
7	G	63	PRO
7	G	74	TYR
7	G	93	SER
7	G	111	THR
7	G	126	ASN
7	G	134	GLU
8	H	7	ASP
8	H	10	PHE
8	H	14	GLU
8	H	15	VAL
8	H	20	TYR
8	H	33	GLN
8	H	53	ASP
8	H	61	SER
8	H	64	ASN
8	H	86	ASP
8	H	89	LEU
8	H	94	ASP
8	H	95	TYR
8	H	102	TYR
8	H	107	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	H	129	TYR
8	H	130	ARG
8	H	138	GLU
8	H	143	LEU
9	I	7	CYS
9	I	8	ARG
9	I	28	GLU
9	I	31	THR
9	I	44	TYR
9	I	49	ILE
9	I	50	THR
9	I	52	ILE
9	I	59	VAL
9	I	72	ASP
9	I	74	GLU
9	I	85	PHE
9	I	93	LYS
9	I	101	PHE
9	I	106	CYS
9	I	111	THR
10	J	22	LEU
10	J	26	GLN
10	J	34	THR
10	J	43	ARG
10	J	44	TYR
10	J	48	ARG
11	K	25	THR
11	K	47	ARG
11	K	51	LEU
11	K	61	TYR
11	K	107	THR
11	K	111	LEU
11	K	113	THR
11	K	114	LEU
12	L	27	LEU
12	L	54	ARG
12	L	55	ILE
12	L	68	GLU
12	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	75	ASN
1	A	169	ASN
1	A	171	GLN
1	A	213	HIS
1	A	225	ASN
1	A	256	GLN
1	A	281	HIS
1	A	282	ASN
1	A	297	GLN
1	A	299	HIS
1	A	316	GLN
1	A	339	ASN
1	A	358	ASN
1	A	394	ASN
1	A	435	HIS
1	A	445	ASN
1	A	447	GLN
1	A	451	HIS
1	A	493	GLN
1	A	515	GLN
1	A	517	ASN
1	A	611	GLN
1	A	640	GLN
1	A	654	ASN
1	A	700	ASN
1	A	723	ASN
1	A	736	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	767	GLN
1	A	786	HIS
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	935	GLN
1	A	959	ASN
1	A	965	GLN
1	A	969	GLN
1	A	1048	ASN
1	A	1078	GLN
1	A	1110	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1187	GLN
1	A	1203	ASN
1	A	1218	GLN
1	A	1270	ASN
1	A	1278	ASN
1	A	1312	ASN
1	A	1354	ASN
1	A	1432	GLN
2	B	121	ASN
2	B	178	ASN
2	B	236	HIS
2	B	325	GLN
2	B	366	GLN
2	B	383	ASN
2	B	465	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	573	GLN
2	B	587	HIS
2	B	706	GLN
2	B	744	HIS
2	B	821	GLN
2	B	842	ASN
2	B	862	GLN
2	B	887	HIS
2	B	957	ASN
2	B	975	GLN
2	B	984	HIS
2	B	986	GLN
2	B	1025	HIS
2	B	1062	HIS
2	B	1065	GLN
2	B	1076	HIS
2	B	1117	GLN
2	B	1141	HIS
2	B	1161	HIS
2	B	1179	GLN
2	B	1193	GLN
3	C	7	GLN
3	C	24	ASN
3	C	65	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	C	79	GLN
3	C	102	GLN
3	C	112	ASN
3	C	123	ASN
3	C	231	ASN
3	C	252	GLN
3	C	267	GLN
4	D	39	ASN
4	D	40	HIS
4	D	138	ASN
4	D	143	ASN
4	D	165	GLN
4	D	200	ASN
5	E	99	HIS
5	E	101	GLN
5	E	106	GLN
5	E	143	ASN
5	E	147	HIS
7	G	14	HIS
7	G	53	ASN
7	G	126	ASN
7	G	131	GLN
7	G	158	HIS
8	H	43	ASN
8	H	128	ASN
8	H	131	ASN
9	I	12	ASN
9	I	46	HIS
9	I	108	HIS
10	J	53	HIS
11	K	44	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	10/18 (55%)	1 (10%)	1 (10%)

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	2	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	1	C

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	BRU	T	23	15,14	15,21,22	4.16	3 (20%)	17,30,33	4.03	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BRU	T	23	15,14	-	0/4/21/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	23	BRU	BR-C5	-13.91	1.50	1.90
