



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2017 – 11:39 PM EST

PDB ID : 1XFX  
Title : Crystal structure of anthrax edema factor (EF) in complex with calmodulin  
in the presence of 10 millimolar exogenously added calcium chloride  
Authors : Shen, Y.; Zhukovskaya, N.L.; Guo, Q.; Florian, J.; Tang, W.J.  
Deposited on : unknown  
Resolution : 3.20 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

<http://wwpdb.org/validation/2016/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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345



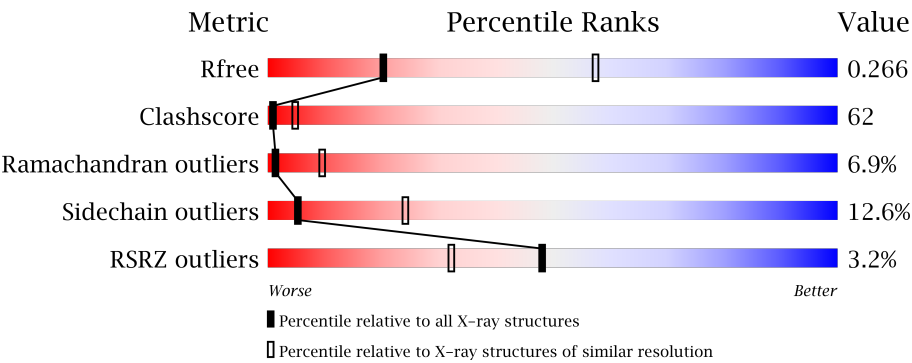
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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>	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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. 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	777	<div><div>4%</div><div><div></div><div>29%</div><div>54%</div><div>10%</div><div>5%</div></div></div>
1	B	777	<div><div>3%</div><div><div></div><div>29%</div><div>54%</div><div>10%</div><div>5%</div></div></div>
1	C	777	<div><div>3%</div><div><div></div><div>29%</div><div>54%</div><div>10%</div><div>5%</div></div></div>
1	D	777	<div><div>4%</div><div><div></div><div>30%</div><div>53%</div><div>10%</div><div>5%</div></div></div>
1	E	777	<div><div>3%</div><div><div></div><div>29%</div><div>54%</div><div>10%</div><div>5%</div></div></div>

Continued on next page...



Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	777	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>4%29%54%10%5%</div></div>
2	O	149	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%24%53%20%..</div></div>
2	P	149	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%25%51%20%..</div></div>
2	Q	149	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%24%53%17%..</div></div>
2	R	149	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%23%54%19%..</div></div>
2	S	149	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%23%54%17%..</div></div>
2	T	149	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%23%54%18%..</div></div>



## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 42858 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 Calmodulin-sensitive adenylate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	B	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	C	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	D	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	E	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	F	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	INITIATING METHIONINE	UNP P40136
A	25	HIS	-	EXPRESSION TAG	UNP P40136
A	26	HIS	-	EXPRESSION TAG	UNP P40136
A	27	HIS	-	EXPRESSION TAG	UNP P40136
A	28	HIS	-	EXPRESSION TAG	UNP P40136
A	29	HIS	-	EXPRESSION TAG	UNP P40136
A	30	HIS	-	EXPRESSION TAG	UNP P40136
A	31	ALA	-	CLONING ARTIFACT	UNP P40136
A	32	ALA	-	CLONING ARTIFACT	UNP P40136
B	24	MET	-	INITIATING METHIONINE	UNP P40136
B	25	HIS	-	EXPRESSION TAG	UNP P40136
B	26	HIS	-	EXPRESSION TAG	UNP P40136
B	27	HIS	-	EXPRESSION TAG	UNP P40136
B	28	HIS	-	EXPRESSION TAG	UNP P40136
B	29	HIS	-	EXPRESSION TAG	UNP P40136
B	30	HIS	-	EXPRESSION TAG	UNP P40136
B	31	ALA	-	CLONING ARTIFACT	UNP P40136

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	32	ALA	-	CLONING ARTIFACT	UNP P40136
C	24	MET	-	INITIATING METHIONINE	UNP P40136
C	25	HIS	-	EXPRESSION TAG	UNP P40136
C	26	HIS	-	EXPRESSION TAG	UNP P40136
C	27	HIS	-	EXPRESSION TAG	UNP P40136
C	28	HIS	-	EXPRESSION TAG	UNP P40136
C	29	HIS	-	EXPRESSION TAG	UNP P40136
C	30	HIS	-	EXPRESSION TAG	UNP P40136
C	31	ALA	-	CLONING ARTIFACT	UNP P40136
C	32	ALA	-	CLONING ARTIFACT	UNP P40136
D	24	MET	-	INITIATING METHIONINE	UNP P40136
D	25	HIS	-	EXPRESSION TAG	UNP P40136
D	26	HIS	-	EXPRESSION TAG	UNP P40136
D	27	HIS	-	EXPRESSION TAG	UNP P40136
D	28	HIS	-	EXPRESSION TAG	UNP P40136
D	29	HIS	-	EXPRESSION TAG	UNP P40136
D	30	HIS	-	EXPRESSION TAG	UNP P40136
D	31	ALA	-	CLONING ARTIFACT	UNP P40136
D	32	ALA	-	CLONING ARTIFACT	UNP P40136
E	24	MET	-	INITIATING METHIONINE	UNP P40136
E	25	HIS	-	EXPRESSION TAG	UNP P40136
E	26	HIS	-	EXPRESSION TAG	UNP P40136
E	27	HIS	-	EXPRESSION TAG	UNP P40136
E	28	HIS	-	EXPRESSION TAG	UNP P40136
E	29	HIS	-	EXPRESSION TAG	UNP P40136
E	30	HIS	-	EXPRESSION TAG	UNP P40136
E	31	ALA	-	CLONING ARTIFACT	UNP P40136
E	32	ALA	-	CLONING ARTIFACT	UNP P40136
F	24	MET	-	INITIATING METHIONINE	UNP P40136
F	25	HIS	-	EXPRESSION TAG	UNP P40136
F	26	HIS	-	EXPRESSION TAG	UNP P40136
F	27	HIS	-	EXPRESSION TAG	UNP P40136
F	28	HIS	-	EXPRESSION TAG	UNP P40136
F	29	HIS	-	EXPRESSION TAG	UNP P40136
F	30	HIS	-	EXPRESSION TAG	UNP P40136
F	31	ALA	-	CLONING ARTIFACT	UNP P40136
F	32	ALA	-	CLONING ARTIFACT	UNP P40136

- Molecule 2 is a protein called Calmodulin 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	146	Total	C	N	O	Se	0	0	0
			1146	702	186	249	9			

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	146	Total 1146	C 702	N 186	O 249	Se 9	0	0	0
2	Q	146	Total 1146	C 702	N 186	O 249	Se 9	0	0	0
2	R	146	Total 1146	C 702	N 186	O 249	Se 9	0	0	0
2	S	146	Total 1146	C 702	N 186	O 249	Se 9	0	0	0
2	T	146	Total 1146	C 702	N 186	O 249	Se 9	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	0	MSE	MET	MODIFIED RESIDUE	UNP P62158
O	36	MSE	MET	MODIFIED RESIDUE	UNP P62158
O	51	MSE	MET	MODIFIED RESIDUE	UNP P62158
O	71	MSE	MET	MODIFIED RESIDUE	UNP P62158
O	72	MSE	MET	MODIFIED RESIDUE	UNP P62158
O	76	MSE	MET	MODIFIED RESIDUE	UNP P62158
O	109	MSE	MET	MODIFIED RESIDUE	UNP P62158
O	124	MSE	MET	MODIFIED RESIDUE	UNP P62158
O	144	MSE	MET	MODIFIED RESIDUE	UNP P62158
O	145	MSE	MET	MODIFIED RESIDUE	UNP P62158
P	0	MSE	MET	MODIFIED RESIDUE	UNP P62158
P	36	MSE	MET	MODIFIED RESIDUE	UNP P62158
P	51	MSE	MET	MODIFIED RESIDUE	UNP P62158
P	71	MSE	MET	MODIFIED RESIDUE	UNP P62158
P	72	MSE	MET	MODIFIED RESIDUE	UNP P62158
P	76	MSE	MET	MODIFIED RESIDUE	UNP P62158
P	109	MSE	MET	MODIFIED RESIDUE	UNP P62158
P	124	MSE	MET	MODIFIED RESIDUE	UNP P62158
P	144	MSE	MET	MODIFIED RESIDUE	UNP P62158
P	145	MSE	MET	MODIFIED RESIDUE	UNP P62158
Q	0	MSE	MET	MODIFIED RESIDUE	UNP P62158
Q	36	MSE	MET	MODIFIED RESIDUE	UNP P62158
Q	51	MSE	MET	MODIFIED RESIDUE	UNP P62158
Q	71	MSE	MET	MODIFIED RESIDUE	UNP P62158
Q	72	MSE	MET	MODIFIED RESIDUE	UNP P62158
Q	76	MSE	MET	MODIFIED RESIDUE	UNP P62158
Q	109	MSE	MET	MODIFIED RESIDUE	UNP P62158
Q	124	MSE	MET	MODIFIED RESIDUE	UNP P62158
Q	144	MSE	MET	MODIFIED RESIDUE	UNP P62158

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
Q	145	MSE	MET	MODIFIED RESIDUE	UNP P62158
R	0	MSE	MET	MODIFIED RESIDUE	UNP P62158
R	36	MSE	MET	MODIFIED RESIDUE	UNP P62158
R	51	MSE	MET	MODIFIED RESIDUE	UNP P62158
R	71	MSE	MET	MODIFIED RESIDUE	UNP P62158
R	72	MSE	MET	MODIFIED RESIDUE	UNP P62158
R	76	MSE	MET	MODIFIED RESIDUE	UNP P62158
R	109	MSE	MET	MODIFIED RESIDUE	UNP P62158
R	124	MSE	MET	MODIFIED RESIDUE	UNP P62158
R	144	MSE	MET	MODIFIED RESIDUE	UNP P62158
R	145	MSE	MET	MODIFIED RESIDUE	UNP P62158
S	0	MSE	MET	MODIFIED RESIDUE	UNP P62158
S	36	MSE	MET	MODIFIED RESIDUE	UNP P62158
S	51	MSE	MET	MODIFIED RESIDUE	UNP P62158
S	71	MSE	MET	MODIFIED RESIDUE	UNP P62158
S	72	MSE	MET	MODIFIED RESIDUE	UNP P62158
S	76	MSE	MET	MODIFIED RESIDUE	UNP P62158
S	109	MSE	MET	MODIFIED RESIDUE	UNP P62158
S	124	MSE	MET	MODIFIED RESIDUE	UNP P62158
S	144	MSE	MET	MODIFIED RESIDUE	UNP P62158
S	145	MSE	MET	MODIFIED RESIDUE	UNP P62158
T	0	MSE	MET	MODIFIED RESIDUE	UNP P62158
T	36	MSE	MET	MODIFIED RESIDUE	UNP P62158
T	51	MSE	MET	MODIFIED RESIDUE	UNP P62158
T	71	MSE	MET	MODIFIED RESIDUE	UNP P62158
T	72	MSE	MET	MODIFIED RESIDUE	UNP P62158
T	76	MSE	MET	MODIFIED RESIDUE	UNP P62158
T	109	MSE	MET	MODIFIED RESIDUE	UNP P62158
T	124	MSE	MET	MODIFIED RESIDUE	UNP P62158
T	144	MSE	MET	MODIFIED RESIDUE	UNP P62158
T	145	MSE	MET	MODIFIED RESIDUE	UNP P62158

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

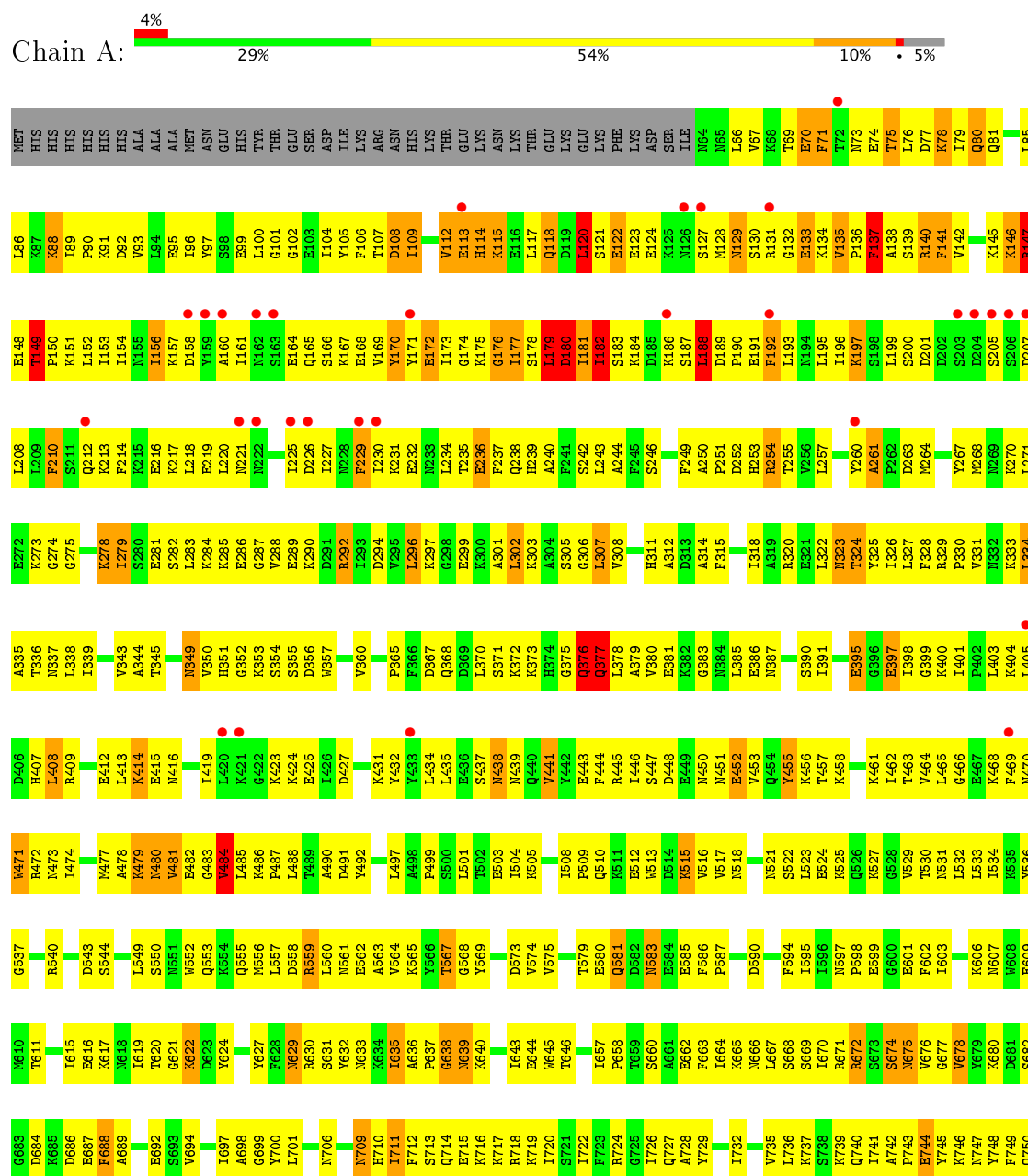
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	4	Total 4	Ca 4	0	0
4	Q	4	Total 4	Ca 4	0	0
4	T	4	Total 4	Ca 4	0	0
4	O	4	Total 4	Ca 4	0	0
4	R	4	Total 4	Ca 4	0	0
4	S	4	Total 4	Ca 4	0	0



### 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.

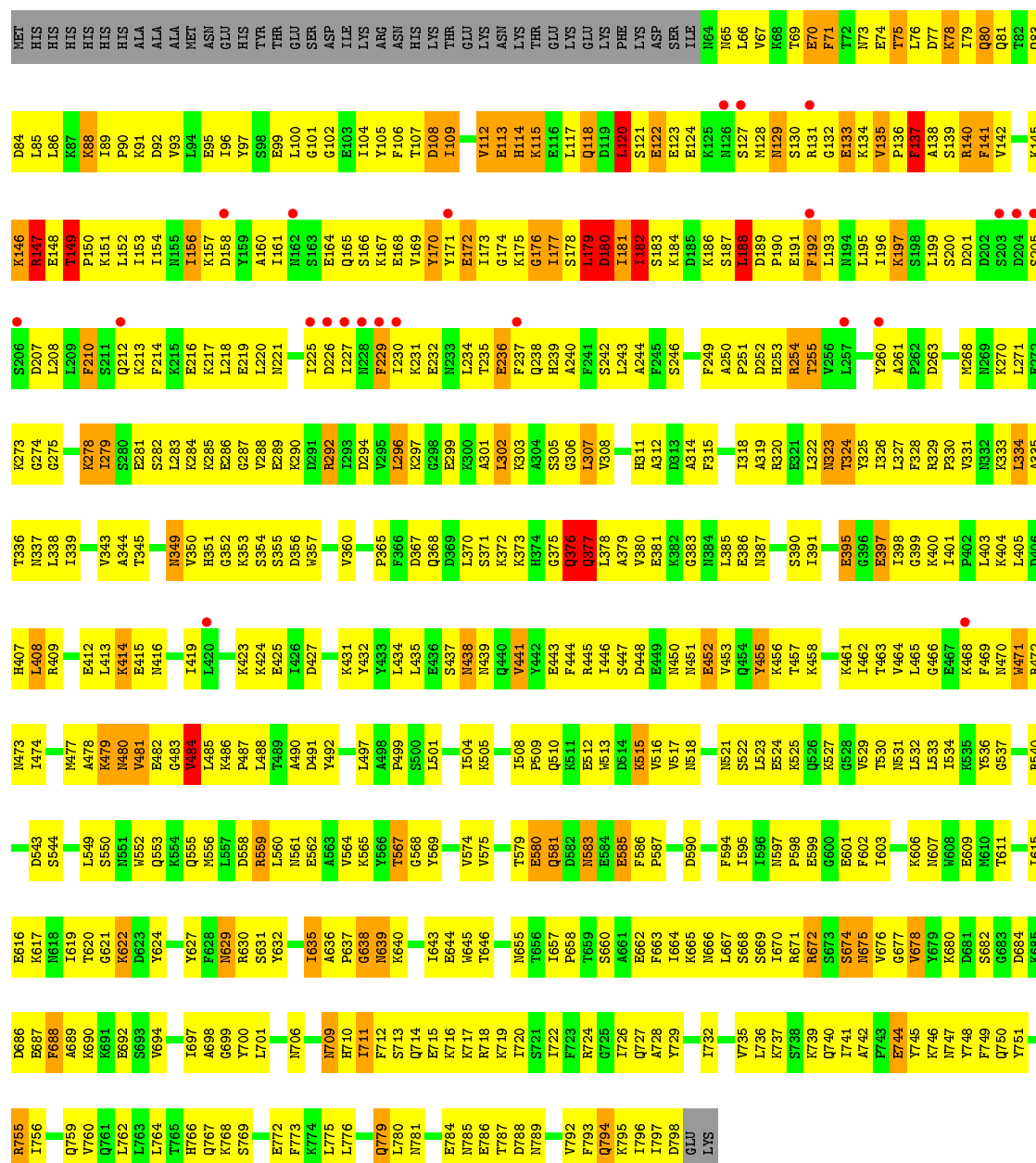
- Molecule 1: Calmodulin-sensitive adenylate cyclase







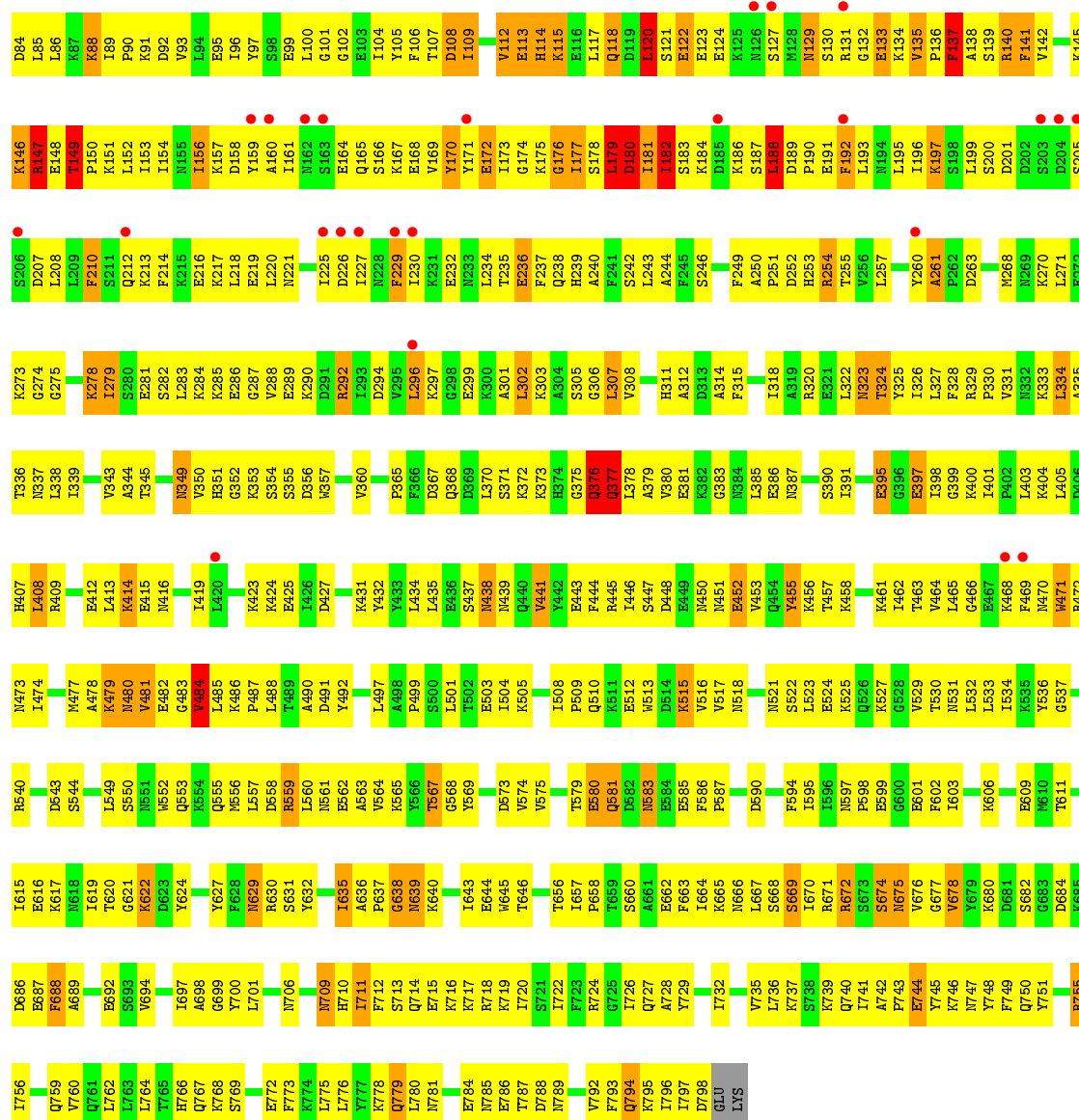
- Molecule 1: Calmodulin-sensitive adenylate cyclase



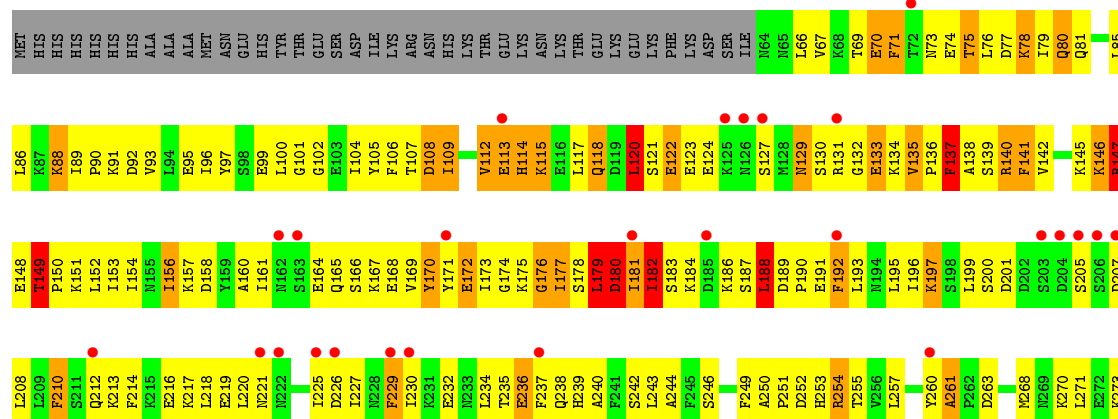
- Molecule 1: Calmodulin-sensitive adenylate cyclase



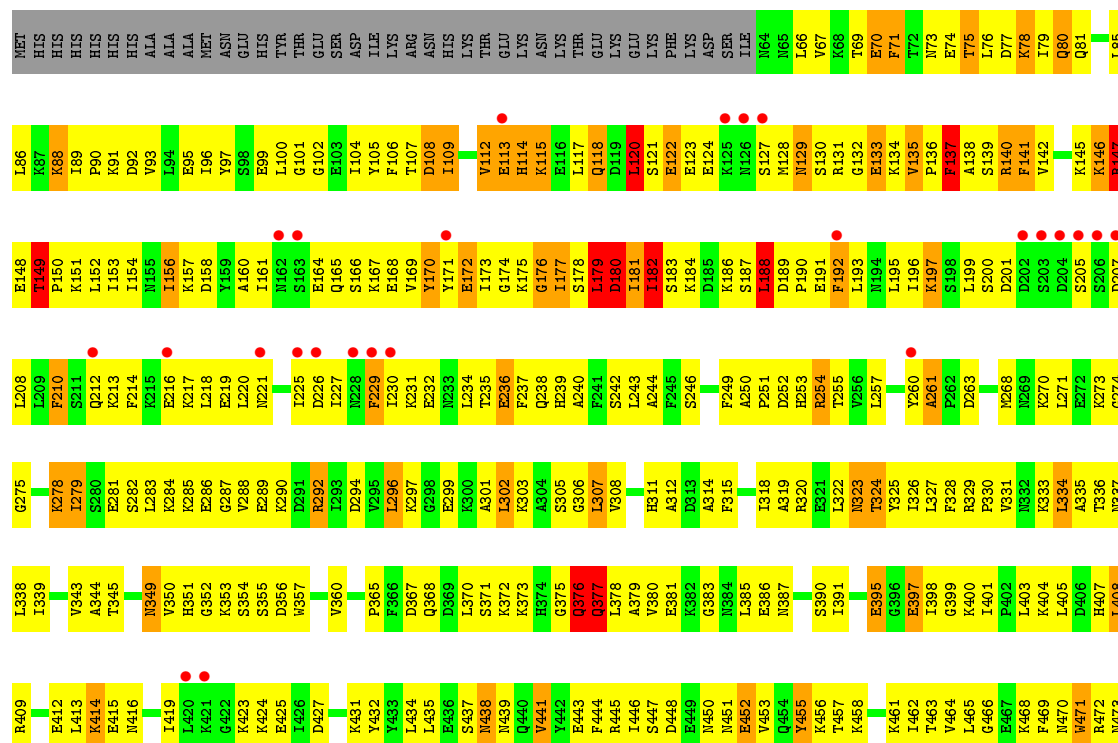




• Molecule 1: Calmodulin-sensitive adenylate cyclase



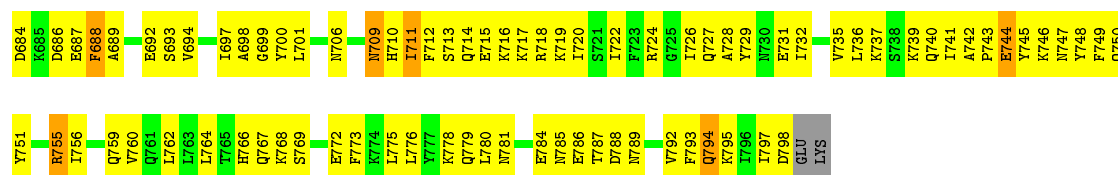




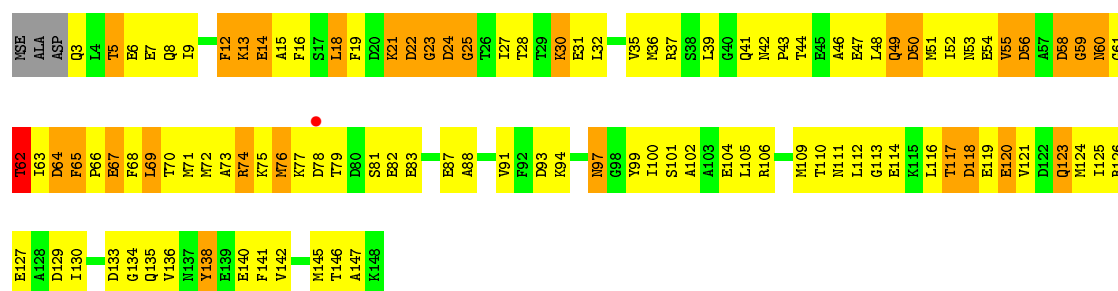




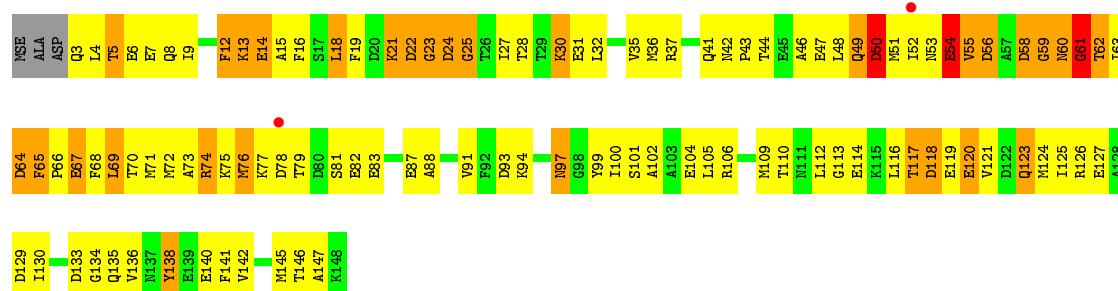




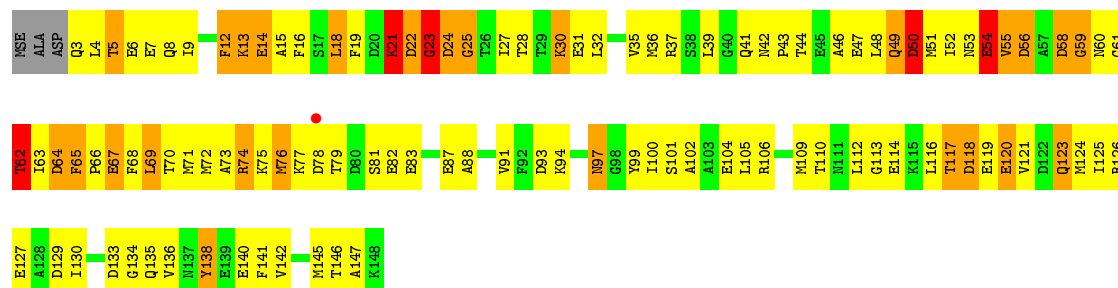
- Molecule 2: Calmodulin 2



- Molecule 2: Calmodulin 2



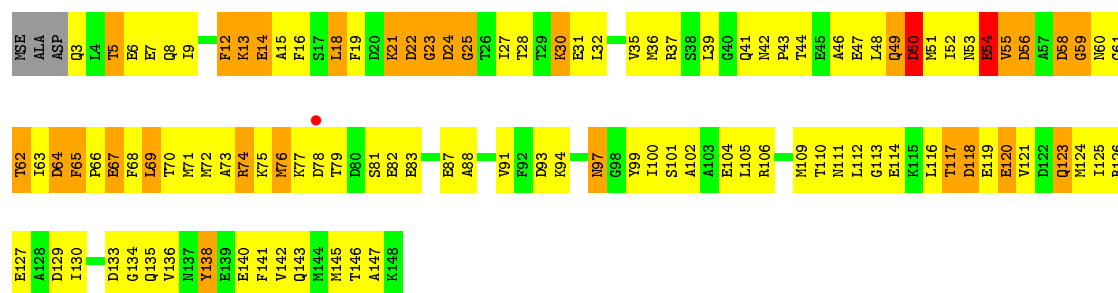
- Molecule 2: Calmodulin 2



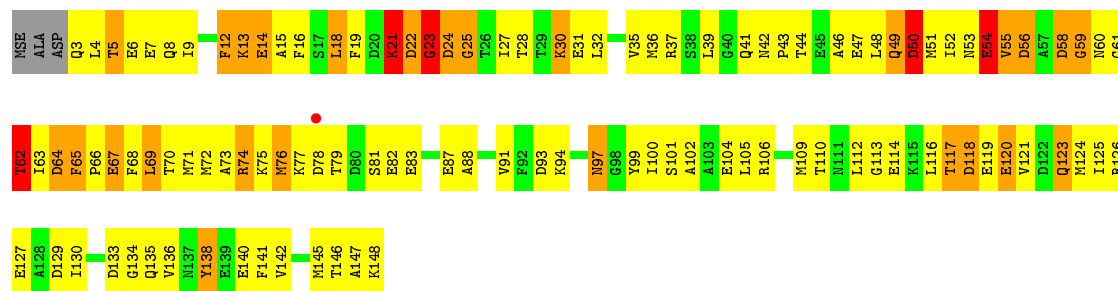
- Molecule 2: Calmodulin 2



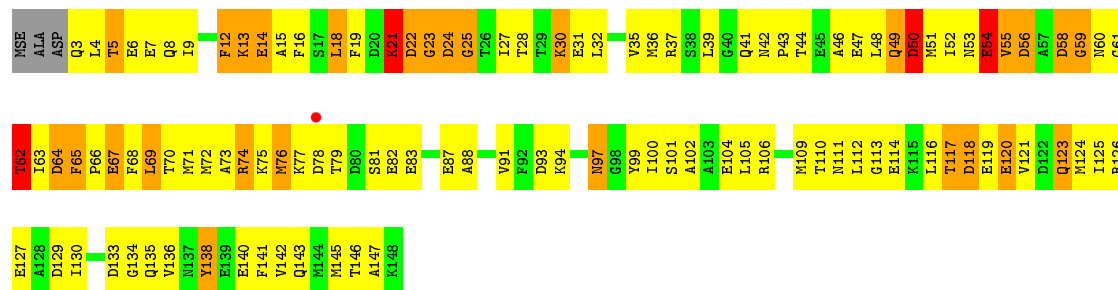




### • Molecule 2: Calmodulin 2



### • Molecule 2: Calmodulin 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	318.30Å 183.76Å 141.52Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	17.45 – 3.20 17.45 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (17.45-3.20) 96.1 (17.45-3.20)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.03	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 3.21Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.262 , 0.278 0.251 , 0.266	Depositor DCC
$R_{free}$ test set	6479 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	97.1	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 39.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.479 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.480 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.478 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.480 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.479 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	42858	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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: CA, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.58	1/6104 (0.0%)	0.81	13/8208 (0.2%)
1	B	0.58	1/6104 (0.0%)	0.81	13/8208 (0.2%)
1	C	0.57	1/6104 (0.0%)	0.81	13/8208 (0.2%)
1	D	0.58	1/6104 (0.0%)	0.81	13/8208 (0.2%)
1	E	0.57	1/6104 (0.0%)	0.81	13/8208 (0.2%)
1	F	0.57	1/6104 (0.0%)	0.81	12/8208 (0.1%)
2	O	0.66	1/1149 (0.1%)	0.86	2/1526 (0.1%)
2	P	0.69	2/1149 (0.2%)	0.88	4/1526 (0.3%)
2	Q	0.64	1/1149 (0.1%)	0.86	4/1526 (0.3%)
2	R	0.66	1/1149 (0.1%)	0.86	4/1526 (0.3%)
2	S	0.65	1/1149 (0.1%)	0.86	3/1526 (0.2%)
2	T	0.67	2/1149 (0.2%)	0.86	3/1526 (0.2%)
All	All	0.59	14/43518 (0.0%)	0.82	97/58404 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
2	O	0	1
2	P	0	3
2	Q	0	3
2	R	0	3
2	S	0	3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
2	T	0	3
All	All	0	22

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	61	GLY	C-O	7.82	1.36	1.23
2	S	62	THR	CB-CG2	6.71	1.74	1.52
2	R	62	THR	CB-CG2	6.62	1.74	1.52
2	T	62	THR	CB-CG2	6.50	1.73	1.52
2	O	62	THR	CB-CG2	6.42	1.73	1.52
2	T	59	GLY	N-CA	-6.18	1.36	1.46
2	P	62	THR	CB-CG2	6.12	1.72	1.52
1	F	179	LEU	C-O	-5.98	1.11	1.23
2	Q	62	THR	CB-CG2	5.89	1.71	1.52
1	B	179	LEU	C-O	-5.86	1.12	1.23
1	E	179	LEU	C-O	-5.86	1.12	1.23
1	A	179	LEU	C-O	-5.82	1.12	1.23
1	D	179	LEU	C-O	-5.81	1.12	1.23
1	C	179	LEU	C-O	-5.81	1.12	1.23

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	LEU	N-CA-C	-11.99	78.63	111.00
1	F	188	LEU	N-CA-C	-11.96	78.71	111.00
1	A	188	LEU	N-CA-C	-11.95	78.73	111.00
1	C	188	LEU	N-CA-C	-11.95	78.75	111.00
1	D	188	LEU	N-CA-C	-11.94	78.75	111.00
1	E	188	LEU	N-CA-C	-11.92	78.82	111.00
2	T	59	GLY	N-CA-C	-9.85	88.47	113.10
1	B	147	ARG	N-CA-C	9.52	136.69	111.00
1	F	147	ARG	N-CA-C	9.40	136.39	111.00
1	E	147	ARG	N-CA-C	9.40	136.38	111.00
1	C	147	ARG	N-CA-C	9.38	136.32	111.00
1	A	147	ARG	N-CA-C	9.37	136.28	111.00
1	D	147	ARG	N-CA-C	9.36	136.28	111.00
2	P	59	GLY	N-CA-C	-9.28	89.90	113.10
2	S	59	GLY	N-CA-C	-9.04	90.49	113.10
2	O	59	GLY	N-CA-C	-8.79	91.13	113.10
1	F	160	ALA	N-CA-C	8.70	134.48	111.00
1	D	160	ALA	N-CA-C	8.67	134.40	111.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	160	ALA	N-CA-C	8.67	134.40	111.00
1	A	160	ALA	N-CA-C	8.66	134.38	111.00
1	C	160	ALA	N-CA-C	8.65	134.36	111.00
1	B	160	ALA	N-CA-C	8.65	134.35	111.00
2	Q	59	GLY	N-CA-C	-8.45	91.98	113.10
2	R	59	GLY	N-CA-C	-8.39	92.11	113.10
1	D	129	ASN	N-CA-C	7.50	131.25	111.00
1	B	129	ASN	N-CA-C	7.47	131.17	111.00
1	C	129	ASN	N-CA-C	7.45	131.11	111.00
1	A	129	ASN	N-CA-C	7.44	131.09	111.00
1	F	129	ASN	N-CA-C	7.43	131.07	111.00
1	E	129	ASN	N-CA-C	7.42	131.03	111.00
1	C	674	SER	N-CA-C	-6.48	93.52	111.00
1	F	674	SER	N-CA-C	-6.47	93.53	111.00
1	A	674	SER	N-CA-C	-6.46	93.57	111.00
1	D	674	SER	N-CA-C	-6.44	93.62	111.00
1	B	674	SER	N-CA-C	-6.43	93.65	111.00
1	E	674	SER	N-CA-C	-6.37	93.81	111.00
2	P	54	GLU	O-C-N	-6.36	112.53	122.70
2	Q	54	GLU	O-C-N	-6.26	112.68	122.70
2	S	54	GLU	O-C-N	-6.17	112.83	122.70
2	R	54	GLU	O-C-N	-6.16	112.85	122.70
1	F	132	GLY	N-CA-C	-6.09	97.87	113.10
1	D	132	GLY	N-CA-C	-6.05	97.97	113.10
1	B	132	GLY	N-CA-C	-6.05	97.98	113.10
1	C	132	GLY	N-CA-C	-6.02	98.05	113.10
1	E	132	GLY	N-CA-C	-5.95	98.23	113.10
1	A	132	GLY	N-CA-C	-5.94	98.25	113.10
1	B	149	THR	N-CA-C	-5.79	95.38	111.00
1	A	149	THR	N-CA-C	-5.75	95.47	111.00
1	E	149	THR	N-CA-C	-5.74	95.51	111.00
1	D	149	THR	N-CA-C	-5.73	95.53	111.00
1	D	146	LYS	N-CA-C	5.72	126.45	111.00
1	F	146	LYS	N-CA-C	5.71	126.42	111.00
1	A	146	LYS	N-CA-C	5.69	126.37	111.00
1	A	261	ALA	N-CA-C	-5.68	95.67	111.00
1	E	261	ALA	N-CA-C	-5.68	95.67	111.00
1	B	261	ALA	N-CA-C	-5.67	95.68	111.00
1	F	261	ALA	N-CA-C	-5.67	95.68	111.00
1	B	768	LYS	N-CA-C	-5.67	95.68	111.00
2	T	54	GLU	O-C-N	-5.67	113.63	122.70
1	E	146	LYS	N-CA-C	5.67	126.30	111.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	146	LYS	N-CA-C	5.66	126.29	111.00
1	C	149	THR	N-CA-C	-5.66	95.71	111.00
1	B	146	LYS	N-CA-C	5.66	126.27	111.00
1	F	149	THR	N-CA-C	-5.65	95.73	111.00
1	E	768	LYS	N-CA-C	-5.65	95.75	111.00
1	F	622	LYS	N-CA-C	-5.64	95.76	111.00
1	D	261	ALA	N-CA-C	-5.63	95.80	111.00
1	B	622	LYS	N-CA-C	-5.63	95.80	111.00
1	D	768	LYS	N-CA-C	-5.63	95.81	111.00
1	E	622	LYS	N-CA-C	-5.62	95.83	111.00
1	C	261	ALA	N-CA-C	-5.61	95.84	111.00
1	F	768	LYS	N-CA-C	-5.61	95.86	111.00
1	C	768	LYS	N-CA-C	-5.60	95.87	111.00
1	A	768	LYS	N-CA-C	-5.57	95.96	111.00
1	A	622	LYS	N-CA-C	-5.57	95.97	111.00
1	C	622	LYS	N-CA-C	-5.57	95.97	111.00
1	D	622	LYS	N-CA-C	-5.54	96.03	111.00
2	Q	23	GLY	N-CA-C	5.35	126.48	113.10
2	P	23	GLY	N-CA-C	5.26	126.26	113.10
2	O	23	GLY	N-CA-C	5.23	126.17	113.10
2	R	23	GLY	N-CA-C	5.22	126.16	113.10
1	E	622	LYS	C-N-CA	-5.22	108.64	121.70
2	T	23	GLY	N-CA-C	5.22	126.15	113.10
2	S	23	GLY	N-CA-C	5.21	126.14	113.10
2	R	62	THR	OG1-CB-CG2	5.20	121.96	110.00
1	D	622	LYS	C-N-CA	-5.19	108.72	121.70
1	E	120	LEU	N-CA-C	5.13	124.86	111.00
2	Q	62	THR	OG1-CB-CG2	5.13	121.81	110.00
1	A	622	LYS	C-N-CA	-5.13	108.88	121.70
1	C	622	LYS	C-N-CA	-5.12	108.89	121.70
1	C	120	LEU	N-CA-C	5.10	124.77	111.00
1	A	120	LEU	N-CA-C	5.08	124.72	111.00
2	P	62	THR	OG1-CB-CG2	5.08	121.67	110.00
1	D	120	LEU	N-CA-C	5.06	124.66	111.00
1	F	120	LEU	N-CA-C	5.06	124.65	111.00
1	B	622	LYS	C-N-CA	-5.06	109.06	121.70
1	B	120	LEU	N-CA-C	5.05	124.64	111.00

There are no chirality outliers.

All (22) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	170	TYR	Sidechain
1	B	170	TYR	Sidechain
1	C	170	TYR	Sidechain
1	D	170	TYR	Sidechain
1	E	170	TYR	Sidechain
1	F	170	TYR	Sidechain
2	O	138	TYR	Sidechain
2	P	138	TYR	Sidechain
2	P	54	GLU	Mainchain,Peptide
2	Q	138	TYR	Sidechain
2	Q	54	GLU	Mainchain,Peptide
2	R	138	TYR	Sidechain
2	R	54	GLU	Mainchain,Peptide
2	S	138	TYR	Sidechain
2	S	54	GLU	Mainchain,Peptide
2	T	138	TYR	Sidechain
2	T	54	GLU	Mainchain,Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5992	0	6010	720	1
1	B	5992	0	6010	721	1
1	C	5992	0	6010	724	1
1	D	5992	0	6010	718	0
1	E	5992	0	6010	708	0
1	F	5992	0	6010	715	1
2	O	1146	0	1071	180	0
2	P	1146	0	1071	182	0
2	Q	1146	0	1071	184	0
2	R	1146	0	1071	185	0
2	S	1146	0	1071	192	0
2	T	1146	0	1071	183	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1	0	0	0	0
4	O	4	0	0	0	0
4	P	4	0	0	0	0
4	Q	4	0	0	0	0
4	R	4	0	0	0	0
4	S	4	0	0	0	0
4	T	4	0	0	0	0
All	All	42858	0	42486	5285	2

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 62.

All (5285) 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:S:62:THR:CG2	2:S:62:THR:CB	1.74	1.60
1:B:179:LEU:O	1:B:183:SER:HB2	1.21	1.35
1:A:179:LEU:O	1:A:183:SER:HB2	1.21	1.35
1:E:179:LEU:O	1:E:183:SER:HB2	1.21	1.32
1:D:179:LEU:O	1:D:183:SER:HB2	1.20	1.32
1:F:179:LEU:O	1:F:183:SER:HB2	1.20	1.29
1:C:179:LEU:O	1:C:183:SER:HB2	1.21	1.28
1:C:127:SER:O	1:C:133:GLU:OE2	1.63	1.17
1:E:127:SER:O	1:E:133:GLU:OE2	1.63	1.17
1:F:127:SER:O	1:F:133:GLU:OE2	1.63	1.17
1:B:127:SER:O	1:B:133:GLU:OE2	1.63	1.16
1:D:127:SER:O	1:D:133:GLU:OE2	1.63	1.16
1:A:127:SER:O	1:A:133:GLU:OE2	1.63	1.16
1:F:296:LEU:H	1:F:296:LEU:HD23	1.11	1.15
1:C:296:LEU:HD23	1:C:296:LEU:H	1.11	1.14
1:A:89:ILE:HG22	1:A:93:VAL:HG11	1.31	1.13
1:D:89:ILE:HG22	1:D:93:VAL:HG11	1.30	1.13
1:E:296:LEU:HD23	1:E:296:LEU:H	1.11	1.13
1:B:179:LEU:O	1:B:183:SER:CB	1.98	1.11
1:C:179:LEU:O	1:C:183:SER:CB	1.99	1.11
1:D:179:LEU:O	1:D:183:SER:CB	1.98	1.11
1:B:89:ILE:HG22	1:B:93:VAL:HG11	1.31	1.11
1:D:296:LEU:HD23	1:D:296:LEU:H	1.12	1.10
1:F:179:LEU:O	1:F:183:SER:CB	1.98	1.10
1:E:179:LEU:O	1:E:183:SER:CB	1.98	1.10
1:A:179:LEU:O	1:A:183:SER:CB	1.99	1.10

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:LEU:HD23	1:B:296:LEU:H	1.11	1.09
1:B:408:LEU:H	1:B:408:LEU:HD12	1.17	1.09
1:E:89:ILE:HG22	1:E:93:VAL:HG11	1.32	1.09
1:C:89:ILE:HG22	1:C:93:VAL:HG11	1.30	1.08
1:A:408:LEU:H	1:A:408:LEU:HD12	1.18	1.08
1:A:296:LEU:HD23	1:A:296:LEU:H	1.11	1.07
1:F:89:ILE:HG22	1:F:93:VAL:HG11	1.31	1.07
1:E:408:LEU:HD12	1:E:408:LEU:H	1.19	1.07
1:E:296:LEU:N	1:E:296:LEU:HD23	1.71	1.06
2:R:13:LYS:NZ	2:R:65:PHE:HB3	1.71	1.06
1:F:408:LEU:H	1:F:408:LEU:HD12	1.18	1.05
1:C:597:ASN:HD21	1:C:601:GLU:HB2	1.21	1.05
1:F:296:LEU:N	1:F:296:LEU:HD23	1.72	1.05
1:A:597:ASN:HD21	1:A:601:GLU:HB2	1.21	1.05
1:B:296:LEU:HD23	1:B:296:LEU:N	1.72	1.05
2:P:55:VAL:HG21	2:P:67:GLU:OE1	1.56	1.05
2:O:13:LYS:NZ	2:O:65:PHE:HB3	1.72	1.05
1:A:296:LEU:HD23	1:A:296:LEU:N	1.72	1.05
1:C:296:LEU:HD23	1:C:296:LEU:N	1.71	1.04
1:D:408:LEU:H	1:D:408:LEU:HD12	1.19	1.04
1:E:597:ASN:HD21	1:E:601:GLU:HB2	1.22	1.04
1:B:501:LEU:HD22	2:P:112:LEU:HD21	1.39	1.04
1:E:479:LYS:HG2	1:E:488:LEU:HD21	1.38	1.04
1:A:501:LEU:HD22	2:O:112:LEU:HD21	1.40	1.03
2:P:13:LYS:NZ	2:P:65:PHE:HB3	1.72	1.03
2:Q:13:LYS:NZ	2:Q:65:PHE:HB3	1.72	1.03
2:S:55:VAL:HG21	2:S:67:GLU:OE1	1.58	1.03
1:F:501:LEU:HD22	2:T:112:LEU:HD21	1.40	1.03
2:S:13:LYS:NZ	2:S:65:PHE:HB3	1.72	1.03
2:T:13:LYS:NZ	2:T:65:PHE:HB3	1.72	1.03
1:D:296:LEU:HD23	1:D:296:LEU:N	1.72	1.03
1:E:501:LEU:HD22	2:S:112:LEU:HD21	1.41	1.03
2:Q:55:VAL:HG21	2:Q:67:GLU:OE1	1.58	1.02
1:C:479:LYS:HG2	1:C:488:LEU:HD21	1.37	1.02
1:F:479:LYS:HG2	1:F:488:LEU:HD21	1.38	1.02
1:D:597:ASN:HD21	1:D:601:GLU:HB2	1.21	1.02
1:C:408:LEU:H	1:C:408:LEU:HD12	1.18	1.02
1:F:597:ASN:HD21	1:F:601:GLU:HB2	1.21	1.02
1:A:479:LYS:HG2	1:A:488:LEU:HD21	1.38	1.01
1:B:597:ASN:HD21	1:B:601:GLU:HB2	1.22	1.01
1:D:501:LEU:HD22	2:R:112:LEU:HD21	1.40	1.01

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:LYS:HG2	1:B:488:LEU:HD21	1.38	1.01
2:R:55:VAL:HG21	2:R:67:GLU:OE1	1.59	1.01
1:C:501:LEU:HD22	2:Q:112:LEU:HD21	1.41	1.00
1:D:479:LYS:HG2	1:D:488:LEU:HD21	1.39	1.00
2:T:55:VAL:HG21	2:T:67:GLU:OE1	1.59	1.00
2:S:30:LYS:HD3	2:S:30:LYS:H	1.27	0.99
2:O:55:VAL:HG21	2:O:67:GLU:OE1	1.59	0.99
1:A:112:VAL:HG12	1:A:113:GLU:H	1.27	0.99
1:C:112:VAL:HG12	1:C:113:GLU:H	1.27	0.99
1:D:90:PRO:O	1:D:93:VAL:HG12	1.62	0.99
1:B:90:PRO:O	1:B:93:VAL:HG12	1.63	0.99
2:Q:30:LYS:H	2:Q:30:LYS:HD3	1.27	0.98
1:B:112:VAL:HG12	1:B:113:GLU:H	1.28	0.98
1:B:657:ILE:HG13	1:B:756:ILE:HD13	1.46	0.98
1:E:112:VAL:HG12	1:E:113:GLU:H	1.26	0.98
1:E:90:PRO:O	1:E:93:VAL:HG12	1.63	0.98
1:F:112:VAL:HG12	1:F:113:GLU:H	1.27	0.98
1:A:182:ILE:C	1:A:187:SER:HB2	1.85	0.97
1:D:122:GLU:HG3	1:D:147:ARG:HB2	1.45	0.97
1:C:90:PRO:O	1:C:93:VAL:HG12	1.64	0.97
1:F:182:ILE:C	1:F:187:SER:HB2	1.85	0.97
1:D:182:ILE:C	1:D:187:SER:HB2	1.85	0.97
1:E:629:ASN:ND2	1:E:631:SER:H	1.63	0.97
1:B:122:GLU:HG3	1:B:147:ARG:HB2	1.45	0.97
1:B:182:ILE:C	1:B:187:SER:HB2	1.84	0.97
1:E:657:ILE:HG13	1:E:756:ILE:HD13	1.46	0.97
1:A:90:PRO:O	1:A:93:VAL:HG12	1.63	0.97
1:E:154:ILE:HG13	1:E:171:TYR:CE1	2.00	0.97
1:F:122:GLU:HG3	1:F:147:ARG:HB2	1.45	0.97
1:F:657:ILE:HG13	1:F:756:ILE:HD13	1.47	0.97
2:R:30:LYS:H	2:R:30:LYS:HD3	1.27	0.96
1:F:90:PRO:O	1:F:93:VAL:HG12	1.63	0.96
2:O:30:LYS:HD3	2:O:30:LYS:H	1.26	0.96
2:T:30:LYS:H	2:T:30:LYS:HD3	1.26	0.96
1:A:122:GLU:HG3	1:A:147:ARG:HB2	1.46	0.96
1:D:112:VAL:HG12	1:D:113:GLU:H	1.27	0.96
1:F:629:ASN:ND2	1:F:631:SER:H	1.63	0.96
1:A:657:ILE:HG13	1:A:756:ILE:HD13	1.47	0.96
1:C:629:ASN:ND2	1:C:631:SER:H	1.63	0.96
2:P:30:LYS:HD3	2:P:30:LYS:H	1.26	0.96
1:C:182:ILE:C	1:C:187:SER:HB2	1.85	0.96

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:657:ILE:HG13	1:C:756:ILE:HD13	1.47	0.96
1:D:629:ASN:ND2	1:D:631:SER:H	1.62	0.96
1:B:154:ILE:HG13	1:B:171:TYR:CE1	2.01	0.96
1:F:161:ILE:CG2	1:F:168:GLU:HB2	1.96	0.96
1:E:182:ILE:C	1:E:187:SER:HB2	1.85	0.95
1:D:657:ILE:HG13	1:D:756:ILE:HD13	1.47	0.95
1:B:161:ILE:CG2	1:B:168:GLU:HB2	1.95	0.95
1:F:154:ILE:HG13	1:F:171:TYR:CE1	2.01	0.95
1:D:154:ILE:HG13	1:D:171:TYR:CE1	2.01	0.95
1:B:629:ASN:ND2	1:B:631:SER:H	1.64	0.95
1:E:161:ILE:CG2	1:E:168:GLU:HB2	1.96	0.95
1:B:472:ARG:HB3	1:B:472:ARG:HH11	1.31	0.95
1:C:472:ARG:HH11	1:C:472:ARG:HB3	1.32	0.95
1:F:472:ARG:HH11	1:F:472:ARG:HB3	1.31	0.95
1:E:472:ARG:HH11	1:E:472:ARG:HB3	1.31	0.94
1:A:154:ILE:HG13	1:A:171:TYR:CE1	2.01	0.94
1:C:122:GLU:HG3	1:C:147:ARG:HB2	1.46	0.94
1:C:180:ASP:OD1	1:C:180:ASP:N	2.00	0.94
1:E:122:GLU:HG3	1:E:147:ARG:HB2	1.45	0.94
1:C:161:ILE:CG2	1:C:168:GLU:HB2	1.97	0.94
1:A:629:ASN:ND2	1:A:631:SER:H	1.64	0.94
1:C:154:ILE:HG13	1:C:171:TYR:CE1	2.01	0.94
1:A:161:ILE:CG2	1:A:168:GLU:HB2	1.96	0.94
1:A:472:ARG:HB3	1:A:472:ARG:HH11	1.33	0.94
1:A:180:ASP:N	1:A:180:ASP:OD1	2.00	0.94
2:R:59:GLY:O	2:R:62:THR:CG2	2.16	0.94
1:D:152:LEU:HD21	1:D:171:TYR:HE1	1.34	0.93
1:D:472:ARG:HB3	1:D:472:ARG:HH11	1.32	0.93
1:F:180:ASP:OD1	1:F:180:ASP:N	2.01	0.92
1:D:161:ILE:CG2	1:D:168:GLU:HB2	1.97	0.92
1:B:180:ASP:N	1:B:180:ASP:OD1	2.00	0.92
1:C:152:LEU:HD21	1:C:171:TYR:HE1	1.34	0.92
1:F:722:ILE:HG23	1:F:760:VAL:HG13	1.51	0.92
1:B:629:ASN:HD22	1:B:631:SER:H	1.18	0.92
1:F:629:ASN:HD22	1:F:631:SER:H	1.17	0.92
1:D:180:ASP:OD1	1:D:180:ASP:N	2.00	0.91
1:C:629:ASN:HD22	1:C:631:SER:H	1.17	0.91
1:D:629:ASN:HD22	1:D:631:SER:H	1.15	0.91
1:B:353:LYS:H	1:B:368:GLN:HE22	1.17	0.91
1:A:615:ILE:HD12	1:A:645:TRP:HH2	1.36	0.91
1:F:152:LEU:HD21	1:F:171:TYR:HE1	1.33	0.91

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:LEU:N	1:E:188:LEU:HD23	1.86	0.91
1:A:152:LEU:HD21	1:A:171:TYR:HE1	1.34	0.91
1:A:722:ILE:HG23	1:A:760:VAL:HG13	1.51	0.91
1:C:722:ILE:HG23	1:C:760:VAL:HG13	1.50	0.91
1:D:615:ILE:HD12	1:D:645:TRP:HH2	1.36	0.90
1:E:353:LYS:H	1:E:368:GLN:HE22	1.17	0.90
2:O:59:GLY:O	2:O:62:THR:CG2	2.19	0.90
1:B:722:ILE:HG23	1:B:760:VAL:HG13	1.51	0.90
1:B:188:LEU:HD23	1:B:188:LEU:N	1.87	0.90
1:C:615:ILE:HD12	1:C:645:TRP:HH2	1.37	0.90
1:D:186:LYS:HE3	1:D:234:LEU:HD12	1.54	0.90
1:B:152:LEU:HD21	1:B:171:TYR:HE1	1.35	0.90
2:S:28:THR:HB	2:S:30:LYS:HZ3	1.37	0.90
1:F:327:LEU:HG	1:F:595:ILE:HG23	1.54	0.90
2:Q:36:MSE:HE3	2:Q:43:PRO:HG3	1.54	0.90
1:C:405:LEU:HD13	1:C:453:VAL:HG21	1.54	0.90
1:F:188:LEU:N	1:F:188:LEU:HD23	1.87	0.90
1:A:327:LEU:HG	1:A:595:ILE:HG23	1.54	0.89
1:E:722:ILE:HG23	1:E:760:VAL:HG13	1.52	0.89
1:A:186:LYS:HE3	1:A:234:LEU:HD12	1.54	0.89
2:R:36:MSE:HE3	2:R:43:PRO:HG3	1.54	0.89
1:A:188:LEU:HD23	1:A:188:LEU:N	1.87	0.89
1:D:405:LEU:HD13	1:D:453:VAL:HG21	1.54	0.89
1:E:152:LEU:HD21	1:E:171:TYR:HE1	1.35	0.89
1:E:405:LEU:HD13	1:E:453:VAL:HG21	1.54	0.89
1:E:327:LEU:HG	1:E:595:ILE:HG23	1.55	0.89
1:F:405:LEU:HD13	1:F:453:VAL:HG21	1.55	0.89
1:C:188:LEU:HD23	1:C:188:LEU:N	1.86	0.89
1:E:615:ILE:HD12	1:E:645:TRP:HH2	1.37	0.89
1:E:629:ASN:HD22	1:E:631:SER:H	1.17	0.89
1:C:186:LYS:HE3	1:C:234:LEU:HD12	1.55	0.89
1:D:722:ILE:HG23	1:D:760:VAL:HG13	1.52	0.89
1:F:615:ILE:HD12	1:F:645:TRP:HH2	1.36	0.89
2:T:36:MSE:HE3	2:T:43:PRO:HG3	1.54	0.89
1:D:188:LEU:N	1:D:188:LEU:HD23	1.87	0.89
1:E:616:GLU:HA	1:E:620:THR:HB	1.55	0.89
2:O:36:MSE:HE3	2:O:43:PRO:HG3	1.54	0.89
1:D:130:SER:HB2	1:D:170:TYR:CE2	2.08	0.88
1:D:327:LEU:HG	1:D:595:ILE:HG23	1.53	0.88
1:B:186:LYS:HE3	1:B:234:LEU:HD12	1.54	0.88
1:A:353:LYS:H	1:A:368:GLN:HE22	1.19	0.88

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:GLU:HA	1:A:620:THR:HB	1.56	0.88
1:D:616:GLU:HA	1:D:620:THR:HB	1.55	0.88
1:E:719:LYS:HE3	1:E:797:ILE:HD11	1.55	0.88
2:R:56:ASP:OD2	2:R:60:ASN:HA	1.74	0.88
1:B:327:LEU:HG	1:B:595:ILE:HG23	1.55	0.88
1:B:550:SER:HB3	1:B:553:GLN:HG3	1.55	0.88
2:Q:56:ASP:OD2	2:Q:60:ASN:HA	1.74	0.88
1:A:550:SER:HB3	1:A:553:GLN:HG3	1.55	0.88
1:C:327:LEU:HG	1:C:595:ILE:HG23	1.54	0.88
1:B:616:GLU:HA	1:B:620:THR:HB	1.55	0.88
2:S:36:MSE:HE3	2:S:43:PRO:HG3	1.54	0.88
1:A:130:SER:HB2	1:A:170:TYR:CE2	2.09	0.88
1:D:275:GLY:HA2	1:D:278:LYS:HE3	1.56	0.88
1:C:275:GLY:HA2	1:C:278:LYS:HE3	1.55	0.87
1:E:275:GLY:HA2	1:E:278:LYS:HE3	1.55	0.87
1:F:616:GLU:HA	1:F:620:THR:HB	1.56	0.87
1:A:405:LEU:HD13	1:A:453:VAL:HG21	1.54	0.87
1:C:130:SER:HB2	1:C:170:TYR:CE2	2.08	0.87
1:C:550:SER:HB3	1:C:553:GLN:HG3	1.57	0.87
1:E:161:ILE:HA	1:E:167:LYS:HD2	1.57	0.87
1:F:353:LYS:H	1:F:368:GLN:HE22	1.18	0.87
1:F:550:SER:HB3	1:F:553:GLN:HG3	1.54	0.87
1:E:186:LYS:HE3	1:E:234:LEU:HD12	1.54	0.87
1:B:405:LEU:HD13	1:B:453:VAL:HG21	1.55	0.87
1:A:630:ARG:CZ	2:O:83:GLU:HG2	2.04	0.87
1:E:130:SER:HB2	1:E:170:TYR:CE2	2.09	0.87
1:B:161:ILE:HA	1:B:167:LYS:HD2	1.56	0.87
2:P:36:MSE:HE3	2:P:43:PRO:HG3	1.54	0.87
1:B:275:GLY:HA2	1:B:278:LYS:HE3	1.57	0.87
1:C:616:GLU:HA	1:C:620:THR:HB	1.56	0.87
1:F:275:GLY:HA2	1:F:278:LYS:HE3	1.56	0.87
1:F:597:ASN:HB2	1:F:598:PRO:HD2	1.57	0.87
2:P:28:THR:HB	2:P:30:LYS:HZ3	1.39	0.87
1:A:719:LYS:HE3	1:A:797:ILE:HD11	1.56	0.86
1:D:597:ASN:HB2	1:D:598:PRO:HD2	1.57	0.86
2:P:65:PHE:HB2	2:P:66:PRO:HD3	1.57	0.86
1:A:611:THR:O	1:A:615:ILE:HG13	1.74	0.86
1:E:611:THR:O	1:E:615:ILE:HG13	1.75	0.86
1:F:719:LYS:HE3	1:F:797:ILE:HD11	1.57	0.86
1:B:611:THR:O	1:B:615:ILE:HG13	1.75	0.86
1:B:615:ILE:HD12	1:B:645:TRP:HH2	1.39	0.86

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:719:LYS:HE3	1:D:797:ILE:HD11	1.56	0.86
1:B:130:SER:HB2	1:B:170:TYR:CE2	2.10	0.86
1:F:611:THR:O	1:F:615:ILE:HG13	1.75	0.86
1:C:719:LYS:HE3	1:C:797:ILE:HD11	1.57	0.86
1:F:161:ILE:HA	1:F:167:LYS:HD2	1.57	0.86
1:F:186:LYS:HE3	1:F:234:LEU:HD12	1.55	0.86
2:O:65:PHE:HB2	2:O:66:PRO:HD3	1.58	0.86
2:Q:65:PHE:HB2	2:Q:66:PRO:HD3	1.58	0.86
2:S:65:PHE:HB2	2:S:66:PRO:HD3	1.57	0.86
1:B:107:THR:HG21	1:B:115:LYS:HD2	1.57	0.86
1:B:719:LYS:HE3	1:B:797:ILE:HD11	1.58	0.86
1:A:275:GLY:HA2	1:A:278:LYS:HE3	1.58	0.86
1:C:611:THR:O	1:C:615:ILE:HG13	1.75	0.86
1:E:180:ASP:N	1:E:180:ASP:OD1	2.01	0.86
1:B:635:ILE:HD12	1:B:635:ILE:H	1.41	0.86
2:P:117:THR:HG23	2:P:120:GLU:HB2	1.58	0.86
2:R:65:PHE:HB2	2:R:66:PRO:HD3	1.58	0.86
1:A:629:ASN:HD22	1:A:631:SER:H	1.19	0.85
1:F:130:SER:HB2	1:F:170:TYR:CE2	2.10	0.85
1:E:630:ARG:CZ	2:S:83:GLU:HG2	2.05	0.85
2:T:65:PHE:HB2	2:T:66:PRO:HD3	1.58	0.85
1:D:89:ILE:HG22	1:D:93:VAL:CG1	2.06	0.85
1:D:353:LYS:H	1:D:368:GLN:HE22	1.17	0.85
1:D:550:SER:HB3	1:D:553:GLN:HG3	1.58	0.85
1:A:597:ASN:HB2	1:A:598:PRO:HD2	1.57	0.85
1:C:353:LYS:H	1:C:368:GLN:HE22	1.19	0.85
1:E:550:SER:HB3	1:E:553:GLN:HG3	1.57	0.85
1:A:107:THR:HG21	1:A:115:LYS:HD2	1.58	0.85
1:B:89:ILE:HG22	1:B:93:VAL:CG1	2.07	0.85
1:C:635:ILE:H	1:C:635:ILE:HD12	1.42	0.85
1:C:89:ILE:HG22	1:C:93:VAL:CG1	2.07	0.85
1:D:161:ILE:HA	1:D:167:LYS:HD2	1.58	0.85
1:A:161:ILE:HA	1:A:167:LYS:HD2	1.57	0.85
1:A:89:ILE:HG22	1:A:93:VAL:CG1	2.07	0.85
1:D:611:THR:O	1:D:615:ILE:HG13	1.76	0.85
2:S:56:ASP:OD2	2:S:60:ASN:HA	1.76	0.84
1:F:107:THR:HG21	1:F:115:LYS:HD2	1.58	0.84
1:A:161:ILE:HG21	1:A:168:GLU:HB2	1.60	0.84
1:E:89:ILE:HG22	1:E:93:VAL:CG1	2.07	0.84
1:C:288:VAL:HG23	1:C:289:GLU:H	1.42	0.84
1:C:472:ARG:NH1	1:C:472:ARG:HB3	1.92	0.84

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:9:ILE:HD12	2:R:69:LEU:HD11	1.59	0.84
1:F:288:VAL:HG23	1:F:289:GLU:H	1.42	0.84
2:R:28:THR:HB	2:R:30:LYS:HZ3	1.43	0.84
1:A:296:LEU:CD2	1:A:296:LEU:H	1.91	0.84
1:D:142:VAL:HG22	1:D:154:ILE:HG23	1.60	0.84
1:E:288:VAL:HG23	1:E:289:GLU:H	1.42	0.84
1:E:597:ASN:HB2	1:E:598:PRO:HD2	1.57	0.84
1:F:142:VAL:HG22	1:F:154:ILE:HG23	1.60	0.84
1:D:107:THR:HG21	1:D:115:LYS:HD2	1.58	0.84
1:D:192:PHE:HA	1:D:195:LEU:HB3	1.60	0.84
1:E:472:ARG:NH1	1:E:472:ARG:HB3	1.92	0.84
2:Q:9:ILE:HD12	2:Q:69:LEU:HD11	1.60	0.84
1:B:161:ILE:HG21	1:B:168:GLU:HB2	1.59	0.83
1:C:597:ASN:HB2	1:C:598:PRO:HD2	1.58	0.83
1:D:746:LYS:O	1:D:750:GLN:HG2	1.78	0.83
2:T:117:THR:HG23	2:T:120:GLU:HB2	1.59	0.83
1:F:89:ILE:HG22	1:F:93:VAL:CG1	2.07	0.83
1:A:142:VAL:HG22	1:A:154:ILE:HG23	1.60	0.83
1:B:597:ASN:HB2	1:B:598:PRO:HD2	1.57	0.83
1:D:630:ARG:CZ	2:R:83:GLU:HG2	2.08	0.83
1:A:635:ILE:HD12	1:A:635:ILE:H	1.41	0.83
1:D:288:VAL:HG23	1:D:289:GLU:H	1.43	0.83
1:F:472:ARG:NH1	1:F:472:ARG:HB3	1.92	0.83
1:C:140:ARG:HA	1:C:140:ARG:HE	1.44	0.83
1:C:161:ILE:HA	1:C:167:LYS:HD2	1.58	0.83
1:E:635:ILE:H	1:E:635:ILE:HD12	1.43	0.83
1:C:142:VAL:HG22	1:C:154:ILE:HG23	1.61	0.83
1:E:746:LYS:O	1:E:750:GLN:HG2	1.78	0.83
2:T:9:ILE:HD12	2:T:69:LEU:HD11	1.60	0.83
1:F:630:ARG:CZ	2:T:83:GLU:HG2	2.08	0.83
1:B:472:ARG:HB3	1:B:472:ARG:NH1	1.92	0.83
1:D:472:ARG:HB3	1:D:472:ARG:NH1	1.92	0.83
2:O:117:THR:HG23	2:O:120:GLU:HB2	1.59	0.83
1:C:630:ARG:CZ	2:Q:83:GLU:HG2	2.08	0.83
2:S:117:THR:HG23	2:S:120:GLU:HB2	1.59	0.83
1:B:746:LYS:O	1:B:750:GLN:HG2	1.78	0.83
1:E:142:VAL:HG22	1:E:154:ILE:HG23	1.61	0.83
1:F:140:ARG:HA	1:F:140:ARG:HE	1.44	0.83
1:F:441:VAL:HG22	1:F:461:LYS:HG2	1.61	0.83
1:B:630:ARG:CZ	2:P:83:GLU:HG2	2.07	0.82
1:E:192:PHE:HA	1:E:195:LEU:HB3	1.60	0.82

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:117:THR:HG23	2:Q:120:GLU:HB2	1.59	0.82
1:A:746:LYS:O	1:A:750:GLN:HG2	1.79	0.82
1:A:93:VAL:HG23	1:A:179:LEU:HD11	1.61	0.82
1:B:89:ILE:HD13	1:B:175:LYS:HE2	1.60	0.82
1:C:441:VAL:HG22	1:C:461:LYS:HG2	1.60	0.82
1:F:746:LYS:O	1:F:750:GLN:HG2	1.79	0.82
2:Q:5:THR:HG23	2:Q:8:GLN:HB2	1.61	0.82
1:A:192:PHE:HA	1:A:195:LEU:HB3	1.60	0.82
1:F:192:PHE:HA	1:F:195:LEU:HB3	1.60	0.82
1:F:635:ILE:H	1:F:635:ILE:HD12	1.42	0.82
1:A:288:VAL:HG23	1:A:289:GLU:H	1.43	0.82
1:B:142:VAL:HG22	1:B:154:ILE:HG23	1.61	0.82
1:C:107:THR:HG21	1:C:115:LYS:HD2	1.58	0.82
2:Q:5:THR:O	2:Q:9:ILE:HG12	1.79	0.82
1:B:288:VAL:HG23	1:B:289:GLU:H	1.42	0.82
1:C:192:PHE:HA	1:C:195:LEU:HB3	1.60	0.82
1:D:140:ARG:HE	1:D:140:ARG:HA	1.44	0.82
1:D:161:ILE:HG21	1:D:168:GLU:HB2	1.61	0.82
2:O:9:ILE:HD12	2:O:69:LEU:HD11	1.60	0.82
2:Q:28:THR:HB	2:Q:30:LYS:HZ3	1.43	0.82
1:A:472:ARG:NH1	1:A:472:ARG:HB3	1.93	0.82
2:T:5:THR:O	2:T:9:ILE:HG12	1.80	0.82
1:A:236:GLU:HA	1:A:239:HIS:CD2	2.15	0.82
1:D:71:PHE:HB3	1:D:108:ASP:HB2	1.62	0.82
1:C:746:LYS:O	1:C:750:GLN:HG2	1.80	0.82
1:D:441:VAL:HG22	1:D:461:LYS:HG2	1.60	0.82
1:E:189:ASP:O	1:E:191:GLU:N	2.13	0.82
1:E:441:VAL:HG22	1:E:461:LYS:HG2	1.61	0.82
2:P:5:THR:HG23	2:P:8:GLN:HB2	1.61	0.82
2:P:9:ILE:HD12	2:P:69:LEU:HD11	1.60	0.82
1:D:236:GLU:HA	1:D:239:HIS:CD2	2.15	0.81
1:E:107:THR:HG21	1:E:115:LYS:HD2	1.60	0.81
1:C:391:ILE:HG12	1:C:399:GLY:HA2	1.62	0.81
1:C:71:PHE:HB3	1:C:108:ASP:HB2	1.61	0.81
1:F:161:ILE:HG21	1:F:168:GLU:HB2	1.60	0.81
1:D:635:ILE:HD12	1:D:635:ILE:H	1.43	0.81
1:A:140:ARG:HA	1:A:140:ARG:HE	1.44	0.81
1:B:140:ARG:HA	1:B:140:ARG:HE	1.44	0.81
1:B:189:ASP:O	1:B:191:GLU:N	2.14	0.81
1:E:296:LEU:CD2	1:E:296:LEU:H	1.90	0.81
1:F:71:PHE:HB3	1:F:108:ASP:HB2	1.61	0.81

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:5:THR:HG23	2:S:8:GLN:HB2	1.61	0.81
1:E:140:ARG:HA	1:E:140:ARG:HE	1.44	0.81
2:P:55:VAL:HB	2:P:67:GLU:OE2	1.79	0.81
1:A:71:PHE:HB3	1:A:108:ASP:HB2	1.61	0.81
2:R:117:THR:HG23	2:R:120:GLU:HB2	1.60	0.81
1:C:161:ILE:HG21	1:C:168:GLU:HB2	1.61	0.81
1:D:93:VAL:HG23	1:D:179:LEU:HD11	1.61	0.81
1:B:93:VAL:HG23	1:B:179:LEU:HD11	1.61	0.81
1:B:192:PHE:HA	1:B:195:LEU:HB3	1.60	0.81
1:B:236:GLU:HA	1:B:239:HIS:CD2	2.16	0.81
1:C:189:ASP:O	1:C:191:GLU:N	2.13	0.81
1:E:161:ILE:HG21	1:E:168:GLU:HB2	1.60	0.81
1:B:71:PHE:HB3	1:B:108:ASP:HB2	1.61	0.81
2:Q:55:VAL:HB	2:Q:67:GLU:OE2	1.81	0.81
2:S:9:ILE:HD12	2:S:69:LEU:HD11	1.61	0.81
1:B:441:VAL:HG22	1:B:461:LYS:HG2	1.60	0.80
1:C:131:ARG:H	1:C:170:TYR:HE2	1.28	0.80
1:C:236:GLU:HA	1:C:239:HIS:CD2	2.15	0.80
1:E:391:ILE:HG12	1:E:399:GLY:HA2	1.63	0.80
1:F:391:ILE:HG12	1:F:399:GLY:HA2	1.63	0.80
1:B:391:ILE:HG12	1:B:399:GLY:HA2	1.63	0.80
2:O:5:THR:HG23	2:O:8:GLN:HB2	1.61	0.80
2:R:5:THR:HG23	2:R:8:GLN:HB2	1.61	0.80
2:T:5:THR:HG23	2:T:8:GLN:HB2	1.61	0.80
1:D:391:ILE:HG12	1:D:399:GLY:HA2	1.62	0.80
2:R:59:GLY:O	2:R:62:THR:HG22	1.80	0.80
2:R:55:VAL:HB	2:R:67:GLU:OE2	1.81	0.80
2:S:5:THR:O	2:S:9:ILE:HG12	1.80	0.80
1:A:441:VAL:HG22	1:A:461:LYS:HG2	1.62	0.80
1:F:93:VAL:HG23	1:F:179:LEU:HD11	1.61	0.80
1:F:89:ILE:HD13	1:F:175:LYS:HE2	1.63	0.80
2:O:55:VAL:HB	2:O:67:GLU:OE2	1.81	0.80
1:A:105:TYR:HB2	1:A:153:ILE:HG12	1.64	0.80
1:A:189:ASP:O	1:A:191:GLU:N	2.14	0.80
2:R:5:THR:O	2:R:9:ILE:HG12	1.80	0.80
1:F:105:TYR:HB2	1:F:153:ILE:HG12	1.64	0.80
1:F:615:ILE:HD12	1:F:645:TRP:CH2	2.16	0.80
1:E:161:ILE:HG23	1:E:168:GLU:HB2	1.63	0.80
1:A:142:VAL:HG13	1:A:154:ILE:CD1	2.12	0.80
1:B:105:TYR:HB2	1:B:153:ILE:HG12	1.63	0.80
1:A:89:ILE:HD13	1:A:175:LYS:HE2	1.62	0.80

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ILE:HD13	1:C:157:LYS:HZ3	1.47	0.80
1:D:189:ASP:O	1:D:191:GLU:N	2.14	0.80
1:E:93:VAL:HG23	1:E:179:LEU:HD11	1.63	0.80
1:F:615:ILE:HG23	1:F:619:ILE:HD12	1.64	0.80
2:P:5:THR:O	2:P:9:ILE:HG12	1.80	0.80
1:A:615:ILE:HD12	1:A:645:TRP:CH2	2.15	0.79
1:B:408:LEU:CD1	1:B:408:LEU:H	1.95	0.79
1:F:409:ARG:NE	1:F:413:LEU:HD21	1.97	0.79
1:A:134:LYS:O	1:A:135:VAL:HG12	1.81	0.79
1:A:736:LEU:HD11	1:A:750:GLN:NE2	1.97	0.79
1:B:409:ARG:NE	1:B:413:LEU:HD21	1.97	0.79
1:C:409:ARG:NE	1:C:413:LEU:HD21	1.97	0.79
1:E:736:LEU:HD11	1:E:750:GLN:NE2	1.97	0.79
1:C:408:LEU:H	1:C:408:LEU:CD1	1.95	0.79
1:C:736:LEU:HD11	1:C:750:GLN:NE2	1.97	0.79
1:E:615:ILE:HD12	1:E:645:TRP:CH2	2.17	0.79
1:E:89:ILE:HD13	1:E:175:LYS:HE2	1.62	0.79
1:F:189:ASP:O	1:F:191:GLU:N	2.14	0.79
2:O:56:ASP:OD2	2:O:60:ASN:HA	1.83	0.79
1:A:408:LEU:H	1:A:408:LEU:CD1	1.96	0.79
1:C:134:LYS:O	1:C:135:VAL:HG12	1.82	0.79
1:D:409:ARG:NE	1:D:413:LEU:HD21	1.98	0.79
1:D:615:ILE:HD12	1:D:645:TRP:CH2	2.16	0.79
1:F:134:LYS:O	1:F:135:VAL:HG12	1.83	0.79
2:T:55:VAL:HB	2:T:67:GLU:OE2	1.81	0.79
1:D:408:LEU:H	1:D:408:LEU:CD1	1.96	0.79
1:E:236:GLU:HA	1:E:239:HIS:CD2	2.15	0.79
1:F:236:GLU:HA	1:F:239:HIS:CD2	2.16	0.79
1:D:446:ILE:HD11	1:D:451:ASN:HB3	1.65	0.79
2:S:55:VAL:HB	2:S:67:GLU:OE2	1.81	0.79
1:B:736:LEU:HD11	1:B:750:GLN:NE2	1.97	0.79
1:C:581:GLN:HE21	1:C:629:ASN:H	1.30	0.79
1:E:134:LYS:O	1:E:135:VAL:HG12	1.82	0.79
1:F:736:LEU:HD11	1:F:750:GLN:NE2	1.97	0.79
2:O:5:THR:O	2:O:9:ILE:HG12	1.81	0.79
2:T:6:GLU:HG3	2:T:7:GLU:N	1.98	0.79
1:C:597:ASN:ND2	1:C:601:GLU:HB2	1.98	0.79
1:C:105:TYR:HB2	1:C:153:ILE:HG12	1.65	0.79
1:F:131:ARG:H	1:F:170:TYR:HE2	1.30	0.79
1:C:89:ILE:HD13	1:C:175:LYS:HE2	1.64	0.79
1:E:409:ARG:NE	1:E:413:LEU:HD21	1.98	0.79

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:PHE:HB3	1:E:108:ASP:HB2	1.62	0.79
2:R:6:GLU:HG3	2:R:7:GLU:N	1.98	0.79
1:C:93:VAL:HG23	1:C:179:LEU:HD11	1.63	0.78
1:C:615:ILE:HD12	1:C:645:TRP:CH2	2.17	0.78
1:E:105:TYR:HB2	1:E:153:ILE:HG12	1.65	0.78
1:E:70:GLU:HB2	1:E:107:THR:HG22	1.65	0.78
1:F:161:ILE:HG23	1:F:168:GLU:HB2	1.65	0.78
1:D:581:GLN:HE21	1:D:629:ASN:H	1.28	0.78
1:D:736:LEU:HD11	1:D:750:GLN:NE2	1.97	0.78
2:Q:6:GLU:HG3	2:Q:7:GLU:N	1.98	0.78
2:O:6:GLU:HG3	2:O:7:GLU:N	1.98	0.78
2:T:56:ASP:OD2	2:T:60:ASN:HA	1.82	0.78
1:D:105:TYR:HB2	1:D:153:ILE:HG12	1.65	0.78
1:D:131:ARG:H	1:D:170:TYR:HE2	1.28	0.78
1:E:446:ILE:HD11	1:E:451:ASN:HB3	1.65	0.78
1:A:391:ILE:HG12	1:A:399:GLY:HA2	1.64	0.78
1:E:131:ARG:H	1:E:170:TYR:HE2	1.30	0.78
1:F:446:ILE:HD11	1:F:451:ASN:HB3	1.66	0.78
1:B:134:LYS:O	1:B:135:VAL:HG12	1.82	0.78
1:D:89:ILE:HD13	1:D:175:LYS:HE2	1.64	0.78
2:O:59:GLY:O	2:O:62:THR:HG22	1.83	0.78
1:B:161:ILE:HG23	1:B:168:GLU:HB2	1.64	0.78
1:B:615:ILE:HD12	1:B:645:TRP:CH2	2.18	0.78
1:B:142:VAL:HG13	1:B:154:ILE:CD1	2.14	0.77
1:D:134:LYS:O	1:D:135:VAL:HG12	1.83	0.77
1:D:142:VAL:HG13	1:D:154:ILE:CD1	2.13	0.77
1:E:186:LYS:HE3	1:E:234:LEU:CD1	2.14	0.77
1:E:615:ILE:HG23	1:E:619:ILE:HD12	1.66	0.77
1:A:409:ARG:NE	1:A:413:LEU:HD21	1.99	0.77
1:A:446:ILE:HD11	1:A:451:ASN:HB3	1.65	0.77
1:B:173:ILE:HG13	1:B:242:SER:HB3	1.66	0.77
1:D:173:ILE:HG13	1:D:242:SER:HB3	1.66	0.77
1:D:409:ARG:CZ	1:D:413:LEU:HD21	2.15	0.77
1:F:581:GLN:HE21	1:F:629:ASN:H	1.32	0.77
2:P:6:GLU:HG3	2:P:7:GLU:N	1.98	0.77
1:C:446:ILE:HD11	1:C:451:ASN:HB3	1.65	0.77
2:S:6:GLU:HG3	2:S:7:GLU:N	1.98	0.77
1:C:142:VAL:HG13	1:C:154:ILE:CD1	2.14	0.77
1:F:409:ARG:CZ	1:F:413:LEU:HD21	2.15	0.77
1:A:131:ARG:H	1:A:170:TYR:HE2	1.31	0.77
1:A:173:ILE:HG13	1:A:242:SER:HB3	1.65	0.77

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:VAL:HG13	1:F:154:ILE:CD1	2.13	0.77
1:B:236:GLU:HA	1:B:239:HIS:HD2	1.50	0.77
1:B:615:ILE:HG23	1:B:619:ILE:HD12	1.66	0.77
1:C:236:GLU:HA	1:C:239:HIS:HD2	1.50	0.77
1:E:597:ASN:ND2	1:E:601:GLU:HB2	1.99	0.77
1:E:581:GLN:HE21	1:E:629:ASN:H	1.32	0.77
1:D:70:GLU:HB2	1:D:107:THR:HG22	1.66	0.77
1:F:450:ASN:HD22	1:F:452:GLU:HG3	1.50	0.77
1:C:70:GLU:HB2	1:C:107:THR:HG22	1.65	0.77
1:A:305:SER:OG	1:A:307:LEU:HD13	1.85	0.77
1:A:597:ASN:ND2	1:A:601:GLU:HB2	1.99	0.77
1:B:446:ILE:HD11	1:B:451:ASN:HB3	1.65	0.76
1:C:769:SER:OG	1:C:769:SER:O	2.00	0.76
1:A:318:ILE:H	1:A:318:ILE:HD12	1.50	0.76
1:B:318:ILE:H	1:B:318:ILE:HD12	1.50	0.76
1:B:70:GLU:HB2	1:B:107:THR:HG22	1.66	0.76
1:D:79:ILE:C	1:D:81:GLN:H	1.87	0.76
1:E:79:ILE:C	1:E:81:GLN:H	1.87	0.76
1:F:186:LYS:HE3	1:F:234:LEU:CD1	2.15	0.76
1:A:236:GLU:HA	1:A:239:HIS:HD2	1.49	0.76
1:B:79:ILE:C	1:B:81:GLN:H	1.87	0.76
1:D:161:ILE:HG23	1:D:168:GLU:HB2	1.65	0.76
1:E:142:VAL:HG13	1:E:154:ILE:CD1	2.14	0.76
1:D:597:ASN:ND2	1:D:601:GLU:HB2	1.98	0.76
1:D:615:ILE:HG23	1:D:619:ILE:HD12	1.66	0.76
1:E:674:SER:O	1:E:676:VAL:N	2.19	0.76
2:T:100:ILE:HB	2:T:136:VAL:CG2	2.15	0.76
1:C:173:ILE:HG13	1:C:242:SER:HB3	1.67	0.76
1:C:550:SER:CB	1:C:553:GLN:HG3	2.16	0.76
1:E:409:ARG:CZ	1:E:413:LEU:HD21	2.15	0.76
1:B:305:SER:OG	1:B:307:LEU:HD13	1.85	0.76
1:C:161:ILE:HG23	1:C:168:GLU:HB2	1.65	0.76
1:D:318:ILE:HD12	1:D:318:ILE:H	1.51	0.76
1:B:409:ARG:CZ	1:B:413:LEU:HD21	2.15	0.76
1:F:318:ILE:H	1:F:318:ILE:HD12	1.51	0.76
1:A:70:GLU:HB2	1:A:107:THR:HG22	1.66	0.76
1:C:217:LYS:HB3	1:C:217:LYS:HZ2	1.51	0.76
1:C:615:ILE:HG23	1:C:619:ILE:HD12	1.66	0.76
1:D:236:GLU:HA	1:D:239:HIS:HD2	1.50	0.76
1:E:318:ILE:H	1:E:318:ILE:HD12	1.51	0.76
1:F:70:GLU:HB2	1:F:107:THR:HG22	1.65	0.76

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:SER:CB	1:B:553:GLN:HG3	2.15	0.76
1:E:172:GLU:HB3	1:E:246:SER:HA	1.68	0.76
1:F:597:ASN:ND2	1:F:601:GLU:HB2	1.98	0.76
1:A:540:ARG:NH2	2:O:87:GLU:OE1	2.19	0.76
1:A:186:LYS:HE3	1:A:234:LEU:CD1	2.15	0.76
1:A:79:ILE:C	1:A:81:GLN:H	1.88	0.76
1:B:186:LYS:HE3	1:B:234:LEU:CD1	2.14	0.76
1:B:769:SER:OG	1:B:769:SER:O	2.00	0.76
1:D:186:LYS:HE3	1:D:234:LEU:CD1	2.14	0.76
1:E:153:ILE:O	1:E:154:ILE:HD13	1.85	0.76
1:E:305:SER:OG	1:E:307:LEU:HD13	1.85	0.76
1:F:173:ILE:HG13	1:F:242:SER:HB3	1.66	0.76
1:A:161:ILE:HG23	1:A:168:GLU:HB2	1.65	0.75
1:B:324:THR:HB	1:B:499:PRO:HA	1.68	0.75
1:B:674:SER:O	1:B:676:VAL:N	2.19	0.75
1:C:409:ARG:CZ	1:C:413:LEU:HD21	2.15	0.75
1:D:305:SER:OG	1:D:307:LEU:HD13	1.86	0.75
1:A:674:SER:O	1:A:676:VAL:N	2.19	0.75
1:B:131:ARG:H	1:B:170:TYR:HE2	1.31	0.75
1:B:172:GLU:HB3	1:B:246:SER:HA	1.68	0.75
1:B:597:ASN:ND2	1:B:601:GLU:HB2	2.00	0.75
1:C:172:GLU:HB3	1:C:246:SER:HA	1.68	0.75
1:B:540:ARG:NH2	2:P:87:GLU:OE1	2.19	0.75
1:B:153:ILE:O	1:B:154:ILE:HD13	1.87	0.75
1:C:186:LYS:HE3	1:C:234:LEU:CD1	2.15	0.75
1:E:173:ILE:HG13	1:E:242:SER:HB3	1.66	0.75
1:F:153:ILE:O	1:F:154:ILE:HD13	1.86	0.75
1:C:549:LEU:HB2	1:C:553:GLN:HE21	1.52	0.75
1:F:172:GLU:HB3	1:F:246:SER:HA	1.68	0.75
1:F:674:SER:O	1:F:676:VAL:N	2.19	0.75
2:S:100:ILE:HB	2:S:136:VAL:CG2	2.16	0.75
1:E:540:ARG:NH2	2:S:87:GLU:OE1	2.20	0.75
1:A:629:ASN:HD22	1:A:629:ASN:C	1.90	0.75
1:D:353:LYS:H	1:D:368:GLN:NE2	1.85	0.75
1:D:549:LEU:HB2	1:D:553:GLN:HE21	1.52	0.75
1:D:674:SER:O	1:D:676:VAL:N	2.19	0.75
1:A:581:GLN:HE21	1:A:629:ASN:H	1.32	0.75
1:B:581:GLN:HE21	1:B:629:ASN:H	1.33	0.75
1:F:540:ARG:NH2	2:T:87:GLU:OE1	2.20	0.75
2:O:109:MSE:HG3	2:O:116:LEU:HD11	1.69	0.75
2:O:22:ASP:O	2:O:24:ASP:N	2.20	0.75

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:SER:CB	1:A:553:GLN:HG3	2.16	0.75
1:A:615:ILE:HG23	1:A:619:ILE:HD12	1.66	0.75
1:C:305:SER:OG	1:C:307:LEU:HD13	1.86	0.75
1:E:296:LEU:N	1:E:296:LEU:CD2	2.48	0.75
2:O:100:ILE:HB	2:O:136:VAL:CG2	2.17	0.75
1:B:549:LEU:HB2	1:B:553:GLN:HE21	1.52	0.75
1:D:71:PHE:CB	1:D:108:ASP:HB2	2.17	0.75
1:E:549:LEU:HB2	1:E:553:GLN:HE21	1.52	0.75
1:F:236:GLU:HA	1:F:239:HIS:HD2	1.50	0.75
1:A:409:ARG:CZ	1:A:413:LEU:HD21	2.16	0.74
1:D:140:ARG:NE	1:D:140:ARG:HA	2.02	0.74
1:F:182:ILE:O	1:F:187:SER:HB2	1.87	0.74
1:A:668:SER:HA	2:O:14:GLU:HG3	1.69	0.74
2:S:109:MSE:HG3	2:S:116:LEU:HD11	1.68	0.74
1:C:71:PHE:CB	1:C:108:ASP:HB2	2.17	0.74
1:F:270:LYS:HD3	1:F:273:LYS:HD2	1.69	0.74
1:B:296:LEU:CD2	1:B:296:LEU:N	2.48	0.74
1:D:769:SER:OG	1:D:769:SER:O	2.00	0.74
1:B:629:ASN:HD22	1:B:629:ASN:C	1.91	0.74
1:C:450:ASN:HD22	1:C:452:GLU:HG3	1.52	0.74
1:D:450:ASN:HD22	1:D:452:GLU:HG3	1.51	0.74
1:E:197:LYS:HB3	1:E:197:LYS:HZ2	1.51	0.74
1:F:353:LYS:H	1:F:368:GLN:NE2	1.85	0.74
2:R:100:ILE:HB	2:R:136:VAL:CG2	2.16	0.74
2:R:22:ASP:O	2:R:24:ASP:N	2.21	0.74
2:T:109:MSE:HG3	2:T:116:LEU:HD11	1.70	0.74
2:T:22:ASP:O	2:T:24:ASP:N	2.20	0.74
1:A:140:ARG:NE	1:A:140:ARG:HA	2.03	0.74
1:A:182:ILE:O	1:A:187:SER:HB2	1.87	0.74
1:A:172:GLU:HB3	1:A:246:SER:HA	1.68	0.74
1:C:182:ILE:O	1:C:187:SER:HB2	1.87	0.74
1:D:172:GLU:HB3	1:D:246:SER:HA	1.68	0.74
1:E:236:GLU:HA	1:E:239:HIS:HD2	1.50	0.74
1:F:79:ILE:C	1:F:81:GLN:H	1.88	0.74
2:Q:100:ILE:HB	2:Q:136:VAL:CG2	2.17	0.74
2:S:22:ASP:O	2:S:24:ASP:N	2.21	0.74
1:B:71:PHE:CB	1:B:108:ASP:HB2	2.17	0.74
1:F:279:ILE:HD13	1:F:279:ILE:H	1.53	0.74
2:P:100:ILE:HB	2:P:136:VAL:CG2	2.17	0.74
2:P:6:GLU:HG3	2:P:7:GLU:H	1.53	0.74
2:S:56:ASP:HB3	2:S:60:ASN:OD1	1.86	0.74