14	T	23	BRU	C4-C5	6.73	1.47	1.38
14	T	23	BRU	C4-N3	3.92	1.39	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	23	BRU	C4-N3-C2	14.08	127.03	115.14
14	T	23	BRU	C5-C4-N3	-7.11	115.12	123.64
14	T	23	BRU	C5-C6-N1	2.91	123.73	119.97
14	T	23	BRU	BR-C5-C6	2.42	122.82	117.31
14	T	23	BRU	C2'-C1'-N1	-2.26	109.06	114.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	23	BRU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1417/1733 (81%)	-0.30	8 (0%) 89 83	18, 67, 100, 123	0
2	B	1113/1224 (90%)	-0.24	9 (0%) 86 77	21, 77, 109, 121	0
3	C	266/347 (76%)	-0.30	0 100 100	34, 66, 93, 107	0
4	D	178/221 (80%)	-0.14	0 100 100	46, 76, 106, 111	0
5	E	214/215 (99%)	-0.08	1 (0%) 91 85	43, 88, 108, 117	0
6	F	87/155 (56%)	-0.62	0 100 100	16, 44, 74, 84	0
7	G	171/171 (100%)	-0.28	0 100 100	47, 63, 94, 101	0
8	H	135/146 (92%)	0.26	3 (2%) 62 48	71, 94, 110, 116	0
9	I	119/122 (97%)	-0.00	3 (2%) 57 43	59, 92, 110, 119	0
10	J	65/70 (92%)	-0.41	0 100 100	45, 62, 87, 98	0
11	K	114/120 (95%)	-0.20	0 100 100	28, 67, 85, 96	0
12	L	46/70 (65%)	-0.04	0 100 100	51, 94, 110, 115	0
13	N	7/12 (58%)	2.06	4 (57%) 0 0	120, 125, 135, 137	0
14	T	17/26 (65%)	1.28	6 (35%) 0 0	99, 119, 135, 136	0
15	P	11/18 (61%)	1.12	2 (18%) 1 1	115, 119, 129, 139	0
All	All	3960/4650 (85%)	-0.22	36 (0%) 84 74	16, 73, 107, 139	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	471	LYS	5.8
15	P	1	C	3.9
2	B	470	LYS	3.7
9	I	116	ASN	3.3
1	A	155	GLU	3.3
14	T	13	DT	3.2
14	T	12	DG	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
14	T	11	DA	3.0
1	A	1455	PRO	2.8
2	B	472	ALA	2.7
2	B	250	PHE	2.7
14	T	14	DA	2.6
13	N	3	DT	2.6
13	N	5	DC	2.6
9	I	120	GLN	2.6
2	B	868	MET	2.5
9	I	119	THR	2.5
1	A	158	PRO	2.4
13	N	6	DT	2.4
2	B	505	ASP	2.3
2	B	882	THR	2.3
1	A	154	SER	2.2
8	H	108	SER	2.2
2	B	433	GLN	2.2
14	T	15	DG	2.2
1	A	159	THR	2.2
14	T	27	DC	2.2
8	H	1	MET	2.2
8	H	36	CYS	2.2
2	B	431	TYR	2.1
1	A	69	THR	2.1
1	A	1188	GLN	2.1
13	N	1	DA	2.1
1	A	160	GLN	2.1
5	E	90	VAL	2.1
15	P	2	A	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
14	BRU	T	23	20/21	0.73	0.29	105,113,118,121	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
17	MG	A	2458	1/1	0.83	0.15	151,151,151,151	0
16	ZN	L	1071	1/1	0.96	0.06	106,106,106,106	0
16	ZN	A	2456	1/1	0.96	0.06	87,87,87,87	0
16	ZN	I	1122	1/1	0.97	0.08	131,131,131,131	0
16	ZN	A	2457	1/1	0.98	0.17	42,42,42,42	0
16	ZN	I	1121	1/1	0.99	0.09	79,79,79,79	0
16	ZN	B	2225	1/1	0.99	0.15	42,42,42,42	0
16	ZN	J	1066	1/1	0.99	0.20	47,47,47,47	0
16	ZN	C	1269	1/1	0.99	0.15	40,40,40,40	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.