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ILE:O	1:B:100:LEU:HG	1.88	0.74
1:E:182:ILE:O	1:E:187:SER:HB2	1.87	0.74
1:F:71:PHE:CB	1:F:108:ASP:HB2	2.17	0.74
2:T:28:THR:HB	2:T:30:LYS:HZ3	1.51	0.74
1:A:152:LEU:HD21	1:A:171:TYR:CE1	2.23	0.74
1:B:182:ILE:O	1:B:187:SER:HB2	1.86	0.74
1:B:353:LYS:H	1:B:368:GLN:NE2	1.84	0.74
1:E:769:SER:OG	1:E:769:SER:O	1.99	0.74
1:C:324:THR:HB	1:C:499:PRO:HA	1.68	0.74
1:C:674:SER:O	1:C:676:VAL:N	2.20	0.74
1:D:540:ARG:NH2	2:R:87:GLU:OE1	2.21	0.74
1:C:140:ARG:HA	1:C:140:ARG:NE	2.02	0.74
1:C:79:ILE:C	1:C:81:GLN:H	1.88	0.74
2:S:62:THR:CG2	2:S:62:THR:CA	2.65	0.74
1:B:497:LEU:HD13	1:B:556:MET:HG2	1.70	0.73
1:D:182:ILE:O	1:D:187:SER:HB2	1.87	0.73
1:D:337:ASN:ND2	1:D:412:GLU:OE2	2.21	0.73
1:E:71:PHE:CB	1:E:108:ASP:HB2	2.18	0.73
1:F:550:SER:CB	1:F:553:GLN:HG3	2.17	0.73
1:F:497:LEU:HD13	1:F:556:MET:HG2	1.70	0.73
1:B:668:SER:HA	2:P:14:GLU:HG3	1.70	0.73
1:A:345:THR:HG22	1:A:490:ALA:O	1.87	0.73
1:A:71:PHE:CB	1:A:108:ASP:HB2	2.17	0.73
1:B:140:ARG:HA	1:B:140:ARG:NE	2.03	0.73
1:F:176:GLY:C	1:F:178:SER:H	1.91	0.73
1:C:540:ARG:NH2	2:Q:87:GLU:OE1	2.22	0.73
1:A:324:THR:HB	1:A:499:PRO:HA	1.69	0.73
1:B:450:ASN:HD22	1:B:452:GLU:HG3	1.53	0.73
1:D:153:ILE:O	1:D:154:ILE:HD13	1.88	0.73
1:E:324:THR:HB	1:E:499:PRO:HA	1.69	0.73
1:A:279:ILE:HD13	1:A:279:ILE:H	1.53	0.73
1:F:450:ASN:ND2	1:F:452:GLU:HG3	2.03	0.73
1:F:549:LEU:HB2	1:F:553:GLN:HE21	1.53	0.73
1:F:629:ASN:C	1:F:629:ASN:HD22	1.92	0.73
2:Q:109:MSE:HG3	2:Q:116:LEU:HD11	1.71	0.73
2:T:6:GLU:HG3	2:T:7:GLU:H	1.52	0.73
1:C:270:LYS:HD3	1:C:273:LYS:HD2	1.70	0.73
1:C:318:ILE:HD12	1:C:318:ILE:H	1.52	0.73
1:C:353:LYS:H	1:C:368:GLN:NE2	1.85	0.73
1:C:96:ILE:O	1:C:100:LEU:HG	1.88	0.73
1:A:153:ILE:O	1:A:154:ILE:HD13	1.88	0.73

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:LEU:HD21	1:F:171:TYR:CE1	2.22	0.73
1:F:217:LYS:HB3	1:F:217:LYS:HZ2	1.54	0.73
1:F:337:ASN:ND2	1:F:412:GLU:OE2	2.22	0.73
2:S:6:GLU:HG3	2:S:7:GLU:H	1.53	0.73
1:F:668:SER:HA	2:T:14:GLU:HG3	1.69	0.73
1:D:270:LYS:HD3	1:D:273:LYS:HD2	1.70	0.73
1:E:353:LYS:H	1:E:368:GLN:NE2	1.84	0.73
2:P:109:MSE:HG3	2:P:116:LEU:HD11	1.70	0.73
2:P:22:ASP:O	2:P:24:ASP:N	2.20	0.73
2:Q:56:ASP:OD2	2:Q:61:GLY:N	2.21	0.73
1:D:308:VAL:HB	1:D:311:HIS:ND1	2.04	0.73
1:E:270:LYS:HD3	1:E:273:LYS:HD2	1.70	0.73
1:F:769:SER:O	1:F:769:SER:OG	2.00	0.73
1:D:629:ASN:C	1:D:629:ASN:HD22	1.92	0.73
1:F:728:ALA:O	1:F:732:ILE:HG12	1.88	0.73
2:R:6:GLU:HG3	2:R:7:GLU:H	1.53	0.73
1:A:296:LEU:CD2	1:A:296:LEU:N	2.49	0.73
1:A:450:ASN:HD22	1:A:452:GLU:HG3	1.52	0.73
1:E:176:GLY:C	1:E:178:SER:H	1.92	0.73
1:D:197:LYS:HZ2	1:D:197:LYS:HB3	1.53	0.72
2:Q:102:ALA:HB2	2:Q:125:ILE:HG13	1.71	0.72
1:A:353:LYS:H	1:A:368:GLN:NE2	1.85	0.72
1:D:550:SER:CB	1:D:553:GLN:HG3	2.18	0.72
1:E:408:LEU:H	1:E:408:LEU:CD1	1.96	0.72
1:E:450:ASN:HD22	1:E:452:GLU:HG3	1.54	0.72
1:D:668:SER:HA	2:R:14:GLU:HG3	1.70	0.72
1:A:549:LEU:HB2	1:A:553:GLN:HE21	1.52	0.72
1:C:279:ILE:H	1:C:279:ILE:HD13	1.54	0.72
1:E:629:ASN:C	1:E:629:ASN:HD22	1.92	0.72
2:Q:6:GLU:HG3	2:Q:7:GLU:H	1.53	0.72
1:E:668:SER:HA	2:S:14:GLU:HG3	1.69	0.72
1:A:450:ASN:ND2	1:A:452:GLU:HG3	2.04	0.72
1:C:728:ALA:O	1:C:732:ILE:HG12	1.89	0.72
1:D:450:ASN:ND2	1:D:452:GLU:HG3	2.04	0.72
1:D:324:THR:HB	1:D:499:PRO:HA	1.70	0.72
1:E:96:ILE:O	1:E:100:LEU:HG	1.89	0.72
1:F:140:ARG:HA	1:F:140:ARG:NE	2.03	0.72
1:F:305:SER:OG	1:F:307:LEU:HD13	1.88	0.72
1:A:694:VAL:HG23	2:O:18:LEU:HD11	1.71	0.72
2:R:102:ALA:HB2	2:R:125:ILE:HG13	1.71	0.72
1:B:152:LEU:HD21	1:B:171:TYR:CE1	2.24	0.72

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:LYS:HB3	1:D:217:LYS:HZ2	1.54	0.72
1:F:179:LEU:C	1:F:183:SER:HB2	2.07	0.72
2:Q:22:ASP:O	2:Q:24:ASP:N	2.21	0.72
2:R:109:MSE:HG3	2:R:116:LEU:HD11	1.72	0.72
1:B:279:ILE:HD13	1:B:279:ILE:H	1.54	0.72
1:C:629:ASN:C	1:C:629:ASN:HD22	1.92	0.72
1:D:728:ALA:O	1:D:732:ILE:HG12	1.89	0.72
1:F:296:LEU:N	1:F:296:LEU:CD2	2.48	0.72
1:F:308:VAL:HB	1:F:311:HIS:ND1	2.04	0.72
1:F:324:THR:HB	1:F:499:PRO:HA	1.70	0.72
1:A:270:LYS:HD3	1:A:273:LYS:HD2	1.70	0.72
1:C:668:SER:HA	2:Q:14:GLU:HG3	1.70	0.72
1:E:152:LEU:HD21	1:E:171:TYR:CE1	2.24	0.72
1:E:279:ILE:HD13	1:E:279:ILE:H	1.54	0.72
1:E:345:THR:HG22	1:E:490:ALA:O	1.90	0.72
1:A:109:ILE:HD13	1:A:157:LYS:HZ3	1.54	0.72
1:A:176:GLY:C	1:A:178:SER:H	1.91	0.72
1:E:140:ARG:HA	1:E:140:ARG:NE	2.03	0.72
2:O:6:GLU:HG3	2:O:7:GLU:H	1.52	0.72
1:A:639:ASN:ND2	1:A:639:ASN:H	1.88	0.72
1:A:728:ALA:O	1:A:732:ILE:HG12	1.89	0.72
1:B:345:THR:HG22	1:B:490:ALA:O	1.90	0.72
1:B:401:ILE:HD13	1:B:485:LEU:O	1.89	0.72
1:C:79:ILE:O	1:C:81:GLN:N	2.23	0.72
1:F:387:ASN:HB3	1:F:477:MET:SD	2.29	0.72
1:A:96:ILE:O	1:A:100:LEU:HG	1.89	0.72
1:C:179:LEU:C	1:C:183:SER:HB2	2.08	0.72
2:S:56:ASP:OD2	2:S:61:GLY:N	2.23	0.72
1:B:270:LYS:HD3	1:B:273:LYS:HD2	1.70	0.71
1:F:96:ILE:O	1:F:100:LEU:HG	1.89	0.71
2:T:56:ASP:OD2	2:T:61:GLY:N	2.23	0.71
1:F:401:ILE:HD13	1:F:485:LEU:O	1.91	0.71
1:A:188:LEU:HD23	1:A:188:LEU:H	1.55	0.71
1:A:308:VAL:HB	1:A:311:HIS:ND1	2.04	0.71
1:A:401:ILE:HD13	1:A:485:LEU:O	1.91	0.71
1:B:109:ILE:CD1	1:B:157:LYS:HZ2	2.04	0.71
1:B:694:VAL:HG23	2:P:18:LEU:HD11	1.72	0.71
1:C:540:ARG:HD3	1:C:627:TYR:CZ	2.25	0.71
1:D:96:ILE:O	1:D:100:LEU:HG	1.89	0.71
1:E:550:SER:CB	1:E:553:GLN:HG3	2.18	0.71
1:A:769:SER:OG	1:A:769:SER:O	1.99	0.71

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:GLY:C	1:B:178:SER:H	1.91	0.71
1:C:188:LEU:HD23	1:C:188:LEU:H	1.55	0.71
1:C:337:ASN:ND2	1:C:412:GLU:OE2	2.23	0.71
1:C:530:THR:O	1:C:534:ILE:HG13	1.90	0.71
1:D:188:LEU:H	1:D:188:LEU:HD23	1.55	0.71
2:T:51:MSE:CB	2:T:71:MSE:HE2	2.21	0.71
1:B:635:ILE:HD12	1:B:635:ILE:N	2.06	0.71
1:C:176:GLY:C	1:C:178:SER:H	1.92	0.71
1:C:308:VAL:HB	1:C:311:HIS:ND1	2.05	0.71
1:D:279:ILE:H	1:D:279:ILE:HD13	1.54	0.71
1:D:79:ILE:O	1:D:81:GLN:N	2.23	0.71
1:E:109:ILE:CD1	1:E:157:LYS:HZ2	2.04	0.71
1:E:337:ASN:ND2	1:E:412:GLU:OE2	2.22	0.71
1:E:694:VAL:HG23	2:S:18:LEU:HD11	1.71	0.71
1:B:728:ALA:O	1:B:732:ILE:HG12	1.89	0.71
1:D:401:ILE:HD13	1:D:485:LEU:O	1.90	0.71
1:E:728:ALA:O	1:E:732:ILE:HG12	1.90	0.71
1:F:109:ILE:HD13	1:F:157:LYS:NZ	2.06	0.71
1:F:694:VAL:HG23	2:T:18:LEU:HD11	1.72	0.71
1:B:337:ASN:ND2	1:B:412:GLU:OE2	2.22	0.71
1:C:401:ILE:HD13	1:C:485:LEU:O	1.90	0.71
1:C:497:LEU:HD13	1:C:556:MET:HG2	1.72	0.71
1:D:109:ILE:HD13	1:D:157:LYS:NZ	2.06	0.71
1:F:345:THR:HG22	1:F:490:ALA:O	1.90	0.71
1:B:308:VAL:HB	1:B:311:HIS:ND1	2.04	0.71
1:C:109:ILE:HD13	1:C:157:LYS:NZ	2.05	0.71
1:D:639:ASN:ND2	1:D:639:ASN:H	1.89	0.71
1:A:109:ILE:HD13	1:A:157:LYS:NZ	2.06	0.71
1:A:497:LEU:HD13	1:A:556:MET:HG2	1.72	0.71
1:A:635:ILE:HD12	1:A:635:ILE:N	2.06	0.71
1:D:270:LYS:O	1:D:273:LYS:HB2	1.91	0.71
1:D:345:THR:HG22	1:D:490:ALA:O	1.89	0.71
1:A:337:ASN:ND2	1:A:412:GLU:OE2	2.22	0.71
1:A:387:ASN:HB3	1:A:477:MET:SD	2.30	0.71
1:B:478:ALA:HB1	1:B:486:LYS:O	1.91	0.71
1:C:296:LEU:CD2	1:C:296:LEU:N	2.48	0.71
1:C:581:GLN:NE2	1:C:629:ASN:H	1.89	0.71
1:C:639:ASN:H	1:C:639:ASN:ND2	1.88	0.71
1:D:462:ILE:HG12	1:D:463:THR:N	2.06	0.71
1:D:540:ARG:HD3	1:D:627:TYR:CZ	2.26	0.71
1:E:109:ILE:HD13	1:E:157:LYS:NZ	2.06	0.71

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:497:LEU:HD13	1:E:556:MET:HG2	1.72	0.71
1:E:639:ASN:ND2	1:E:639:ASN:H	1.88	0.71
1:F:90:PRO:HD3	1:F:249:PHE:CE2	2.26	0.71
2:R:56:ASP:HB3	2:R:60:ASN:OD1	1.91	0.71
1:A:540:ARG:HD3	1:A:627:TYR:CZ	2.26	0.70
1:B:296:LEU:CD2	1:B:296:LEU:H	1.91	0.70
1:D:296:LEU:CD2	1:D:296:LEU:N	2.49	0.70
2:O:58:ASP:HB2	2:O:62:THR:HG23	1.73	0.70
2:P:58:ASP:HB2	2:P:62:THR:HG23	1.73	0.70
2:Q:56:ASP:OD2	2:Q:60:ASN:CA	2.39	0.70
1:A:197:LYS:HZ2	1:A:197:LYS:HB3	1.56	0.70
1:C:462:ILE:HG12	1:C:463:THR:N	2.06	0.70
1:E:179:LEU:C	1:E:183:SER:HB2	2.07	0.70
1:E:308:VAL:HB	1:E:311:HIS:ND1	2.05	0.70
1:E:530:THR:O	1:E:534:ILE:HG13	1.91	0.70
2:O:56:ASP:HB3	2:O:60:ASN:OD1	1.91	0.70
1:A:118:GLN:HA	1:A:118:GLN:OE1	1.92	0.70
1:A:79:ILE:O	1:A:81:GLN:N	2.23	0.70
1:B:188:LEU:HD23	1:B:188:LEU:H	1.55	0.70
1:F:188:LEU:H	1:F:188:LEU:HD23	1.55	0.70
2:Q:36:MSE:CE	2:Q:43:PRO:HG3	2.21	0.70
2:Q:51:MSE:CB	2:Q:71:MSE:HE2	2.21	0.70
1:E:630:ARG:NH1	2:S:83:GLU:HG2	2.07	0.70
1:B:450:ASN:ND2	1:B:452:GLU:HG3	2.05	0.70
1:C:635:ILE:HD12	1:C:635:ILE:N	2.06	0.70
1:E:79:ILE:O	1:E:81:GLN:N	2.24	0.70
1:C:694:VAL:HG23	2:Q:18:LEU:HD11	1.73	0.70
1:B:118:GLN:HA	1:B:118:GLN:OE1	1.90	0.70
1:D:152:LEU:HD21	1:D:171:TYR:CE1	2.22	0.70
1:E:76:LEU:HD22	1:E:76:LEU:H	1.57	0.70
2:T:102:ALA:HB2	2:T:125:ILE:HG13	1.73	0.70
1:B:197:LYS:HB3	1:B:197:LYS:HZ2	1.55	0.70
1:B:288:VAL:HG23	1:B:289:GLU:N	2.06	0.70
1:C:218:LEU:HD11	1:C:225:ILE:HD11	1.74	0.70
1:C:450:ASN:ND2	1:C:452:GLU:HG3	2.05	0.70
1:D:635:ILE:N	1:D:635:ILE:HD12	2.07	0.70
2:Q:59:GLY:O	2:Q:62:THR:CG2	2.39	0.70
1:B:79:ILE:O	1:B:81:GLN:N	2.23	0.70
1:E:401:ILE:HD13	1:E:485:LEU:O	1.91	0.70
1:F:118:GLN:OE1	1:F:118:GLN:HA	1.92	0.70
1:F:478:ALA:HB1	1:F:486:LYS:O	1.91	0.70

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:630:ARG:NH1	2:R:83:GLU:HG2	2.06	0.70
1:B:109:ILE:HD13	1:B:157:LYS:NZ	2.06	0.70
1:E:225:ILE:HG22	1:E:225:ILE:O	1.92	0.70
1:E:450:ASN:ND2	1:E:452:GLU:HG3	2.06	0.70
1:F:79:ILE:O	1:F:81:GLN:N	2.25	0.70
2:P:30:LYS:H	2:P:30:LYS:CD	2.04	0.70
2:S:36:MSE:CE	2:S:43:PRO:HG3	2.22	0.70
1:A:462:ILE:HG12	1:A:463:THR:N	2.07	0.70
1:A:517:VAL:HG23	1:A:518:ASN:ND2	2.06	0.70
1:B:472:ARG:HH11	1:B:472:ARG:CB	2.05	0.70
1:D:218:LEU:HD11	1:D:225:ILE:HD11	1.74	0.70
1:D:581:GLN:NE2	1:D:629:ASN:H	1.89	0.70
1:E:288:VAL:HG23	1:E:289:GLU:N	2.07	0.70
1:F:462:ILE:HG12	1:F:463:THR:N	2.07	0.70
2:R:36:MSE:CE	2:R:43:PRO:HG3	2.22	0.70
2:S:102:ALA:HB2	2:S:125:ILE:HG13	1.73	0.70
1:C:152:LEU:HD21	1:C:171:TYR:CE1	2.23	0.69
1:D:472:ARG:HH11	1:D:472:ARG:CB	2.05	0.69
1:E:635:ILE:N	1:E:635:ILE:HD12	2.07	0.69
1:E:90:PRO:HD3	1:E:249:PHE:CE2	2.27	0.69
2:T:30:LYS:H	2:T:30:LYS:CD	2.04	0.69
1:B:639:ASN:H	1:B:639:ASN:ND2	1.89	0.69
1:C:153:ILE:O	1:C:154:ILE:HD13	1.90	0.69
1:D:497:LEU:HD13	1:D:556:MET:HG2	1.71	0.69
1:F:288:VAL:HG23	1:F:289:GLU:N	2.07	0.69
2:O:28:THR:HB	2:O:30:LYS:HZ3	1.57	0.69
2:P:51:MSE:CB	2:P:71:MSE:HE2	2.22	0.69
1:E:501:LEU:CD2	2:S:112:LEU:HD21	2.22	0.69
1:A:630:ARG:NH1	2:O:83:GLU:HG2	2.07	0.69
1:B:517:VAL:HG23	1:B:518:ASN:ND2	2.07	0.69
1:D:130:SER:HB2	1:D:170:TYR:HE2	1.57	0.69
1:D:288:VAL:HG23	1:D:289:GLU:N	2.07	0.69
1:D:517:VAL:HG23	1:D:518:ASN:ND2	2.07	0.69
1:D:90:PRO:HD3	1:D:249:PHE:CE2	2.26	0.69
1:F:639:ASN:H	1:F:639:ASN:ND2	1.89	0.69
2:P:36:MSE:CE	2:P:43:PRO:HG3	2.23	0.69
2:S:56:ASP:OD2	2:S:60:ASN:CA	2.39	0.69
2:S:51:MSE:CB	2:S:71:MSE:HE2	2.23	0.69
1:D:176:GLY:C	1:D:178:SER:H	1.92	0.69
1:F:472:ARG:CB	1:F:472:ARG:HH11	2.05	0.69
2:R:51:MSE:CB	2:R:71:MSE:HE2	2.22	0.69

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:30:LYS:H	2:S:30:LYS:CD	2.05	0.69
1:F:501:LEU:CD2	2:T:112:LEU:HD21	2.21	0.69
1:A:478:ALA:HB1	1:A:486:LYS:O	1.92	0.69
1:B:90:PRO:HD3	1:B:249:PHE:CE2	2.27	0.69
1:C:478:ALA:HB1	1:C:486:LYS:O	1.91	0.69
1:C:715:GLU:HA	1:C:718:ARG:NH1	2.07	0.69
1:E:188:LEU:H	1:E:188:LEU:HD23	1.54	0.69
1:F:530:THR:O	1:F:534:ILE:HG13	1.91	0.69
1:F:76:LEU:HD22	1:F:76:LEU:H	1.57	0.69
1:B:387:ASN:HB3	1:B:477:MET:SD	2.32	0.69
1:B:540:ARG:HD3	1:B:627:TYR:CZ	2.27	0.69
1:B:76:LEU:HD22	1:B:76:LEU:H	1.57	0.69
1:E:540:ARG:HD3	1:E:627:TYR:CZ	2.27	0.69
1:F:540:ARG:HD3	1:F:627:TYR:CZ	2.27	0.69
2:P:56:ASP:OD2	2:P:60:ASN:HA	1.92	0.69
2:T:58:ASP:HB2	2:T:62:THR:HG23	1.72	0.69
1:A:288:VAL:HG23	1:A:289:GLU:N	2.08	0.69
1:B:225:ILE:HG22	1:B:225:ILE:O	1.92	0.69
1:B:530:THR:O	1:B:534:ILE:HG13	1.92	0.69
1:C:225:ILE:HG22	1:C:225:ILE:O	1.92	0.69
1:E:387:ASN:HB3	1:E:477:MET:SD	2.33	0.69
1:F:517:VAL:HG23	1:F:518:ASN:ND2	2.06	0.69
2:O:51:MSE:CB	2:O:71:MSE:HE2	2.22	0.69
2:P:5:THR:CG2	2:P:8:GLN:HB2	2.23	0.69
1:B:462:ILE:HG12	1:B:463:THR:N	2.07	0.69
1:C:345:THR:HG22	1:C:490:ALA:O	1.92	0.69
1:C:387:ASN:HB3	1:C:477:MET:SD	2.32	0.69
1:D:86:LEU:HA	1:D:89:ILE:HD12	1.75	0.69
1:E:218:LEU:HD11	1:E:225:ILE:HD11	1.75	0.69
1:F:175:LYS:HB2	1:F:175:LYS:NZ	2.07	0.69
2:O:30:LYS:H	2:O:30:LYS:CD	2.04	0.69
1:C:148:GLU:HG3	1:C:149:THR:HG22	1.75	0.69
2:O:102:ALA:HB2	2:O:125:ILE:HG13	1.74	0.69
1:A:480:ASN:HD21	1:A:483:GLY:H	1.38	0.69
1:B:279:ILE:CD1	1:B:279:ILE:H	2.06	0.69
1:C:403:LEU:HG	1:C:405:LEU:CD1	2.23	0.69
1:C:517:VAL:HG23	1:C:518:ASN:ND2	2.07	0.69
1:D:148:GLU:HG3	1:D:149:THR:HG22	1.75	0.69
1:D:175:LYS:HB2	1:D:175:LYS:NZ	2.08	0.69
1:D:275:GLY:HA2	1:D:278:LYS:HG3	1.75	0.69
1:D:403:LEU:HG	1:D:405:LEU:CD1	2.23	0.69

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:LYS:NZ	1:E:175:LYS:HB2	2.08	0.69
1:F:218:LEU:HD11	1:F:225:ILE:HD11	1.75	0.69
1:F:635:ILE:N	1:F:635:ILE:HD12	2.07	0.69
1:A:501:LEU:CD2	2:O:112:LEU:HD21	2.20	0.69
2:P:102:ALA:HB2	2:P:125:ILE:HG13	1.74	0.69
2:Q:63:ILE:HB	2:Q:67:GLU:HB3	1.75	0.69
1:A:175:LYS:HB2	1:A:175:LYS:NZ	2.08	0.69
1:B:480:ASN:HD21	1:B:483:GLY:H	1.39	0.69
1:C:118:GLN:HA	1:C:118:GLN:OE1	1.92	0.69
2:P:13:LYS:HZ3	2:P:65:PHE:HB3	1.58	0.69
1:B:270:LYS:O	1:B:273:LYS:HB2	1.93	0.68
1:C:630:ARG:NH1	2:Q:83:GLU:HG2	2.08	0.68
1:E:118:GLN:HA	1:E:118:GLN:OE1	1.92	0.68
1:E:122:GLU:HG3	1:E:147:ARG:CB	2.23	0.68
1:E:148:GLU:HG3	1:E:149:THR:HG22	1.75	0.68
1:A:218:LEU:HD11	1:A:225:ILE:HD11	1.75	0.68
1:B:148:GLU:HG3	1:B:149:THR:HG22	1.75	0.68
1:C:288:VAL:HG23	1:C:289:GLU:N	2.07	0.68
1:C:90:PRO:HD3	1:C:249:PHE:CE2	2.27	0.68
1:D:118:GLN:HA	1:D:118:GLN:OE1	1.93	0.68
1:E:270:LYS:O	1:E:273:LYS:HB2	1.93	0.68
1:F:480:ASN:HD21	1:F:483:GLY:H	1.39	0.68
1:F:630:ARG:NH1	2:T:83:GLU:HG2	2.08	0.68
1:A:90:PRO:HD3	1:A:249:PHE:CE2	2.27	0.68
1:B:175:LYS:HB2	1:B:175:LYS:NZ	2.07	0.68
1:B:715:GLU:HA	1:B:718:ARG:NH1	2.08	0.68
1:E:480:ASN:HD21	1:E:483:GLY:H	1.40	0.68
1:E:74:GLU:HB2	1:E:78:LYS:HB3	1.76	0.68
2:O:36:MSE:HE1	2:O:51:MSE:HE1	1.75	0.68
2:Q:36:MSE:HE1	2:Q:51:MSE:HE1	1.76	0.68
1:C:130:SER:HB2	1:C:170:TYR:HE2	1.58	0.68
1:C:175:LYS:NZ	1:C:175:LYS:HB2	2.08	0.68
1:D:225:ILE:HG22	1:D:225:ILE:O	1.92	0.68
1:D:480:ASN:HD21	1:D:483:GLY:H	1.40	0.68
1:D:715:GLU:HA	1:D:718:ARG:NH1	2.08	0.68
2:O:5:THR:CG2	2:O:8:GLN:HB2	2.23	0.68
2:Q:5:THR:CG2	2:Q:8:GLN:HB2	2.24	0.68
1:A:715:GLU:HA	1:A:718:ARG:NH1	2.09	0.68
1:B:179:LEU:C	1:B:183:SER:HB2	2.07	0.68
1:D:387:ASN:HB3	1:D:477:MET:SD	2.32	0.68
1:E:478:ALA:HB1	1:E:486:LYS:O	1.93	0.68

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:517:VAL:HG23	1:E:518:ASN:ND2	2.08	0.68
1:F:403:LEU:HG	1:F:405:LEU:CD1	2.24	0.68
2:P:36:MSE:HE1	2:P:51:MSE:HE1	1.76	0.68
2:Q:30:LYS:H	2:Q:30:LYS:CD	2.05	0.68
2:Q:28:THR:HB	2:Q:30:LYS:NZ	2.09	0.68
1:D:694:VAL:HG23	2:R:18:LEU:HD11	1.73	0.68
1:A:186:LYS:O	1:A:188:LEU:O	2.12	0.68
1:A:275:GLY:HA2	1:A:278:LYS:HG3	1.76	0.68
1:B:217:LYS:HZ2	1:B:217:LYS:HB3	1.58	0.68
1:B:403:LEU:HG	1:B:405:LEU:CD1	2.24	0.68
1:D:478:ALA:HB1	1:D:486:LYS:O	1.92	0.68
1:E:715:GLU:HA	1:E:718:ARG:NH1	2.08	0.68
2:O:36:MSE:CE	2:O:43:PRO:HG3	2.22	0.68
2:R:30:LYS:CD	2:R:30:LYS:H	2.05	0.68
2:S:5:THR:CG2	2:S:8:GLN:HB2	2.24	0.68
1:A:76:LEU:HD22	1:A:76:LEU:H	1.58	0.68
1:C:270:LYS:O	1:C:273:LYS:HB2	1.93	0.68
1:C:76:LEU:O	1:C:80:GLN:N	2.27	0.68
1:E:186:LYS:O	1:E:188:LEU:O	2.11	0.68
1:E:462:ILE:HG12	1:E:463:THR:N	2.07	0.68
1:F:279:ILE:CD1	1:F:279:ILE:H	2.05	0.68
1:F:86:LEU:HA	1:F:89:ILE:HD12	1.76	0.68
1:C:76:LEU:HD22	1:C:76:LEU:H	1.58	0.68
1:D:516:VAL:HG21	1:D:532:LEU:HD11	1.75	0.68
1:F:715:GLU:HA	1:F:718:ARG:NH1	2.09	0.68
2:P:56:ASP:HB3	2:P:60:ASN:OD1	1.93	0.68
1:C:515:LYS:HZ2	1:C:515:LYS:HB3	1.58	0.68
2:O:63:ILE:HB	2:O:67:GLU:HB3	1.75	0.68
1:B:630:ARG:NH1	2:P:83:GLU:HG2	2.09	0.68
2:R:63:ILE:HB	2:R:67:GLU:HB3	1.75	0.68
2:R:94:LYS:NZ	2:R:94:LYS:HB3	2.09	0.68
1:B:218:LEU:HD11	1:B:225:ILE:HD11	1.76	0.68
1:D:76:LEU:H	1:D:76:LEU:HD22	1.58	0.68
1:D:76:LEU:O	1:D:80:GLN:N	2.27	0.68
1:F:74:GLU:HB2	1:F:78:LYS:HB3	1.76	0.68
2:Q:94:LYS:NZ	2:Q:94:LYS:HB3	2.09	0.68
2:T:28:THR:HB	2:T:30:LYS:NZ	2.09	0.68
1:C:480:ASN:HD21	1:C:483:GLY:H	1.39	0.67
1:D:186:LYS:O	1:D:188:LEU:O	2.12	0.67
1:E:581:GLN:NE2	1:E:629:ASN:H	1.91	0.67
2:R:49:GLN:NE2	2:R:49:GLN:H	1.92	0.67

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:5:THR:CG2	2:R:8:GLN:HB2	2.24	0.67
2:S:62:THR:CG2	2:S:62:THR:N	2.57	0.67
1:A:130:SER:HB2	1:A:170:TYR:HE2	1.58	0.67
1:A:403:LEU:HG	1:A:405:LEU:CD1	2.25	0.67
1:E:403:LEU:HG	1:E:405:LEU:CD1	2.24	0.67
1:E:76:LEU:O	1:E:80:GLN:N	2.28	0.67
1:F:225:ILE:HG22	1:F:225:ILE:O	1.93	0.67
2:P:63:ILE:HB	2:P:67:GLU:HB3	1.76	0.67
2:Q:13:LYS:HZ2	2:Q:65:PHE:HB3	1.59	0.67
1:A:270:LYS:O	1:A:273:LYS:HB2	1.93	0.67
1:C:186:LYS:O	1:C:188:LEU:O	2.11	0.67
1:F:581:GLN:NE2	1:F:629:ASN:H	1.93	0.67
1:F:76:LEU:O	1:F:80:GLN:N	2.27	0.67
2:Q:58:ASP:HB2	2:Q:62:THR:HG23	1.75	0.67
1:A:788:ASP:O	1:A:792:VAL:HG23	1.95	0.67
1:B:122:GLU:HG3	1:B:147:ARG:CB	2.23	0.67
2:O:28:THR:HB	2:O:30:LYS:NZ	2.08	0.67
2:R:106:ARG:O	2:R:110:THR:HG23	1.94	0.67
2:R:36:MSE:HE1	2:R:51:MSE:HE1	1.76	0.67
2:T:36:MSE:CE	2:T:43:PRO:HG3	2.22	0.67
2:T:63:ILE:HB	2:T:67:GLU:HB3	1.76	0.67
1:C:472:ARG:HH11	1:C:472:ARG:CB	2.06	0.67
1:D:165:GLN:HE21	1:D:251:PRO:HG2	1.59	0.67
1:D:718:ARG:HH11	1:D:767:GLN:HE21	1.42	0.67
1:E:472:ARG:HH11	1:E:472:ARG:CB	2.05	0.67
1:E:739:LYS:HG2	1:E:740:GLN:H	1.60	0.67
1:F:165:GLN:HE21	1:F:251:PRO:HG2	1.59	0.67
1:F:275:GLY:HA2	1:F:278:LYS:HG3	1.75	0.67
2:R:56:ASP:OD2	2:R:61:GLY:N	2.28	0.67
2:T:5:THR:CG2	2:T:8:GLN:HB2	2.24	0.67
1:A:739:LYS:HG2	1:A:740:GLN:H	1.59	0.67
1:B:165:GLN:HE21	1:B:251:PRO:HG2	1.59	0.67
1:C:275:GLY:HA2	1:C:278:LYS:HG3	1.76	0.67
1:C:671:ARG:NH1	1:C:677:GLY:HA3	2.10	0.67
2:S:63:ILE:HB	2:S:67:GLU:HB3	1.75	0.67
1:A:472:ARG:CB	1:A:472:ARG:HH11	2.06	0.67
1:A:609:GLU:OE2	1:A:609:GLU:N	2.25	0.67
1:A:671:ARG:NH1	1:A:677:GLY:HA3	2.10	0.67
1:E:175:LYS:O	1:E:178:SER:N	2.28	0.67
1:F:109:ILE:HD13	1:F:157:LYS:HZ3	1.59	0.67
1:F:186:LYS:O	1:F:188:LEU:O	2.12	0.67

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:SER:O	1:F:187:SER:HB3	1.94	0.67
2:R:13:LYS:HZ3	2:R:65:PHE:HB3	1.59	0.67
1:A:148:GLU:HG3	1:A:149:THR:HG22	1.75	0.67
1:E:788:ASP:O	1:E:792:VAL:HG23	1.95	0.67
2:Q:106:ARG:O	2:Q:110:THR:HG23	1.95	0.67
1:B:186:LYS:O	1:B:188:LEU:O	2.12	0.67
1:B:671:ARG:NH1	1:B:677:GLY:HA3	2.10	0.67
1:C:183:SER:O	1:C:187:SER:HB3	1.95	0.67
1:C:86:LEU:HA	1:C:89:ILE:HD12	1.76	0.67
1:D:462:ILE:HD11	1:D:466:GLY:HA2	1.77	0.67
2:P:49:GLN:H	2:P:49:GLN:NE2	1.93	0.67
1:A:86:LEU:HA	1:A:89:ILE:HD12	1.76	0.67
1:C:165:GLN:HE21	1:C:251:PRO:HG2	1.60	0.67
1:D:609:GLU:OE2	1:D:609:GLU:N	2.26	0.67
1:F:385:LEU:O	1:F:385:LEU:HD13	1.95	0.67
1:F:739:LYS:HG2	1:F:740:GLN:H	1.60	0.67
1:F:788:ASP:O	1:F:792:VAL:HG23	1.95	0.67
2:O:49:GLN:NE2	2:O:49:GLN:H	1.93	0.67
2:Q:5:THR:HG23	2:Q:8:GLN:CB	2.25	0.67
1:A:279:ILE:CD1	1:A:279:ILE:H	2.05	0.66
1:A:581:GLN:NE2	1:A:629:ASN:H	1.92	0.66
1:B:164:GLU:O	1:B:167:LYS:HG2	1.96	0.66
1:B:199:LEU:C	1:B:201:ASP:H	1.99	0.66
1:B:246:SER:O	1:B:250:ALA:HB2	1.95	0.66
1:B:275:GLY:HA2	1:B:278:LYS:HG3	1.76	0.66
1:B:739:LYS:HG2	1:B:740:GLN:H	1.59	0.66
1:C:737:LYS:HE2	1:C:737:LYS:HA	1.76	0.66
1:D:183:SER:O	1:D:187:SER:HB3	1.94	0.66
1:E:275:GLY:HA2	1:E:278:LYS:CE	2.25	0.66
1:F:397:GLU:HG3	1:F:480:ASN:HB3	1.78	0.66
1:D:501:LEU:CD2	2:R:112:LEU:HD21	2.21	0.66
2:S:49:GLN:H	2:S:49:GLN:NE2	1.93	0.66
2:T:36:MSE:HE1	2:T:51:MSE:HE1	1.76	0.66
2:O:106:ARG:O	2:O:110:THR:HG23	1.95	0.66
2:O:28:THR:HG21	2:O:30:LYS:HZ1	1.59	0.66
1:A:183:SER:O	1:A:187:SER:HB3	1.95	0.66
1:B:142:VAL:HG13	1:B:154:ILE:HD12	1.76	0.66
1:C:516:VAL:HG21	1:C:532:LEU:HD11	1.77	0.66
1:C:788:ASP:O	1:C:792:VAL:HG23	1.95	0.66
2:T:49:GLN:NE2	2:T:49:GLN:H	1.93	0.66
1:A:142:VAL:HG13	1:A:154:ILE:HD12	1.75	0.66

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:SER:O	1:B:187:SER:HB3	1.95	0.66
1:B:385:LEU:O	1:B:385:LEU:HD13	1.96	0.66
1:C:175:LYS:O	1:C:178:SER:N	2.29	0.66
1:C:74:GLU:HB2	1:C:78:LYS:HB3	1.76	0.66
1:D:175:LYS:O	1:D:178:SER:N	2.28	0.66
1:D:275:GLY:HA2	1:D:278:LYS:CE	2.26	0.66
1:D:74:GLU:HB2	1:D:78:LYS:HB3	1.77	0.66
2:O:94:LYS:NZ	2:O:94:LYS:HB3	2.11	0.66
2:P:94:LYS:HB3	2:P:94:LYS:NZ	2.10	0.66
2:S:28:THR:HB	2:S:30:LYS:NZ	2.09	0.66
1:A:175:LYS:O	1:A:178:SER:N	2.28	0.66
1:A:165:GLN:HE21	1:A:251:PRO:HG2	1.60	0.66
1:B:609:GLU:N	1:B:609:GLU:OE2	2.26	0.66
1:B:76:LEU:O	1:B:80:GLN:N	2.28	0.66
1:C:697:ILE:C	1:C:699:GLY:H	1.98	0.66
1:C:739:LYS:HG2	1:C:740:GLN:H	1.60	0.66
1:D:530:THR:O	1:D:534:ILE:HG13	1.95	0.66
1:F:148:GLU:HG3	1:F:149:THR:HG22	1.76	0.66
1:F:175:LYS:O	1:F:178:SER:N	2.28	0.66
1:F:737:LYS:HA	1:F:737:LYS:HE2	1.76	0.66
1:A:530:THR:O	1:A:534:ILE:HG13	1.95	0.66
1:A:74:GLU:HB2	1:A:78:LYS:HB3	1.77	0.66
1:B:175:LYS:O	1:B:178:SER:N	2.28	0.66
1:B:737:LYS:HE2	1:B:737:LYS:HA	1.76	0.66
1:E:462:ILE:HD11	1:E:466:GLY:HA2	1.78	0.66
1:E:516:VAL:HG21	1:E:532:LEU:HD11	1.77	0.66
1:E:86:LEU:HA	1:E:89:ILE:HD12	1.77	0.66
1:F:270:LYS:O	1:F:273:LYS:HB2	1.94	0.66
2:Q:49:GLN:NE2	2:Q:49:GLN:H	1.93	0.66
1:B:788:ASP:O	1:B:792:VAL:HG23	1.94	0.66
1:D:122:GLU:HG3	1:D:147:ARG:CB	2.23	0.66
1:D:199:LEU:C	1:D:201:ASP:H	1.99	0.66
1:D:694:VAL:HA	1:D:697:ILE:HD12	1.78	0.66
1:E:130:SER:HB2	1:E:170:TYR:HE2	1.58	0.66
1:E:76:LEU:CD2	1:E:76:LEU:H	2.09	0.66
1:F:142:VAL:HG13	1:F:154:ILE:HD12	1.76	0.66
2:O:5:THR:HG23	2:O:8:GLN:CB	2.26	0.66
2:R:5:THR:HG23	2:R:8:GLN:CB	2.26	0.66
1:A:225:ILE:O	1:A:225:ILE:HG22	1.93	0.66
1:B:718:ARG:HH11	1:B:767:GLN:HE21	1.44	0.66
1:C:275:GLY:HA2	1:C:278:LYS:CE	2.25	0.66

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:788:ASP:O	1:D:792:VAL:HG23	1.95	0.66
1:F:90:PRO:HG2	1:F:93:VAL:HB	1.77	0.66
2:R:28:THR:HB	2:R:30:LYS:NZ	2.10	0.66
1:B:74:GLU:HB2	1:B:78:LYS:HB3	1.77	0.66
1:E:217:LYS:HB3	1:E:217:LYS:HZ2	1.61	0.66
1:E:165:GLN:HE21	1:E:251:PRO:HG2	1.60	0.66
1:E:671:ARG:NH1	1:E:677:GLY:HA3	2.10	0.66
1:F:671:ARG:NH1	1:F:677:GLY:HA3	2.11	0.66
2:T:5:THR:HG23	2:T:8:GLN:CB	2.26	0.66
1:B:581:GLN:NE2	1:B:629:ASN:H	1.92	0.66
1:D:246:SER:O	1:D:250:ALA:HB2	1.96	0.66
1:D:385:LEU:O	1:D:385:LEU:HD13	1.96	0.66
1:D:397:GLU:HG3	1:D:480:ASN:HB3	1.78	0.66
1:D:737:LYS:HA	1:D:737:LYS:HE2	1.76	0.66
1:D:776:LEU:O	1:D:776:LEU:HD23	1.96	0.66
1:A:122:GLU:HG3	1:A:147:ARG:CB	2.23	0.65
1:A:246:SER:O	1:A:250:ALA:HB2	1.96	0.65
1:B:130:SER:HB2	1:B:170:TYR:HE2	1.58	0.65
1:C:246:SER:O	1:C:250:ALA:HB2	1.95	0.65
1:C:718:ARG:HH11	1:C:767:GLN:HE21	1.43	0.65
1:D:739:LYS:HG2	1:D:740:GLN:H	1.59	0.65
1:E:154:ILE:HG13	1:E:171:TYR:HE1	1.61	0.65
2:P:106:ARG:O	2:P:110:THR:HG23	1.94	0.65
1:B:501:LEU:CD2	2:P:112:LEU:HD21	2.21	0.65
1:B:89:ILE:CG2	1:B:93:VAL:HG11	2.20	0.65
1:C:517:VAL:HB	1:C:525:LYS:HZ1	1.61	0.65
1:E:275:GLY:HA2	1:E:278:LYS:HG3	1.77	0.65
1:F:516:VAL:HG21	1:F:532:LEU:HD11	1.78	0.65
2:S:58:ASP:HB2	2:S:62:THR:HG23	1.78	0.65
1:A:397:GLU:HG3	1:A:480:ASN:HB3	1.78	0.65
1:A:499:PRO:HG2	1:A:504:ILE:HD11	1.79	0.65
1:A:718:ARG:HH11	1:A:767:GLN:HE21	1.44	0.65
1:A:76:LEU:H	1:A:76:LEU:CD2	2.10	0.65
1:A:76:LEU:O	1:A:80:GLN:N	2.27	0.65
1:B:462:ILE:HD11	1:B:466:GLY:HA2	1.78	0.65
1:B:697:ILE:C	1:B:699:GLY:H	1.99	0.65
1:C:397:GLU:HG3	1:C:480:ASN:HB3	1.79	0.65
1:F:246:SER:O	1:F:250:ALA:HB2	1.95	0.65
2:T:94:LYS:NZ	2:T:94:LYS:HB3	2.11	0.65
1:C:776:LEU:HD23	1:C:776:LEU:O	1.97	0.65
1:D:671:ARG:NH1	1:D:677:GLY:HA3	2.11	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:SER:O	1:E:250:ALA:HB2	1.96	0.65
1:E:345:THR:HB	1:E:491:ASP:HB3	1.78	0.65
1:F:199:LEU:C	1:F:201:ASP:H	2.00	0.65
2:R:58:ASP:HB2	2:R:62:THR:HG23	1.79	0.65
1:C:122:GLU:HG3	1:C:147:ARG:CB	2.23	0.65
1:C:142:VAL:HG13	1:C:154:ILE:HD12	1.77	0.65
1:C:199:LEU:C	1:C:201:ASP:H	2.00	0.65
1:C:385:LEU:HD13	1:C:385:LEU:O	1.96	0.65
1:D:697:ILE:C	1:D:699:GLY:H	2.00	0.65
2:T:106:ARG:O	2:T:110:THR:HG23	1.95	0.65
1:B:372:LYS:HD2	1:B:373:LYS:HE2	1.79	0.65
1:B:405:LEU:HD12	1:B:405:LEU:H	1.62	0.65
1:C:90:PRO:HG2	1:C:93:VAL:HB	1.78	0.65
1:E:397:GLU:HG3	1:E:480:ASN:HB3	1.79	0.65
1:A:674:SER:OG	1:A:674:SER:O	2.15	0.65
1:B:76:LEU:H	1:B:76:LEU:CD2	2.09	0.65
1:B:90:PRO:HG2	1:B:93:VAL:HB	1.78	0.65
1:D:109:ILE:CD1	1:D:157:LYS:HZ2	2.10	0.65
1:E:164:GLU:O	1:E:167:LYS:HG2	1.97	0.65
1:F:609:GLU:N	1:F:609:GLU:OE2	2.26	0.65
2:Q:52:ILE:HG13	2:Q:63:ILE:HG23	1.79	0.65
1:A:385:LEU:HD13	1:A:385:LEU:O	1.96	0.65
1:A:462:ILE:HD11	1:A:466:GLY:HA2	1.78	0.65
1:C:164:GLU:O	1:C:167:LYS:HG2	1.96	0.65
1:D:76:LEU:H	1:D:76:LEU:CD2	2.10	0.65
1:F:164:GLU:O	1:F:167:LYS:HG2	1.97	0.65
2:R:52:ILE:HG13	2:R:63:ILE:HG23	1.79	0.65
1:A:164:GLU:O	1:A:167:LYS:HG2	1.97	0.65
1:A:275:GLY:HA2	1:A:278:LYS:CE	2.27	0.65
1:A:697:ILE:C	1:A:699:GLY:H	1.99	0.65
1:A:737:LYS:HA	1:A:737:LYS:HE2	1.77	0.65
1:B:360:VAL:HG21	1:B:365:PRO:HB3	1.79	0.65
1:C:268:MET:O	1:C:271:LEU:HB2	1.97	0.65
1:E:142:VAL:HG13	1:E:154:ILE:HD12	1.77	0.65
1:F:776:LEU:HD23	1:F:776:LEU:O	1.97	0.65
2:P:28:THR:HB	2:P:30:LYS:NZ	2.09	0.65
2:R:56:ASP:OD2	2:R:60:ASN:CA	2.45	0.65
2:S:36:MSE:HE1	2:S:51:MSE:HE1	1.77	0.65
1:A:694:VAL:HA	1:A:697:ILE:HD12	1.79	0.65
1:A:776:LEU:O	1:A:776:LEU:HD23	1.97	0.65
1:B:397:GLU:HG3	1:B:480:ASN:HB3	1.79	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LEU:HA	1:B:89:ILE:HD12	1.77	0.65
1:C:148:GLU:HG3	1:C:149:THR:N	2.12	0.65
1:D:109:ILE:HD13	1:D:157:LYS:HZ3	1.60	0.65
1:E:183:SER:O	1:E:187:SER:HB3	1.95	0.65
1:E:776:LEU:O	1:E:776:LEU:HD23	1.97	0.65
1:F:694:VAL:HA	1:F:697:ILE:HD12	1.78	0.65
1:F:76:LEU:H	1:F:76:LEU:CD2	2.10	0.65
2:S:5:THR:HG23	2:S:8:GLN:CB	2.26	0.65
1:A:148:GLU:HG3	1:A:149:THR:N	2.12	0.64
1:C:405:LEU:H	1:C:405:LEU:HD12	1.61	0.64
2:S:106:ARG:O	2:S:110:THR:HG23	1.95	0.64
1:B:516:VAL:HG21	1:B:532:LEU:HD11	1.77	0.64
1:C:360:VAL:HG21	1:C:365:PRO:HB3	1.78	0.64
1:C:462:ILE:HD11	1:C:466:GLY:HA2	1.78	0.64
1:D:142:VAL:HG13	1:D:154:ILE:HD12	1.77	0.64
1:F:718:ARG:HH11	1:F:767:GLN:HE21	1.43	0.64
2:O:51:MSE:HB2	2:O:71:MSE:HE2	1.80	0.64
2:T:51:MSE:HB2	2:T:71:MSE:HE2	1.79	0.64
1:A:199:LEU:C	1:A:201:ASP:H	1.99	0.64
1:B:122:GLU:CG	1:B:147:ARG:HB2	2.26	0.64
1:C:345:THR:HB	1:C:491:ASP:HB3	1.79	0.64
1:C:76:LEU:H	1:C:76:LEU:CD2	2.10	0.64
1:D:164:GLU:O	1:D:167:LYS:HG2	1.97	0.64
1:D:372:LYS:HD2	1:D:373:LYS:HE2	1.78	0.64
1:D:90:PRO:HG2	1:D:93:VAL:HB	1.78	0.64
1:F:499:PRO:HG2	1:F:504:ILE:HD11	1.79	0.64
2:O:52:ILE:HG13	2:O:63:ILE:HG23	1.79	0.64
1:A:179:LEU:C	1:A:183:SER:HB2	2.08	0.64
1:A:516:VAL:HG21	1:A:532:LEU:HD11	1.78	0.64
1:C:609:GLU:N	1:C:609:GLU:OE2	2.26	0.64
1:E:737:LYS:HA	1:E:737:LYS:HE2	1.76	0.64
1:F:130:SER:HB2	1:F:170:TYR:HE2	1.59	0.64
1:F:697:ILE:C	1:F:699:GLY:H	1.99	0.64
2:S:52:ILE:HG13	2:S:63:ILE:HG23	1.79	0.64
2:T:13:LYS:HZ2	2:T:65:PHE:HB3	1.60	0.64
1:B:345:THR:HB	1:B:491:ASP:HB3	1.78	0.64
1:B:776:LEU:HD23	1:B:776:LEU:O	1.96	0.64
1:E:279:ILE:H	1:E:279:ILE:CD1	2.06	0.64
1:C:501:LEU:CD2	2:Q:112:LEU:HD21	2.23	0.64
2:S:94:LYS:HB3	2:S:94:LYS:NZ	2.11	0.64
2:T:52:ILE:HG13	2:T:63:ILE:HG23	1.79	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PRO:HG2	1:A:93:VAL:HB	1.78	0.64
1:C:109:ILE:CD1	1:C:157:LYS:NZ	2.61	0.64
1:C:694:VAL:HA	1:C:697:ILE:HD12	1.80	0.64
1:D:499:PRO:HG2	1:D:504:ILE:HD11	1.79	0.64
1:E:268:MET:O	1:E:271:LEU:HB2	1.97	0.64
1:E:405:LEU:HD12	1:E:405:LEU:H	1.63	0.64
1:E:697:ILE:C	1:E:699:GLY:H	1.99	0.64
1:F:345:THR:HB	1:F:491:ASP:HB3	1.79	0.64
1:B:275:GLY:HA2	1:B:278:LYS:CE	2.26	0.64
1:E:112:VAL:HG12	1:E:113:GLU:N	2.08	0.64
1:F:268:MET:O	1:F:271:LEU:HB2	1.97	0.64
1:F:462:ILE:HD11	1:F:466:GLY:HA2	1.78	0.64
2:S:51:MSE:HB2	2:S:71:MSE:HE2	1.80	0.64
1:A:517:VAL:HB	1:A:525:LYS:HZ1	1.63	0.64
1:E:199:LEU:C	1:E:201:ASP:H	2.00	0.64
1:E:674:SER:OG	1:E:674:SER:O	2.15	0.64
1:E:694:VAL:HA	1:E:697:ILE:HD12	1.78	0.64
1:E:90:PRO:HG2	1:E:93:VAL:HB	1.78	0.64
1:F:109:ILE:CD1	1:F:157:LYS:HZ2	2.11	0.64
1:C:499:PRO:HG2	1:C:504:ILE:HD11	1.80	0.64
1:F:148:GLU:HG3	1:F:149:THR:N	2.13	0.64
1:F:360:VAL:HG21	1:F:365:PRO:HB3	1.79	0.64
1:F:405:LEU:H	1:F:405:LEU:HD12	1.63	0.64
1:A:217:LYS:HB3	1:A:217:LYS:HZ2	1.63	0.64
1:A:360:VAL:HG21	1:A:365:PRO:HB3	1.79	0.64
1:B:148:GLU:HG3	1:B:149:THR:N	2.13	0.64
1:E:385:LEU:O	1:E:385:LEU:HD13	1.97	0.64
2:R:51:MSE:HB2	2:R:71:MSE:HE2	1.79	0.64
1:E:360:VAL:HG21	1:E:365:PRO:HB3	1.79	0.63
2:P:5:THR:HG23	2:P:8:GLN:CB	2.26	0.63
1:C:89:ILE:CG2	1:C:93:VAL:HG11	2.20	0.63
1:D:148:GLU:HG3	1:D:149:THR:N	2.13	0.63
1:E:504:ILE:HD12	1:E:504:ILE:H	1.63	0.63
1:E:718:ARG:HH11	1:E:767:GLN:HE21	1.44	0.63
1:F:109:ILE:CD1	1:F:157:LYS:NZ	2.61	0.63
1:F:372:LYS:HD2	1:F:373:LYS:HE2	1.80	0.63
2:O:68:PHE:O	2:O:71:MSE:HB3	1.99	0.63
1:A:405:LEU:HD12	1:A:405:LEU:H	1.63	0.63
1:B:109:ILE:CD1	1:B:157:LYS:NZ	2.61	0.63
1:C:678:VAL:HG13	1:C:745:TYR:CD2	2.34	0.63
1:D:345:THR:HB	1:D:491:ASP:HB3	1.79	0.63

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:435:LEU:HG	1:E:446:ILE:HG22	1.81	0.63
2:P:102:ALA:HB1	2:P:121:VAL:HG12	1.80	0.63
2:P:52:ILE:HG13	2:P:63:ILE:HG23	1.79	0.63
1:A:109:ILE:CD1	1:A:157:LYS:NZ	2.61	0.63
1:A:268:MET:O	1:A:271:LEU:HB2	1.98	0.63
1:B:499:PRO:HG2	1:B:504:ILE:HD11	1.80	0.63
1:B:694:VAL:HA	1:B:697:ILE:HD12	1.80	0.63
1:C:307:LEU:HD12	1:C:331:VAL:HG21	1.81	0.63
1:E:305:SER:HB2	1:E:594:PHE:CD1	2.34	0.63
1:E:372:LYS:HD2	1:E:373:LYS:HE2	1.80	0.63
1:E:499:PRO:HG2	1:E:504:ILE:HD11	1.79	0.63
1:C:279:ILE:H	1:C:279:ILE:CD1	2.06	0.63
1:D:268:MET:O	1:D:271:LEU:HB2	1.98	0.63
1:E:122:GLU:CG	1:E:147:ARG:HB2	2.26	0.63
1:E:148:GLU:HG3	1:E:149:THR:N	2.12	0.63
1:B:193:LEU:O	1:B:197:LYS:HB2	1.99	0.63
1:B:268:MET:O	1:B:271:LEU:HB2	1.97	0.63
1:C:372:LYS:HD2	1:C:373:LYS:HE2	1.79	0.63
1:D:109:ILE:CD1	1:D:157:LYS:NZ	2.62	0.63
1:F:504:ILE:HD12	1:F:504:ILE:H	1.64	0.63
2:Q:51:MSE:HB2	2:Q:71:MSE:HE2	1.80	0.63
1:A:372:LYS:HD2	1:A:373:LYS:HE2	1.79	0.63
1:B:107:THR:CG2	1:B:115:LYS:HD2	2.29	0.63
1:C:338:LEU:O	1:C:343:VAL:HG23	1.99	0.63
1:D:179:LEU:C	1:D:183:SER:HB2	2.07	0.63
1:D:461:LYS:HG3	1:D:462:ILE:H	1.64	0.63
1:D:305:SER:HB2	1:D:594:PHE:CD1	2.34	0.63
1:F:435:LEU:HG	1:F:446:ILE:HG22	1.81	0.63
2:Q:18:LEU:HB3	2:Q:19:PHE:CD1	2.34	0.63
1:A:193:LEU:O	1:A:197:LYS:HB2	1.99	0.63
1:A:89:ILE:CG2	1:A:93:VAL:HG11	2.20	0.63
1:D:89:ILE:CG2	1:D:93:VAL:HG11	2.19	0.63
2:O:56:ASP:OD2	2:O:60:ASN:CA	2.47	0.63
2:O:13:LYS:HZ3	2:O:65:PHE:HB3	1.59	0.63
2:P:73:ALA:O	2:P:76:MSE:N	2.32	0.63
2:T:56:ASP:OD2	2:T:60:ASN:CA	2.47	0.63
1:D:307:LEU:HD12	1:D:307:LEU:H	1.64	0.63
1:E:456:LYS:HD3	1:E:471:TRP:NE1	2.14	0.63
1:F:461:LYS:HG3	1:F:462:ILE:H	1.64	0.63
1:B:344:ALA:HA	1:B:569:TYR:OH	1.99	0.62
1:B:504:ILE:H	1:B:504:ILE:HD12	1.65	0.62

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:LEU:O	1:B:533:LEU:HD23	1.99	0.62
1:C:461:LYS:HG3	1:C:462:ILE:H	1.64	0.62
1:D:435:LEU:HG	1:D:446:ILE:HG22	1.81	0.62
2:S:102:ALA:HB1	2:S:121:VAL:HG12	1.81	0.62
1:A:305:SER:HB2	1:A:594:PHE:CD1	2.34	0.62
1:D:122:GLU:CG	1:D:147:ARG:HB2	2.25	0.62
1:D:338:LEU:O	1:D:343:VAL:HG23	1.99	0.62
1:E:104:ILE:HG23	1:E:152:LEU:HD22	1.81	0.62
2:P:51:MSE:HB2	2:P:71:MSE:HE2	1.80	0.62
1:A:345:THR:HB	1:A:491:ASP:HB3	1.79	0.62
1:A:461:LYS:HG3	1:A:462:ILE:H	1.64	0.62
1:B:789:ASN:O	1:B:792:VAL:HB	1.99	0.62
1:D:360:VAL:HG21	1:D:365:PRO:HB3	1.79	0.62
1:F:122:GLU:HG3	1:F:147:ARG:CB	2.23	0.62
2:Q:52:ILE:HG13	2:Q:63:ILE:CG2	2.29	0.62
2:Q:68:PHE:O	2:Q:71:MSE:HB3	1.99	0.62
1:A:435:LEU:HG	1:A:446:ILE:HG22	1.81	0.62
1:A:456:LYS:HD3	1:A:471:TRP:NE1	2.14	0.62
1:A:504:ILE:HD12	1:A:504:ILE:H	1.64	0.62
1:B:435:LEU:HG	1:B:446:ILE:HG22	1.81	0.62
1:D:193:LEU:O	1:D:197:LYS:HB2	1.99	0.62
1:D:405:LEU:H	1:D:405:LEU:HD12	1.63	0.62
1:E:179:LEU:O	1:E:183:SER:CA	2.47	0.62
1:F:197:LYS:HZ2	1:F:197:LYS:HB3	1.64	0.62
1:A:104:ILE:HG23	1:A:152:LEU:HD22	1.81	0.62
1:A:107:THR:CG2	1:A:115:LYS:HD2	2.29	0.62
1:A:307:LEU:HD12	1:A:307:LEU:H	1.64	0.62
1:B:104:ILE:HG23	1:B:152:LEU:HD22	1.82	0.62
1:D:678:VAL:HG13	1:D:745:TYR:CD2	2.35	0.62
1:E:109:ILE:CD1	1:E:157:LYS:NZ	2.63	0.62
1:E:193:LEU:O	1:E:197:LYS:HB2	1.98	0.62
1:F:748:TYR:O	1:F:751:TYR:N	2.32	0.62
2:R:102:ALA:HB1	2:R:121:VAL:HG12	1.80	0.62
2:T:68:PHE:O	2:T:71:MSE:HB3	2.00	0.62
1:A:164:GLU:O	1:A:167:LYS:HE3	2.00	0.62
1:A:678:VAL:HG13	1:A:745:TYR:CD2	2.34	0.62
1:A:789:ASN:O	1:A:792:VAL:HB	2.00	0.62
1:C:193:LEU:O	1:C:197:LYS:HB2	1.98	0.62
1:E:461:LYS:HG3	1:E:462:ILE:H	1.64	0.62
1:F:179:LEU:O	1:F:183:SER:CA	2.48	0.62
2:P:55:VAL:CG2	2:P:67:GLU:OE1	2.41	0.62

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:68:PHE:O	2:P:71:MSE:HB3	1.99	0.62
2:Q:102:ALA:HB1	2:Q:121:VAL:HG12	1.80	0.62
2:R:18:LEU:HB3	2:R:19:PHE:CD1	2.35	0.62
2:S:68:PHE:O	2:S:71:MSE:HB3	1.99	0.62
2:T:28:THR:HG21	2:T:30:LYS:HZ1	1.63	0.62
1:B:732:ILE:HG23	1:B:749:PHE:HD1	1.64	0.62
1:C:344:ALA:HA	1:C:569:TYR:OH	1.99	0.62
1:C:504:ILE:H	1:C:504:ILE:HD12	1.64	0.62
1:F:275:GLY:HA2	1:F:278:LYS:CE	2.26	0.62
2:R:8:GLN:O	2:R:12:PHE:HD2	1.81	0.62
1:A:480:ASN:HD21	1:A:483:GLY:N	1.98	0.62
1:A:732:ILE:HG23	1:A:749:PHE:HD1	1.65	0.62
1:B:115:LYS:NZ	1:B:115:LYS:HB3	2.14	0.62
1:B:154:ILE:HG13	1:B:171:TYR:HE1	1.61	0.62
1:C:115:LYS:HB3	1:C:115:LYS:NZ	2.14	0.62
1:D:732:ILE:HG23	1:D:749:PHE:HD1	1.64	0.62
1:F:107:THR:CG2	1:F:115:LYS:HD2	2.29	0.62
1:F:122:GLU:CG	1:F:147:ARG:HB2	2.25	0.62
1:F:344:ALA:HA	1:F:569:TYR:OH	1.99	0.62
1:F:732:ILE:HG23	1:F:749:PHE:HD1	1.65	0.62
2:O:102:ALA:HB1	2:O:121:VAL:HG12	1.81	0.62
2:P:117:THR:HG23	2:P:120:GLU:CB	2.30	0.62
1:B:637:PRO:O	1:B:640:LYS:HG3	2.00	0.62
1:C:104:ILE:HG23	1:C:152:LEU:HD22	1.81	0.62
1:E:344:ALA:HA	1:E:569:TYR:OH	2.00	0.62
1:F:305:SER:HB2	1:F:594:PHE:CD1	2.35	0.62
1:F:789:ASN:O	1:F:792:VAL:HB	2.00	0.62
1:F:89:ILE:CG2	1:F:93:VAL:HG11	2.20	0.62
2:Q:73:ALA:O	2:Q:76:MSE:N	2.32	0.62
2:T:18:LEU:HB3	2:T:19:PHE:CD1	2.35	0.62
1:A:189:ASP:HB3	1:A:190:PRO:CD	2.30	0.62
1:A:443:GLU:OE2	1:A:458:LYS:HG2	2.00	0.62
1:A:748:TYR:O	1:A:751:TYR:N	2.32	0.62
1:B:724:ARG:HG3	1:B:724:ARG:HH11	1.64	0.62
1:C:305:SER:HB2	1:C:594:PHE:CD1	2.34	0.62
1:E:307:LEU:HD12	1:E:331:VAL:HG21	1.82	0.62
1:F:307:LEU:H	1:F:307:LEU:HD12	1.65	0.62
1:A:724:ARG:HH11	1:A:724:ARG:HG3	1.65	0.61
1:C:189:ASP:HB3	1:C:190:PRO:CD	2.30	0.61
1:C:456:LYS:HD3	1:C:471:TRP:NE1	2.15	0.61
1:D:718:ARG:NH1	1:D:767:GLN:HE21	1.98	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:LYS:HB3	1:E:115:LYS:NZ	2.15	0.61
1:E:307:LEU:HD12	1:E:307:LEU:H	1.64	0.61
1:F:307:LEU:HD12	1:F:331:VAL:HG21	1.82	0.61
2:S:13:LYS:HZ3	2:S:65:PHE:HB3	1.59	0.61
2:T:102:ALA:HB1	2:T:121:VAL:HG12	1.82	0.61
1:A:122:GLU:CG	1:A:147:ARG:HB2	2.26	0.61
1:C:279:ILE:O	1:C:283:LEU:HB2	2.01	0.61
1:D:115:LYS:HB3	1:D:115:LYS:NZ	2.14	0.61
1:D:307:LEU:HD12	1:D:331:VAL:HG21	1.83	0.61
1:F:678:VAL:HG13	1:F:745:TYR:CD2	2.35	0.61
1:F:722:ILE:HG23	1:F:760:VAL:CG1	2.28	0.61
2:O:73:ALA:O	2:O:76:MSE:N	2.33	0.61
2:R:68:PHE:O	2:R:71:MSE:HB3	2.00	0.61
2:T:52:ILE:HG13	2:T:63:ILE:CG2	2.30	0.61
1:A:412:GLU:HG2	1:A:413:LEU:HD23	1.82	0.61
1:B:480:ASN:HD21	1:B:483:GLY:N	1.98	0.61
1:D:443:GLU:OE2	1:D:458:LYS:HG2	2.01	0.61
1:D:344:ALA:HA	1:D:569:TYR:OH	2.00	0.61
1:D:724:ARG:HH11	1:D:724:ARG:HG3	1.65	0.61
1:F:193:LEU:O	1:F:197:LYS:HB2	1.99	0.61
1:F:338:LEU:O	1:F:343:VAL:HG23	1.99	0.61
1:F:748:TYR:O	1:F:751:TYR:HB3	2.01	0.61
2:R:52:ILE:HG13	2:R:63:ILE:CG2	2.30	0.61
1:A:165:GLN:CD	1:A:252:ASP:HB3	2.21	0.61
1:A:722:ILE:HG23	1:A:760:VAL:CG1	2.28	0.61
1:B:182:ILE:O	1:B:187:SER:CB	2.48	0.61
1:B:307:LEU:HD12	1:B:307:LEU:H	1.65	0.61
1:C:179:LEU:O	1:C:183:SER:CA	2.48	0.61
1:C:217:LYS:CB	1:C:236:GLU:HG3	2.31	0.61
1:C:296:LEU:CD2	1:C:296:LEU:H	1.90	0.61
1:E:182:ILE:O	1:E:187:SER:CB	2.49	0.61
1:F:456:LYS:HD3	1:F:471:TRP:NE1	2.14	0.61
2:O:18:LEU:HB3	2:O:19:PHE:CD1	2.35	0.61
1:B:412:GLU:HG2	1:B:413:LEU:HD23	1.82	0.61
1:B:565:LYS:C	1:B:567:THR:H	2.04	0.61
1:E:338:LEU:O	1:E:343:VAL:HG23	2.00	0.61
1:E:637:PRO:O	1:E:640:LYS:HG3	2.00	0.61
1:F:188:LEU:N	1:F:188:LEU:CD2	2.63	0.61
1:F:480:ASN:HD21	1:F:483:GLY:N	1.99	0.61
2:P:52:ILE:HG13	2:P:63:ILE:CG2	2.30	0.61
2:Q:8:GLN:O	2:Q:12:PHE:HD2	1.83	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LEU:HD23	1:A:533:LEU:O	2.00	0.61
1:B:305:SER:HB2	1:B:594:PHE:CD1	2.36	0.61
1:C:197:LYS:HB3	1:C:197:LYS:HZ2	1.65	0.61
1:C:412:GLU:HG2	1:C:413:LEU:HD23	1.82	0.61
1:C:480:ASN:HD21	1:C:483:GLY:N	1.99	0.61
1:C:724:ARG:HG3	1:C:724:ARG:HH11	1.64	0.61
1:C:718:ARG:NH1	1:C:767:GLN:HE21	1.99	0.61
1:D:104:ILE:HG23	1:D:152:LEU:HD22	1.82	0.61
1:D:189:ASP:HB3	1:D:190:PRO:CD	2.30	0.61
1:E:165:GLN:CD	1:E:252:ASP:HB3	2.21	0.61
1:E:732:ILE:HG23	1:E:749:PHE:HD1	1.65	0.61
1:E:678:VAL:HG13	1:E:745:TYR:CD2	2.36	0.61
2:S:52:ILE:HG13	2:S:63:ILE:CG2	2.29	0.61
1:A:637:PRO:O	1:A:640:LYS:HG3	2.01	0.61
1:B:461:LYS:HG3	1:B:462:ILE:H	1.65	0.61
1:C:789:ASN:O	1:C:792:VAL:HB	2.01	0.61
1:D:517:VAL:HB	1:D:525:LYS:HZ1	1.65	0.61
1:E:609:GLU:N	1:E:609:GLU:OE2	2.27	0.61
1:E:789:ASN:O	1:E:792:VAL:HB	2.00	0.61
1:F:718:ARG:NH1	1:F:767:GLN:HE21	1.98	0.61
1:A:344:ALA:HA	1:A:569:TYR:OH	2.01	0.61
1:B:279:ILE:O	1:B:283:LEU:HB2	2.01	0.61
1:C:307:LEU:HD12	1:C:307:LEU:H	1.64	0.61
1:C:637:PRO:O	1:C:640:LYS:HG3	2.00	0.61
1:C:732:ILE:HG23	1:C:749:PHE:HD1	1.65	0.61
1:E:412:GLU:HG2	1:E:413:LEU:HD23	1.82	0.61
1:E:443:GLU:OE2	1:E:458:LYS:HG2	2.01	0.61
1:E:565:LYS:C	1:E:567:THR:H	2.04	0.61
1:F:182:ILE:O	1:F:187:SER:CB	2.49	0.61
1:F:189:ASP:HB3	1:F:190:PRO:CD	2.30	0.61
1:F:478:ALA:HA	1:F:488:LEU:HG	1.83	0.61
2:P:50:ASP:O	2:P:54:GLU:HB2	2.01	0.61
2:S:50:ASP:O	2:S:54:GLU:HB2	2.01	0.61
1:A:307:LEU:HD12	1:A:331:VAL:HG21	1.82	0.61
1:B:678:VAL:HG13	1:B:745:TYR:CD2	2.36	0.61
1:C:182:ILE:O	1:C:187:SER:CB	2.49	0.61
1:C:435:LEU:HG	1:C:446:ILE:HG22	1.81	0.61
1:C:443:GLU:OE2	1:C:458:LYS:HG2	2.01	0.61
1:C:478:ALA:HA	1:C:488:LEU:HG	1.83	0.61
1:D:353:LYS:N	1:D:368:GLN:HE22	1.95	0.61
1:E:164:GLU:O	1:E:167:LYS:HE3	2.01	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:408:LEU:H	1:F:408:LEU:CD1	1.95	0.61
1:F:565:LYS:C	1:F:567:THR:H	2.03	0.61
2:P:8:GLN:O	2:P:12:PHE:HD2	1.83	0.61
1:A:736:LEU:HD21	1:A:750:GLN:HE22	1.66	0.61
1:D:456:LYS:HD3	1:D:471:TRP:NE1	2.16	0.61
1:F:112:VAL:HG12	1:F:113:GLU:N	2.09	0.61
1:A:115:LYS:HB3	1:A:115:LYS:NZ	2.15	0.60
1:B:179:LEU:O	1:B:183:SER:CA	2.48	0.60
1:B:515:LYS:HB3	1:B:515:LYS:HZ2	1.65	0.60
1:C:736:LEU:HD21	1:C:750:GLN:HE22	1.66	0.60
1:D:165:GLN:CD	1:D:252:ASP:HB3	2.21	0.60
1:D:480:ASN:HD21	1:D:483:GLY:N	1.99	0.60
1:D:504:ILE:HD12	1:D:504:ILE:H	1.64	0.60
1:D:533:LEU:HD23	1:D:533:LEU:O	2.01	0.60
1:F:279:ILE:O	1:F:283:LEU:HB2	2.01	0.60
2:O:117:THR:HG23	2:O:120:GLU:CB	2.30	0.60
2:O:8:GLN:O	2:O:12:PHE:HD2	1.83	0.60
2:S:8:GLN:O	2:S:12:PHE:HD2	1.82	0.60
2:S:55:VAL:CG2	2:S:67:GLU:OE1	2.43	0.60
1:A:279:ILE:O	1:A:283:LEU:HB2	2.01	0.60
1:A:338:LEU:O	1:A:343:VAL:HG23	2.01	0.60
1:D:182:ILE:O	1:D:187:SER:CB	2.49	0.60
1:E:189:ASP:HB3	1:E:190:PRO:CD	2.31	0.60
1:F:104:ILE:HG23	1:F:152:LEU:HD22	1.82	0.60
1:F:78:LYS:O	1:F:81:GLN:HB3	2.00	0.60
2:O:52:ILE:HG13	2:O:63:ILE:CG2	2.30	0.60
2:P:18:LEU:HB3	2:P:19:PHE:CD1	2.35	0.60
2:R:66:PRO:O	2:R:68:PHE:N	2.34	0.60
1:A:639:ASN:HD22	1:A:639:ASN:H	1.48	0.60
1:B:189:ASP:HB3	1:B:190:PRO:CD	2.31	0.60
1:B:165:GLN:CD	1:B:252:ASP:HB3	2.21	0.60
1:B:338:LEU:O	1:B:343:VAL:HG23	2.01	0.60
1:B:517:VAL:HB	1:B:525:LYS:HZ1	1.65	0.60
1:C:107:THR:CG2	1:C:115:LYS:HD2	2.29	0.60
1:C:196:ILE:O	1:C:199:LEU:HB2	2.02	0.60
1:D:789:ASN:O	1:D:792:VAL:HB	2.00	0.60
1:E:179:LEU:O	1:E:183:SER:N	2.34	0.60
1:F:443:GLU:OE2	1:F:458:LYS:HG2	2.00	0.60
2:Q:50:ASP:O	2:Q:54:GLU:HB2	2.01	0.60
2:R:73:ALA:O	2:R:76:MSE:N	2.33	0.60
1:A:179:LEU:O	1:A:183:SER:CA	2.48	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:GLU:CG	1:C:147:ARG:HB2	2.26	0.60
1:C:188:LEU:CD2	1:C:188:LEU:N	2.62	0.60
1:C:343:VAL:HG13	1:C:487:PRO:HG2	1.83	0.60
1:D:637:PRO:O	1:D:640:LYS:HG3	2.01	0.60
1:D:78:LYS:O	1:D:81:GLN:HB3	2.01	0.60
1:E:196:ILE:O	1:E:199:LEU:HB2	2.01	0.60
1:E:279:ILE:O	1:E:283:LEU:HB2	2.01	0.60
1:F:217:LYS:CB	1:F:236:GLU:HG3	2.32	0.60
1:F:165:GLN:CD	1:F:252:ASP:HB3	2.21	0.60
2:Q:66:PRO:O	2:Q:68:PHE:N	2.34	0.60
2:R:8:GLN:O	2:R:12:PHE:CD2	2.54	0.60
2:R:50:ASP:O	2:R:54:GLU:HB2	2.02	0.60
1:A:515:LYS:NZ	1:A:515:LYS:HB3	2.17	0.60
1:B:587:PRO:HB2	1:B:643:ILE:HD12	1.84	0.60
1:B:718:ARG:NH1	1:B:767:GLN:HE21	2.00	0.60
1:E:353:LYS:N	1:E:368:GLN:HE22	1.94	0.60
1:E:639:ASN:HD22	1:E:639:ASN:N	1.99	0.60
1:E:748:TYR:O	1:E:751:TYR:N	2.35	0.60
2:Q:117:THR:HG23	2:Q:120:GLU:CB	2.31	0.60
1:A:718:ARG:NH1	1:A:767:GLN:HE21	1.99	0.60
1:C:736:LEU:HD21	1:C:750:GLN:NE2	2.17	0.60
1:D:279:ILE:O	1:D:283:LEU:HB2	2.01	0.60
1:E:480:ASN:HD21	1:E:483:GLY:N	2.00	0.60
1:E:567:THR:CG2	1:E:568:GLY:N	2.65	0.60
1:E:718:ARG:NH1	1:E:767:GLN:HE21	1.99	0.60
1:E:724:ARG:HG3	1:E:724:ARG:HH11	1.65	0.60
1:F:637:PRO:O	1:F:640:LYS:HG3	2.01	0.60
2:S:8:GLN:O	2:S:12:PHE:CD2	2.55	0.60
2:T:56:ASP:HB3	2:T:60:ASN:OD1	2.02	0.60
2:T:66:PRO:O	2:T:68:PHE:N	2.35	0.60
1:A:195:LEU:HD11	1:A:226:ASP:O	2.01	0.60
1:B:195:LEU:HD11	1:B:226:ASP:O	2.02	0.60
1:B:217:LYS:CB	1:B:236:GLU:HG3	2.31	0.60
1:B:307:LEU:HD12	1:B:331:VAL:HG21	1.84	0.60
1:D:179:LEU:O	1:D:183:SER:CA	2.48	0.60
1:E:748:TYR:O	1:E:751:TYR:HB3	2.01	0.60
1:E:78:LYS:O	1:E:81:GLN:HB3	2.01	0.60
2:P:66:PRO:O	2:P:68:PHE:N	2.34	0.60
2:S:18:LEU:HB3	2:S:19:PHE:CD1	2.36	0.60
1:B:353:LYS:N	1:B:368:GLN:HE22	1.95	0.60
1:C:639:ASN:HD22	1:C:639:ASN:H	1.48	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:688:PHE:C	1:C:688:PHE:CD2	2.75	0.60
1:D:736:LEU:HD21	1:D:750:GLN:HE22	1.67	0.60
2:O:66:PRO:O	2:O:68:PHE:N	2.35	0.60
2:T:117:THR:HG21	2:T:120:GLU:OE2	2.02	0.60
1:A:182:ILE:O	1:A:187:SER:CB	2.49	0.60
1:A:196:ILE:O	1:A:199:LEU:HB2	2.02	0.60
1:A:630:ARG:HH11	1:A:630:ARG:HG3	1.66	0.60
1:A:729:TYR:HB2	1:A:756:ILE:HG21	1.84	0.60
1:B:179:LEU:O	1:B:183:SER:N	2.35	0.60
1:B:196:ILE:O	1:B:199:LEU:HB2	2.02	0.60
1:C:587:PRO:HB2	1:C:643:ILE:HD12	1.84	0.60
1:C:748:TYR:O	1:C:751:TYR:N	2.33	0.60
1:D:217:LYS:CB	1:D:236:GLU:HG3	2.32	0.60
1:F:164:GLU:O	1:F:167:LYS:HE3	2.01	0.60
1:F:688:PHE:CD2	1:F:688:PHE:C	2.75	0.60
2:T:8:GLN:O	2:T:12:PHE:HD2	1.83	0.60
1:A:112:VAL:HG12	1:A:113:GLU:N	2.09	0.60
1:A:179:LEU:O	1:A:183:SER:N	2.35	0.60
1:A:565:LYS:C	1:A:567:THR:H	2.04	0.60
1:D:639:ASN:N	1:D:639:ASN:HD22	2.00	0.60
1:E:217:LYS:CB	1:E:236:GLU:HG3	2.32	0.60
1:F:97:TYR:CE1	1:F:178:SER:HB2	2.37	0.60
1:B:456:LYS:HD3	1:B:471:TRP:NE1	2.16	0.59
1:B:567:THR:CG2	1:B:568:GLY:N	2.65	0.59
1:C:515:LYS:NZ	1:C:515:LYS:HB3	2.16	0.59
1:C:748:TYR:O	1:C:751:TYR:HB3	2.01	0.59
1:D:674:SER:OG	1:D:674:SER:O	2.15	0.59
1:F:412:GLU:HG2	1:F:413:LEU:HD23	1.83	0.59
1:A:353:LYS:N	1:A:368:GLN:HE22	1.96	0.59
1:A:748:TYR:O	1:A:751:TYR:HB3	2.02	0.59
1:B:164:GLU:O	1:B:167:LYS:HE3	2.01	0.59
1:B:379:ALA:O	1:B:383:GLY:N	2.36	0.59
1:B:748:TYR:O	1:B:751:TYR:N	2.35	0.59
1:C:379:ALA:O	1:C:383:GLY:N	2.35	0.59
1:D:107:THR:CG2	1:D:115:LYS:HD2	2.30	0.59
1:D:377:GLN:O	1:D:381:GLU:HB2	2.02	0.59
1:D:412:GLU:HG2	1:D:413:LEU:HD23	1.82	0.59
1:D:516:VAL:HG21	1:D:532:LEU:CD1	2.32	0.59
1:E:196:ILE:HA	1:E:199:LEU:HD12	1.82	0.59
1:E:533:LEU:HD23	1:E:533:LEU:O	2.03	0.59
1:F:115:LYS:NZ	1:F:115:LYS:HB3	2.16	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:LEU:HD11	1:F:226:ASP:O	2.01	0.59
1:F:515:LYS:HB3	1:F:515:LYS:NZ	2.17	0.59
1:F:567:THR:CG2	1:F:568:GLY:N	2.65	0.59
2:O:43:PRO:CG	2:O:48:LEU:HD13	2.32	0.59
2:R:59:GLY:O	2:R:62:THR:HG23	2.00	0.59
2:S:66:PRO:O	2:S:68:PHE:N	2.35	0.59
1:B:97:TYR:CE1	1:B:178:SER:HB2	2.37	0.59
1:B:478:ALA:HA	1:B:488:LEU:HG	1.83	0.59
1:B:78:LYS:O	1:B:81:GLN:HB3	2.02	0.59
1:C:112:VAL:HG12	1:C:113:GLU:N	2.09	0.59
1:C:195:LEU:HD11	1:C:226:ASP:O	2.02	0.59
1:C:165:GLN:CD	1:C:252:ASP:HB3	2.22	0.59
1:C:353:LYS:N	1:C:368:GLN:HE22	1.96	0.59
2:P:8:GLN:O	2:P:12:PHE:CD2	2.55	0.59
2:R:117:THR:HG23	2:R:120:GLU:CB	2.32	0.59
2:T:8:GLN:O	2:T:12:PHE:CD2	2.55	0.59
2:T:73:ALA:O	2:T:76:MSE:N	2.32	0.59
1:C:164:GLU:O	1:C:167:LYS:HE3	2.01	0.59
1:C:567:THR:CG2	1:C:568:GLY:N	2.65	0.59
1:D:478:ALA:HA	1:D:488:LEU:HG	1.84	0.59
1:E:478:ALA:HA	1:E:488:LEU:HG	1.84	0.59
1:E:517:VAL:HB	1:E:525:LYS:HZ1	1.66	0.59
1:F:379:ALA:O	1:F:383:GLY:N	2.35	0.59
2:Q:117:THR:HG21	2:Q:120:GLU:OE2	2.03	0.59
2:R:117:THR:HG21	2:R:120:GLU:OE2	2.03	0.59
2:T:50:ASP:O	2:T:54:GLU:HB2	2.01	0.59
1:A:154:ILE:HG13	1:A:171:TYR:HE1	1.62	0.59
1:A:515:LYS:HZ2	1:A:515:LYS:HB3	1.66	0.59
1:B:443:GLU:OE2	1:B:458:LYS:HG2	2.02	0.59
1:B:515:LYS:NZ	1:B:515:LYS:HB3	2.18	0.59
1:C:179:LEU:O	1:C:183:SER:N	2.36	0.59
1:C:711:ILE:HG13	1:C:712:PHE:CD2	2.38	0.59
1:D:97:TYR:CE1	1:D:178:SER:HB2	2.37	0.59
1:D:688:PHE:C	1:D:688:PHE:CD2	2.76	0.59
1:E:175:LYS:HB2	1:E:175:LYS:HZ3	1.68	0.59
2:O:97:ASN:N	2:O:97:ASN:HD22	2.01	0.59
1:A:78:LYS:O	1:A:81:GLN:HB3	2.01	0.59
1:D:196:ILE:O	1:D:199:LEU:HB2	2.02	0.59
1:E:688:PHE:C	1:E:688:PHE:CD2	2.75	0.59
1:E:736:LEU:HD21	1:E:750:GLN:HE22	1.67	0.59
1:F:343:VAL:HG13	1:F:487:PRO:HG2	1.85	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LYS:CB	1:A:236:GLU:HG3	2.32	0.59
1:D:565:LYS:C	1:D:567:THR:H	2.04	0.59
1:F:196:ILE:O	1:F:199:LEU:HB2	2.02	0.59
2:Q:8:GLN:O	2:Q:12:PHE:CD2	2.56	0.59
2:R:13:LYS:HZ1	2:R:65:PHE:HB3	1.66	0.59
1:B:343:VAL:HG13	1:B:487:PRO:HG2	1.83	0.59
1:B:688:PHE:CD2	1:B:688:PHE:C	2.75	0.59
1:D:748:TYR:O	1:D:751:TYR:N	2.35	0.59
1:E:379:ALA:O	1:E:383:GLY:N	2.36	0.59
1:E:515:LYS:HB3	1:E:515:LYS:NZ	2.17	0.59
1:F:196:ILE:HA	1:F:199:LEU:HD12	1.84	0.59
2:P:43:PRO:CG	2:P:48:LEU:HD13	2.33	0.59
2:Q:56:ASP:HB3	2:Q:60:ASN:OD1	2.02	0.59
1:A:97:TYR:CE1	1:A:178:SER:HB2	2.38	0.59
1:A:243:LEU:HA	1:A:246:SER:OG	2.03	0.59
1:C:565:LYS:C	1:C:567:THR:H	2.04	0.59
1:C:639:ASN:HD22	1:C:639:ASN:N	1.99	0.59
1:C:78:LYS:O	1:C:81:GLN:HB3	2.02	0.59
1:C:92:ASP:O	1:C:96:ILE:HG13	2.03	0.59
1:D:164:GLU:O	1:D:167:LYS:HE3	2.01	0.59
1:D:179:LEU:O	1:D:183:SER:N	2.36	0.59
1:E:195:LEU:HD11	1:E:226:ASP:O	2.02	0.59
1:F:639:ASN:H	1:F:639:ASN:HD22	1.49	0.59
2:Q:43:PRO:CG	2:Q:48:LEU:HD13	2.33	0.59
2:R:43:PRO:CG	2:R:48:LEU:HD13	2.32	0.59
2:S:117:THR:HG21	2:S:120:GLU:OE2	2.02	0.59
2:T:117:THR:HG23	2:T:120:GLU:CB	2.31	0.59
1:A:377:GLN:O	1:A:381:GLU:HB2	2.03	0.59
1:B:700:TYR:HD1	1:B:728:ALA:HA	1.68	0.59
1:B:92:ASP:O	1:B:96:ILE:HG13	2.03	0.59
1:C:131:ARG:HG3	1:C:243:LEU:CD2	2.33	0.59
1:E:700:TYR:HD1	1:E:728:ALA:HA	1.67	0.59
1:F:353:LYS:N	1:F:368:GLN:HE22	1.96	0.59
1:F:501:LEU:HD22	2:T:112:LEU:CD2	2.27	0.59
2:T:13:LYS:HZ1	2:T:65:PHE:HB3	1.68	0.59
1:A:478:ALA:HA	1:A:488:LEU:HG	1.84	0.58
1:A:587:PRO:HB2	1:A:643:ILE:HD12	1.85	0.58
1:B:243:LEU:HA	1:B:246:SER:OG	2.03	0.58
1:B:639:ASN:HD22	1:B:639:ASN:N	2.00	0.58
1:B:748:TYR:O	1:B:751:TYR:HB3	2.02	0.58
1:B:776:LEU:O	1:B:780:LEU:HD13	2.03	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ILE:C	1:B:81:GLN:N	2.56	0.58
1:C:307:LEU:HD12	1:C:331:VAL:CG2	2.33	0.58
1:C:674:SER:OG	1:C:674:SER:O	2.14	0.58
1:D:515:LYS:NZ	1:D:515:LYS:HB3	2.18	0.58
1:D:722:ILE:HG23	1:D:760:VAL:CG1	2.30	0.58
2:O:55:VAL:CG2	2:O:67:GLU:OE1	2.44	0.58
2:T:51:MSE:HB3	2:T:71:MSE:HE2	1.85	0.58
1:A:711:ILE:HG13	1:A:712:PHE:CD2	2.39	0.58
1:F:179:LEU:O	1:F:183:SER:N	2.35	0.58
1:F:377:GLN:O	1:F:381:GLU:HB2	2.03	0.58
1:F:630:ARG:HH11	1:F:630:ARG:HG3	1.69	0.58
2:O:100:ILE:HB	2:O:136:VAL:HG22	1.85	0.58
2:P:117:THR:HG21	2:P:120:GLU:OE2	2.03	0.58
1:B:176:GLY:C	1:B:178:SER:N	2.57	0.58
1:B:480:ASN:ND2	1:B:481:VAL:N	2.51	0.58
1:B:88:LYS:NZ	1:B:172:GLU:OE2	2.36	0.58
1:D:154:ILE:HG13	1:D:171:TYR:HE1	1.62	0.58
1:D:379:ALA:O	1:D:383:GLY:N	2.35	0.58
1:D:700:TYR:HD1	1:D:728:ALA:HA	1.68	0.58
1:E:79:ILE:C	1:E:81:GLN:N	2.57	0.58
1:F:711:ILE:HG13	1:F:712:PHE:CD2	2.38	0.58
2:O:117:THR:HG21	2:O:120:GLU:OE2	2.03	0.58
2:S:43:PRO:CG	2:S:48:LEU:HD13	2.33	0.58
1:B:711:ILE:HG13	1:B:712:PHE:CD2	2.39	0.58
1:D:196:ILE:HA	1:D:199:LEU:HD12	1.85	0.58
1:E:729:TYR:HB2	1:E:756:ILE:HG21	1.85	0.58
1:F:533:LEU:HD23	1:F:533:LEU:O	2.04	0.58
1:F:639:ASN:HD22	1:F:639:ASN:N	2.00	0.58
1:F:736:LEU:HD21	1:F:750:GLN:HE22	1.68	0.58
2:O:8:GLN:O	2:O:12:PHE:CD2	2.56	0.58
2:R:49:GLN:NE2	2:R:49:GLN:N	2.51	0.58
1:A:196:ILE:HA	1:A:199:LEU:HD12	1.85	0.58
1:A:688:PHE:CD2	1:A:688:PHE:C	2.75	0.58
1:A:700:TYR:HD1	1:A:728:ALA:HA	1.69	0.58
1:B:639:ASN:HD22	1:B:639:ASN:H	1.49	0.58
1:B:736:LEU:HD21	1:B:750:GLN:HE22	1.69	0.58
1:C:197:LYS:HZ3	1:C:197:LYS:C	2.05	0.58
1:C:533:LEU:HD23	1:C:533:LEU:O	2.03	0.58
1:C:700:TYR:HD1	1:C:728:ALA:HA	1.67	0.58
1:D:711:ILE:HG13	1:D:712:PHE:CD2	2.39	0.58
1:D:736:LEU:HD21	1:D:750:GLN:NE2	2.18	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:LEU:HD12	1:E:331:VAL:CG2	2.33	0.58
1:F:736:LEU:HD21	1:F:750:GLN:NE2	2.19	0.58
1:A:446:ILE:HG13	1:A:452:GLU:O	2.04	0.58
1:A:736:LEU:HD21	1:A:750:GLN:NE2	2.17	0.58
1:D:243:LEU:HA	1:D:246:SER:OG	2.03	0.58
1:D:748:TYR:O	1:D:751:TYR:HB3	2.03	0.58
1:D:776:LEU:O	1:D:780:LEU:HD13	2.04	0.58
1:D:92:ASP:O	1:D:96:ILE:HG13	2.04	0.58
1:E:97:TYR:CE1	1:E:178:SER:HB2	2.38	0.58
1:E:301:ALA:O	1:E:303:LYS:N	2.37	0.58
1:E:515:LYS:HB3	1:E:515:LYS:HZ2	1.67	0.58
1:E:88:LYS:NZ	1:E:172:GLU:OE2	2.37	0.58
1:F:243:LEU:HA	1:F:246:SER:OG	2.04	0.58
1:F:88:LYS:NZ	1:F:172:GLU:OE2	2.37	0.58
2:T:49:GLN:NE2	2:T:49:GLN:N	2.52	0.58
2:T:52:ILE:HG23	2:T:53:ASN:N	2.19	0.58
1:A:88:LYS:NZ	1:A:172:GLU:OE2	2.37	0.58
1:D:88:LYS:NZ	1:D:172:GLU:OE2	2.37	0.58
1:D:97:TYR:HE1	1:D:178:SER:HB2	1.69	0.58
1:D:195:LEU:HD11	1:D:226:ASP:O	2.03	0.58
1:E:131:ARG:HG3	1:E:243:LEU:CD2	2.32	0.58
1:F:175:LYS:O	1:F:177:ILE:N	2.36	0.58
1:F:724:ARG:HG3	1:F:724:ARG:HH11	1.67	0.58
2:P:56:ASP:OD2	2:P:60:ASN:CA	2.51	0.58
2:Q:52:ILE:HG23	2:Q:53:ASN:N	2.19	0.58
1:B:729:TYR:HB2	1:B:756:ILE:HG21	1.84	0.58
1:C:196:ILE:HA	1:C:199:LEU:HD12	1.84	0.58
1:D:372:LYS:HG3	1:D:373:LYS:N	2.19	0.58
2:Q:49:GLN:NE2	2:Q:49:GLN:N	2.52	0.58
2:T:41:GLN:O	2:T:42:ASN:HB3	2.04	0.58
2:T:43:PRO:CG	2:T:48:LEU:HD13	2.33	0.58
1:A:188:LEU:CD2	1:A:188:LEU:N	2.63	0.58
1:A:567:THR:CG2	1:A:568:GLY:N	2.66	0.58
1:B:175:LYS:O	1:B:177:ILE:N	2.36	0.58
1:B:196:ILE:HA	1:B:199:LEU:HD12	1.85	0.58
1:C:243:LEU:HA	1:C:246:SER:OG	2.03	0.58
1:C:377:GLN:O	1:C:381:GLU:HB2	2.04	0.58
1:D:587:PRO:HB2	1:D:643:ILE:HD12	1.85	0.58
1:E:107:THR:CG2	1:E:115:LYS:HD2	2.31	0.58
1:F:97:TYR:HE1	1:F:178:SER:HB2	1.69	0.58
1:A:176:GLY:C	1:A:178:SER:N	2.57	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:722:ILE:HG23	1:B:760:VAL:CG1	2.29	0.58
1:B:97:TYR:HE1	1:B:178:SER:HB2	1.68	0.58
1:C:154:ILE:HG13	1:C:171:TYR:HE1	1.62	0.58
1:C:175:LYS:O	1:C:177:ILE:N	2.37	0.58
1:C:776:LEU:O	1:C:780:LEU:HD13	2.03	0.58
1:D:630:ARG:HG3	1:D:630:ARG:HH11	1.68	0.58
1:D:657:ILE:HD11	1:D:701:LEU:HD23	1.86	0.58
1:D:729:TYR:HB2	1:D:756:ILE:HG21	1.86	0.58
1:E:175:LYS:O	1:E:177:ILE:N	2.37	0.58
1:F:729:TYR:HB2	1:F:756:ILE:HG21	1.84	0.58
2:O:56:ASP:OD2	2:O:61:GLY:N	2.37	0.58
2:Q:97:ASN:HD22	2:Q:97:ASN:N	2.01	0.58
1:A:307:LEU:HD12	1:A:331:VAL:CG2	2.34	0.57
1:C:697:ILE:CD1	1:C:732:ILE:HD13	2.34	0.57
1:D:446:ILE:HG13	1:D:452:GLU:O	2.04	0.57
1:E:508:ILE:HG23	1:E:536:TYR:CD2	2.39	0.57
1:F:480:ASN:HD22	1:F:481:VAL:H	1.52	0.57
1:F:515:LYS:HB3	1:F:515:LYS:HZ2	1.68	0.57
2:S:121:VAL:C	2:S:123:GLN:N	2.57	0.57
1:B:377:GLN:O	1:B:381:GLU:HB2	2.03	0.57
1:B:324:THR:CB	1:B:499:PRO:HA	2.34	0.57
1:C:282:SER:HA	1:C:285:LYS:HD3	1.87	0.57
1:C:516:VAL:HG21	1:C:532:LEU:CD1	2.34	0.57
1:E:372:LYS:HG3	1:E:373:LYS:N	2.19	0.57
1:E:587:PRO:HB2	1:E:643:ILE:HD12	1.86	0.57
1:E:776:LEU:O	1:E:780:LEU:HD13	2.04	0.57
1:F:480:ASN:ND2	1:F:481:VAL:N	2.52	0.57
1:F:587:PRO:HB2	1:F:643:ILE:HD12	1.85	0.57
2:P:100:ILE:HB	2:P:136:VAL:HG22	1.86	0.57
2:S:49:GLN:NE2	2:S:49:GLN:N	2.52	0.57
2:S:52:ILE:HG23	2:S:53:ASN:N	2.19	0.57
2:T:100:ILE:HB	2:T:136:VAL:HG22	1.84	0.57
1:A:109:ILE:CD1	1:A:157:LYS:HZ2	2.15	0.57
1:A:324:THR:CB	1:A:499:PRO:HA	2.34	0.57
1:A:657:ILE:HD11	1:A:701:LEU:HD23	1.87	0.57
1:B:630:ARG:HG3	1:B:630:ARG:HH11	1.69	0.57
1:C:301:ALA:O	1:C:303:LYS:N	2.37	0.57
1:C:729:TYR:HB2	1:C:756:ILE:HG21	1.84	0.57
1:D:301:ALA:O	1:D:303:LYS:N	2.37	0.57
1:E:176:GLY:C	1:E:178:SER:N	2.57	0.57
1:E:736:LEU:HD21	1:E:750:GLN:NE2	2.18	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:688:PHE:HD2	1:F:688:PHE:C	2.07	0.57
2:R:102:ALA:CB	2:R:125:ILE:HG13	2.34	0.57
1:A:354:SER:O	1:A:371:SER:HB2	2.05	0.57
1:A:379:ALA:O	1:A:383:GLY:N	2.36	0.57
1:A:480:ASN:ND2	1:A:481:VAL:N	2.51	0.57
1:A:697:ILE:CD1	1:A:732:ILE:HD13	2.34	0.57
1:A:776:LEU:O	1:A:780:LEU:HD13	2.05	0.57
1:B:131:ARG:HG3	1:B:243:LEU:CD2	2.34	0.57
1:C:88:LYS:NZ	1:C:172:GLU:OE2	2.37	0.57
1:C:446:ILE:HG13	1:C:452:GLU:O	2.04	0.57
1:D:171:TYR:O	1:D:175:LYS:NZ	2.38	0.57
1:E:377:GLN:O	1:E:381:GLU:HB2	2.03	0.57
1:E:480:ASN:ND2	1:E:481:VAL:N	2.53	0.57
1:E:639:ASN:HD22	1:E:639:ASN:H	1.48	0.57
2:S:97:ASN:N	2:S:97:ASN:HD22	2.01	0.57
1:A:372:LYS:HG3	1:A:373:LYS:N	2.19	0.57
1:A:79:ILE:C	1:A:81:GLN:N	2.57	0.57
1:C:252:ASP:O	1:C:254:ARG:HD2	2.05	0.57
1:D:214:PHE:HB3	1:D:218:LEU:HB3	1.87	0.57
1:E:252:ASP:O	1:E:254:ARG:HD2	2.05	0.57
1:F:307:LEU:HD12	1:F:331:VAL:CG2	2.34	0.57
2:Q:51:MSE:HB3	2:Q:71:MSE:HE2	1.85	0.57
2:Q:97:ASN:H	2:Q:97:ASN:ND2	2.02	0.57
1:A:516:VAL:HG21	1:A:532:LEU:CD1	2.35	0.57
1:A:508:ILE:HG23	1:A:536:TYR:CD2	2.39	0.57
1:B:480:ASN:HD22	1:B:481:VAL:N	2.03	0.57
1:B:697:ILE:CD1	1:B:732:ILE:HD13	2.34	0.57
1:C:657:ILE:HD11	1:C:701:LEU:HD23	1.86	0.57
1:E:97:TYR:HE1	1:E:178:SER:HB2	1.69	0.57
1:E:243:LEU:HA	1:E:246:SER:OG	2.03	0.57
1:E:282:SER:HA	1:E:285:LYS:HD3	1.87	0.57
1:E:89:ILE:CG2	1:E:93:VAL:HG11	2.20	0.57
1:F:176:GLY:C	1:F:178:SER:N	2.57	0.57
1:F:700:TYR:HD1	1:F:728:ALA:HA	1.68	0.57
2:O:59:GLY:O	2:O:62:THR:HG23	2.02	0.57
2:P:59:GLY:O	2:P:62:THR:CG2	2.52	0.57
1:A:214:PHE:HB3	1:A:218:LEU:HB3	1.86	0.57
1:B:516:VAL:HG21	1:B:532:LEU:CD1	2.34	0.57
1:C:372:LYS:HG3	1:C:373:LYS:N	2.19	0.57
1:C:480:ASN:HD22	1:C:481:VAL:H	1.52	0.57
1:C:688:PHE:C	1:C:688:PHE:HD2	2.08	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:ARG:HG3	1:D:243:LEU:CD2	2.35	0.57
1:D:175:LYS:O	1:D:177:ILE:N	2.37	0.57
1:D:567:THR:CG2	1:D:568:GLY:N	2.66	0.57
1:E:137:PHE:HD2	1:E:137:PHE:C	2.08	0.57
1:E:343:VAL:HG13	1:E:487:PRO:HG2	1.86	0.57
2:O:52:ILE:HG23	2:O:53:ASN:N	2.18	0.57
2:S:97:ASN:ND2	2:S:97:ASN:H	2.02	0.57
2:T:13:LYS:HZ3	2:T:65:PHE:HB3	1.68	0.57
1:A:112:VAL:O	1:A:114:HIS:N	2.38	0.57
1:A:326:ILE:HG22	1:A:328:PHE:CE1	2.40	0.57
1:B:137:PHE:C	1:B:137:PHE:HD2	2.08	0.57
1:B:372:LYS:HG3	1:B:373:LYS:N	2.19	0.57
1:C:480:ASN:HD22	1:C:481:VAL:N	2.03	0.57
1:C:722:ILE:HG23	1:C:760:VAL:CG1	2.28	0.57
1:E:354:SER:O	1:E:371:SER:HB2	2.05	0.57
1:E:722:ILE:HG23	1:E:760:VAL:CG1	2.30	0.57
1:F:197:LYS:HZ3	1:F:197:LYS:C	2.06	0.57
1:F:372:LYS:HG3	1:F:373:LYS:N	2.19	0.57
1:F:657:ILE:HD11	1:F:701:LEU:HD23	1.86	0.57
2:P:121:VAL:C	2:P:123:GLN:N	2.57	0.57
2:P:49:GLN:N	2:P:49:GLN:NE2	2.52	0.57
2:P:97:ASN:N	2:P:97:ASN:HD22	2.02	0.57
2:Q:102:ALA:CB	2:Q:125:ILE:HG13	2.34	0.57
2:Q:49:GLN:HE21	2:Q:49:GLN:H	1.52	0.57
2:R:121:VAL:C	2:R:123:GLN:N	2.57	0.57
2:R:52:ILE:HG23	2:R:53:ASN:N	2.19	0.57
2:R:97:ASN:HD22	2:R:97:ASN:N	2.02	0.57
1:A:97:TYR:HE1	1:A:178:SER:HB2	1.70	0.57
1:A:282:SER:HA	1:A:285:LYS:HD3	1.86	0.57
1:A:639:ASN:HD22	1:A:639:ASN:N	1.99	0.57
1:B:446:ILE:HG13	1:B:452:GLU:O	2.05	0.57
1:C:137:PHE:HD2	1:C:137:PHE:C	2.08	0.57
1:C:97:TYR:CE1	1:C:178:SER:HB2	2.38	0.57
1:C:354:SER:O	1:C:371:SER:HB2	2.05	0.57
1:E:480:ASN:HD22	1:E:481:VAL:N	2.03	0.57
1:E:630:ARG:HH11	1:E:630:ARG:HG3	1.69	0.57
2:P:55:VAL:HG21	2:P:67:GLU:CD	2.24	0.57
2:R:51:MSE:HB3	2:R:71:MSE:HE2	1.86	0.57
2:T:49:GLN:H	2:T:49:GLN:HE21	1.52	0.57
1:B:93:VAL:CG2	1:B:179:LEU:HD11	2.35	0.57
1:B:282:SER:HA	1:B:285:LYS:HD3	1.87	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ALA:O	1:B:303:LYS:N	2.38	0.57
1:B:480:ASN:HD22	1:B:481:VAL:H	1.51	0.57
1:B:657:ILE:HD11	1:B:701:LEU:HD23	1.87	0.57
1:B:674:SER:OG	1:B:674:SER:O	2.15	0.57
1:B:688:PHE:HD2	1:B:688:PHE:C	2.08	0.57
1:E:480:ASN:HD22	1:E:481:VAL:H	1.53	0.57
1:E:516:VAL:HG21	1:E:532:LEU:CD1	2.34	0.57
1:F:776:LEU:O	1:F:780:LEU:HD13	2.04	0.57
2:P:51:MSE:HB3	2:P:71:MSE:HE2	1.86	0.57
2:R:41:GLN:O	2:R:42:ASN:HB3	2.04	0.57
2:S:100:ILE:HB	2:S:136:VAL:HG22	1.85	0.57
1:A:615:ILE:CD1	1:A:645:TRP:HH2	2.16	0.56
1:A:697:ILE:CG2	1:A:732:ILE:HD11	2.35	0.56
1:C:508:ILE:HG23	1:C:536:TYR:CD2	2.40	0.56
1:D:639:ASN:H	1:D:639:ASN:HD22	1.49	0.56
1:E:171:TYR:O	1:E:175:LYS:NZ	2.38	0.56
1:F:137:PHE:C	1:F:137:PHE:HD2	2.07	0.56
1:F:171:TYR:O	1:F:175:LYS:NZ	2.38	0.56
1:F:92:ASP:O	1:F:96:ILE:HG13	2.05	0.56
2:S:51:MSE:HB3	2:S:71:MSE:HE2	1.87	0.56
1:F:668:SER:CA	2:T:14:GLU:HG3	2.35	0.56
1:A:137:PHE:HD2	1:A:137:PHE:C	2.08	0.56
1:A:175:LYS:O	1:A:177:ILE:N	2.37	0.56
1:A:343:VAL:HG13	1:A:487:PRO:HG2	1.86	0.56
1:A:688:PHE:HD2	1:A:688:PHE:C	2.08	0.56
1:B:122:GLU:H	1:B:122:GLU:CD	2.09	0.56
1:B:307:LEU:HD12	1:B:331:VAL:CG2	2.35	0.56
1:B:354:SER:O	1:B:371:SER:HB2	2.04	0.56
1:C:214:PHE:HB3	1:C:218:LEU:HB3	1.87	0.56
1:C:480:ASN:ND2	1:C:481:VAL:N	2.52	0.56
1:D:131:ARG:HB3	1:D:170:TYR:OH	2.05	0.56
1:D:137:PHE:HD2	1:D:137:PHE:C	2.08	0.56
1:D:343:VAL:HG13	1:D:487:PRO:HG2	1.86	0.56
1:F:279:ILE:N	1:F:279:ILE:HD13	2.20	0.56
1:F:446:ILE:HG13	1:F:452:GLU:O	2.05	0.56
1:F:516:VAL:HG21	1:F:532:LEU:CD1	2.35	0.56
2:O:41:GLN:O	2:O:42:ASN:HB3	2.05	0.56
2:P:13:LYS:HZ2	2:P:65:PHE:HB3	1.68	0.56
1:C:668:SER:CA	2:Q:14:GLU:HG3	2.36	0.56
2:S:102:ALA:CB	2:S:125:ILE:HG13	2.35	0.56
2:S:73:ALA:O	2:S:76:MSE:N	2.33	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:97:ASN:N	2:T:97:ASN:HD22	2.03	0.56
1:A:92:ASP:O	1:A:96:ILE:HG13	2.05	0.56
1:B:109:ILE:HD13	1:B:157:LYS:HZ3	1.69	0.56
1:B:515:LYS:NZ	1:B:516:VAL:HG23	2.20	0.56
1:D:175:LYS:HZ1	1:D:175:LYS:HB2	1.69	0.56
1:D:307:LEU:HD12	1:D:331:VAL:CG2	2.35	0.56
1:D:405:LEU:HD13	1:D:453:VAL:CG2	2.33	0.56
1:D:697:ILE:CG2	1:D:732:ILE:HD11	2.35	0.56
1:E:697:ILE:CG2	1:E:732:ILE:HD11	2.35	0.56
1:E:657:ILE:HD11	1:E:701:LEU:HD23	1.87	0.56
1:F:480:ASN:HD22	1:F:481:VAL:N	2.03	0.56
2:O:49:GLN:NE2	2:O:49:GLN:N	2.52	0.56
2:P:28:THR:HG21	2:P:30:LYS:HZ1	1.70	0.56
2:Q:28:THR:HG21	2:Q:30:LYS:HZ1	1.68	0.56
2:Q:41:GLN:O	2:Q:42:ASN:HB3	2.05	0.56
1:A:131:ARG:HG3	1:A:243:LEU:CD2	2.35	0.56
1:A:93:VAL:CG2	1:A:179:LEU:HD11	2.34	0.56
1:B:413:LEU:HB2	1:B:419:ILE:HG12	1.87	0.56
1:C:176:GLY:C	1:C:178:SER:N	2.58	0.56
1:C:180:ASP:O	1:C:183:SER:N	2.32	0.56
1:C:279:ILE:HD13	1:C:279:ILE:N	2.21	0.56
1:D:697:ILE:CD1	1:D:732:ILE:HD13	2.36	0.56
1:E:324:THR:CB	1:E:499:PRO:HA	2.34	0.56
1:E:360:VAL:HG11	1:E:370:LEU:HD22	1.88	0.56
1:E:711:ILE:HG13	1:E:712:PHE:CD2	2.40	0.56
1:E:697:ILE:CD1	1:E:732:ILE:HD13	2.36	0.56
1:E:92:ASP:O	1:E:96:ILE:HG13	2.05	0.56
1:F:282:SER:HA	1:F:285:LYS:HD3	1.87	0.56
1:F:697:ILE:CD1	1:F:732:ILE:HD13	2.36	0.56
2:P:97:ASN:ND2	2:P:97:ASN:H	2.03	0.56
1:B:137:PHE:CD2	1:B:137:PHE:C	2.79	0.56
1:B:508:ILE:HG23	1:B:536:TYR:CD2	2.41	0.56
1:D:176:GLY:C	1:D:178:SER:N	2.57	0.56
1:D:279:ILE:N	1:D:279:ILE:HD13	2.21	0.56
1:D:450:ASN:ND2	1:D:452:GLU:CG	2.69	0.56
1:D:464:VAL:HG23	1:D:465:LEU:HD12	1.87	0.56
1:D:480:ASN:ND2	1:D:481:VAL:N	2.53	0.56
1:E:501:LEU:HD22	2:S:112:LEU:CD2	2.28	0.56
1:F:324:THR:CB	1:F:499:PRO:HA	2.35	0.56
2:Q:13:LYS:HZ3	2:Q:65:PHE:HB3	1.69	0.56
2:S:49:GLN:H	2:S:49:GLN:HE21	1.51	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:LEU:N	1:D:188:LEU:CD2	2.63	0.56
1:D:354:SER:O	1:D:371:SER:HB2	2.04	0.56
1:E:137:PHE:CD2	1:E:137:PHE:C	2.79	0.56
1:F:184:LYS:HE3	1:F:191:GLU:HB2	1.88	0.56
1:F:301:ALA:O	1:F:303:LYS:N	2.39	0.56
1:F:354:SER:O	1:F:371:SER:HB2	2.06	0.56
2:O:97:ASN:ND2	2:O:97:ASN:H	2.02	0.56
2:R:28:THR:HG21	2:R:30:LYS:HZ1	1.69	0.56
2:R:97:ASN:ND2	2:R:97:ASN:H	2.03	0.56
2:T:102:ALA:CB	2:T:125:ILE:HG13	2.35	0.56
1:A:480:ASN:HD22	1:A:481:VAL:H	1.52	0.56
1:A:480:ASN:HD22	1:A:481:VAL:N	2.03	0.56
1:C:252:ASP:CG	1:C:253:HIS:H	2.09	0.56
1:D:282:SER:HA	1:D:285:LYS:HD3	1.88	0.56
1:D:296:LEU:CD2	1:D:296:LEU:H	1.91	0.56
1:D:480:ASN:HD22	1:D:481:VAL:N	2.04	0.56
1:E:184:LYS:HE3	1:E:191:GLU:HB2	1.87	0.56
1:F:234:LEU:HD23	1:F:235:THR:H	1.71	0.56
2:O:102:ALA:CB	2:O:125:ILE:HG13	2.36	0.56
2:P:41:GLN:O	2:P:42:ASN:HB3	2.04	0.56
1:B:360:VAL:HG11	1:B:370:LEU:HD22	1.87	0.56
1:C:97:TYR:HE1	1:C:178:SER:HB2	1.70	0.56
1:C:413:LEU:HB2	1:C:419:ILE:HG12	1.87	0.56
1:C:630:ARG:HG3	1:C:630:ARG:HH11	1.71	0.56
1:C:697:ILE:CG2	1:C:732:ILE:HD11	2.36	0.56
1:D:252:ASP:CG	1:D:253:HIS:H	2.09	0.56
1:D:470:ASN:O	1:D:472:ARG:HG3	2.06	0.56
1:D:688:PHE:HD2	1:D:688:PHE:C	2.09	0.56
1:F:214:PHE:HB3	1:F:218:LEU:HB3	1.87	0.56
2:P:52:ILE:HG23	2:P:53:ASN:N	2.20	0.56
2:Q:100:ILE:HB	2:Q:136:VAL:HG22	1.87	0.56
2:R:13:LYS:HZ2	2:R:65:PHE:HB3	1.68	0.56
1:A:667:LEU:HB3	2:O:14:GLU:OE2	2.06	0.56
1:A:80:GLN:HG3	1:A:80:GLN:O	2.06	0.56
1:B:697:ILE:CG2	1:B:732:ILE:HD11	2.35	0.56
1:C:80:GLN:HG3	1:C:80:GLN:O	2.06	0.56
1:D:501:LEU:HD22	2:R:112:LEU:CD2	2.27	0.56
1:D:678:VAL:HG22	1:D:745:TYR:CE2	2.41	0.56
1:E:252:ASP:CG	1:E:253:HIS:H	2.09	0.56
1:E:446:ILE:HG13	1:E:452:GLU:O	2.06	0.56
1:E:666:ASN:O	1:E:670:ILE:HG13	2.06	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:684:ASP:C	1:E:686:ASP:H	2.09	0.56
1:F:450:ASN:ND2	1:F:452:GLU:CG	2.69	0.56
1:F:684:ASP:C	1:F:686:ASP:H	2.10	0.56
2:S:13:LYS:HZ2	2:S:65:PHE:HB3	1.67	0.56
1:A:252:ASP:O	1:A:254:ARG:HD2	2.06	0.56
1:B:214:PHE:HB3	1:B:218:LEU:HB3	1.86	0.56
1:C:470:ASN:O	1:C:472:ARG:HG3	2.06	0.56
1:D:508:ILE:HG23	1:D:536:TYR:CD2	2.41	0.56
1:E:464:VAL:HG23	1:E:465:LEU:HD12	1.87	0.56
1:E:470:ASN:O	1:E:472:ARG:HG3	2.06	0.56
1:F:252:ASP:O	1:F:254:ARG:HD2	2.06	0.56
2:O:121:VAL:C	2:O:123:GLN:N	2.58	0.56
1:B:252:ASP:CG	1:B:253:HIS:H	2.10	0.56
1:C:184:LYS:HE3	1:C:191:GLU:HB2	1.88	0.56
1:C:324:THR:CB	1:C:499:PRO:HA	2.34	0.56
1:C:464:VAL:HG23	1:C:465:LEU:HD12	1.88	0.56
1:C:515:LYS:NZ	1:C:516:VAL:HG23	2.21	0.56
1:D:79:ILE:C	1:D:81:GLN:N	2.57	0.56
1:E:413:LEU:HB2	1:E:419:ILE:HG12	1.88	0.56
1:F:137:PHE:C	1:F:137:PHE:CD2	2.79	0.56
2:Q:121:VAL:C	2:Q:123:GLN:N	2.57	0.56
2:R:49:GLN:HE21	2:R:49:GLN:H	1.51	0.56
1:A:137:PHE:CD2	1:A:137:PHE:C	2.79	0.55
1:A:450:ASN:ND2	1:A:452:GLU:CG	2.70	0.55
1:A:629:ASN:HD22	1:A:630:ARG:N	2.02	0.55
1:C:122:GLU:CD	1:C:122:GLU:H	2.09	0.55
1:C:171:TYR:O	1:C:175:LYS:NZ	2.39	0.55
1:D:480:ASN:HD22	1:D:481:VAL:H	1.53	0.55
1:E:515:LYS:NZ	1:E:516:VAL:HG23	2.22	0.55
1:F:505:LYS:HD3	2:T:112:LEU:O	2.07	0.55
2:Q:55:VAL:CG2	2:Q:67:GLU:OE1	2.43	0.55
2:S:117:THR:HG23	2:S:120:GLU:CB	2.31	0.55
1:A:184:LYS:HE3	1:A:191:GLU:HB2	1.87	0.55
1:A:464:VAL:HG23	1:A:465:LEU:HD12	1.87	0.55
1:B:629:ASN:HD22	1:B:630:ARG:N	2.04	0.55
1:B:736:LEU:HD21	1:B:750:GLN:NE2	2.19	0.55
1:D:252:ASP:O	1:D:254:ARG:HD2	2.05	0.55
1:D:360:VAL:HG11	1:D:370:LEU:HD22	1.88	0.55
1:E:142:VAL:HG22	1:E:154:ILE:HD12	1.88	0.55
2:O:55:VAL:HG21	2:O:67:GLU:CD	2.27	0.55
2:O:51:MSE:HB3	2:O:71:MSE:HE2	1.86	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:13:LYS:HZ1	2:Q:65:PHE:HB3	1.69	0.55
2:R:100:ILE:HB	2:R:136:VAL:HG23	1.88	0.55
2:T:55:VAL:CG2	2:T:67:GLU:OE1	2.44	0.55
1:A:252:ASP:CG	1:A:253:HIS:H	2.09	0.55
1:C:234:LEU:HD23	1:C:235:THR:H	1.71	0.55
1:C:678:VAL:HG22	1:C:745:TYR:CE2	2.40	0.55
1:D:80:GLN:HG3	1:D:80:GLN:O	2.06	0.55
1:E:122:GLU:H	1:E:122:GLU:CD	2.09	0.55
1:E:688:PHE:HD2	1:E:688:PHE:C	2.08	0.55
1:F:517:VAL:HB	1:F:525:LYS:HZ1	1.70	0.55
1:F:602:PHE:C	1:F:603:ILE:HG13	2.27	0.55
1:F:80:GLN:HG3	1:F:80:GLN:O	2.06	0.55
2:P:102:ALA:CB	2:P:125:ILE:HG13	2.35	0.55
2:S:59:GLY:O	2:S:62:THR:CG2	2.55	0.55
2:T:97:ASN:ND2	2:T:97:ASN:H	2.04	0.55
1:A:171:TYR:O	1:A:175:LYS:NZ	2.39	0.55
1:A:301:ALA:O	1:A:303:LYS:N	2.39	0.55
1:D:326:ILE:HG22	1:D:328:PHE:CE1	2.41	0.55
1:E:188:LEU:N	1:E:188:LEU:CD2	2.62	0.55
1:E:279:ILE:HD13	1:E:279:ILE:N	2.21	0.55
1:E:462:ILE:HG12	1:E:463:THR:H	1.72	0.55
1:F:122:GLU:CD	1:F:122:GLU:H	2.09	0.55
1:F:123:GLU:HG2	1:F:124:GLU:N	2.22	0.55
1:D:668:SER:CA	2:R:14:GLU:HG3	2.36	0.55
2:S:55:VAL:HG21	2:S:67:GLU:CD	2.26	0.55
1:D:112:VAL:O	1:D:114:HIS:N	2.38	0.55
1:D:123:GLU:HG2	1:D:124:GLU:N	2.21	0.55
1:D:413:LEU:HB2	1:D:419:ILE:HG12	1.88	0.55
1:E:214:PHE:HB3	1:E:218:LEU:HB3	1.88	0.55
1:E:234:LEU:HD23	1:E:235:THR:H	1.72	0.55
1:F:131:ARG:HG3	1:F:243:LEU:CD2	2.35	0.55
1:F:252:ASP:CG	1:F:253:HIS:H	2.10	0.55
1:F:360:VAL:HG11	1:F:370:LEU:HD22	1.88	0.55
1:F:443:GLU:HG3	1:F:458:LYS:HG2	1.89	0.55
1:F:77:ASP:O	1:F:81:GLN:HB2	2.07	0.55
2:O:13:LYS:HZ2	2:O:65:PHE:HB3	1.67	0.55
2:Q:59:GLY:O	2:Q:62:THR:HG22	2.05	0.55
2:T:32:LEU:HG	2:T:36:MSE:HE2	1.89	0.55
1:A:234:LEU:HD23	1:A:235:THR:H	1.72	0.55
1:A:360:VAL:HG11	1:A:370:LEU:HD22	1.89	0.55
1:A:413:LEU:HB2	1:A:419:ILE:HG12	1.88	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:GLU:HG2	1:B:124:GLU:N	2.21	0.55
1:B:443:GLU:HG3	1:B:458:LYS:HG2	1.88	0.55
1:C:112:VAL:O	1:C:114:HIS:N	2.39	0.55
1:D:137:PHE:CD2	1:D:137:PHE:C	2.80	0.55
1:E:629:ASN:HD22	1:E:630:ARG:N	2.04	0.55
1:E:697:ILE:HG21	1:E:732:ILE:HD11	1.88	0.55
1:E:80:GLN:O	1:E:80:GLN:HG3	2.06	0.55
1:F:639:ASN:ND2	1:F:639:ASN:N	2.52	0.55
2:O:28:THR:CB	2:O:30:LYS:NZ	2.68	0.55
2:S:32:LEU:HG	2:S:36:MSE:HE2	1.89	0.55
2:S:41:GLN:O	2:S:42:ASN:HB3	2.05	0.55
1:A:123:GLU:HG2	1:A:124:GLU:N	2.22	0.55
1:A:443:GLU:HG3	1:A:458:LYS:HG2	1.89	0.55
1:A:515:LYS:NZ	1:A:516:VAL:HG23	2.21	0.55
1:A:666:ASN:O	1:A:670:ILE:HG13	2.05	0.55
1:B:184:LYS:HE3	1:B:191:GLU:HB2	1.88	0.55
1:C:405:LEU:HD13	1:C:453:VAL:CG2	2.33	0.55
1:D:109:ILE:HD11	1:D:157:LYS:HZ2	1.72	0.55
1:E:443:GLU:HG3	1:E:458:LYS:HG2	1.88	0.55
1:F:407:HIS:HB2	1:F:408:LEU:HD12	1.88	0.55
1:F:508:ILE:HG23	1:F:536:TYR:CD2	2.40	0.55
2:O:28:THR:CG2	2:O:30:LYS:HZ1	2.19	0.55
2:R:55:VAL:CG2	2:R:67:GLU:OE1	2.44	0.55
1:A:470:ASN:O	1:A:472:ARG:HG3	2.06	0.55
1:A:602:PHE:C	1:A:603:ILE:HG13	2.28	0.55
1:B:171:TYR:O	1:B:175:LYS:NZ	2.39	0.55
1:B:252:ASP:O	1:B:254:ARG:HD2	2.06	0.55
1:B:462:ILE:HG12	1:B:463:THR:H	1.72	0.55
1:B:666:ASN:O	1:B:670:ILE:HG13	2.06	0.55
1:D:74:GLU:HB2	1:D:78:LYS:CB	2.37	0.55
1:E:173:ILE:HG13	1:E:242:SER:CB	2.37	0.55
1:F:296:LEU:H	1:F:296:LEU:CD2	1.91	0.55
2:S:94:LYS:HB3	2:S:94:LYS:HZ2	1.71	0.55
1:A:175:LYS:HZ2	1:A:175:LYS:HB2	1.72	0.55
1:A:505:LYS:HD3	2:O:112:LEU:O	2.07	0.55
1:A:697:ILE:HG21	1:A:732:ILE:HD11	1.89	0.55
1:B:326:ILE:HG22	1:B:328:PHE:CE1	2.42	0.55
1:B:470:ASN:O	1:B:472:ARG:HG3	2.06	0.55
1:B:77:ASP:O	1:B:81:GLN:HB2	2.07	0.55
1:C:443:GLU:HG3	1:C:458:LYS:HG2	1.88	0.55
1:C:446:ILE:HG13	1:C:451:ASN:O	2.07	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:LYS:HE3	1:D:191:GLU:HB2	1.89	0.55
1:D:443:GLU:HG3	1:D:458:LYS:HG2	1.88	0.55
1:D:77:ASP:O	1:D:81:GLN:HB2	2.07	0.55
1:E:668:SER:CA	2:S:14:GLU:HG3	2.36	0.55
1:F:154:ILE:HG13	1:F:171:TYR:HE1	1.62	0.55
1:F:462:ILE:HG12	1:F:463:THR:H	1.72	0.55
1:A:668:SER:CA	2:O:14:GLU:HG3	2.36	0.55
2:P:12:PHE:CE1	2:P:72:MSE:SE	3.10	0.55
2:Q:28:THR:CB	2:Q:30:LYS:NZ	2.70	0.55
1:A:122:GLU:CD	1:A:122:GLU:H	2.09	0.55
1:C:131:ARG:HB3	1:C:170:TYR:OH	2.06	0.55
1:D:515:LYS:NZ	1:D:516:VAL:HG23	2.22	0.55
1:D:658:PRO:HD3	1:D:755:ARG:NH1	2.21	0.55
1:D:93:VAL:CG2	1:D:179:LEU:HD11	2.35	0.55
1:E:123:GLU:HG2	1:E:124:GLU:N	2.22	0.55
1:E:602:PHE:C	1:E:603:ILE:HG13	2.27	0.55
1:E:77:ASP:O	1:E:81:GLN:HB2	2.07	0.55
1:F:278:LYS:HB2	1:F:279:ILE:HD13	1.89	0.55
1:F:326:ILE:HG22	1:F:328:PHE:CE1	2.42	0.55
1:F:470:ASN:O	1:F:472:ARG:HG3	2.07	0.55
1:F:597:ASN:HD21	1:F:601:GLU:CB	2.08	0.55
1:F:678:VAL:HG22	1:F:745:TYR:CE2	2.42	0.55
1:F:697:ILE:CG2	1:F:732:ILE:HD11	2.36	0.55
2:T:117:THR:OG1	2:T:119:GLU:HG2	2.07	0.55
1:A:254:ARG:HD2	1:A:254:ARG:H	1.72	0.54
1:B:450:ASN:ND2	1:B:452:GLU:CG	2.71	0.54
1:B:464:VAL:HG23	1:B:465:LEU:HD12	1.88	0.54
1:B:697:ILE:HG21	1:B:732:ILE:HD11	1.89	0.54
1:C:329:ARG:HD2	1:C:590:ASP:OD2	2.07	0.54
1:C:77:ASP:O	1:C:81:GLN:HB2	2.07	0.54
1:D:122:GLU:CD	1:D:122:GLU:H	2.09	0.54
1:D:324:THR:CB	1:D:499:PRO:HA	2.36	0.54
1:E:786:GLU:O	1:E:789:ASN:HB3	2.07	0.54
2:P:49:GLN:H	2:P:49:GLN:HE21	1.52	0.54
2:T:28:THR:CB	2:T:30:LYS:NZ	2.70	0.54
1:A:462:ILE:HG12	1:A:463:THR:H	1.72	0.54
1:C:137:PHE:CD2	1:C:137:PHE:C	2.79	0.54
1:C:450:ASN:ND2	1:C:452:GLU:CG	2.71	0.54
1:C:684:ASP:C	1:C:686:ASP:H	2.10	0.54
1:D:234:LEU:HD23	1:D:235:THR:H	1.72	0.54
1:D:446:ILE:HG13	1:D:451:ASN:O	2.07	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:697:ILE:HG21	1:D:732:ILE:HD11	1.90	0.54
1:D:786:GLU:O	1:D:789:ASN:HB3	2.08	0.54
1:E:505:LYS:HD3	2:S:112:LEU:O	2.07	0.54
1:F:413:LEU:HB2	1:F:419:ILE:HG12	1.88	0.54
1:A:446:ILE:HG13	1:A:451:ASN:O	2.07	0.54
1:B:123:GLU:O	1:B:146:LYS:NZ	2.40	0.54
1:B:188:LEU:CD2	1:B:188:LEU:N	2.62	0.54
1:E:407:HIS:HB2	1:E:408:LEU:HD12	1.88	0.54
1:F:515:LYS:NZ	1:F:516:VAL:HG23	2.23	0.54
1:F:629:ASN:HD22	1:F:630:ARG:N	2.04	0.54
1:A:678:VAL:HG22	1:A:745:TYR:CE2	2.42	0.54
1:B:80:GLN:O	1:B:80:GLN:HG3	2.07	0.54
1:C:407:HIS:HB2	1:C:408:LEU:HD12	1.89	0.54
1:C:424:LYS:HB3	1:C:424:LYS:HZ2	1.72	0.54
1:C:666:ASN:O	1:C:670:ILE:HG13	2.07	0.54
1:C:76:LEU:HD22	1:C:76:LEU:N	2.22	0.54
1:D:112:VAL:HG12	1:D:113:GLU:N	2.09	0.54
1:D:666:ASN:O	1:D:670:ILE:HG13	2.06	0.54
1:E:217:LYS:HB3	1:E:217:LYS:NZ	2.23	0.54
1:E:678:VAL:HG22	1:E:745:TYR:CE2	2.42	0.54
1:F:131:ARG:HB3	1:F:170:TYR:OH	2.07	0.54
1:F:230:ILE:HG13	1:F:237:PHE:CE2	2.43	0.54
1:F:464:VAL:HG23	1:F:465:LEU:HD12	1.88	0.54
2:O:32:LEU:HG	2:O:36:MSE:HE2	1.89	0.54
2:P:13:LYS:HZ1	2:P:65:PHE:HB3	1.69	0.54
2:S:97:ASN:HD22	2:S:97:ASN:H	1.56	0.54
2:T:55:VAL:HG21	2:T:67:GLU:CD	2.27	0.54
1:A:142:VAL:HG22	1:A:154:ILE:HD12	1.88	0.54
1:A:335:ALA:O	1:A:339:ILE:HG13	2.07	0.54
1:A:794:GLN:NE2	1:A:795:LYS:N	2.56	0.54
1:C:123:GLU:HG2	1:C:124:GLU:N	2.21	0.54
1:F:350:VAL:HG12	1:F:352:GLY:H	1.73	0.54
1:F:666:ASN:O	1:F:670:ILE:HG13	2.08	0.54
1:F:786:GLU:O	1:F:789:ASN:HB3	2.08	0.54
2:O:129:ASP:OD2	2:O:140:GLU:OE2	2.26	0.54
2:P:32:LEU:HG	2:P:36:MSE:HE2	1.90	0.54
1:A:279:ILE:HD13	1:A:279:ILE:N	2.20	0.54
1:A:786:GLU:O	1:A:789:ASN:HB3	2.08	0.54
1:B:446:ILE:HG13	1:B:451:ASN:O	2.08	0.54
1:B:678:VAL:HG22	1:B:745:TYR:CE2	2.42	0.54
1:B:786:GLU:O	1:B:789:ASN:HB3	2.08	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:602:PHE:C	1:C:603:ILE:HG13	2.28	0.54
2:O:49:GLN:HE21	2:O:49:GLN:H	1.52	0.54
2:R:110:THR:O	2:R:113:GLY:N	2.39	0.54
1:A:165:GLN:HE21	1:A:251:PRO:CG	2.20	0.54
1:A:407:HIS:HB2	1:A:408:LEU:HD12	1.89	0.54
1:B:658:PRO:HD3	1:B:755:ARG:NH1	2.23	0.54
1:C:217:LYS:HB3	1:C:217:LYS:NZ	2.22	0.54
1:C:165:GLN:HE21	1:C:251:PRO:CG	2.20	0.54
1:C:515:LYS:HZ3	1:C:516:VAL:HG23	1.72	0.54
1:C:794:GLN:NE2	1:C:795:LYS:N	2.56	0.54
1:D:602:PHE:C	1:D:603:ILE:HG13	2.28	0.54
1:E:306:GLY:O	1:E:336:THR:HG23	2.07	0.54
1:F:74:GLU:HB2	1:F:78:LYS:CB	2.37	0.54
2:O:136:VAL:HG23	2:O:136:VAL:O	2.08	0.54
2:O:65:PHE:HB2	2:O:66:PRO:CD	2.35	0.54
2:Q:136:VAL:HG23	2:Q:136:VAL:O	2.08	0.54
2:R:100:ILE:HB	2:R:136:VAL:HG22	1.87	0.54
2:R:65:PHE:HB2	2:R:66:PRO:CD	2.36	0.54
1:A:131:ARG:HB3	1:A:170:TYR:OH	2.08	0.54
1:A:413:LEU:N	1:A:413:LEU:HD23	2.23	0.54
1:B:407:HIS:HB2	1:B:408:LEU:HD12	1.89	0.54
1:C:142:VAL:HG22	1:C:154:ILE:HD12	1.89	0.54
1:C:275:GLY:HA2	1:C:278:LYS:CD	2.38	0.54
1:C:697:ILE:HG21	1:C:732:ILE:HD11	1.90	0.54
1:F:196:ILE:HG23	1:F:199:LEU:HD12	1.90	0.54
2:P:110:THR:O	2:P:113:GLY:N	2.37	0.54
1:A:350:VAL:HG12	1:A:352:GLY:H	1.73	0.54
1:A:713:SER:O	1:A:717:LYS:HG3	2.08	0.54
1:B:134:LYS:HG2	1:B:136:PRO:HD3	1.90	0.54
1:C:709:ASN:HB2	2:Q:130:ILE:HG23	1.90	0.54
1:D:217:LYS:HB3	1:D:217:LYS:NZ	2.23	0.54
1:D:515:LYS:HB3	1:D:515:LYS:HZ2	1.71	0.54
1:F:254:ARG:HD2	1:F:254:ARG:H	1.73	0.54
2:O:12:PHE:CE1	2:O:72:MSE:SE	3.11	0.54
2:O:97:ASN:H	2:O:97:ASN:HD22	1.56	0.54
2:Q:24:ASP:OD1	2:Q:25:GLY:N	2.40	0.54
2:T:110:THR:O	2:T:113:GLY:N	2.39	0.54
1:B:165:GLN:HE21	1:B:251:PRO:CG	2.20	0.54
1:B:794:GLN:NE2	1:B:795:LYS:N	2.56	0.54
1:C:74:GLU:HB2	1:C:78:LYS:CB	2.37	0.54
1:D:403:LEU:HG	1:D:405:LEU:HD12	1.90	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:HIS:HB2	1:D:408:LEU:HD12	1.89	0.54
1:D:709:ASN:HB2	2:R:130:ILE:HG23	1.90	0.54
1:F:165:GLN:HE21	1:F:251:PRO:CG	2.20	0.54
1:F:329:ARG:HD2	1:F:590:ASP:OD2	2.08	0.54
1:F:615:ILE:CD1	1:F:645:TRP:HH2	2.16	0.54
2:O:58:ASP:OD2	2:O:58:ASP:N	2.41	0.54
2:P:58:ASP:N	2:P:58:ASP:OD2	2.41	0.54
2:Q:55:VAL:HG21	2:Q:67:GLU:CD	2.26	0.54
2:T:100:ILE:HB	2:T:136:VAL:HG23	1.89	0.54
1:A:123:GLU:O	1:A:146:LYS:NZ	2.40	0.53
1:A:145:LYS:HB3	1:A:151:LYS:HB2	1.90	0.53
1:A:329:ARG:HD2	1:A:590:ASP:OD2	2.09	0.53
1:A:74:GLU:HB2	1:A:78:LYS:CB	2.38	0.53
1:A:77:ASP:O	1:A:81:GLN:HB2	2.07	0.53
1:B:109:ILE:HD11	1:B:157:LYS:HZ2	1.72	0.53
1:B:684:ASP:C	1:B:686:ASP:H	2.10	0.53
1:C:254:ARG:H	1:C:254:ARG:HD2	1.73	0.53
1:C:301:ALA:C	1:C:303:LYS:N	2.62	0.53
1:C:629:ASN:HD22	1:C:630:ARG:N	2.05	0.53
1:D:165:GLN:HE21	1:D:251:PRO:CG	2.20	0.53
1:E:74:GLU:HB2	1:E:78:LYS:CB	2.37	0.53
1:F:180:ASP:O	1:F:183:SER:N	2.33	0.53
2:O:117:THR:OG1	2:O:119:GLU:HG2	2.08	0.53
1:A:173:ILE:HD12	1:A:243:LEU:CD2	2.38	0.53
1:A:515:LYS:HZ3	1:A:516:VAL:N	2.06	0.53
1:B:112:VAL:HG12	1:B:113:GLU:N	2.10	0.53
1:B:234:LEU:HD23	1:B:235:THR:H	1.71	0.53
1:C:137:PHE:O	1:C:139:SER:N	2.42	0.53
1:C:176:GLY:O	1:C:180:ASP:OD1	2.27	0.53
1:C:230:ILE:HG13	1:C:237:PHE:CE2	2.43	0.53
1:D:196:ILE:HG23	1:D:199:LEU:HD12	1.90	0.53
1:D:350:VAL:HG12	1:D:352:GLY:H	1.73	0.53
1:E:123:GLU:O	1:E:146:LYS:NZ	2.41	0.53
1:E:794:GLN:NE2	1:E:795:LYS:N	2.56	0.53
1:F:135:VAL:O	1:F:135:VAL:HG22	2.08	0.53
1:F:109:ILE:HD11	1:F:157:LYS:HZ2	1.72	0.53
1:F:176:GLY:O	1:F:180:ASP:OD1	2.26	0.53
2:P:28:THR:CB	2:P:30:LYS:NZ	2.70	0.53
2:P:65:PHE:HB2	2:P:66:PRO:CD	2.35	0.53
2:Q:43:PRO:HG3	2:Q:48:LEU:HD13	1.91	0.53
2:S:117:THR:OG1	2:S:119:GLU:HG2	2.08	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:VAL:HG12	1:C:352:GLY:H	1.74	0.53
1:D:142:VAL:HG22	1:D:154:ILE:HD12	1.89	0.53
1:D:275:GLY:HA2	1:D:278:LYS:CG	2.38	0.53
1:E:196:ILE:HG23	1:E:199:LEU:HD12	1.90	0.53
1:E:275:GLY:HA2	1:E:278:LYS:CD	2.39	0.53
1:F:123:GLU:O	1:F:146:LYS:NZ	2.41	0.53
2:O:110:THR:O	2:O:113:GLY:N	2.38	0.53
2:R:28:THR:CB	2:R:30:LYS:NZ	2.71	0.53
2:R:58:ASP:OD2	2:R:58:ASP:N	2.41	0.53
2:S:12:PHE:CE1	2:S:72:MSE:SE	3.11	0.53
2:S:58:ASP:OD2	2:S:58:ASP:N	2.41	0.53
2:T:43:PRO:HG3	2:T:48:LEU:HD13	1.91	0.53
1:A:217:LYS:HB3	1:A:217:LYS:NZ	2.23	0.53
1:A:684:ASP:C	1:A:686:ASP:H	2.10	0.53
1:A:747:ASN:O	1:A:750:GLN:HB2	2.08	0.53
1:B:275:GLY:HA2	1:B:278:LYS:CG	2.39	0.53
1:B:275:GLY:HA2	1:B:278:LYS:CD	2.39	0.53
1:C:196:ILE:HG23	1:C:199:LEU:HD12	1.89	0.53
1:C:405:LEU:HD12	1:C:405:LEU:N	2.24	0.53
1:D:279:ILE:H	1:D:279:ILE:CD1	2.06	0.53
1:E:326:ILE:HG22	1:E:328:PHE:CE1	2.43	0.53
1:F:674:SER:OG	1:F:674:SER:O	2.16	0.53
2:P:129:ASP:OD2	2:P:140:GLU:OE2	2.27	0.53
1:B:668:SER:CA	2:P:14:GLU:HG3	2.37	0.53
2:P:28:THR:OG1	2:P:31:GLU:HB2	2.09	0.53
1:C:667:LEU:HB3	2:Q:14:GLU:OE2	2.08	0.53
1:A:275:GLY:HA2	1:A:278:LYS:CD	2.38	0.53
1:A:561:ASN:HA	1:A:564:VAL:HG22	1.91	0.53
1:A:794:GLN:HE22	1:A:795:LYS:HG3	1.74	0.53
1:B:230:ILE:HG13	1:B:237:PHE:CE2	2.43	0.53
1:B:271:LEU:HA	1:B:275:GLY:HA3	1.90	0.53
1:B:279:ILE:N	1:B:279:ILE:HD13	2.21	0.53
1:B:413:LEU:HD23	1:B:413:LEU:N	2.24	0.53
1:B:561:ASN:HA	1:B:564:VAL:HG22	1.91	0.53
1:B:602:PHE:C	1:B:603:ILE:HG13	2.28	0.53
1:C:123:GLU:O	1:C:146:LYS:NZ	2.42	0.53
1:D:123:GLU:O	1:D:146:LYS:NZ	2.41	0.53
1:D:176:GLY:O	1:D:180:ASP:OD1	2.25	0.53
1:D:636:ALA:O	1:D:640:LYS:HA	2.08	0.53
1:E:137:PHE:O	1:E:139:SER:N	2.42	0.53
1:E:109:ILE:HD13	1:E:157:LYS:HZ3	1.71	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:450:ASN:ND2	1:E:452:GLU:CG	2.71	0.53
1:F:142:VAL:HG22	1:F:154:ILE:HD12	1.91	0.53
1:F:93:VAL:CG2	1:F:179:LEU:HD11	2.35	0.53
2:P:9:ILE:CD1	2:P:69:LEU:HD11	2.37	0.53
2:Q:100:ILE:HB	2:Q:136:VAL:HG23	1.90	0.53
2:R:28:THR:OG1	2:R:31:GLU:HB2	2.08	0.53
1:A:137:PHE:O	1:A:139:SER:N	2.42	0.53
1:A:196:ILE:HG23	1:A:199:LEU:HD12	1.91	0.53
1:A:482:GLU:O	1:A:484:VAL:HG23	2.09	0.53
1:B:254:ARG:HD2	1:B:254:ARG:H	1.73	0.53
1:B:306:GLY:O	1:B:336:THR:HG23	2.09	0.53
1:C:324:THR:HB	1:C:499:PRO:CA	2.37	0.53
1:C:636:ALA:O	1:C:640:LYS:HA	2.08	0.53
1:D:684:ASP:C	1:D:686:ASP:H	2.11	0.53
1:E:747:ASN:O	1:E:750:GLN:HB2	2.09	0.53
1:F:629:ASN:HD22	1:F:631:SER:N	1.98	0.53
1:F:794:GLN:NE2	1:F:795:LYS:N	2.57	0.53
2:P:136:VAL:HG23	2:P:136:VAL:O	2.08	0.53
2:P:65:PHE:H	2:P:65:PHE:HD1	1.54	0.53
2:Q:117:THR:OG1	2:Q:119:GLU:HG2	2.08	0.53
2:R:65:PHE:H	2:R:65:PHE:HD1	1.55	0.53
2:R:97:ASN:HD22	2:R:97:ASN:H	1.57	0.53
2:S:28:THR:HG21	2:S:30:LYS:HZ1	1.73	0.53
2:S:28:THR:CB	2:S:30:LYS:NZ	2.70	0.53
2:S:43:PRO:HG3	2:S:48:LEU:HD13	1.90	0.53
1:A:636:ALA:O	1:A:640:LYS:HA	2.09	0.53
1:B:335:ALA:O	1:B:339:ILE:HG13	2.09	0.53
1:C:403:LEU:HG	1:C:405:LEU:HD12	1.90	0.53
1:D:301:ALA:C	1:D:303:LYS:N	2.62	0.53
1:D:515:LYS:HZ3	1:D:516:VAL:N	2.07	0.53
1:D:76:LEU:HD22	1:D:76:LEU:N	2.22	0.53
1:F:636:ALA:O	1:F:640:LYS:HA	2.08	0.53
1:F:713:SER:O	1:F:717:LYS:HG3	2.08	0.53
1:F:697:ILE:HG21	1:F:732:ILE:HD11	1.90	0.53
1:F:747:ASN:O	1:F:750:GLN:HB2	2.09	0.53
1:F:76:LEU:HD22	1:F:76:LEU:N	2.22	0.53
2:Q:32:LEU:HG	2:Q:36:MSE:HE2	1.91	0.53
2:Q:58:ASP:N	2:Q:58:ASP:OD2	2.41	0.53
2:Q:65:PHE:HB2	2:Q:66:PRO:CD	2.35	0.53
2:Q:65:PHE:HD1	2:Q:65:PHE:H	1.55	0.53
2:Q:97:ASN:HD22	2:Q:97:ASN:H	1.57	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:136:VAL:O	2:R:136:VAL:HG23	2.08	0.53
2:R:43:PRO:HG3	2:R:48:LEU:HD13	1.90	0.53
2:S:110:THR:O	2:S:113:GLY:N	2.39	0.53
2:T:58:ASP:OD2	2:T:58:ASP:N	2.41	0.53
1:A:109:ILE:HD11	1:A:157:LYS:HZ2	1.73	0.53
1:A:275:GLY:HA2	1:A:278:LYS:CG	2.38	0.53
1:A:403:LEU:HG	1:A:405:LEU:HD12	1.91	0.53
1:A:405:LEU:N	1:A:405:LEU:HD12	2.24	0.53
1:A:671:ARG:HH12	1:A:677:GLY:HA3	1.72	0.53
1:B:176:GLY:O	1:B:180:ASP:OD1	2.26	0.53
1:B:405:LEU:HD12	1:B:405:LEU:N	2.24	0.53
1:C:326:ILE:HG22	1:C:328:PHE:CE1	2.44	0.53
1:C:327:LEU:HD12	1:C:327:LEU:N	2.24	0.53
1:C:462:ILE:HG12	1:C:463:THR:H	1.72	0.53
1:D:306:GLY:O	1:D:336:THR:HG23	2.09	0.53
1:E:230:ILE:HG13	1:E:237:PHE:CE2	2.44	0.53
1:E:658:PRO:HD3	1:E:755:ARG:NH1	2.24	0.53
1:E:794:GLN:HE22	1:E:795:LYS:HG3	1.73	0.53
1:F:499:PRO:HD3	1:F:552:TRP:CH2	2.44	0.53
2:Q:9:ILE:HG23	2:Q:69:LEU:HD21	1.91	0.53
1:A:197:LYS:HZ3	1:A:197:LYS:C	2.12	0.53
1:B:403:LEU:HG	1:B:405:LEU:HD12	1.90	0.53
1:B:636:ALA:O	1:B:640:LYS:HA	2.08	0.53
1:C:131:ARG:HG3	1:C:243:LEU:HD22	1.91	0.53
1:C:360:VAL:HG11	1:C:370:LEU:HD22	1.89	0.53
1:C:671:ARG:HH12	1:C:677:GLY:HA3	1.73	0.53
1:D:335:ALA:O	1:D:339:ILE:HG13	2.08	0.53
1:A:709:ASN:HB2	2:O:130:ILE:HG23	1.90	0.53
2:O:56:ASP:OD2	2:O:60:ASN:C	2.46	0.53
1:D:667:LEU:HB3	2:R:14:GLU:OE2	2.09	0.53
2:R:32:LEU:HG	2:R:36:MSE:HE2	1.90	0.53
2:S:129:ASP:OD2	2:S:140:GLU:OE2	2.27	0.53
1:A:230:ILE:HG13	1:A:237:PHE:CE2	2.43	0.53
1:A:501:LEU:HD22	2:O:112:LEU:CD2	2.26	0.53
1:A:795:LYS:HA	1:A:798:ASP:OD2	2.09	0.53
1:B:794:GLN:HE22	1:B:795:LYS:HG3	1.74	0.53
1:C:413:LEU:HD23	1:C:413:LEU:N	2.24	0.53
1:C:505:LYS:HD3	2:Q:112:LEU:O	2.09	0.53
1:C:629:ASN:HD22	1:C:631:SER:N	1.98	0.53
1:C:79:ILE:C	1:C:81:GLN:N	2.57	0.53
1:D:218:LEU:HD21	1:D:225:ILE:CD1	2.39	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:ILE:HG13	1:D:237:PHE:CE2	2.43	0.53
1:E:134:LYS:HG2	1:E:136:PRO:HD3	1.91	0.53
1:E:76:LEU:HD22	1:E:76:LEU:N	2.21	0.53
1:F:173:ILE:HD12	1:F:243:LEU:CD2	2.39	0.53
1:F:275:GLY:HA2	1:F:278:LYS:CG	2.39	0.53
1:F:446:ILE:HG13	1:F:451:ASN:O	2.07	0.53
2:O:43:PRO:HG3	2:O:48:LEU:HD13	1.90	0.53
2:O:65:PHE:H	2:O:65:PHE:HD1	1.56	0.53
2:P:70:THR:O	2:P:70:THR:HG22	2.08	0.53
2:Q:12:PHE:CE1	2:Q:72:MSE:SE	3.12	0.53
2:T:12:PHE:CE1	2:T:72:MSE:SE	3.12	0.53
1:A:558:ASP:O	1:A:560:LEU:N	2.43	0.52
1:A:630:ARG:HG3	1:A:630:ARG:NH1	2.24	0.52
1:B:350:VAL:HG12	1:B:352:GLY:H	1.73	0.52
1:B:515:LYS:HZ3	1:B:516:VAL:N	2.07	0.52
1:B:558:ASP:O	1:B:560:LEU:N	2.42	0.52
1:C:173:ILE:HG23	1:C:174:GLY:H	1.74	0.52
1:D:279:ILE:C	1:D:281:GLU:H	2.12	0.52
1:D:561:ASN:HA	1:D:564:VAL:HG22	1.91	0.52
1:D:629:ASN:HD22	1:D:630:ARG:N	2.06	0.52
1:E:176:GLY:O	1:E:180:ASP:OD1	2.26	0.52
1:E:308:VAL:O	1:E:311:HIS:HB2	2.10	0.52
2:O:100:ILE:HB	2:O:136:VAL:HG23	1.91	0.52
2:O:28:THR:OG1	2:O:31:GLU:HB2	2.08	0.52
2:S:136:VAL:HG23	2:S:136:VAL:O	2.08	0.52
2:T:94:LYS:HB3	2:T:94:LYS:HZ2	1.74	0.52
1:A:306:GLY:O	1:A:336:THR:HG23	2.09	0.52
1:A:76:LEU:N	1:A:76:LEU:HD22	2.22	0.52
1:B:137:PHE:O	1:B:139:SER:N	2.42	0.52
1:B:279:ILE:C	1:B:281:GLU:H	2.12	0.52
1:B:499:PRO:HD3	1:B:552:TRP:CH2	2.44	0.52
1:B:329:ARG:HD2	1:B:590:ASP:OD2	2.09	0.52
1:C:275:GLY:HA2	1:C:278:LYS:CG	2.39	0.52
1:C:558:ASP:O	1:C:560:LEU:N	2.42	0.52
1:C:786:GLU:O	1:C:789:ASN:HB3	2.08	0.52
1:D:172:GLU:CB	1:D:246:SER:HA	2.39	0.52
1:D:629:ASN:HD22	1:D:631:SER:N	1.96	0.52
1:E:131:ARG:HG3	1:E:243:LEU:HD22	1.90	0.52
1:E:254:ARG:HD2	1:E:254:ARG:H	1.73	0.52
1:E:279:ILE:C	1:E:281:GLU:H	2.12	0.52
1:F:482:GLU:O	1:F:484:VAL:HG23	2.09	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:9:ILE:CD1	2:O:69:LEU:HD11	2.38	0.52
2:P:117:THR:OG1	2:P:119:GLU:HG2	2.08	0.52
2:P:56:ASP:OD2	2:P:60:ASN:C	2.48	0.52
2:S:28:THR:OG1	2:S:31:GLU:HB2	2.08	0.52
2:T:121:VAL:C	2:T:123:GLN:N	2.58	0.52
2:T:52:ILE:HG23	2:T:53:ASN:H	1.74	0.52
2:T:65:PHE:H	2:T:65:PHE:HD1	1.55	0.52
2:T:64:ASP:OD2	2:T:67:GLU:HG3	2.09	0.52
2:T:70:THR:O	2:T:70:THR:HG22	2.08	0.52
1:A:134:LYS:HG2	1:A:136:PRO:HD3	1.91	0.52
1:A:278:LYS:HB2	1:A:279:ILE:HD13	1.91	0.52
1:B:671:ARG:HH12	1:B:677:GLY:HA3	1.73	0.52
1:B:74:GLU:HB2	1:B:78:LYS:CB	2.38	0.52
1:D:254:ARG:HD2	1:D:254:ARG:H	1.74	0.52
1:D:278:LYS:HB2	1:D:279:ILE:HD13	1.92	0.52
1:D:329:ARG:HD2	1:D:590:ASP:OD2	2.10	0.52
1:D:597:ASN:HD21	1:D:601:GLU:CB	2.08	0.52
1:D:678:VAL:HG22	1:D:745:TYR:HE2	1.74	0.52
1:E:131:ARG:HB3	1:E:170:TYR:OH	2.09	0.52
1:E:271:LEU:HA	1:E:275:GLY:HA3	1.90	0.52
1:F:173:ILE:HG23	1:F:174:GLY:H	1.75	0.52
1:F:279:ILE:C	1:F:281:GLU:H	2.12	0.52
1:F:335:ALA:O	1:F:339:ILE:HG13	2.08	0.52
1:F:405:LEU:HD12	1:F:405:LEU:N	2.24	0.52
2:Q:94:LYS:HB3	2:Q:94:LYS:HZ2	1.74	0.52
2:R:129:ASP:OD2	2:R:140:GLU:OE2	2.28	0.52
2:T:28:THR:OG1	2:T:31:GLU:HB2	2.09	0.52
1:B:504:ILE:HD12	1:B:504:ILE:N	2.25	0.52
1:B:515:LYS:NZ	1:B:516:VAL:CG2	2.72	0.52
1:C:278:LYS:HB2	1:C:279:ILE:HD13	1.92	0.52
1:C:499:PRO:HD3	1:C:552:TRP:CH2	2.44	0.52
1:C:658:PRO:HD3	1:C:755:ARG:NH1	2.24	0.52
1:C:795:LYS:HA	1:C:798:ASP:OD2	2.09	0.52
1:D:137:PHE:O	1:D:139:SER:N	2.42	0.52
1:D:324:THR:HB	1:D:499:PRO:CA	2.39	0.52
1:D:482:GLU:O	1:D:484:VAL:HG23	2.10	0.52
1:D:747:ASN:O	1:D:750:GLN:HB2	2.09	0.52
1:D:794:GLN:NE2	1:D:795:LYS:N	2.57	0.52
1:E:165:GLN:HE21	1:E:251:PRO:CG	2.21	0.52
1:E:446:ILE:HG13	1:E:451:ASN:O	2.08	0.52
1:E:561:ASN:HA	1:E:564:VAL:HG22	1.91	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:403:LEU:HG	1:F:405:LEU:HD12	1.90	0.52
2:T:129:ASP:OD2	2:T:140:GLU:OE2	2.27	0.52
1:A:176:GLY:O	1:A:180:ASP:OD1	2.27	0.52
1:A:529:VAL:HG21	2:O:109:MSE:HE1	1.91	0.52
1:B:217:LYS:HB3	1:B:217:LYS:NZ	2.24	0.52
1:C:93:VAL:CG2	1:C:179:LEU:HD11	2.37	0.52
1:C:335:ALA:O	1:C:339:ILE:HG13	2.08	0.52
1:D:165:GLN:NE2	1:D:251:PRO:HG2	2.23	0.52
1:D:271:LEU:HA	1:D:275:GLY:HA3	1.91	0.52
1:D:275:GLY:HA2	1:D:278:LYS:CD	2.38	0.52
1:D:462:ILE:HG12	1:D:463:THR:H	1.72	0.52
1:D:505:LYS:HD3	2:R:112:LEU:O	2.08	0.52
1:D:794:GLN:HE22	1:D:795:LYS:HG3	1.75	0.52
1:E:121:SER:O	1:E:123:GLU:OE2	2.28	0.52
1:E:413:LEU:N	1:E:413:LEU:HD23	2.24	0.52
1:F:217:LYS:HB3	1:F:217:LYS:NZ	2.23	0.52
1:F:275:GLY:HA2	1:F:278:LYS:CD	2.39	0.52
1:F:515:LYS:HZ3	1:F:516:VAL:N	2.08	0.52
1:F:795:LYS:HA	1:F:798:ASP:OD2	2.10	0.52
2:P:31:GLU:O	2:P:35:VAL:HG23	2.10	0.52
2:Q:70:THR:HG22	2:Q:70:THR:O	2.09	0.52
2:R:70:THR:HG22	2:R:70:THR:O	2.08	0.52
2:R:9:ILE:HG23	2:R:69:LEU:HD21	1.91	0.52
2:S:100:ILE:HB	2:S:136:VAL:HG23	1.90	0.52
1:B:121:SER:O	1:B:123:GLU:OE2	2.28	0.52
1:C:747:ASN:O	1:C:750:GLN:HB2	2.09	0.52
1:D:145:LYS:HB3	1:D:151:LYS:HB2	1.91	0.52
1:D:499:PRO:HD3	1:D:552:TRP:CH2	2.44	0.52
1:E:112:VAL:O	1:E:114:HIS:N	2.37	0.52
1:E:180:ASP:O	1:E:183:SER:N	2.33	0.52
1:E:173:ILE:HD12	1:E:243:LEU:CD2	2.40	0.52
1:E:278:LYS:HB2	1:E:279:ILE:HD13	1.91	0.52
1:E:515:LYS:HZ3	1:E:516:VAL:N	2.08	0.52
1:E:713:SER:O	1:E:717:LYS:HG3	2.09	0.52
1:F:306:GLY:O	1:F:336:THR:HG23	2.09	0.52
2:O:70:THR:HG22	2:O:70:THR:O	2.08	0.52
1:B:709:ASN:HB2	2:P:130:ILE:HG23	1.90	0.52
2:R:31:GLU:O	2:R:35:VAL:HG23	2.10	0.52
2:S:24:ASP:OD1	2:S:25:GLY:N	2.41	0.52
1:F:709:ASN:HB2	2:T:130:ILE:HG23	1.91	0.52
1:A:499:PRO:HD3	1:A:552:TRP:CH2	2.44	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:VAL:HG22	1:B:154:ILE:HD12	1.90	0.52
1:B:517:VAL:O	1:B:525:LYS:NZ	2.43	0.52
1:B:747:ASN:O	1:B:750:GLN:HB2	2.09	0.52
1:B:795:LYS:HA	1:B:798:ASP:OD2	2.10	0.52
1:C:109:ILE:CD1	1:C:157:LYS:HZ2	2.23	0.52
1:C:218:LEU:HD21	1:C:225:ILE:CD1	2.40	0.52
1:D:173:ILE:HD12	1:D:243:LEU:CD2	2.39	0.52
1:D:558:ASP:O	1:D:560:LEU:N	2.42	0.52
1:D:615:ILE:CD1	1:D:645:TRP:HH2	2.16	0.52
1:E:558:ASP:O	1:E:560:LEU:N	2.43	0.52
1:E:597:ASN:OD1	1:E:599:GLU:HB2	2.10	0.52
1:E:671:ARG:HH12	1:E:677:GLY:HA3	1.72	0.52
1:F:301:ALA:C	1:F:303:LYS:N	2.62	0.52
1:F:531:ASN:HA	1:F:534:ILE:HD12	1.92	0.52
1:F:667:LEU:HB3	2:T:14:GLU:OE2	2.09	0.52
2:O:13:LYS:HZ1	2:O:65:PHE:HB3	1.68	0.52
2:O:9:ILE:HG23	2:O:69:LEU:HD21	1.92	0.52
2:R:12:PHE:CE1	2:R:72:MSE:SE	3.13	0.52
2:R:9:ILE:CD1	2:R:69:LEU:HD11	2.38	0.52
2:S:64:ASP:OD2	2:S:67:GLU:HG3	2.10	0.52
2:T:9:ILE:HG23	2:T:69:LEU:HD21	1.92	0.52
1:A:301:ALA:C	1:A:303:LYS:N	2.62	0.52
1:A:658:PRO:HD3	1:A:755:ARG:NH1	2.25	0.52
1:B:238:GLN:C	1:B:240:ALA:N	2.63	0.52
1:B:713:SER:O	1:B:717:LYS:HG3	2.09	0.52
1:C:197:LYS:HD3	1:C:263:ASP:OD1	2.10	0.52
1:C:306:GLY:O	1:C:336:THR:HG23	2.09	0.52
1:D:197:LYS:HD3	1:D:263:ASP:OD1	2.10	0.52
1:D:405:LEU:N	1:D:405:LEU:HD12	2.24	0.52
1:D:795:LYS:HA	1:D:798:ASP:OD2	2.09	0.52
1:E:175:LYS:HZ3	1:E:175:LYS:CB	2.22	0.52
1:E:218:LEU:HD21	1:E:225:ILE:CD1	2.40	0.52
1:E:172:GLU:CB	1:E:246:SER:HA	2.40	0.52
1:E:301:ALA:C	1:E:303:LYS:H	2.14	0.52
1:E:350:VAL:HG12	1:E:352:GLY:H	1.74	0.52
1:E:504:ILE:HD12	1:E:504:ILE:N	2.25	0.52
1:E:517:VAL:O	1:E:525:LYS:NZ	2.43	0.52
1:F:558:ASP:O	1:F:560:LEU:N	2.43	0.52
2:O:24:ASP:OD1	2:O:25:GLY:N	2.42	0.52
2:S:110:THR:HG22	2:S:114:GLU:O	2.10	0.52
2:S:65:PHE:HB2	2:S:66:PRO:CD	2.35	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ARG:HG3	1:A:243:LEU:HD22	1.92	0.52
1:A:169:VAL:CG2	1:A:246:SER:HB2	2.40	0.52
1:B:131:ARG:HB3	1:B:170:TYR:OH	2.09	0.52
1:B:180:ASP:C	1:B:182:ILE:H	2.13	0.52
1:B:405:LEU:HD13	1:B:453:VAL:CG2	2.34	0.52
1:B:424:LYS:HB3	1:B:424:LYS:HZ2	1.75	0.52
1:B:531:ASN:HA	1:B:534:ILE:HD12	1.92	0.52
1:C:678:VAL:HG22	1:C:745:TYR:HE2	1.74	0.52
1:D:131:ARG:HG3	1:D:243:LEU:HD22	1.92	0.52
1:E:109:ILE:HD11	1:E:157:LYS:HZ2	1.73	0.52
1:E:499:PRO:HD3	1:E:552:TRP:CH2	2.45	0.52
1:E:795:LYS:HA	1:E:798:ASP:OD2	2.09	0.52
1:F:197:LYS:NZ	1:F:197:LYS:HB3	2.25	0.52
1:F:197:LYS:HD3	1:F:263:ASP:OD1	2.09	0.52
1:F:165:GLN:NE2	1:F:251:PRO:HG2	2.23	0.52
2:O:64:ASP:OD2	2:O:67:GLU:HG3	2.09	0.52
2:Q:64:ASP:OD2	2:Q:67:GLU:HG3	2.09	0.52
1:E:709:ASN:HB2	2:S:130:ILE:HG23	1.91	0.52
1:A:135:VAL:O	1:A:135:VAL:HG22	2.10	0.52
1:A:173:ILE:HG23	1:A:174:GLY:H	1.74	0.52
1:A:218:LEU:HD21	1:A:225:ILE:CD1	2.40	0.52
1:A:271:LEU:HA	1:A:275:GLY:HA3	1.91	0.52
1:A:504:ILE:N	1:A:504:ILE:HD12	2.25	0.52
1:B:173:ILE:HG23	1:B:174:GLY:H	1.74	0.52
1:B:169:VAL:CG2	1:B:246:SER:HB2	2.40	0.52
1:B:76:LEU:HD22	1:B:76:LEU:N	2.21	0.52
1:C:217:LYS:HB2	1:C:236:GLU:HG3	1.92	0.52
1:C:165:GLN:NE2	1:C:251:PRO:HG2	2.24	0.52
1:D:301:ALA:C	1:D:303:LYS:H	2.14	0.52
1:E:288:VAL:CG2	1:E:289:GLU:H	2.20	0.52
1:E:629:ASN:HD22	1:E:631:SER:N	1.98	0.52
1:F:121:SER:O	1:F:123:GLU:OE2	2.28	0.52
1:F:288:VAL:CG2	1:F:289:GLU:H	2.20	0.52
2:Q:31:GLU:O	2:Q:35:VAL:HG23	2.09	0.52
2:R:117:THR:OG1	2:R:119:GLU:HG2	2.10	0.52
2:S:52:ILE:HG23	2:S:53:ASN:H	1.74	0.52
2:S:9:ILE:HG23	2:S:69:LEU:HD21	1.92	0.52
1:C:238:GLN:C	1:C:240:ALA:N	2.63	0.51
1:C:271:LEU:HA	1:C:275:GLY:HA3	1.91	0.51
1:C:561:ASN:HA	1:C:564:VAL:HG22	1.91	0.51
1:D:173:ILE:HG13	1:D:242:SER:CB	2.37	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:LEU:HD23	1:D:413:LEU:N	2.24	0.51
1:E:180:ASP:C	1:E:182:ILE:H	2.14	0.51
1:E:403:LEU:HG	1:E:405:LEU:HD12	1.91	0.51
1:F:137:PHE:O	1:F:139:SER:N	2.42	0.51
1:F:170:TYR:HA	1:F:173:ILE:HG22	1.92	0.51
1:F:405:LEU:HD13	1:F:453:VAL:CG2	2.34	0.51
1:F:658:PRO:HD3	1:F:755:ARG:NH1	2.24	0.51
2:O:31:GLU:O	2:O:35:VAL:HG23	2.10	0.51
2:O:52:ILE:HG23	2:O:53:ASN:H	1.74	0.51
2:Q:28:THR:OG1	2:Q:31:GLU:HB2	2.09	0.51
2:Q:66:PRO:C	2:Q:68:PHE:N	2.63	0.51
2:T:66:PRO:C	2:T:68:PHE:N	2.64	0.51
1:A:170:TYR:HA	1:A:173:ILE:HG22	1.92	0.51
1:A:173:ILE:HG13	1:A:242:SER:CB	2.37	0.51
1:A:279:ILE:C	1:A:281:GLU:H	2.12	0.51
1:A:597:ASN:OD1	1:A:599:GLU:HB2	2.10	0.51
1:B:667:LEU:HB3	2:P:14:GLU:OE2	2.10	0.51
1:C:172:GLU:CB	1:C:246:SER:HA	2.40	0.51
1:C:95:GLU:O	1:C:99:GLU:HB2	2.10	0.51
1:E:112:VAL:CG1	1:E:113:GLU:H	2.07	0.51
1:E:170:TYR:HA	1:E:173:ILE:HG22	1.93	0.51
1:E:187:SER:C	1:E:188:LEU:O	2.44	0.51
1:F:413:LEU:HD23	1:F:413:LEU:N	2.24	0.51
1:F:78:LYS:HG3	1:F:79:ILE:N	2.26	0.51
2:Q:129:ASP:OD2	2:Q:140:GLU:OE2	2.28	0.51
2:R:52:ILE:HG23	2:R:53:ASN:H	1.74	0.51
2:T:31:GLU:O	2:T:35:VAL:HG23	2.10	0.51
1:A:515:LYS:NZ	1:A:516:VAL:CG2	2.74	0.51
1:B:170:TYR:HA	1:B:173:ILE:HG22	1.92	0.51
1:B:173:ILE:HG23	1:B:174:GLY:N	2.25	0.51
1:B:218:LEU:HD21	1:B:225:ILE:CD1	2.41	0.51
1:B:165:GLN:NE2	1:B:252:ASP:HB3	2.26	0.51
1:B:197:LYS:HD3	1:B:263:ASP:OD1	2.09	0.51
1:B:288:VAL:CG2	1:B:289:GLU:H	2.20	0.51
1:B:513:TRP:CZ3	1:B:517:VAL:HG11	2.46	0.51
1:C:134:LYS:HG2	1:C:136:PRO:HD3	1.91	0.51
1:C:515:LYS:HZ3	1:C:516:VAL:N	2.09	0.51
1:C:794:GLN:HE22	1:C:795:LYS:HG3	1.75	0.51
1:E:405:LEU:HD12	1:E:405:LEU:N	2.24	0.51
1:E:636:ALA:O	1:E:640:LYS:HA	2.09	0.51
1:F:145:LYS:HB3	1:F:151:LYS:HB2	1.92	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:308:VAL:O	1:F:311:HIS:HB2	2.11	0.51
2:P:64:ASP:OD2	2:P:67:GLU:HG3	2.09	0.51
2:P:97:ASN:H	2:P:97:ASN:HD22	1.58	0.51
2:S:31:GLU:O	2:S:35:VAL:HG23	2.10	0.51
2:S:37:ARG:HA	2:S:41:GLN:O	2.10	0.51
2:T:65:PHE:HB2	2:T:66:PRO:CD	2.35	0.51
1:A:197:LYS:HD3	1:A:263:ASP:OD1	2.10	0.51
1:A:517:VAL:O	1:A:525:LYS:NZ	2.44	0.51
1:B:145:LYS:HB3	1:B:151:LYS:HB2	1.92	0.51
1:B:196:ILE:HG23	1:B:199:LEU:HD12	1.91	0.51
1:B:308:VAL:O	1:B:311:HIS:HB2	2.10	0.51
1:B:483:GLY:O	1:B:484:VAL:HG22	2.10	0.51
1:C:145:LYS:HB3	1:C:151:LYS:HB2	1.91	0.51
1:C:515:LYS:NZ	1:C:516:VAL:CG2	2.74	0.51
1:C:724:ARG:O	1:C:727:GLN:HB2	2.10	0.51
1:D:135:VAL:HG22	1:D:135:VAL:O	2.11	0.51
1:D:238:GLN:C	1:D:240:ALA:N	2.63	0.51
1:D:630:ARG:CZ	2:R:83:GLU:CG	2.87	0.51
1:E:135:VAL:HG22	1:E:135:VAL:O	2.11	0.51
1:E:165:GLN:NE2	1:E:252:ASP:HB3	2.25	0.51
1:E:329:ARG:HD2	1:E:590:ASP:OD2	2.10	0.51
1:F:671:ARG:HH12	1:F:677:GLY:HA3	1.74	0.51
1:F:71:PHE:O	1:F:78:LYS:NZ	2.43	0.51
2:P:9:ILE:HG23	2:P:69:LEU:HD21	1.92	0.51
2:S:70:THR:HG22	2:S:70:THR:O	2.09	0.51
1:B:387:ASN:O	1:B:390:SER:HB2	2.10	0.51
1:C:121:SER:O	1:C:123:GLU:OE2	2.28	0.51
1:C:173:ILE:HD12	1:C:243:LEU:CD2	2.40	0.51
1:C:308:VAL:O	1:C:311:HIS:HB2	2.10	0.51
1:D:107:THR:HG21	1:D:115:LYS:CD	2.37	0.51
1:D:597:ASN:OD1	1:D:599:GLU:HB2	2.10	0.51
1:E:165:GLN:NE2	1:E:251:PRO:HG2	2.24	0.51
1:F:324:THR:HB	1:F:499:PRO:CA	2.39	0.51
1:F:597:ASN:OD1	1:F:599:GLU:HB2	2.11	0.51
2:O:110:THR:HG22	2:O:114:GLU:O	2.11	0.51
2:P:43:PRO:HG3	2:P:48:LEU:HD13	1.91	0.51
2:S:9:ILE:CD1	2:S:69:LEU:HD11	2.38	0.51
1:A:165:GLN:NE2	1:A:252:ASP:HB3	2.26	0.51
1:A:629:ASN:C	1:A:629:ASN:ND2	2.62	0.51
1:C:135:VAL:O	1:C:135:VAL:HG22	2.10	0.51
1:C:482:GLU:O	1:C:484:VAL:HG23	2.11	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:531:ASN:HA	1:C:534:ILE:HD12	1.92	0.51
1:D:170:TYR:HA	1:D:173:ILE:HG22	1.93	0.51
1:D:214:PHE:CD1	1:D:218:LEU:HD23	2.46	0.51
1:D:662:GLU:OE2	1:D:755:ARG:NH2	2.38	0.51
1:D:713:SER:O	1:D:717:LYS:HG3	2.10	0.51
1:E:156:ILE:N	1:E:156:ILE:HD12	2.26	0.51
1:E:165:GLN:C	1:E:167:LYS:H	2.14	0.51
1:E:173:ILE:HG23	1:E:174:GLY:H	1.75	0.51
1:E:169:VAL:CG2	1:E:246:SER:HB2	2.40	0.51
1:E:275:GLY:HA2	1:E:278:LYS:CG	2.39	0.51
1:E:513:TRP:CZ3	1:E:517:VAL:HG11	2.46	0.51
1:F:173:ILE:HG23	1:F:174:GLY:N	2.26	0.51
1:F:483:GLY:O	1:F:484:VAL:HG22	2.11	0.51
1:F:497:LEU:CD1	1:F:556:MET:HG2	2.40	0.51
1:F:517:VAL:O	1:F:525:LYS:NZ	2.44	0.51
2:S:56:ASP:OD2	2:S:60:ASN:C	2.49	0.51
2:S:65:PHE:HD1	2:S:65:PHE:H	1.56	0.51
1:B:278:LYS:HB2	1:B:279:ILE:HD13	1.92	0.51
1:B:301:ALA:C	1:B:303:LYS:N	2.63	0.51
1:B:324:THR:HB	1:B:499:PRO:CA	2.37	0.51
1:B:629:ASN:ND2	1:B:629:ASN:C	2.63	0.51
1:B:630:ARG:HG3	1:B:630:ARG:NH1	2.26	0.51
1:C:189:ASP:C	1:C:191:GLU:N	2.64	0.51
1:C:244:ALA:HB3	1:C:268:MET:HE3	1.93	0.51
1:C:279:ILE:C	1:C:281:GLU:H	2.13	0.51
1:D:197:LYS:NZ	1:D:197:LYS:HB3	2.25	0.51
1:E:324:THR:HB	1:E:499:PRO:CA	2.39	0.51
1:F:134:LYS:HG2	1:F:136:PRO:HD3	1.92	0.51
1:F:338:LEU:HD21	1:F:409:ARG:CZ	2.41	0.51
2:Q:110:THR:HG22	2:Q:114:GLU:O	2.11	0.51
2:R:64:ASP:OD2	2:R:67:GLU:HG3	2.09	0.51
2:S:13:LYS:HZ1	2:S:65:PHE:HB3	1.69	0.51
1:F:529:VAL:HG21	2:T:109:MSE:HE1	1.92	0.51
1:A:797:ILE:HG13	1:A:797:ILE:O	2.11	0.51
1:B:95:GLU:O	1:B:99:GLU:HB2	2.11	0.51
1:C:288:VAL:CG2	1:C:289:GLU:H	2.20	0.51
1:D:387:ASN:O	1:D:390:SER:HB2	2.11	0.51
1:D:504:ILE:HD12	1:D:504:ILE:N	2.25	0.51
1:D:741:ILE:O	1:D:742:ALA:C	2.49	0.51
1:E:387:ASN:O	1:E:390:SER:HB2	2.10	0.51
1:E:667:LEU:HB3	2:S:14:GLU:OE2	2.10	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:ARG:HG3	1:F:243:LEU:HD22	1.93	0.51
2:S:66:PRO:C	2:S:68:PHE:N	2.64	0.51
1:A:173:ILE:HG23	1:A:174:GLY:N	2.25	0.51
1:A:238:GLN:C	1:A:240:ALA:N	2.63	0.51
1:A:318:ILE:N	1:A:318:ILE:HD12	2.24	0.51
1:A:710:HIS:C	1:A:712:PHE:H	2.13	0.51
1:B:197:LYS:HZ3	1:B:197:LYS:C	2.14	0.51
1:C:107:THR:HG21	1:C:115:LYS:CD	2.37	0.51
1:C:408:LEU:HD12	1:C:408:LEU:N	2.03	0.51
1:C:797:ILE:HG13	1:C:797:ILE:O	2.11	0.51
1:D:165:GLN:NE2	1:D:252:ASP:HB3	2.26	0.51
1:D:710:HIS:C	1:D:712:PHE:H	2.14	0.51
1:E:482:GLU:O	1:E:484:VAL:HG23	2.10	0.51
1:E:615:ILE:CD1	1:E:645:TRP:HH2	2.17	0.51
1:F:180:ASP:C	1:F:182:ILE:H	2.14	0.51
1:F:214:PHE:CD1	1:F:218:LEU:HD23	2.46	0.51
1:F:271:LEU:HA	1:F:275:GLY:HA3	1.92	0.51
1:F:327:LEU:N	1:F:327:LEU:HD12	2.26	0.51
1:F:513:TRP:CZ3	1:F:517:VAL:HG11	2.46	0.51
1:F:561:ASN:HA	1:F:564:VAL:HG22	1.92	0.51
1:F:715:GLU:OE1	1:F:767:GLN:NE2	2.44	0.51
2:Q:37:ARG:HA	2:Q:41:GLN:O	2.11	0.51
2:R:55:VAL:HG21	2:R:67:GLU:CD	2.27	0.51
2:T:136:VAL:HG23	2:T:136:VAL:O	2.10	0.51
1:A:121:SER:O	1:A:123:GLU:OE2	2.28	0.51
1:A:531:ASN:HA	1:A:534:ILE:HD12	1.93	0.51
1:A:741:ILE:O	1:A:742:ALA:C	2.50	0.51
1:B:482:GLU:O	1:B:484:VAL:HG23	2.10	0.51
1:B:497:LEU:CD1	1:B:556:MET:HG2	2.40	0.51
1:B:630:ARG:CZ	2:P:83:GLU:CG	2.87	0.51
1:C:170:TYR:HA	1:C:173:ILE:HG22	1.93	0.51
1:C:517:VAL:O	1:C:525:LYS:NZ	2.44	0.51
1:D:121:SER:O	1:D:123:GLU:OE2	2.28	0.51
1:D:97:TYR:HE1	1:D:178:SER:CB	2.24	0.51
1:E:173:ILE:HG23	1:E:174:GLY:N	2.26	0.51
1:E:376:GLN:HB3	1:E:379:ALA:HB3	1.94	0.51
1:E:515:LYS:NZ	1:E:516:VAL:CG2	2.74	0.51
1:E:78:LYS:HG3	1:E:79:ILE:N	2.26	0.51
1:F:217:LYS:HB2	1:F:236:GLU:HG3	1.93	0.51
1:F:424:LYS:HB3	1:F:424:LYS:HZ2	1.76	0.51
1:F:794:GLN:HE22	1:F:795:LYS:HG3	1.75	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:664:ILE:HG21	2:R:15:ALA:HB2	1.93	0.51
1:E:692:GLU:OE1	2:S:21:LYS:NZ	2.43	0.51
2:T:110:THR:HG22	2:T:114:GLU:O	2.11	0.51
1:A:197:LYS:NZ	1:A:197:LYS:HB3	2.25	0.50
1:A:214:PHE:CD1	1:A:218:LEU:HD23	2.46	0.50
1:A:71:PHE:O	1:A:78:LYS:NZ	2.43	0.50
1:B:180:ASP:O	1:B:182:ILE:N	2.44	0.50
1:C:148:GLU:HG3	1:C:149:THR:H	1.76	0.50
1:C:173:ILE:HG23	1:C:174:GLY:N	2.25	0.50
1:C:387:ASN:O	1:C:390:SER:HB2	2.11	0.50
1:C:513:TRP:CZ3	1:C:517:VAL:HG11	2.47	0.50
1:D:169:VAL:CG2	1:D:246:SER:HB2	2.40	0.50
1:D:71:PHE:O	1:D:78:LYS:NZ	2.42	0.50
1:E:153:ILE:C	1:E:154:ILE:HD13	2.31	0.50
1:E:335:ALA:O	1:E:339:ILE:HG13	2.10	0.50
1:E:508:ILE:HG23	1:E:536:TYR:CE2	2.47	0.50
1:F:218:LEU:HD21	1:F:225:ILE:CD1	2.41	0.50
1:F:504:ILE:HD12	1:F:504:ILE:N	2.25	0.50
1:F:635:ILE:CD1	1:F:635:ILE:N	2.72	0.50
1:F:662:GLU:OE2	1:F:755:ARG:NH2	2.38	0.50
1:F:95:GLU:O	1:F:99:GLU:HB2	2.12	0.50
2:R:66:PRO:C	2:R:68:PHE:N	2.63	0.50
2:S:62:THR:N	2:S:62:THR:HG22	2.26	0.50
1:A:107:THR:HG21	1:A:115:LYS:CD	2.37	0.50
1:A:275:GLY:CA	1:A:278:LYS:HE3	2.37	0.50
1:A:301:ALA:C	1:A:303:LYS:H	2.14	0.50
1:A:513:TRP:CZ3	1:A:517:VAL:HG11	2.46	0.50
1:A:629:ASN:HD22	1:A:631:SER:N	1.99	0.50
1:B:197:LYS:NZ	1:B:197:LYS:HB3	2.26	0.50
1:B:356:ASP:N	1:B:356:ASP:OD2	2.44	0.50
1:B:501:LEU:HD22	2:P:112:LEU:CD2	2.26	0.50
1:C:165:GLN:C	1:C:167:LYS:H	2.14	0.50
1:C:175:LYS:HB2	1:C:175:LYS:HZ3	1.74	0.50
1:C:169:VAL:CG2	1:C:246:SER:HB2	2.40	0.50
1:C:301:ALA:C	1:C:303:LYS:H	2.14	0.50
1:C:504:ILE:HD12	1:C:504:ILE:N	2.25	0.50
1:D:349:ASN:HD22	1:D:350:VAL:N	2.08	0.50
1:D:424:LYS:HZ2	1:D:424:LYS:HB3	1.76	0.50
1:D:515:LYS:NZ	1:D:516:VAL:CG2	2.74	0.50
1:D:797:ILE:HG13	1:D:797:ILE:O	2.12	0.50
1:E:180:ASP:O	1:E:182:ILE:N	2.45	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:ASP:C	1:E:191:GLU:N	2.64	0.50
1:F:189:ASP:C	1:F:191:GLU:N	2.65	0.50
1:F:408:LEU:N	1:F:408:LEU:HD12	2.04	0.50
1:F:79:ILE:C	1:F:81:GLN:N	2.57	0.50
2:S:44:THR:OG1	2:S:47:GLU:HB2	2.12	0.50
2:T:58:ASP:HB2	2:T:62:THR:O	2.11	0.50
1:A:189:ASP:C	1:A:191:GLU:N	2.64	0.50
1:A:327:LEU:HD12	1:A:327:LEU:N	2.25	0.50
1:A:497:LEU:CD1	1:A:556:MET:HG2	2.40	0.50
1:B:217:LYS:HB2	1:B:236:GLU:HG3	1.93	0.50
1:B:173:ILE:HD12	1:B:243:LEU:CD2	2.41	0.50
1:B:301:ALA:C	1:B:303:LYS:H	2.14	0.50
1:B:515:LYS:HZ3	1:B:516:VAL:HG23	1.76	0.50
1:B:741:ILE:O	1:B:742:ALA:C	2.50	0.50
1:C:180:ASP:C	1:C:182:ILE:H	2.14	0.50
1:C:349:ASN:HD22	1:C:350:VAL:N	2.08	0.50
1:C:700:TYR:HD1	1:C:728:ALA:CA	2.25	0.50
1:D:189:ASP:HB3	1:D:190:PRO:HD2	1.94	0.50
1:E:214:PHE:CD1	1:E:218:LEU:HD23	2.47	0.50
1:E:431:LYS:O	1:E:432:TYR:HD2	1.94	0.50
1:E:710:HIS:C	1:E:712:PHE:H	2.14	0.50
2:T:37:ARG:HA	2:T:41:GLN:O	2.12	0.50
1:A:180:ASP:C	1:A:182:ILE:H	2.14	0.50
1:A:302:LEU:HD22	1:A:602:PHE:HE1	1.77	0.50
1:A:97:TYR:HE1	1:A:178:SER:CB	2.25	0.50
1:B:189:ASP:C	1:B:191:GLU:N	2.65	0.50
1:B:327:LEU:HD12	1:B:327:LEU:N	2.25	0.50
1:C:154:ILE:CG1	1:C:171:TYR:CE1	2.87	0.50
1:C:597:ASN:OD1	1:C:599:GLU:HB2	2.11	0.50
1:C:713:SER:O	1:C:717:LYS:HG3	2.11	0.50
1:C:78:LYS:HG3	1:C:79:ILE:N	2.26	0.50
1:D:288:VAL:CG2	1:D:289:GLU:H	2.20	0.50
1:D:513:TRP:CZ3	1:D:517:VAL:HG11	2.46	0.50
1:D:715:GLU:OE1	1:D:767:GLN:NE2	2.44	0.50
1:D:95:GLU:O	1:D:99:GLU:HB2	2.10	0.50
1:E:93:VAL:CG2	1:E:179:LEU:HD11	2.37	0.50
1:E:238:GLN:C	1:E:240:ALA:N	2.63	0.50
1:E:531:ASN:HA	1:E:534:ILE:HD12	1.94	0.50
1:F:165:GLN:NE2	1:F:252:ASP:HB3	2.26	0.50
1:F:356:ASP:OD2	1:F:356:ASP:N	2.44	0.50
1:F:351:HIS:HB2	1:F:386:GLU:HG2	1.94	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:397:GLU:HA	1:F:480:ASN:CB	2.42	0.50
1:F:431:LYS:O	1:F:432:TYR:HD2	1.94	0.50
1:F:776:LEU:HD23	1:F:776:LEU:C	2.32	0.50
2:P:101:SER:OG	2:P:104:GLU:HG2	2.12	0.50
2:Q:52:ILE:HG23	2:Q:53:ASN:H	1.74	0.50
1:A:165:GLN:C	1:A:167:LYS:H	2.14	0.50
1:A:376:GLN:HB3	1:A:379:ALA:HB3	1.94	0.50
1:A:483:GLY:O	1:A:484:VAL:HG22	2.11	0.50
1:A:630:ARG:CZ	2:O:83:GLU:CG	2.84	0.50
1:B:107:THR:HG21	1:B:115:LYS:CD	2.37	0.50
1:B:135:VAL:O	1:B:135:VAL:HG22	2.12	0.50
1:B:131:ARG:HG3	1:B:243:LEU:HD22	1.92	0.50
1:B:505:LYS:HD3	2:P:112:LEU:O	2.11	0.50
1:B:710:HIS:C	1:B:712:PHE:H	2.14	0.50
1:B:678:VAL:HG22	1:B:745:TYR:HE2	1.76	0.50
1:C:187:SER:C	1:C:188:LEU:O	2.44	0.50
1:C:165:GLN:NE2	1:C:252:ASP:HB3	2.26	0.50
1:C:376:GLN:HB3	1:C:379:ALA:HB3	1.93	0.50
1:D:134:LYS:HG2	1:D:136:PRO:HD3	1.92	0.50
1:D:217:LYS:HB2	1:D:236:GLU:HG3	1.94	0.50
1:D:308:VAL:O	1:D:311:HIS:HB2	2.11	0.50
1:D:327:LEU:HD12	1:D:327:LEU:N	2.26	0.50
1:D:351:HIS:HB2	1:D:386:GLU:HG2	1.94	0.50
1:E:197:LYS:HD3	1:E:263:ASP:OD1	2.10	0.50
1:E:301:ALA:C	1:E:303:LYS:N	2.62	0.50
1:E:403:LEU:HD22	1:E:474:ILE:HG21	1.94	0.50
1:E:630:ARG:CZ	2:S:83:GLU:CG	2.85	0.50
1:E:630:ARG:NH1	1:E:630:ARG:HG3	2.26	0.50
1:E:678:VAL:HG22	1:E:745:TYR:HE2	1.77	0.50
2:O:73:ALA:O	2:O:74:ARG:C	2.50	0.50
1:A:112:VAL:HG12	1:A:113:GLU:HG3	1.94	0.50
1:A:165:GLN:NE2	1:A:251:PRO:HG2	2.24	0.50
1:A:356:ASP:N	1:A:356:ASP:OD2	2.44	0.50
1:A:431:LYS:O	1:A:432:TYR:HD2	1.94	0.50
1:A:735:VAL:O	1:A:741:ILE:HD13	2.12	0.50
1:B:115:LYS:HZ1	1:B:117:LEU:HB2	1.76	0.50
1:B:376:GLN:HB3	1:B:379:ALA:HB3	1.94	0.50
1:B:97:TYR:HE1	1:B:178:SER:CB	2.24	0.50
1:C:156:ILE:HD12	1:C:156:ILE:N	2.26	0.50
1:C:180:ASP:O	1:C:182:ILE:N	2.45	0.50
1:E:351:HIS:HB2	1:E:386:GLU:HG2	1.94	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:741:ILE:O	1:E:742:ALA:C	2.49	0.50
1:F:349:ASN:HD22	1:F:350:VAL:N	2.09	0.50
1:F:376:GLN:HB3	1:F:379:ALA:HB3	1.94	0.50
1:F:443:GLU:HG3	1:F:458:LYS:CG	2.42	0.50
1:F:678:VAL:HG22	1:F:745:TYR:HE2	1.76	0.50
2:R:24:ASP:OD1	2:R:25:GLY:N	2.40	0.50
1:A:349:ASN:HD22	1:A:350:VAL:N	2.09	0.50
1:A:351:HIS:HB2	1:A:386:GLU:HG2	1.94	0.50
1:B:165:GLN:C	1:B:167:LYS:H	2.15	0.50
1:B:165:GLN:NE2	1:B:251:PRO:HG2	2.23	0.50
1:B:214:PHE:CD1	1:B:218:LEU:HD23	2.47	0.50
1:B:78:LYS:HG3	1:B:79:ILE:N	2.26	0.50
1:C:109:ILE:HD11	1:C:157:LYS:HZ2	1.76	0.50
1:C:173:ILE:HG13	1:C:242:SER:CB	2.38	0.50
1:C:197:LYS:HB3	1:C:197:LYS:NZ	2.26	0.50
1:C:214:PHE:CD1	1:C:218:LEU:HD23	2.46	0.50
1:C:529:VAL:HG21	2:Q:109:MSE:HE1	1.93	0.50
1:C:715:GLU:OE1	1:C:767:GLN:NE2	2.45	0.50
1:D:187:SER:C	1:D:188:LEU:O	2.44	0.50
1:D:189:ASP:C	1:D:191:GLU:N	2.65	0.50
1:D:78:LYS:HG3	1:D:79:ILE:N	2.26	0.50
1:E:145:LYS:HB3	1:E:151:LYS:HB2	1.93	0.50
1:E:217:LYS:HB2	1:E:236:GLU:HG3	1.94	0.50
1:E:462:ILE:CD1	1:E:466:GLY:HA2	2.42	0.50
1:F:153:ILE:C	1:F:154:ILE:HD13	2.32	0.50
1:F:301:ALA:C	1:F:303:LYS:H	2.14	0.50
1:F:710:HIS:C	1:F:712:PHE:H	2.14	0.50
2:O:37:ARG:HA	2:O:41:GLN:O	2.11	0.50
2:Q:49:GLN:O	2:Q:51:MSE:N	2.45	0.50
2:T:5:THR:HG23	2:T:8:GLN:H	1.77	0.50
1:B:153:ILE:C	1:B:154:ILE:HD13	2.31	0.50
1:B:173:ILE:HG13	1:B:242:SER:CB	2.37	0.50
1:C:189:ASP:HB3	1:C:190:PRO:HD2	1.94	0.50
1:C:218:LEU:O	1:C:218:LEU:HG	2.12	0.50
1:C:630:ARG:CZ	2:Q:83:GLU:CG	2.87	0.50
1:D:244:ALA:HB3	1:D:268:MET:HE3	1.94	0.50
1:D:529:VAL:HG21	2:R:109:MSE:HE1	1.93	0.50
1:E:71:PHE:O	1:E:78:LYS:NZ	2.45	0.50
1:F:112:VAL:CG1	1:F:113:GLU:H	2.07	0.50
1:F:156:ILE:HD12	1:F:156:ILE:N	2.27	0.50
2:Q:44:THR:OG1	2:Q:47:GLU:HB2	2.12	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:64:ASP:H	2:T:67:GLU:HB2	1.77	0.50
1:A:217:LYS:HB2	1:A:236:GLU:HG3	1.94	0.50
1:A:288:VAL:CG2	1:A:289:GLU:H	2.21	0.50
1:A:664:ILE:HG21	2:O:15:ALA:HB2	1.94	0.50
1:A:692:GLU:HA	1:A:692:GLU:OE2	2.12	0.50
1:A:78:LYS:HG3	1:A:79:ILE:N	2.26	0.50
1:B:112:VAL:O	1:B:114:HIS:N	2.38	0.50
1:B:281:GLU:O	1:B:285:LYS:HG2	2.12	0.50
1:B:724:ARG:NH1	1:B:724:ARG:HG3	2.27	0.50
1:C:741:ILE:O	1:C:742:ALA:C	2.50	0.50
1:D:156:ILE:HD12	1:D:156:ILE:N	2.26	0.50
1:E:244:ALA:HB3	1:E:268:MET:HE3	1.94	0.50
1:E:529:VAL:HG21	2:S:109:MSE:HE1	1.92	0.50
1:E:95:GLU:O	1:E:99:GLU:HB2	2.12	0.50
1:F:180:ASP:O	1:F:182:ILE:N	2.45	0.50
1:F:716:LYS:O	1:F:720:ILE:HG22	2.12	0.50
2:O:5:THR:HG23	2:O:8:GLN:H	1.76	0.50
2:P:37:ARG:HA	2:P:41:GLN:O	2.12	0.50
2:P:66:PRO:C	2:P:68:PHE:N	2.64	0.50
2:S:73:ALA:O	2:S:74:ARG:C	2.51	0.50
2:T:97:ASN:HD22	2:T:97:ASN:H	1.60	0.50
1:A:180:ASP:O	1:A:183:SER:N	2.33	0.49
1:A:180:ASP:O	1:A:182:ILE:N	2.45	0.49
1:A:387:ASN:O	1:A:390:SER:HB2	2.11	0.49
1:B:172:GLU:CB	1:B:246:SER:HA	2.40	0.49
1:B:397:GLU:HA	1:B:480:ASN:CB	2.42	0.49
1:B:338:LEU:HD21	1:B:409:ARG:CZ	2.41	0.49
1:B:443:GLU:HG3	1:B:458:LYS:CG	2.42	0.49
1:C:318:ILE:HD12	1:C:318:ILE:N	2.25	0.49
1:C:356:ASP:N	1:C:356:ASP:OD2	2.45	0.49
1:D:446:ILE:HD11	1:D:451:ASN:CB	2.40	0.49
1:D:671:ARG:HH12	1:D:677:GLY:HA3	1.73	0.49
1:F:462:ILE:CD1	1:F:466:GLY:HA2	2.42	0.49
2:P:110:THR:HG22	2:P:114:GLU:O	2.12	0.49
2:Q:73:ALA:O	2:Q:74:ARG:C	2.50	0.49
2:R:37:ARG:HA	2:R:41:GLN:O	2.12	0.49
1:F:664:ILE:HG21	2:T:15:ALA:HB2	1.94	0.49
2:T:49:GLN:O	2:T:51:MSE:N	2.45	0.49
1:A:106:PHE:HA	1:A:154:ILE:O	2.11	0.49
1:A:189:ASP:HB3	1:A:190:PRO:HD2	1.94	0.49
1:A:323:ASN:O	1:A:324:THR:HG22	2.13	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LEU:HD21	1:A:409:ARG:CZ	2.42	0.49
1:A:508:ILE:HG23	1:A:536:TYR:CE2	2.47	0.49
1:A:776:LEU:C	1:A:776:LEU:HD23	2.33	0.49
1:B:156:ILE:HD12	1:B:156:ILE:N	2.27	0.49
1:B:431:LYS:O	1:B:432:TYR:HD2	1.94	0.49
1:B:735:VAL:O	1:B:741:ILE:HD13	2.13	0.49
1:C:106:PHE:HA	1:C:154:ILE:O	2.12	0.49
1:C:431:LYS:O	1:C:432:TYR:HD2	1.94	0.49
1:C:483:GLY:O	1:C:484:VAL:HG22	2.11	0.49
1:C:71:PHE:O	1:C:78:LYS:NZ	2.44	0.49
1:D:431:LYS:O	1:D:432:TYR:HD2	1.94	0.49
1:D:517:VAL:O	1:D:525:LYS:NZ	2.45	0.49
1:D:581:GLN:HB3	1:D:627:TYR:CE1	2.47	0.49
1:E:338:LEU:HD21	1:E:409:ARG:CZ	2.42	0.49
1:E:735:VAL:O	1:E:741:ILE:HD13	2.12	0.49
1:E:742:ALA:HB1	1:E:744:GLU:OE1	2.12	0.49
1:F:165:GLN:C	1:F:167:LYS:H	2.15	0.49
1:F:169:VAL:CG2	1:F:246:SER:HB2	2.42	0.49
1:F:437:SER:O	1:F:439:ASN:N	2.45	0.49
1:A:706:ASN:O	2:O:130:ILE:HG23	2.13	0.49
2:T:101:SER:OG	2:T:104:GLU:HG2	2.12	0.49
1:A:678:VAL:HG22	1:A:745:TYR:HE2	1.76	0.49
1:B:148:GLU:HG3	1:B:149:THR:H	1.77	0.49
1:B:244:ALA:HB3	1:B:268:MET:HE3	1.93	0.49
1:B:351:HIS:HB2	1:B:386:GLU:HG2	1.94	0.49
1:B:797:ILE:HG13	1:B:797:ILE:O	2.12	0.49
1:C:164:GLU:HG2	1:C:166:SER:HB3	1.94	0.49
1:C:351:HIS:HB2	1:C:386:GLU:HG2	1.94	0.49
1:D:483:GLY:O	1:D:484:VAL:HG22	2.11	0.49
1:E:327:LEU:HD12	1:E:327:LEU:N	2.27	0.49
1:E:397:GLU:HA	1:E:480:ASN:CB	2.42	0.49
1:E:797:ILE:HG13	1:E:797:ILE:O	2.11	0.49
1:F:148:GLU:HG3	1:F:149:THR:H	1.77	0.49
1:F:164:GLU:HG2	1:F:166:SER:HB3	1.94	0.49
1:F:238:GLN:C	1:F:240:ALA:N	2.63	0.49
1:F:797:ILE:O	1:F:797:ILE:HG13	2.11	0.49
2:P:24:ASP:OD1	2:P:25:GLY:N	2.42	0.49
2:Q:64:ASP:H	2:Q:67:GLU:HB2	1.77	0.49
2:R:44:THR:OG1	2:R:47:GLU:HB2	2.12	0.49
2:R:76:MSE:C	2:R:78:ASP:H	2.16	0.49
2:S:126:ARG:HH21	2:S:126:ARG:HG3	1.77	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:64:ASP:H	2:S:67:GLU:HB2	1.77	0.49
1:A:355:SER:HB2	1:A:371:SER:HA	1.94	0.49
1:A:403:LEU:HD22	1:A:474:ILE:HG21	1.95	0.49
1:C:664:ILE:HG21	2:Q:15:ALA:HB2	1.95	0.49
1:C:776:LEU:HD23	1:C:776:LEU:C	2.32	0.49
1:D:173:ILE:HG23	1:D:174:GLY:H	1.76	0.49
1:D:356:ASP:OD2	1:D:356:ASP:N	2.45	0.49
1:E:349:ASN:HD22	1:E:350:VAL:N	2.09	0.49
1:E:405:LEU:HD13	1:E:453:VAL:CG2	2.33	0.49
1:E:437:SER:O	1:E:439:ASN:N	2.45	0.49
1:E:716:LYS:O	1:E:720:ILE:HG22	2.12	0.49
1:F:515:LYS:NZ	1:F:516:VAL:CG2	2.75	0.49
1:F:630:ARG:NH1	1:F:630:ARG:HG3	2.26	0.49
1:F:686:ASP:O	1:F:689:ALA:HB3	2.13	0.49
1:F:700:TYR:HD1	1:F:728:ALA:CA	2.26	0.49
2:O:64:ASP:H	2:O:67:GLU:HB2	1.77	0.49
2:P:73:ALA:O	2:P:74:ARG:C	2.50	0.49
2:Q:126:ARG:HG3	2:Q:126:ARG:HH21	1.76	0.49
2:R:64:ASP:H	2:R:67:GLU:HB2	1.77	0.49
2:T:146:THR:O	2:T:147:ALA:C	2.49	0.49
1:A:308:VAL:O	1:A:311:HIS:HB2	2.12	0.49
1:A:397:GLU:O	1:A:479:LYS:HA	2.13	0.49
1:B:776:LEU:HD23	1:B:776:LEU:C	2.33	0.49
1:C:338:LEU:HD21	1:C:409:ARG:CZ	2.43	0.49
1:C:716:LYS:O	1:C:720:ILE:HG22	2.13	0.49
1:D:106:PHE:HA	1:D:154:ILE:O	2.13	0.49
1:D:165:GLN:C	1:D:167:LYS:H	2.14	0.49
1:D:154:ILE:CG1	1:D:171:TYR:CE1	2.87	0.49
1:D:462:ILE:CD1	1:D:466:GLY:HA2	2.42	0.49
1:D:635:ILE:N	1:D:635:ILE:CD1	2.72	0.49
1:E:581:GLN:HB3	1:E:627:TYR:CE1	2.48	0.49
1:B:706:ASN:O	2:P:130:ILE:HG23	2.13	0.49
2:S:49:GLN:O	2:S:51:MSE:N	2.46	0.49
2:T:126:ARG:HG3	2:T:126:ARG:HH21	1.77	0.49
1:A:156:ILE:N	1:A:156:ILE:HD12	2.26	0.49
1:B:567:THR:HG22	1:B:568:GLY:N	2.28	0.49
1:B:724:ARG:O	1:B:727:GLN:HB2	2.12	0.49
1:D:180:ASP:O	1:D:182:ILE:N	2.46	0.49
1:D:192:PHE:HD1	1:D:192:PHE:H	1.61	0.49
1:D:216:GLU:HG3	1:D:217:LYS:HG2	1.95	0.49
1:D:338:LEU:HD21	1:D:409:ARG:CZ	2.43	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:LEU:HD22	1:D:474:ILE:HG21	1.94	0.49
1:D:686:ASP:O	1:D:689:ALA:HB3	2.13	0.49
1:E:106:PHE:HA	1:E:154:ILE:O	2.12	0.49
1:E:597:ASN:HB2	1:E:598:PRO:CD	2.37	0.49
1:E:662:GLU:OE2	1:E:755:ARG:NH2	2.37	0.49
1:F:387:ASN:O	1:F:390:SER:HB2	2.12	0.49
1:F:741:ILE:O	1:F:742:ALA:C	2.50	0.49
2:O:101:SER:OG	2:O:104:GLU:HG2	2.13	0.49
2:O:44:THR:OG1	2:O:47:GLU:HB2	2.13	0.49
2:P:100:ILE:HB	2:P:136:VAL:HG23	1.91	0.49
2:P:25:GLY:HA3	2:P:65:PHE:CZ	2.48	0.49
2:P:44:THR:OG1	2:P:47:GLU:HB2	2.12	0.49
2:Q:65:PHE:CD1	2:Q:65:PHE:N	2.81	0.49
2:S:146:THR:O	2:S:147:ALA:C	2.50	0.49
2:S:5:THR:HG23	2:S:8:GLN:H	1.77	0.49
2:T:9:ILE:CD1	2:T:69:LEU:HD11	2.38	0.49
1:B:397:GLU:O	1:B:479:LYS:HA	2.13	0.49
1:B:671:ARG:HG3	1:B:671:ARG:HH11	1.77	0.49
1:C:311:HIS:O	1:C:312:ALA:C	2.51	0.49
1:C:412:GLU:C	1:C:414:LYS:H	2.16	0.49
1:D:180:ASP:C	1:D:182:ILE:H	2.15	0.49
1:D:437:SER:O	1:D:439:ASN:N	2.46	0.49
1:D:716:LYS:O	1:D:720:ILE:HG22	2.12	0.49
1:D:717:LYS:O	1:D:720:ILE:HG22	2.13	0.49
1:E:397:GLU:O	1:E:479:LYS:HA	2.13	0.49
1:E:567:THR:HG22	1:E:568:GLY:N	2.28	0.49
1:E:700:TYR:HD1	1:E:728:ALA:CA	2.25	0.49
1:F:172:GLU:CB	1:F:246:SER:HA	2.39	0.49
2:P:13:LYS:NZ	2:P:65:PHE:CB	2.61	0.49
2:R:110:THR:HG22	2:R:114:GLU:O	2.12	0.49
1:D:706:ASN:O	2:R:130:ILE:HG23	2.13	0.49
2:R:73:ALA:O	2:R:74:ARG:C	2.50	0.49
2:T:73:ALA:O	2:T:74:ARG:C	2.50	0.49
1:A:218:LEU:O	1:A:218:LEU:HG	2.13	0.49
1:A:715:GLU:OE1	1:A:767:GLN:NE2	2.45	0.49
1:B:218:LEU:O	1:B:218:LEU:HG	2.13	0.49
1:B:629:ASN:HD22	1:B:631:SER:N	1.99	0.49
1:C:281:GLU:O	1:C:285:LYS:HG2	2.13	0.49
1:C:397:GLU:O	1:C:479:LYS:HA	2.12	0.49
1:C:443:GLU:HG3	1:C:458:LYS:HZ2	1.77	0.49
1:D:153:ILE:C	1:D:154:ILE:HD13	2.33	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:508:ILE:HG23	1:D:536:TYR:CE2	2.48	0.49
1:D:630:ARG:HG3	1:D:630:ARG:NH1	2.25	0.49
1:E:115:LYS:HZ1	1:E:117:LEU:HB2	1.78	0.49
1:E:216:GLU:HG3	1:E:217:LYS:HG2	1.95	0.49
1:E:311:HIS:O	1:E:312:ALA:C	2.51	0.49
1:F:97:TYR:HE1	1:F:178:SER:CB	2.25	0.49
2:O:49:GLN:O	2:O:51:MSE:N	2.46	0.49
2:P:16:PHE:CE1	2:P:27:ILE:CD1	2.96	0.49
2:R:94:LYS:HB3	2:R:94:LYS:HZ2	1.76	0.49
2:T:24:ASP:OD1	2:T:25:GLY:N	2.42	0.49
1:A:141:PHE:N	1:A:141:PHE:CD1	2.81	0.49
1:A:424:LYS:HZ2	1:A:424:LYS:HB3	1.78	0.49
1:B:189:ASP:HB3	1:B:190:PRO:HD2	1.94	0.49
1:B:308:VAL:CG2	1:B:336:THR:O	2.61	0.49
1:B:355:SER:HB2	1:B:371:SER:HA	1.95	0.49
1:B:742:ALA:HB1	1:B:744:GLU:OE1	2.13	0.49
1:C:697:ILE:C	1:C:699:GLY:N	2.65	0.49
1:D:376:GLN:HB3	1:D:379:ALA:HB3	1.94	0.49
1:D:724:ARG:O	1:D:727:GLN:HB2	2.13	0.49
1:E:106:PHE:CZ	1:E:171:TYR:OH	2.62	0.49
1:E:446:ILE:HD11	1:E:451:ASN:CB	2.40	0.49
1:E:443:GLU:HG3	1:E:458:LYS:CG	2.42	0.49
1:E:722:ILE:O	1:E:726:ILE:HG13	2.13	0.49
1:F:218:LEU:HG	1:F:218:LEU:O	2.12	0.49
1:F:397:GLU:O	1:F:479:LYS:HA	2.13	0.49
2:Q:19:PHE:CD1	2:Q:19:PHE:N	2.81	0.49
1:A:148:GLU:HG3	1:A:149:THR:H	1.76	0.49
1:A:308:VAL:CG2	1:A:336:THR:O	2.61	0.49
1:B:192:PHE:HD1	1:B:192:PHE:H	1.61	0.49
1:B:405:LEU:CD1	1:B:405:LEU:H	2.26	0.49
1:C:112:VAL:HG12	1:C:113:GLU:HG3	1.94	0.49
1:C:308:VAL:CG2	1:C:336:THR:O	2.61	0.49
1:D:397:GLU:HA	1:D:480:ASN:CB	2.42	0.49
1:D:671:ARG:HH11	1:D:671:ARG:HG3	1.77	0.49
1:D:742:ALA:HB1	1:D:744:GLU:OE1	2.13	0.49
1:E:81:GLN:CD	1:E:156:ILE:HG21	2.33	0.49
1:E:483:GLY:O	1:E:484:VAL:HG22	2.13	0.49
1:E:629:ASN:ND2	1:E:629:ASN:C	2.64	0.49
1:E:715:GLU:OE1	1:E:767:GLN:NE2	2.45	0.49
1:F:107:THR:HG21	1:F:115:LYS:CD	2.37	0.49
1:F:189:ASP:HB3	1:F:190:PRO:HD2	1.94	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:403:LEU:HD22	1:F:474:ILE:HG21	1.94	0.49
1:F:742:ALA:HB1	1:F:744:GLU:OE1	2.13	0.49
2:P:49:GLN:O	2:P:51:MSE:N	2.45	0.49
2:P:56:ASP:OD2	2:P:61:GLY:N	2.46	0.49
2:R:25:GLY:HA3	2:R:65:PHE:CZ	2.48	0.49
2:T:76:MSE:C	2:T:78:ASP:H	2.16	0.49
1:B:112:VAL:CG1	1:B:113:GLU:H	2.08	0.48
1:B:112:VAL:HG12	1:B:113:GLU:HG3	1.95	0.48
1:B:134:LYS:NZ	1:B:136:PRO:HG3	2.28	0.48
1:B:216:GLU:HG3	1:B:217:LYS:HG2	1.95	0.48
1:B:225:ILE:HG23	1:B:229:PHE:CD2	2.48	0.48
1:B:615:ILE:CD1	1:B:645:TRP:HH2	2.19	0.48
1:C:404:LYS:O	1:C:405:LEU:C	2.52	0.48
1:C:597:ASN:HD21	1:C:601:GLU:CB	2.08	0.48
1:C:717:LYS:O	1:C:720:ILE:HG22	2.13	0.48
1:D:173:ILE:HG23	1:D:174:GLY:N	2.27	0.48
1:D:180:ASP:O	1:D:183:SER:N	2.33	0.48
1:D:218:LEU:HG	1:D:218:LEU:O	2.13	0.48
1:D:322:LEU:O	1:D:323:ASN:HB3	2.13	0.48
1:D:397:GLU:O	1:D:479:LYS:HA	2.13	0.48
1:D:443:GLU:HG3	1:D:458:LYS:CG	2.42	0.48
1:D:776:LEU:C	1:D:776:LEU:HD23	2.33	0.48
1:E:192:PHE:HD1	1:E:192:PHE:H	1.61	0.48
1:E:365:PRO:HB2	1:E:367:ASP:O	2.13	0.48
1:E:88:LYS:HD2	1:E:89:ILE:HG13	1.94	0.48
1:F:173:ILE:HG13	1:F:242:SER:CB	2.38	0.48
1:F:308:VAL:CG2	1:F:336:THR:O	2.61	0.48
1:F:355:SER:HB2	1:F:371:SER:HA	1.95	0.48
1:F:583:ASN:O	1:F:587:PRO:HD3	2.13	0.48
2:P:126:ARG:HH21	2:P:126:ARG:HG3	1.77	0.48
1:B:664:ILE:HG21	2:P:15:ALA:HB2	1.95	0.48
2:P:64:ASP:H	2:P:67:GLU:HB2	1.78	0.48
2:R:126:ARG:HH21	2:R:126:ARG:HG3	1.77	0.48
2:S:13:LYS:NZ	2:S:65:PHE:CB	2.61	0.48
1:A:443:GLU:HG3	1:A:458:LYS:CG	2.42	0.48
1:A:742:ALA:HB1	1:A:744:GLU:OE1	2.13	0.48
1:A:75:THR:O	1:A:76:LEU:C	2.52	0.48
1:B:106:PHE:HA	1:B:154:ILE:O	2.12	0.48
1:B:141:PHE:N	1:B:141:PHE:CD1	2.81	0.48
1:B:323:ASN:O	1:B:324:THR:HG22	2.13	0.48
1:B:403:LEU:HD22	1:B:474:ILE:HG21	1.94	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:581:GLN:HB3	1:B:627:TYR:CE1	2.48	0.48
1:C:437:SER:O	1:C:439:ASN:N	2.46	0.48
1:C:445:ARG:HG2	1:C:471:TRP:CZ3	2.48	0.48
1:D:112:VAL:HG12	1:D:113:GLU:HG3	1.95	0.48
1:D:164:GLU:HG2	1:D:166:SER:HB3	1.94	0.48
1:D:199:LEU:C	1:D:201:ASP:N	2.67	0.48
1:D:205:SER:C	1:D:207:ASP:H	2.17	0.48
1:D:622:LYS:HA	1:D:622:LYS:HD3	1.50	0.48
1:E:112:VAL:HG12	1:E:113:GLU:HG3	1.95	0.48
1:E:164:GLU:HG2	1:E:166:SER:HB3	1.94	0.48
1:E:445:ARG:HG2	1:E:471:TRP:CZ3	2.49	0.48
1:E:776:LEU:HD23	1:E:776:LEU:C	2.33	0.48
1:F:192:PHE:HD1	1:F:192:PHE:H	1.61	0.48
1:F:322:LEU:O	1:F:323:ASN:HB3	2.13	0.48
1:F:365:PRO:HB2	1:F:367:ASP:O	2.13	0.48
1:F:724:ARG:O	1:F:727:GLN:HB2	2.13	0.48
2:O:93:ASP:OD1	2:O:97:ASN:ND2	2.46	0.48
2:P:5:THR:HG23	2:P:8:GLN:H	1.78	0.48
2:Q:101:SER:OG	2:Q:104:GLU:HG2	2.13	0.48
2:R:101:SER:OG	2:R:104:GLU:HG2	2.13	0.48
2:R:49:GLN:O	2:R:51:MSE:N	2.46	0.48
2:S:58:ASP:HB2	2:S:62:THR:O	2.12	0.48
1:A:154:ILE:CG1	1:A:171:TYR:CE1	2.87	0.48
1:A:192:PHE:HD1	1:A:192:PHE:H	1.61	0.48
1:A:281:GLU:O	1:A:285:LYS:HG2	2.13	0.48
1:B:199:LEU:C	1:B:201:ASP:N	2.66	0.48
1:B:169:VAL:HG22	1:B:246:SER:HB2	1.96	0.48
1:B:597:ASN:OD1	1:B:599:GLU:HB2	2.12	0.48
1:B:71:PHE:O	1:B:78:LYS:NZ	2.46	0.48
1:C:192:PHE:H	1:C:192:PHE:HD1	1.61	0.48
1:C:355:SER:HB2	1:C:371:SER:HA	1.95	0.48
1:C:462:ILE:CD1	1:C:466:GLY:HA2	2.43	0.48
1:C:581:GLN:HB3	1:C:627:TYR:CE1	2.49	0.48
1:C:615:ILE:CD1	1:C:645:TRP:HH2	2.17	0.48
1:C:97:TYR:HE1	1:C:178:SER:CB	2.26	0.48
1:D:437:SER:C	1:D:439:ASN:H	2.17	0.48
1:E:141:PHE:N	1:E:141:PHE:CD1	2.81	0.48
1:E:205:SER:C	1:E:207:ASP:H	2.17	0.48
1:E:312:ALA:O	1:E:315:PHE:HB2	2.14	0.48
1:E:671:ARG:HH11	1:E:671:ARG:HG3	1.77	0.48
1:F:281:GLU:O	1:F:285:LYS:HG2	2.13	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:404:LYS:O	1:F:405:LEU:C	2.52	0.48
1:F:567:THR:HG22	1:F:568:GLY:N	2.28	0.48
1:F:722:ILE:O	1:F:726:ILE:HG13	2.13	0.48
1:F:735:VAL:O	1:F:741:ILE:HD13	2.12	0.48
2:O:138:TYR:CZ	2:O:142:VAL:CG2	2.97	0.48
2:P:52:ILE:HG23	2:P:53:ASN:H	1.75	0.48
2:R:146:THR:O	2:R:147:ALA:C	2.51	0.48
2:T:25:GLY:HA3	2:T:65:PHE:CZ	2.48	0.48
1:A:205:SER:C	1:A:207:ASP:H	2.17	0.48
1:A:324:THR:HB	1:A:499:PRO:CA	2.38	0.48
1:A:397:GLU:HA	1:A:480:ASN:CB	2.42	0.48
1:B:172:GLU:O	1:B:176:GLY:N	2.34	0.48
1:B:187:SER:C	1:B:188:LEU:O	2.44	0.48
1:C:205:SER:C	1:C:207:ASP:H	2.17	0.48
1:C:397:GLU:HA	1:C:480:ASN:CB	2.42	0.48
1:C:443:GLU:HG3	1:C:458:LYS:CG	2.42	0.48
1:C:508:ILE:HG23	1:C:536:TYR:CE2	2.48	0.48
1:C:497:LEU:CD1	1:C:556:MET:HG2	2.40	0.48
1:C:671:ARG:HG3	1:C:671:ARG:HH11	1.77	0.48
1:C:781:ASN:O	1:C:789:ASN:ND2	2.46	0.48
1:D:218:LEU:C	1:D:220:LEU:H	2.16	0.48
1:D:404:LYS:O	1:D:405:LEU:C	2.52	0.48
1:D:700:TYR:HD1	1:D:728:ALA:CA	2.26	0.48
1:E:355:SER:HB2	1:E:371:SER:HA	1.95	0.48
1:E:724:ARG:O	1:E:727:GLN:HB2	2.13	0.48
2:O:117:THR:O	2:O:119:GLU:N	2.46	0.48
2:O:19:PHE:CD1	2:O:19:PHE:N	2.82	0.48
2:R:19:PHE:CD1	2:R:19:PHE:N	2.82	0.48
2:R:65:PHE:N	2:R:65:PHE:CD1	2.81	0.48
2:S:101:SER:OG	2:S:104:GLU:HG2	2.14	0.48
2:S:19:PHE:N	2:S:19:PHE:CD1	2.81	0.48
2:S:25:GLY:HA3	2:S:65:PHE:CZ	2.49	0.48
1:A:199:LEU:C	1:A:201:ASP:N	2.67	0.48
1:A:225:ILE:HG23	1:A:229:PHE:CD2	2.48	0.48
1:A:404:LYS:O	1:A:405:LEU:C	2.52	0.48
1:A:437:SER:O	1:A:439:ASN:N	2.46	0.48
1:A:533:LEU:HD23	1:A:533:LEU:C	2.33	0.48
1:A:95:GLU:O	1:A:99:GLU:HB2	2.12	0.48
1:B:175:LYS:NZ	1:B:175:LYS:CB	2.76	0.48
1:B:205:SER:C	1:B:207:ASP:H	2.17	0.48
1:B:349:ASN:HD22	1:B:350:VAL:N	2.11	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:ILE:HG23	1:B:536:TYR:CE2	2.48	0.48
1:B:75:THR:O	1:B:76:LEU:C	2.51	0.48
1:C:323:ASN:O	1:C:324:THR:HG22	2.13	0.48
1:C:482:GLU:HA	1:C:482:GLU:OE2	2.13	0.48
1:C:630:ARG:HG3	1:C:630:ARG:NH1	2.27	0.48
1:C:662:GLU:OE2	1:C:755:ARG:NH2	2.39	0.48
1:D:225:ILE:HG23	1:D:229:PHE:CD2	2.48	0.48
1:D:482:GLU:OE2	1:D:482:GLU:HA	2.14	0.48
1:E:323:ASN:O	1:E:324:THR:HG22	2.13	0.48
1:E:724:ARG:HG3	1:E:724:ARG:NH1	2.29	0.48
1:E:97:TYR:HE1	1:E:178:SER:CB	2.26	0.48
1:F:216:GLU:HG3	1:F:217:LYS:HG2	1.95	0.48
1:F:88:LYS:HD2	1:F:89:ILE:HG13	1.95	0.48
2:O:25:GLY:HA3	2:O:65:PHE:CZ	2.49	0.48
2:P:16:PHE:CE1	2:P:27:ILE:HD13	2.48	0.48
2:P:76:MSE:C	2:P:78:ASP:H	2.17	0.48
2:Q:76:MSE:C	2:Q:78:ASP:H	2.16	0.48
1:E:706:ASN:O	2:S:130:ILE:HG23	2.14	0.48
2:T:28:THR:CG2	2:T:30:LYS:HZ1	2.26	0.48
1:A:172:GLU:O	1:A:176:GLY:N	2.34	0.48
1:A:405:LEU:H	1:A:405:LEU:CD1	2.27	0.48
1:B:445:ARG:HG2	1:B:471:TRP:CZ3	2.49	0.48
1:B:715:GLU:OE1	1:B:767:GLN:NE2	2.46	0.48
1:C:365:PRO:HB2	1:C:367:ASP:O	2.14	0.48
1:C:405:LEU:H	1:C:405:LEU:CD1	2.26	0.48
1:D:148:GLU:HG3	1:D:149:THR:H	1.77	0.48
1:D:412:GLU:C	1:D:414:LYS:H	2.16	0.48
1:D:531:ASN:HA	1:D:534:ILE:HD12	1.95	0.48
1:D:302:LEU:HD22	1:D:602:PHE:HE1	1.79	0.48
1:E:356:ASP:N	1:E:356:ASP:OD2	2.46	0.48
1:F:437:SER:C	1:F:439:ASN:H	2.17	0.48
2:P:19:PHE:CD1	2:P:19:PHE:N	2.82	0.48
2:Q:16:PHE:CE1	2:Q:27:ILE:CD1	2.97	0.48
1:A:445:ARG:HG2	1:A:471:TRP:CZ3	2.48	0.48
1:A:671:ARG:HH11	1:A:671:ARG:HG3	1.78	0.48
1:B:717:LYS:O	1:B:720:ILE:HG22	2.13	0.48
1:C:115:LYS:HZ1	1:C:117:LEU:HB2	1.78	0.48
1:C:697:ILE:O	1:C:699:GLY:N	2.47	0.48
1:C:742:ALA:HB1	1:C:744:GLU:OE1	2.13	0.48
1:D:141:PHE:CD1	1:D:141:PHE:N	2.81	0.48
1:D:355:SER:HB2	1:D:371:SER:HA	1.96	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:LEU:C	1:E:220:LEU:H	2.15	0.48
1:E:664:ILE:HG21	2:S:15:ALA:HB2	1.95	0.48
1:F:323:ASN:O	1:F:324:THR:HG22	2.13	0.48
1:F:508:ILE:HG23	1:F:536:TYR:CE2	2.49	0.48
2:O:66:PRO:C	2:O:68:PHE:N	2.64	0.48
1:B:529:VAL:HG21	2:P:109:MSE:HE1	1.94	0.48
2:P:117:THR:O	2:P:119:GLU:N	2.47	0.48
2:Q:129:ASP:OD1	2:Q:134:GLY:N	2.47	0.48
2:Q:5:THR:HG23	2:Q:8:GLN:H	1.77	0.48
2:R:5:THR:HG23	2:R:8:GLN:H	1.77	0.48
2:T:44:THR:OG1	2:T:47:GLU:HB2	2.13	0.48
2:T:65:PHE:CD1	2:T:65:PHE:N	2.81	0.48
1:A:482:GLU:HA	1:A:482:GLU:OE2	2.14	0.48
1:B:154:ILE:CG1	1:B:171:TYR:CE1	2.88	0.48
1:B:365:PRO:HB2	1:B:367:ASP:O	2.14	0.48
1:C:437:SER:C	1:C:439:ASN:H	2.17	0.48
1:C:478:ALA:CB	1:C:486:LYS:O	2.62	0.48
1:C:710:HIS:C	1:C:712:PHE:H	2.16	0.48
1:D:497:LEU:CD1	1:D:556:MET:HG2	2.41	0.48
1:D:735:VAL:O	1:D:741:ILE:HD13	2.13	0.48
1:D:781:ASN:O	1:D:789:ASN:ND2	2.46	0.48
1:E:412:GLU:C	1:E:414:LYS:H	2.16	0.48
1:E:497:LEU:CD1	1:E:556:MET:HG2	2.41	0.48
1:F:112:VAL:O	1:F:114:HIS:N	2.39	0.48
1:F:141:PHE:CD1	1:F:141:PHE:N	2.80	0.48
2:O:97:ASN:ND2	2:O:97:ASN:N	2.60	0.48
2:Q:39:LEU:HD23	2:Q:39:LEU:HA	1.75	0.48
2:R:117:THR:O	2:R:119:GLU:N	2.47	0.48
1:A:169:VAL:HG22	1:A:246:SER:HB2	1.96	0.48
1:A:216:GLU:HG3	1:A:217:LYS:HG2	1.96	0.48
1:A:437:SER:C	1:A:439:ASN:H	2.18	0.48
1:B:620:THR:HG22	1:B:621:GLY:N	2.29	0.48
1:C:141:PHE:CD1	1:C:141:PHE:N	2.81	0.48
1:C:403:LEU:HD22	1:C:474:ILE:HG21	1.95	0.48
1:D:311:HIS:O	1:D:312:ALA:C	2.52	0.48
1:E:154:ILE:CG1	1:E:171:TYR:CE1	2.86	0.48
1:E:189:ASP:HB3	1:E:190:PRO:HD2	1.94	0.48
1:E:308:VAL:CG2	1:E:336:THR:O	2.62	0.48
1:E:482:GLU:OE2	1:E:482:GLU:HA	2.14	0.48
1:E:717:LYS:O	1:E:720:ILE:HG22	2.14	0.48
1:F:302:LEU:HD22	1:F:602:PHE:HE1	1.78	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:482:GLU:HA	1:F:482:GLU:OE2	2.14	0.48
1:F:671:ARG:HG3	1:F:671:ARG:HH11	1.78	0.48
2:O:76:MSE:C	2:O:78:ASP:H	2.16	0.48
2:O:88:ALA:O	2:O:91:VAL:HB	2.14	0.48
1:C:706:ASN:O	2:Q:130:ILE:HG23	2.13	0.48
2:R:9:ILE:HG23	2:R:69:LEU:CD2	2.43	0.48
2:T:13:LYS:NZ	2:T:65:PHE:CB	2.62	0.48
1:A:115:LYS:HB3	1:A:115:LYS:HZ3	1.77	0.48
1:A:153:ILE:C	1:A:154:ILE:HD13	2.33	0.48
1:A:164:GLU:HG2	1:A:166:SER:HB3	1.95	0.48
1:A:175:LYS:O	1:A:176:GLY:C	2.52	0.48
1:A:462:ILE:CD1	1:A:466:GLY:HA2	2.42	0.48
1:A:567:THR:HG22	1:A:568:GLY:N	2.29	0.48
1:B:322:LEU:O	1:B:323:ASN:HB3	2.14	0.48
1:B:437:SER:O	1:B:439:ASN:N	2.47	0.48
1:C:722:ILE:O	1:C:726:ILE:HG13	2.13	0.48
1:D:210:PHE:HZ	1:D:221:ASN:OD1	1.97	0.48
1:D:281:GLU:O	1:D:285:LYS:HG2	2.13	0.48
1:D:692:GLU:HA	1:D:692:GLU:OE2	2.14	0.48
1:D:722:ILE:O	1:D:726:ILE:HG13	2.14	0.48
1:E:175:LYS:O	1:E:176:GLY:C	2.53	0.48
1:E:225:ILE:HG23	1:E:229:PHE:CD2	2.49	0.48
1:E:437:SER:C	1:E:439:ASN:H	2.17	0.48
1:F:141:PHE:H	1:F:141:PHE:HD1	1.62	0.48
1:F:199:LEU:C	1:F:201:ASP:N	2.67	0.48
1:F:275:GLY:CA	1:F:278:LYS:HE3	2.35	0.48
2:Q:25:GLY:HA3	2:Q:65:PHE:CZ	2.49	0.48
2:S:93:ASP:OD1	2:S:97:ASN:ND2	2.47	0.48
1:A:175:LYS:CB	1:A:175:LYS:NZ	2.76	0.47
1:A:176:GLY:O	1:A:178:SER:N	2.47	0.47
1:A:397:GLU:HA	1:A:480:ASN:HB2	1.96	0.47
1:A:620:THR:HG22	1:A:621:GLY:N	2.28	0.47
1:B:700:TYR:HD1	1:B:728:ALA:CA	2.25	0.47
1:C:127:SER:O	1:C:133:GLU:CD	2.47	0.47
1:C:153:ILE:C	1:C:154:ILE:HD13	2.34	0.47
1:C:567:THR:HG22	1:C:568:GLY:N	2.28	0.47
1:D:115:LYS:HB3	1:D:115:LYS:HZ3	1.76	0.47
1:D:724:ARG:HG3	1:D:724:ARG:NH1	2.29	0.47
1:E:218:LEU:O	1:E:218:LEU:HG	2.13	0.47
1:E:281:GLU:O	1:E:285:LYS:HG2	2.13	0.47
1:E:686:ASP:O	1:E:689:ALA:HB3	2.13	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:58:ASP:HB2	2:P:62:THR:O	2.13	0.47
2:R:49:GLN:O	2:R:53:ASN:N	2.43	0.47
2:R:88:ALA:O	2:R:91:VAL:HB	2.14	0.47
2:R:93:ASP:OD1	2:R:97:ASN:ND2	2.46	0.47
1:A:81:GLN:CD	1:A:156:ILE:HG21	2.35	0.47
1:B:164:GLU:HG2	1:B:166:SER:HB3	1.95	0.47
1:B:311:HIS:O	1:B:312:ALA:C	2.52	0.47
1:B:315:PHE:HA	1:B:318:ILE:HD13	1.96	0.47
1:B:482:GLU:OE2	1:B:482:GLU:HA	2.14	0.47
1:C:322:LEU:O	1:C:323:ASN:HB3	2.15	0.47
1:C:501:LEU:HD22	2:Q:112:LEU:CD2	2.28	0.47
1:D:191:GLU:O	1:D:193:LEU:N	2.48	0.47
1:E:148:GLU:HG3	1:E:149:THR:H	1.77	0.47
1:E:169:VAL:HG22	1:E:246:SER:HB2	1.96	0.47
1:F:112:VAL:HG12	1:F:113:GLU:HG3	1.95	0.47
1:F:106:PHE:HA	1:F:154:ILE:O	2.14	0.47
1:F:282:SER:HA	1:F:285:LYS:CD	2.44	0.47
2:Q:121:VAL:C	2:Q:123:GLN:H	2.17	0.47
2:Q:76:MSE:HE3	2:Q:76:MSE:HB2	1.64	0.47
2:T:117:THR:O	2:T:119:GLU:N	2.47	0.47
2:T:121:VAL:C	2:T:123:GLN:H	2.17	0.47
2:T:42:ASN:O	2:T:42:ASN:CG	2.53	0.47
1:A:412:GLU:C	1:A:414:LYS:H	2.16	0.47
1:B:697:ILE:C	1:B:699:GLY:N	2.66	0.47
1:C:191:GLU:O	1:C:193:LEU:N	2.47	0.47
1:C:620:THR:HG22	1:C:621:GLY:N	2.30	0.47
1:C:75:THR:O	1:C:76:LEU:C	2.52	0.47
1:D:275:GLY:CA	1:D:278:LYS:HG3	2.43	0.47
1:D:337:ASN:C	1:D:339:ILE:N	2.67	0.47
1:D:75:THR:O	1:D:76:LEU:C	2.52	0.47
1:D:88:LYS:HD2	1:D:89:ILE:HG13	1.95	0.47
1:E:282:SER:HA	1:E:285:LYS:CD	2.44	0.47
1:F:115:LYS:HZ1	1:F:117:LEU:HB2	1.78	0.47
1:F:115:LYS:NZ	1:F:117:LEU:HB2	2.30	0.47
1:F:191:GLU:O	1:F:193:LEU:N	2.48	0.47
1:F:412:GLU:C	1:F:414:LYS:H	2.16	0.47
1:F:445:ARG:HG2	1:F:471:TRP:CZ3	2.49	0.47
1:F:581:GLN:HB3	1:F:627:TYR:CE1	2.48	0.47
1:F:629:ASN:C	1:F:629:ASN:ND2	2.64	0.47
1:F:717:LYS:O	1:F:720:ILE:HG22	2.14	0.47
2:Q:56:ASP:OD2	2:Q:60:ASN:C	2.52	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:55:VAL:CB	2:R:67:GLU:OE2	2.60	0.47
1:A:173:ILE:C	1:A:175:LYS:N	2.67	0.47
1:A:583:ASN:O	1:A:587:PRO:HD3	2.14	0.47
1:A:700:TYR:HD1	1:A:728:ALA:CA	2.26	0.47
1:A:724:ARG:HG3	1:A:724:ARG:NH1	2.28	0.47
1:B:275:GLY:CA	1:B:278:LYS:HG3	2.43	0.47
1:B:437:SER:C	1:B:439:ASN:H	2.18	0.47
1:B:481:VAL:O	1:B:482:GLU:HB2	2.14	0.47
1:D:197:LYS:C	1:D:197:LYS:HZ3	2.17	0.47
1:D:405:LEU:H	1:D:405:LEU:CD1	2.27	0.47
1:D:445:ARG:HG2	1:D:471:TRP:CZ3	2.49	0.47
1:D:629:ASN:C	1:D:629:ASN:ND2	2.65	0.47
1:E:134:LYS:NZ	1:E:136:PRO:HG3	2.30	0.47
1:F:175:LYS:CB	1:F:175:LYS:NZ	2.76	0.47
1:F:318:ILE:N	1:F:318:ILE:HD12	2.25	0.47
1:F:315:PHE:HA	1:F:318:ILE:HD13	1.96	0.47
2:O:65:PHE:CD1	2:O:65:PHE:N	2.82	0.47
2:P:129:ASP:OD1	2:P:134:GLY:N	2.47	0.47
2:Q:117:THR:O	2:Q:119:GLU:N	2.48	0.47
2:S:109:MSE:HG3	2:S:116:LEU:CD1	2.41	0.47
2:T:16:PHE:CE1	2:T:27:ILE:CD1	2.97	0.47
1:A:102:GLY:HA3	1:A:150:PRO:HG2	1.96	0.47
1:A:191:GLU:O	1:A:193:LEU:N	2.47	0.47
1:A:581:GLN:HB3	1:A:627:TYR:CE1	2.49	0.47
1:A:662:GLU:OE2	1:A:755:ARG:NH2	2.38	0.47
1:A:700:TYR:CD1	1:A:727:GLN:HB3	2.50	0.47
1:B:597:ASN:HB2	1:B:598:PRO:CD	2.37	0.47
1:C:115:LYS:NZ	1:C:117:LEU:HB2	2.30	0.47
1:C:169:VAL:HG22	1:C:246:SER:HB2	1.97	0.47
1:C:175:LYS:O	1:C:176:GLY:C	2.53	0.47
1:C:216:GLU:HG3	1:C:217:LYS:HG2	1.95	0.47
1:C:225:ILE:HG23	1:C:229:PHE:CD2	2.48	0.47
1:C:282:SER:HA	1:C:285:LYS:CD	2.44	0.47
1:D:323:ASN:O	1:D:324:THR:HG22	2.15	0.47
1:E:515:LYS:HZ3	1:E:516:VAL:HG23	1.79	0.47
1:F:102:GLY:HA3	1:F:150:PRO:HG2	1.96	0.47
1:F:397:GLU:HA	1:F:480:ASN:HB2	1.95	0.47
1:F:697:ILE:C	1:F:699:GLY:N	2.67	0.47
2:O:126:ARG:HG3	2:O:126:ARG:HH21	1.78	0.47
2:O:49:GLN:O	2:O:53:ASN:N	2.43	0.47
2:P:9:ILE:HG23	2:P:69:LEU:CD2	2.44	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:9:ILE:HG23	2:Q:69:LEU:CD2	2.44	0.47
2:S:117:THR:O	2:S:119:GLU:N	2.47	0.47
2:S:42:ASN:O	2:S:42:ASN:CG	2.52	0.47
2:T:19:PHE:N	2:T:19:PHE:CD1	2.81	0.47
1:A:134:LYS:NZ	1:A:136:PRO:HG3	2.29	0.47
1:A:165:GLN:OE1	1:A:252:ASP:HB3	2.15	0.47
1:A:275:GLY:CA	1:A:278:LYS:HG3	2.43	0.47
1:A:312:ALA:O	1:A:315:PHE:HB2	2.14	0.47
1:A:322:LEU:O	1:A:323:ASN:HB3	2.14	0.47
1:A:365:PRO:HB2	1:A:367:ASP:O	2.14	0.47
1:B:180:ASP:O	1:B:183:SER:N	2.33	0.47
1:B:191:GLU:O	1:B:193:LEU:N	2.48	0.47
1:B:412:GLU:C	1:B:414:LYS:H	2.16	0.47
1:C:540:ARG:NH1	1:C:627:TYR:CE1	2.83	0.47
1:C:686:ASP:O	1:C:689:ALA:HB3	2.14	0.47
1:D:312:ALA:O	1:D:315:PHE:HB2	2.14	0.47
1:D:432:TYR:CD1	1:D:445:ARG:NE	2.82	0.47
1:D:583:ASN:O	1:D:587:PRO:HD3	2.14	0.47
1:D:581:GLN:HB3	1:D:627:TYR:HE1	1.80	0.47
1:E:115:LYS:NZ	1:E:117:LEU:HB2	2.29	0.47
1:E:173:ILE:O	1:E:174:GLY:C	2.53	0.47
1:E:191:GLU:O	1:E:193:LEU:N	2.48	0.47
1:E:302:LEU:HD22	1:E:602:PHE:HE1	1.79	0.47
1:E:318:ILE:N	1:E:318:ILE:HD12	2.25	0.47
1:E:424:LYS:HB3	1:E:424:LYS:HZ2	1.80	0.47
1:E:397:GLU:HA	1:E:480:ASN:HB2	1.96	0.47
1:E:697:ILE:C	1:E:699:GLY:N	2.67	0.47
1:E:781:ASN:O	1:E:789:ASN:ND2	2.46	0.47
1:F:217:LYS:HB2	1:F:236:GLU:CD	2.35	0.47
2:Q:102:ALA:HB1	2:Q:121:VAL:CG1	2.45	0.47
2:Q:42:ASN:CG	2:Q:42:ASN:O	2.53	0.47
2:Q:58:ASP:HB2	2:Q:62:THR:O	2.15	0.47
1:D:523:LEU:HD22	2:R:127:GLU:HG2	1.97	0.47
2:T:9:ILE:HG23	2:T:69:LEU:CD2	2.44	0.47
1:A:115:LYS:NZ	1:A:117:LEU:HB2	2.29	0.47
1:A:311:HIS:O	1:A:312:ALA:C	2.51	0.47
1:A:722:ILE:O	1:A:726:ILE:HG13	2.15	0.47
1:B:115:LYS:NZ	1:B:117:LEU:HB2	2.29	0.47
1:B:533:LEU:C	1:B:533:LEU:HD23	2.34	0.47
1:B:597:ASN:CB	1:B:598:PRO:HD2	2.36	0.47
1:B:302:LEU:HD22	1:B:602:PHE:HE1	1.79	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:716:LYS:O	1:B:720:ILE:HG22	2.15	0.47
1:C:302:LEU:HD22	1:C:602:PHE:HE1	1.79	0.47
1:D:509:PRO:HG2	1:D:512:GLU:HG3	1.96	0.47
1:D:533:LEU:HD23	1:D:533:LEU:C	2.35	0.47
1:E:107:THR:HG21	1:E:115:LYS:CD	2.38	0.47
1:E:217:LYS:HB2	1:E:236:GLU:CD	2.34	0.47
1:E:404:LYS:O	1:E:405:LEU:C	2.51	0.47
1:E:432:TYR:CD1	1:E:445:ARG:NE	2.83	0.47
1:F:175:LYS:O	1:F:176:GLY:C	2.52	0.47
1:F:527:LYS:HG2	2:T:145:MSE:SE	2.65	0.47
1:F:75:THR:O	1:F:76:LEU:C	2.52	0.47
2:P:97:ASN:ND2	2:P:97:ASN:N	2.61	0.47
2:R:129:ASP:OD1	2:R:134:GLY:N	2.47	0.47
1:F:706:ASN:O	2:T:130:ILE:HG23	2.14	0.47
2:T:88:ALA:O	2:T:91:VAL:HB	2.14	0.47
1:A:172:GLU:CB	1:A:246:SER:HA	2.40	0.47
1:A:724:ARG:O	1:A:727:GLN:HB2	2.15	0.47
1:B:218:LEU:C	1:B:220:LEU:H	2.15	0.47
1:B:217:LYS:HB2	1:B:236:GLU:CD	2.35	0.47
1:C:692:GLU:HA	1:C:692:GLU:OE2	2.15	0.47
1:D:165:GLN:OE1	1:D:252:ASP:HB3	2.15	0.47
1:D:217:LYS:HB2	1:D:236:GLU:CD	2.35	0.47
1:D:666:ASN:HB2	1:D:748:TYR:OH	2.15	0.47
1:E:322:LEU:O	1:E:323:ASN:HB3	2.15	0.47
1:E:597:ASN:HD21	1:E:601:GLU:CB	2.09	0.47
1:F:175:LYS:HB2	1:F:175:LYS:HZ3	1.77	0.47
1:F:225:ILE:HG23	1:F:229:PHE:CD2	2.48	0.47
1:F:509:PRO:HG2	1:F:512:GLU:HG3	1.96	0.47
1:F:630:ARG:CZ	2:T:83:GLU:CG	2.88	0.47
1:F:692:GLU:OE1	2:T:21:LYS:NZ	2.47	0.47
2:O:9:ILE:HG23	2:O:69:LEU:CD2	2.44	0.47
2:P:102:ALA:HB1	2:P:121:VAL:CG1	2.45	0.47
2:P:138:TYR:CZ	2:P:142:VAL:CG2	2.98	0.47
2:P:93:ASP:OD1	2:P:97:ASN:ND2	2.48	0.47
2:Q:55:VAL:CB	2:Q:67:GLU:OE2	2.59	0.47
2:S:138:TYR:CZ	2:S:142:VAL:CG2	2.98	0.47
2:S:9:ILE:HG23	2:S:69:LEU:CD2	2.44	0.47
1:A:217:LYS:HB2	1:A:236:GLU:CD	2.35	0.47
1:B:165:GLN:OE1	1:B:252:ASP:HB3	2.14	0.47
1:B:175:LYS:HZ1	1:B:175:LYS:HB2	1.77	0.47
1:B:583:ASN:O	1:B:587:PRO:HD3	2.14	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:VAL:CG1	1:C:113:GLU:H	2.07	0.47
1:C:78:LYS:HD2	1:C:156:ILE:HD13	1.97	0.47
1:C:481:VAL:O	1:C:482:GLU:HB2	2.15	0.47
1:C:724:ARG:NH1	1:C:724:ARG:HG3	2.27	0.47
1:D:115:LYS:NZ	1:D:117:LEU:HB2	2.30	0.47
1:D:175:LYS:O	1:D:176:GLY:C	2.53	0.47
1:D:169:VAL:HG22	1:D:246:SER:HB2	1.96	0.47
1:D:365:PRO:HB2	1:D:367:ASP:O	2.14	0.47
1:E:620:THR:HG22	1:E:621:GLY:N	2.29	0.47
1:F:620:THR:HG22	1:F:621:GLY:N	2.30	0.47
1:F:692:GLU:HA	1:F:692:GLU:OE2	2.15	0.47
1:F:81:GLN:CD	1:F:156:ILE:HG21	2.35	0.47
2:O:42:ASN:O	2:O:42:ASN:CG	2.52	0.47
2:O:55:VAL:CB	2:O:67:GLU:OE2	2.59	0.47
2:P:146:THR:O	2:P:147:ALA:C	2.51	0.47
2:R:141:PHE:CZ	2:R:145:MSE:HE3	2.50	0.47
2:R:16:PHE:CE1	2:R:27:ILE:CD1	2.97	0.47
2:S:65:PHE:CD1	2:S:65:PHE:N	2.82	0.47
2:S:76:MSE:C	2:S:78:ASP:H	2.17	0.47
1:A:515:LYS:HZ3	1:A:516:VAL:HG23	1.79	0.47
1:A:509:PRO:HD2	1:A:536:TYR:CE2	2.50	0.47
1:A:565:LYS:C	1:A:567:THR:N	2.68	0.47
1:A:781:ASN:O	1:A:789:ASN:ND2	2.47	0.47
1:A:88:LYS:HD2	1:A:89:ILE:HG13	1.95	0.47
1:B:175:LYS:O	1:B:176:GLY:C	2.53	0.47
1:B:432:TYR:CD1	1:B:445:ARG:NE	2.83	0.47
1:B:686:ASP:O	1:B:689:ALA:HB3	2.14	0.47
1:B:692:GLU:HA	1:B:692:GLU:OE2	2.15	0.47
1:C:318:ILE:HG23	1:C:322:LEU:HD12	1.96	0.47
1:D:127:SER:O	1:D:133:GLU:CD	2.48	0.47
1:D:515:LYS:HZ1	1:D:516:VAL:CG2	2.27	0.47
1:D:567:THR:HG22	1:D:568:GLY:N	2.30	0.47
1:E:252:ASP:OD2	1:E:253:HIS:CD2	2.68	0.47
1:F:205:SER:C	1:F:207:ASP:H	2.17	0.47
1:F:597:ASN:HB2	1:F:598:PRO:CD	2.37	0.47
2:O:58:ASP:HB2	2:O:62:THR:O	2.15	0.47
2:O:81:SER:O	2:O:83:GLU:N	2.47	0.47
2:R:16:PHE:CE1	2:R:27:ILE:HD13	2.50	0.47
2:S:88:ALA:O	2:S:91:VAL:HB	2.15	0.47
2:T:109:MSE:HG3	2:T:116:LEU:CD1	2.43	0.47
1:A:127:SER:O	1:A:133:GLU:CD	2.48	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:PHE:H	1:A:141:PHE:HD1	1.63	0.47
1:A:315:PHE:HA	1:A:318:ILE:HD13	1.97	0.47
1:A:716:LYS:O	1:A:720:ILE:HG22	2.14	0.47
1:B:296:LEU:HD22	1:B:606:LYS:HE2	1.97	0.47
1:B:345:THR:O	1:B:479:LYS:HE2	2.15	0.47
1:C:176:GLY:O	1:C:178:SER:N	2.48	0.47
1:C:312:ALA:O	1:C:315:PHE:HB2	2.15	0.47
1:C:509:PRO:HG2	1:C:512:GLU:HG3	1.97	0.47
1:C:533:LEU:HD23	1:C:533:LEU:C	2.36	0.47
1:D:173:ILE:C	1:D:175:LYS:N	2.66	0.47
1:D:414:LYS:HZ3	1:D:414:LYS:HA	1.79	0.47
1:D:697:ILE:C	1:D:699:GLY:N	2.67	0.47
1:E:684:ASP:C	1:E:686:ASP:N	2.68	0.47
2:T:129:ASP:OD1	2:T:134:GLY:N	2.48	0.47
1:A:282:SER:HA	1:A:285:LYS:CD	2.44	0.46
1:A:509:PRO:HG2	1:A:512:GLU:HG3	1.96	0.46
1:B:102:GLY:HA3	1:B:150:PRO:HG2	1.97	0.46
1:C:175:LYS:HZ3	1:C:175:LYS:CB	2.28	0.46
1:C:275:GLY:CA	1:C:278:LYS:HE3	2.35	0.46
1:C:285:LYS:O	1:C:288:VAL:HG22	2.14	0.46
1:D:102:GLY:HA3	1:D:150:PRO:HG2	1.97	0.46
1:E:141:PHE:H	1:E:141:PHE:HD1	1.64	0.46
1:E:175:LYS:NZ	1:E:175:LYS:CB	2.76	0.46
1:E:329:ARG:HB3	1:E:330:PRO:CD	2.46	0.46
1:E:523:LEU:HD22	2:S:127:GLU:HG2	1.98	0.46
1:E:75:THR:O	1:E:76:LEU:C	2.52	0.46
1:F:176:GLY:O	1:F:178:SER:N	2.48	0.46
2:O:16:PHE:CE1	2:O:27:ILE:CD1	2.98	0.46
1:E:527:LYS:HG2	2:S:145:MSE:SE	2.65	0.46
2:T:97:ASN:ND2	2:T:99:TYR:H	2.13	0.46
1:A:357:TRP:CZ3	1:A:439:ASN:ND2	2.84	0.46
1:A:432:TYR:CD1	1:A:445:ARG:NE	2.84	0.46
1:A:481:VAL:O	1:A:482:GLU:HB2	2.15	0.46
1:A:697:ILE:O	1:A:699:GLY:N	2.47	0.46
1:B:173:ILE:O	1:B:174:GLY:C	2.53	0.46
1:B:462:ILE:CD1	1:B:466:GLY:HA2	2.42	0.46
1:C:210:PHE:HZ	1:C:221:ASN:OD1	1.99	0.46
1:C:217:LYS:HB2	1:C:236:GLU:CD	2.35	0.46
1:C:629:ASN:C	1:C:629:ASN:ND2	2.65	0.46
1:C:88:LYS:HD2	1:C:89:ILE:HG13	1.97	0.46
1:D:308:VAL:CG2	1:D:336:THR:O	2.63	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:481:VAL:O	1:D:482:GLU:HB2	2.16	0.46
1:E:275:GLY:CA	1:E:278:LYS:HE3	2.36	0.46
1:E:285:LYS:O	1:E:288:VAL:HG22	2.16	0.46
1:E:296:LEU:HD22	1:E:606:LYS:HE2	1.97	0.46
1:E:315:PHE:HA	1:E:318:ILE:HD13	1.98	0.46
1:E:357:TRP:CZ3	1:E:439:ASN:ND2	2.84	0.46
1:E:583:ASN:O	1:E:587:PRO:HD3	2.15	0.46
1:F:311:HIS:O	1:F:312:ALA:C	2.54	0.46
2:O:129:ASP:OD1	2:O:134:GLY:N	2.48	0.46
1:A:527:LYS:HG2	2:O:145:MSE:SE	2.65	0.46
2:P:121:VAL:C	2:P:123:GLN:H	2.17	0.46
2:P:81:SER:O	2:P:83:GLU:N	2.48	0.46
2:P:94:LYS:HB3	2:P:94:LYS:HZ2	1.79	0.46
2:Q:110:THR:O	2:Q:113:GLY:N	2.39	0.46
2:Q:81:SER:O	2:Q:83:GLU:N	2.47	0.46
2:Q:93:ASP:OD1	2:Q:97:ASN:ND2	2.48	0.46
1:A:244:ALA:HB3	1:A:268:MET:HE3	1.96	0.46
1:A:285:LYS:O	1:A:288:VAL:HG22	2.15	0.46
1:A:329:ARG:HB3	1:A:330:PRO:CD	2.46	0.46
1:A:597:ASN:CB	1:A:598:PRO:HD2	2.36	0.46
1:B:127:SER:O	1:B:133:GLU:CD	2.48	0.46
1:B:176:GLY:O	1:B:178:SER:N	2.48	0.46
1:B:700:TYR:CD1	1:B:727:GLN:HB3	2.51	0.46
1:C:175:LYS:NZ	1:C:175:LYS:CB	2.76	0.46
1:C:180:ASP:CG	1:C:181:ILE:H	2.18	0.46
1:C:583:ASN:O	1:C:587:PRO:HD3	2.15	0.46
1:C:639:ASN:N	1:C:639:ASN:ND2	2.52	0.46
1:C:735:VAL:O	1:C:741:ILE:HD13	2.14	0.46
1:D:106:PHE:CZ	1:D:171:TYR:OH	2.64	0.46
1:E:172:GLU:O	1:E:176:GLY:N	2.34	0.46
1:F:244:ALA:HB3	1:F:268:MET:HE3	1.97	0.46
1:F:169:VAL:HG22	1:F:246:SER:HB2	1.97	0.46
1:F:329:ARG:HB3	1:F:330:PRO:CD	2.46	0.46
2:O:109:MSE:HG3	2:O:116:LEU:CD1	2.42	0.46
2:O:146:THR:O	2:O:147:ALA:C	2.52	0.46
2:Q:59:GLY:O	2:Q:62:THR:HG23	2.12	0.46
2:R:58:ASP:HB2	2:R:62:THR:O	2.16	0.46
2:T:93:ASP:OD1	2:T:97:ASN:ND2	2.48	0.46
1:A:187:SER:C	1:A:188:LEU:O	2.44	0.46
1:A:337:ASN:C	1:A:339:ILE:N	2.67	0.46
1:A:602:PHE:N	1:A:602:PHE:CD2	2.83	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ASN:HB2	1:A:748:TYR:OH	2.15	0.46
1:B:446:ILE:HD11	1:B:451:ASN:CB	2.41	0.46
1:B:718:ARG:O	1:B:722:ILE:HG13	2.15	0.46
1:C:447:SER:OG	1:C:448:ASP:N	2.48	0.46
1:C:597:ASN:HB2	1:C:598:PRO:CD	2.38	0.46
1:D:81:GLN:CD	1:D:156:ILE:HG21	2.35	0.46
1:E:165:GLN:OE1	1:E:252:ASP:HB3	2.15	0.46
1:E:602:PHE:N	1:E:602:PHE:CD2	2.84	0.46
1:E:540:ARG:NH1	1:E:627:TYR:CE1	2.83	0.46
1:F:210:PHE:HZ	1:F:221:ASN:OD1	1.98	0.46
1:F:296:LEU:HD22	1:F:606:LYS:HE2	1.98	0.46
1:F:481:VAL:O	1:F:482:GLU:HB2	2.15	0.46
2:O:28:THR:CB	2:O:30:LYS:HZ1	2.29	0.46
2:P:65:PHE:CD1	2:P:65:PHE:N	2.81	0.46
2:Q:146:THR:O	2:Q:147:ALA:C	2.51	0.46
2:Q:88:ALA:O	2:Q:91:VAL:HB	2.15	0.46
2:R:121:VAL:C	2:R:123:GLN:H	2.16	0.46
2:S:121:VAL:C	2:S:123:GLN:H	2.17	0.46
2:T:39:LEU:HD23	2:T:39:LEU:HA	1.75	0.46
1:A:717:LYS:O	1:A:720:ILE:HG22	2.15	0.46
1:B:115:LYS:HB3	1:B:115:LYS:HZ3	1.80	0.46
1:B:141:PHE:HD1	1:B:141:PHE:H	1.64	0.46
1:B:282:SER:HA	1:B:285:LYS:CD	2.44	0.46
1:B:329:ARG:HB3	1:B:330:PRO:CD	2.46	0.46
1:B:722:ILE:O	1:B:726:ILE:HG13	2.16	0.46
1:C:165:GLN:C	1:C:167:LYS:N	2.69	0.46
1:C:227:ILE:HG22	1:C:227:ILE:O	2.15	0.46
1:C:329:ARG:HB3	1:C:330:PRO:CD	2.45	0.46
1:C:565:LYS:C	1:C:567:THR:N	2.69	0.46
1:C:666:ASN:HB2	1:C:748:TYR:OH	2.16	0.46
1:C:81:GLN:CD	1:C:156:ILE:HG21	2.36	0.46
1:D:175:LYS:CB	1:D:175:LYS:NZ	2.76	0.46
1:D:176:GLY:O	1:D:178:SER:N	2.48	0.46
1:D:397:GLU:HA	1:D:480:ASN:HB2	1.96	0.46
1:D:565:LYS:C	1:D:567:THR:N	2.68	0.46
1:E:227:ILE:HG22	1:E:227:ILE:O	2.15	0.46
1:E:692:GLU:OE2	1:E:692:GLU:HA	2.15	0.46
1:E:709:ASN:O	1:E:717:LYS:HE3	2.16	0.46
1:F:173:ILE:O	1:F:174:GLY:C	2.54	0.46
1:F:180:ASP:CG	1:F:181:ILE:H	2.19	0.46
1:F:187:SER:C	1:F:188:LEU:O	2.44	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:323:ASN:C	1:F:324:THR:CG2	2.84	0.46
1:F:432:TYR:CD1	1:F:445:ARG:NE	2.84	0.46
1:F:529:VAL:O	1:F:532:LEU:HB2	2.16	0.46
1:F:602:PHE:CD2	1:F:602:PHE:N	2.83	0.46
1:F:540:ARG:NH1	1:F:627:TYR:CE1	2.83	0.46
1:F:697:ILE:HG12	1:F:732:ILE:HD13	1.98	0.46
1:F:746:LYS:HG2	1:F:750:GLN:HE21	1.81	0.46
2:P:66:PRO:O	2:P:67:GLU:C	2.54	0.46
2:R:66:PRO:O	2:R:67:GLU:C	2.54	0.46
2:S:13:LYS:O	2:S:14:GLU:C	2.54	0.46
2:T:66:PRO:O	2:T:67:GLU:C	2.54	0.46
2:T:81:SER:O	2:T:83:GLU:N	2.48	0.46
1:A:112:VAL:CG1	1:A:113:GLU:H	2.07	0.46
1:B:285:LYS:O	1:B:288:VAL:HG22	2.16	0.46
1:B:529:VAL:O	1:B:532:LEU:HB2	2.16	0.46
1:B:81:GLN:CD	1:B:156:ILE:HG21	2.35	0.46
1:C:134:LYS:NZ	1:C:136:PRO:HG3	2.30	0.46
1:C:397:GLU:HA	1:C:480:ASN:HB2	1.97	0.46
1:C:515:LYS:HZ3	1:C:516:VAL:CG2	2.29	0.46
1:C:527:LYS:HG2	2:Q:145:MSE:SE	2.66	0.46
1:D:134:LYS:NZ	1:D:136:PRO:HG3	2.31	0.46
1:D:282:SER:HA	1:D:285:LYS:CD	2.45	0.46
1:E:180:ASP:CG	1:E:181:ILE:H	2.19	0.46
1:F:183:SER:HB3	1:F:184:LYS:H	1.51	0.46
1:F:218:LEU:C	1:F:220:LEU:H	2.15	0.46
1:B:533:LEU:HD12	2:P:112:LEU:HD11	1.97	0.46
2:Q:141:PHE:CZ	2:Q:145:MSE:HE3	2.51	0.46
2:R:28:THR:OG1	2:R:30:LYS:HE2	2.16	0.46
1:A:218:LEU:C	1:A:220:LEU:H	2.16	0.46
1:A:210:PHE:HZ	1:A:221:ASN:OD1	1.98	0.46
1:A:238:GLN:O	1:A:240:ALA:N	2.49	0.46
1:A:93:VAL:HG23	1:A:179:LEU:CD1	2.40	0.46
1:B:210:PHE:HZ	1:B:221:ASN:OD1	1.98	0.46
1:B:337:ASN:C	1:B:339:ILE:N	2.67	0.46
1:B:509:PRO:HD2	1:B:536:TYR:CE2	2.51	0.46
1:B:602:PHE:N	1:B:602:PHE:CD2	2.84	0.46
1:B:662:GLU:OE2	1:B:755:ARG:NH2	2.39	0.46
1:C:102:GLY:HA3	1:C:150:PRO:HG2	1.97	0.46
1:C:141:PHE:HD1	1:C:141:PHE:H	1.63	0.46
1:C:172:GLU:O	1:C:176:GLY:N	2.34	0.46
1:C:173:ILE:O	1:C:174:GLY:C	2.54	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:PHE:HA	1:C:318:ILE:HD13	1.97	0.46
1:C:446:ILE:HD11	1:C:451:ASN:CB	2.41	0.46
1:D:315:PHE:HA	1:D:318:ILE:HD13	1.97	0.46
1:E:102:GLY:HA3	1:E:150:PRO:HG2	1.96	0.46
1:E:357:TRP:CH2	1:E:439:ASN:ND2	2.84	0.46
1:E:509:PRO:HD2	1:E:536:TYR:CE2	2.51	0.46
1:E:718:ARG:O	1:E:722:ILE:HG13	2.15	0.46
1:F:134:LYS:NZ	1:F:136:PRO:HG3	2.31	0.46
1:F:312:ALA:O	1:F:315:PHE:HB2	2.16	0.46
1:F:552:TRP:O	1:F:553:GLN:C	2.54	0.46
1:F:700:TYR:CD1	1:F:727:GLN:HB3	2.50	0.46
2:P:55:VAL:CB	2:P:67:GLU:OE2	2.57	0.46
2:Q:49:GLN:O	2:Q:53:ASN:N	2.43	0.46
2:Q:66:PRO:O	2:Q:67:GLU:C	2.54	0.46
2:R:105:LEU:HD21	2:R:124:MSE:SE	2.66	0.46
2:R:138:TYR:CZ	2:R:142:VAL:CG2	2.99	0.46
1:A:281:GLU:C	1:A:283:LEU:N	2.69	0.46
1:A:323:ASN:C	1:A:324:THR:CG2	2.84	0.46
1:A:529:VAL:O	1:A:532:LEU:HB2	2.16	0.46
1:A:492:TYR:CE2	1:A:574:VAL:HG21	2.51	0.46
1:A:597:ASN:HB2	1:A:598:PRO:CD	2.37	0.46
1:A:684:ASP:C	1:A:686:ASP:N	2.69	0.46
1:B:78:LYS:HD2	1:B:156:ILE:HD13	1.98	0.46
1:B:403:LEU:CD2	1:B:474:ILE:HG21	2.46	0.46
1:B:684:ASP:C	1:B:686:ASP:N	2.69	0.46
1:B:88:LYS:HD2	1:B:89:ILE:HG13	1.97	0.46
1:D:115:LYS:HZ1	1:D:117:LEU:HB2	1.81	0.46
1:D:141:PHE:HD1	1:D:141:PHE:N	2.14	0.46
1:D:620:THR:HG22	1:D:621:GLY:N	2.30	0.46
1:E:357:TRP:CZ3	1:E:439:ASN:HB2	2.51	0.46
1:E:357:TRP:HZ3	1:E:439:ASN:HB2	1.81	0.46
1:E:533:LEU:C	1:E:533:LEU:HD23	2.36	0.46
1:F:285:LYS:O	1:F:288:VAL:HG22	2.16	0.46
1:F:405:LEU:H	1:F:405:LEU:CD1	2.27	0.46
1:F:724:ARG:NH1	1:F:724:ARG:HG3	2.30	0.46
1:F:781:ASN:O	1:F:789:ASN:ND2	2.47	0.46
2:Q:9:ILE:CD1	2:Q:69:LEU:HD11	2.38	0.46
2:R:81:SER:O	2:R:83:GLU:N	2.48	0.46
1:A:115:LYS:HZ1	1:A:117:LEU:HB2	1.80	0.46
1:A:123:GLU:CG	1:A:124:GLU:N	2.79	0.46
1:A:165:GLN:C	1:A:167:LYS:N	2.69	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:ILE:HG12	1:A:732:ILE:HD13	1.98	0.46
1:A:99:GLU:C	1:A:101:GLY:H	2.19	0.46
1:B:173:ILE:C	1:B:175:LYS:N	2.66	0.46
1:B:312:ALA:O	1:B:315:PHE:HB2	2.16	0.46
1:B:404:LYS:O	1:B:405:LEU:C	2.52	0.46
1:B:781:ASN:O	1:B:789:ASN:ND2	2.46	0.46
1:C:323:ASN:C	1:C:324:THR:CG2	2.84	0.46
1:C:357:TRP:HZ3	1:C:439:ASN:HB2	1.81	0.46
1:D:318:ILE:HD12	1:D:318:ILE:N	2.25	0.46
1:D:492:TYR:CE2	1:D:574:VAL:HG21	2.51	0.46
1:D:602:PHE:N	1:D:602:PHE:CD2	2.84	0.46
1:E:176:GLY:O	1:E:178:SER:N	2.48	0.46
1:E:197:LYS:HB3	1:E:197:LYS:NZ	2.26	0.46
1:E:299:GLU:HA	1:E:302:LEU:HB3	1.98	0.46
1:E:403:LEU:CD2	1:E:474:ILE:HG21	2.46	0.46
1:E:565:LYS:C	1:E:567:THR:N	2.69	0.46
1:E:635:ILE:N	1:E:635:ILE:CD1	2.72	0.46
1:E:746:LYS:HG2	1:E:750:GLN:HE21	1.81	0.46
1:F:552:TRP:HA	1:F:555:GLN:HG2	1.98	0.46
2:P:13:LYS:O	2:P:14:GLU:C	2.54	0.46
2:P:42:ASN:O	2:P:42:ASN:CG	2.53	0.46
2:Q:56:ASP:CG	2:Q:60:ASN:HA	2.34	0.46
2:R:24:ASP:CG	2:R:25:GLY:H	2.19	0.46
1:E:533:LEU:HD12	2:S:112:LEU:HD11	1.97	0.46
2:S:66:PRO:O	2:S:67:GLU:C	2.54	0.46
1:A:180:ASP:CG	1:A:181:ILE:H	2.18	0.46
1:A:405:LEU:HD13	1:A:453:VAL:CG2	2.33	0.46
1:A:357:TRP:CZ3	1:A:439:ASN:HB2	2.52	0.46
1:A:357:TRP:HZ3	1:A:439:ASN:HB2	1.81	0.46
1:A:552:TRP:O	1:A:553:GLN:C	2.53	0.46
1:B:318:ILE:HG23	1:B:322:LEU:HD12	1.98	0.46
1:B:478:ALA:CB	1:B:486:LYS:O	2.61	0.46
1:B:581:GLN:HB3	1:B:627:TYR:HE1	1.81	0.46
1:B:739:LYS:CG	1:B:740:GLN:H	2.26	0.46
1:C:173:ILE:C	1:C:175:LYS:N	2.67	0.46
1:C:414:LYS:HA	1:C:414:LYS:HZ3	1.81	0.46
1:C:432:TYR:CD1	1:C:445:ARG:NE	2.84	0.46
1:D:281:GLU:C	1:D:283:LEU:N	2.69	0.46
1:D:552:TRP:O	1:D:553:GLN:C	2.53	0.46
1:D:629:ASN:HB3	1:D:632:TYR:CE1	2.51	0.46
1:D:700:TYR:CD1	1:D:727:GLN:HB3	2.51	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:492:TYR:CE2	1:E:574:VAL:HG21	2.51	0.46
1:F:165:GLN:OE1	1:F:252:ASP:HB3	2.15	0.46
1:F:227:ILE:O	1:F:227:ILE:HG22	2.16	0.46
1:F:515:LYS:HZ3	1:F:516:VAL:HG23	1.81	0.46
1:F:533:LEU:HD23	1:F:533:LEU:C	2.36	0.46
1:F:565:LYS:C	1:F:567:THR:N	2.68	0.46
2:Q:16:PHE:CE1	2:Q:27:ILE:HD13	2.50	0.46
2:Q:28:THR:OG1	2:Q:30:LYS:HE2	2.16	0.46
2:T:28:THR:OG1	2:T:30:LYS:HE2	2.16	0.46
2:T:59:GLY:O	2:T:62:THR:CG2	2.64	0.46
1:A:299:GLU:HA	1:A:302:LEU:HB3	1.99	0.45
1:A:395:GLU:O	1:A:395:GLU:OE1	2.34	0.45
1:B:278:LYS:O	1:B:281:GLU:N	2.49	0.45
1:B:323:ASN:C	1:B:324:THR:CG2	2.84	0.45
1:B:527:LYS:HG2	2:P:145:MSE:SE	2.65	0.45
1:B:756:ILE:HG12	1:B:756:ILE:H	1.64	0.45
1:C:492:TYR:CE2	1:C:574:VAL:HG21	2.51	0.45
1:C:580:GLU:O	1:C:583:ASN:HB2	2.16	0.45
1:C:778:LYS:HB3	1:C:778:LYS:HE3	1.76	0.45
1:E:141:PHE:N	1:E:141:PHE:HD1	2.14	0.45
1:E:210:PHE:HZ	1:E:221:ASN:OD1	1.98	0.45
1:E:296:LEU:O	1:E:301:ALA:HB2	2.17	0.45
1:E:323:ASN:C	1:E:324:THR:CG2	2.84	0.45
1:E:337:ASN:C	1:E:339:ILE:N	2.69	0.45
1:E:700:TYR:CD1	1:E:727:GLN:HB3	2.52	0.45
2:O:138:TYR:CZ	2:O:142:VAL:HG21	2.51	0.45
2:S:129:ASP:OD1	2:S:134:GLY:N	2.48	0.45
2:S:16:PHE:CE1	2:S:27:ILE:HD13	2.52	0.45
2:T:138:TYR:CZ	2:T:142:VAL:CG2	2.99	0.45
1:A:345:THR:O	1:A:479:LYS:HE2	2.17	0.45
1:A:391:ILE:CG1	1:A:399:GLY:HA2	2.43	0.45
1:A:443:GLU:HG3	1:A:458:LYS:HZ2	1.82	0.45
1:A:478:ALA:CB	1:A:486:LYS:O	2.62	0.45
1:A:686:ASP:O	1:A:689:ALA:HB3	2.15	0.45
1:B:318:ILE:N	1:B:318:ILE:HD12	2.24	0.45
1:C:234:LEU:HD23	1:C:234:LEU:N	2.32	0.45
1:C:252:ASP:OD2	1:C:253:HIS:CD2	2.70	0.45
1:D:180:ASP:CG	1:D:181:ILE:H	2.19	0.45
1:D:684:ASP:C	1:D:686:ASP:N	2.70	0.45
1:F:152:LEU:HD21	1:F:154:ILE:HD11	1.99	0.45
1:F:279:ILE:HG22	1:F:283:LEU:HD13	1.99	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:443:GLU:HG3	1:F:458:LYS:HZ2	1.79	0.45
2:O:13:LYS:O	2:O:14:GLU:C	2.53	0.45
2:O:16:PHE:CE1	2:O:27:ILE:HD13	2.52	0.45
2:O:94:LYS:HB3	2:O:94:LYS:HZ2	1.80	0.45
2:P:28:THR:OG1	2:P:30:LYS:HE2	2.16	0.45
1:C:533:LEU:HD12	2:Q:112:LEU:HD11	1.98	0.45
2:S:102:ALA:HB1	2:S:121:VAL:CG1	2.46	0.45
2:S:16:PHE:CE1	2:S:27:ILE:CD1	2.98	0.45
1:A:296:LEU:O	1:A:301:ALA:HB2	2.16	0.45
1:A:552:TRP:HA	1:A:555:GLN:HG2	1.97	0.45
1:A:581:GLN:HB3	1:A:627:TYR:HE1	1.82	0.45
1:A:629:ASN:HB3	1:A:632:TYR:CE1	2.51	0.45
1:B:175:LYS:HB2	1:B:175:LYS:HZ2	1.82	0.45
1:B:357:TRP:CZ3	1:B:439:ASN:HB2	2.52	0.45
1:C:104:ILE:HG23	1:C:152:LEU:CD2	2.47	0.45
1:C:141:PHE:N	1:C:141:PHE:HD1	2.14	0.45
1:C:307:LEU:H	1:C:307:LEU:CD1	2.29	0.45
1:D:529:VAL:O	1:D:532:LEU:HB2	2.16	0.45
1:D:697:ILE:O	1:D:699:GLY:N	2.50	0.45
1:E:311:HIS:O	1:E:314:ALA:N	2.49	0.45
1:E:611:THR:HG22	1:E:615:ILE:HD11	1.98	0.45
1:F:141:PHE:N	1:F:141:PHE:HD1	2.14	0.45
1:F:333:LYS:HA	1:F:336:THR:OG1	2.17	0.45
1:F:357:TRP:CH2	1:F:439:ASN:ND2	2.85	0.45
1:F:550:SER:HB3	1:F:553:GLN:CG	2.38	0.45
1:F:778:LYS:HE3	1:F:778:LYS:HB3	1.76	0.45
2:P:24:ASP:CG	2:P:25:GLY:H	2.20	0.45
2:Q:138:TYR:CZ	2:Q:142:VAL:CG2	2.99	0.45
2:T:16:PHE:CE1	2:T:27:ILE:HD13	2.51	0.45
1:A:227:ILE:HG22	1:A:227:ILE:O	2.16	0.45
1:A:357:TRP:CH2	1:A:439:ASN:ND2	2.84	0.45
1:A:515:LYS:HZ1	1:A:516:VAL:CG2	2.30	0.45
1:A:597:ASN:HD21	1:A:601:GLU:CB	2.09	0.45
1:B:238:GLN:O	1:B:240:ALA:N	2.50	0.45
1:B:299:GLU:HA	1:B:302:LEU:HB3	1.99	0.45
1:B:492:TYR:CE2	1:B:574:VAL:HG21	2.52	0.45
1:B:509:PRO:HG2	1:B:512:GLU:HG3	1.98	0.45
1:B:660:SER:O	1:B:663:PHE:HB3	2.17	0.45
1:C:684:ASP:C	1:C:686:ASP:N	2.69	0.45
1:D:141:PHE:H	1:D:141:PHE:HD1	1.63	0.45
1:D:299:GLU:HA	1:D:302:LEU:HB3	1.98	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:LYS:HB3	1:E:115:LYS:HZ3	1.81	0.45
1:E:78:LYS:HD2	1:E:156:ILE:HD13	1.99	0.45
1:E:345:THR:O	1:E:479:LYS:HE2	2.16	0.45
1:E:481:VAL:O	1:E:482:GLU:HB2	2.15	0.45
1:E:552:TRP:O	1:E:553:GLN:C	2.54	0.45
1:E:629:ASN:HB3	1:E:632:TYR:CE1	2.52	0.45
1:F:684:ASP:C	1:F:686:ASP:N	2.69	0.45
1:F:739:LYS:HG2	1:F:740:GLN:N	2.30	0.45
2:O:66:PRO:O	2:O:67:GLU:C	2.54	0.45
2:P:97:ASN:ND2	2:P:99:TYR:H	2.14	0.45
1:A:375:GLY:O	1:A:377:GLN:N	2.49	0.45
1:A:611:THR:HG22	1:A:615:ILE:HD11	1.97	0.45
1:C:165:GLN:OE1	1:C:252:ASP:HB3	2.16	0.45
1:C:700:TYR:CD1	1:C:727:GLN:HB3	2.51	0.45
1:D:104:ILE:HG23	1:D:152:LEU:CD2	2.47	0.45
1:D:165:GLN:C	1:D:167:LYS:N	2.70	0.45
1:D:709:ASN:O	1:D:717:LYS:HE3	2.16	0.45
1:E:281:GLU:C	1:E:283:LEU:N	2.70	0.45
1:E:278:LYS:O	1:E:281:GLU:N	2.49	0.45
1:E:297:LYS:NZ	1:E:297:LYS:HB3	2.32	0.45
1:E:325:TYR:CD1	1:E:598:PRO:HD3	2.52	0.45
1:E:478:ALA:CB	1:E:486:LYS:O	2.63	0.45
1:F:278:LYS:CB	1:F:279:ILE:HD13	2.47	0.45
2:O:102:ALA:HB1	2:O:121:VAL:CG1	2.46	0.45
2:O:28:THR:OG1	2:O:30:LYS:HE2	2.17	0.45
2:P:69:LEU:O	2:P:69:LEU:HD12	2.17	0.45
1:D:527:LYS:HG2	2:R:145:MSE:SE	2.66	0.45
2:R:42:ASN:O	2:R:42:ASN:CG	2.53	0.45
2:S:105:LEU:HD21	2:S:124:MSE:SE	2.67	0.45
1:F:523:LEU:HD22	2:T:127:GLU:HG2	1.99	0.45
1:A:403:LEU:CD2	1:A:474:ILE:HG21	2.47	0.45
1:C:602:PHE:N	1:C:602:PHE:CD2	2.84	0.45
1:D:278:LYS:O	1:D:281:GLU:N	2.49	0.45
1:D:318:ILE:HG23	1:D:322:LEU:HD12	1.97	0.45
1:D:611:THR:HG22	1:D:615:ILE:HD11	1.98	0.45
1:D:697:ILE:HG12	1:D:732:ILE:HD13	1.99	0.45
1:F:238:GLN:C	1:F:240:ALA:H	2.20	0.45
1:F:238:GLN:O	1:F:240:ALA:N	2.50	0.45
1:F:296:LEU:O	1:F:301:ALA:HB2	2.17	0.45
2:O:121:VAL:C	2:O:123:GLN:H	2.18	0.45
2:Q:24:ASP:CG	2:Q:25:GLY:H	2.20	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:46:ALA:HA	2:Q:49:GLN:NE2	2.32	0.45
2:S:56:ASP:CG	2:S:60:ASN:HA	2.36	0.45
2:S:3:GLN:N	2:S:77:LYS:HD3	2.32	0.45
2:S:81:SER:O	2:S:83:GLU:N	2.50	0.45
2:T:13:LYS:O	2:T:14:GLU:C	2.55	0.45
1:A:307:LEU:CD1	1:A:307:LEU:H	2.29	0.45
1:A:759:GLN:NE2	1:A:762:LEU:HD23	2.32	0.45
1:B:100:LEU:HD13	1:B:182:ILE:HG21	1.99	0.45
1:B:447:SER:OG	1:B:448:ASP:N	2.49	0.45
1:B:565:LYS:C	1:B:567:THR:N	2.68	0.45
1:C:275:GLY:CA	1:C:278:LYS:HG3	2.43	0.45
1:C:278:LYS:O	1:C:281:GLU:N	2.49	0.45
1:C:279:ILE:HG22	1:C:283:LEU:HD13	1.98	0.45
1:C:337:ASN:C	1:C:339:ILE:N	2.67	0.45
1:C:357:TRP:CH2	1:C:439:ASN:ND2	2.85	0.45
1:C:709:ASN:O	1:C:717:LYS:HE3	2.16	0.45
1:D:112:VAL:CG1	1:D:113:GLU:H	2.07	0.45
1:D:238:GLN:O	1:D:240:ALA:N	2.49	0.45
1:D:307:LEU:CD1	1:D:307:LEU:H	2.30	0.45
1:D:357:TRP:CZ3	1:D:439:ASN:HB2	2.51	0.45
1:D:357:TRP:CH2	1:D:439:ASN:ND2	2.85	0.45
1:E:183:SER:HB3	1:E:184:LYS:H	1.51	0.45
1:E:275:GLY:CA	1:E:278:LYS:HG3	2.44	0.45
1:E:552:TRP:HA	1:E:555:GLN:HG2	1.99	0.45
1:F:123:GLU:CG	1:F:124:GLU:N	2.80	0.45
1:F:165:GLN:C	1:F:167:LYS:N	2.69	0.45
1:F:278:LYS:HB2	1:F:279:ILE:CD1	2.47	0.45
1:F:318:ILE:HG23	1:F:322:LEU:HD12	1.98	0.45
2:Q:109:MSE:HG3	2:Q:116:LEU:CD1	2.44	0.45
2:R:61:GLY:C	2:R:62:THR:HG22	2.36	0.45
2:S:24:ASP:CG	2:S:25:GLY:H	2.19	0.45
2:S:69:LEU:O	2:S:69:LEU:HD12	2.17	0.45
1:A:141:PHE:N	1:A:141:PHE:HD1	2.14	0.45
1:A:718:ARG:O	1:A:722:ILE:HG13	2.17	0.45
1:B:122:GLU:HG3	1:B:147:ARG:H	1.81	0.45
1:B:397:GLU:HA	1:B:480:ASN:HB2	1.98	0.45
1:B:746:LYS:HG2	1:B:750:GLN:HE21	1.82	0.45
1:B:759:GLN:NE2	1:B:762:LEU:HD23	2.32	0.45
1:C:238:GLN:C	1:C:240:ALA:H	2.20	0.45
1:C:281:GLU:C	1:C:283:LEU:N	2.70	0.45
1:C:299:GLU:HA	1:C:302:LEU:HB3	1.98	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:SER:O	1:C:331:VAL:HG23	2.17	0.45
1:C:403:LEU:CD2	1:C:474:ILE:HG21	2.46	0.45
1:C:529:VAL:O	1:C:532:LEU:HB2	2.17	0.45
1:D:285:LYS:O	1:D:288:VAL:HG22	2.16	0.45
1:D:403:LEU:CD2	1:D:474:ILE:HG21	2.46	0.45
1:D:515:LYS:HZ3	1:D:516:VAL:HG23	1.82	0.45
1:D:579:THR:O	1:D:581:GLN:N	2.49	0.45
1:E:199:LEU:C	1:E:201:ASP:N	2.67	0.45
1:E:279:ILE:HG22	1:E:283:LEU:HD13	1.99	0.45
1:E:666:ASN:HB2	1:E:748:TYR:OH	2.16	0.45
1:F:78:LYS:HD2	1:F:156:ILE:HD13	1.98	0.45
1:F:275:GLY:O	1:F:278:LYS:HB2	2.17	0.45
1:F:297:LYS:NZ	1:F:297:LYS:HB3	2.32	0.45
1:F:398:ILE:HD13	1:F:479:LYS:HA	1.99	0.45
1:F:447:SER:OG	1:F:448:ASP:N	2.50	0.45
1:F:666:ASN:HB2	1:F:748:TYR:OH	2.16	0.45
2:O:141:PHE:CZ	2:O:145:MSE:HE3	2.52	0.45
1:D:533:LEU:HD12	2:R:112:LEU:HD11	1.99	0.45
2:T:49:GLN:O	2:T:53:ASN:N	2.44	0.45
1:A:104:ILE:HG23	1:A:152:LEU:CD2	2.47	0.45
1:A:275:GLY:O	1:A:278:LYS:HB2	2.17	0.45
1:A:709:ASN:O	1:A:717:LYS:HE3	2.16	0.45
1:B:552:TRP:HA	1:B:555:GLN:HG2	1.98	0.45
1:C:697:ILE:HD13	1:C:732:ILE:HD13	1.99	0.45
1:D:123:GLU:CG	1:D:124:GLU:N	2.79	0.45
1:D:329:ARG:HB3	1:D:330:PRO:CD	2.46	0.45
1:E:165:GLN:C	1:E:167:LYS:N	2.69	0.45
1:E:238:GLN:C	1:E:240:ALA:H	2.20	0.45
1:E:307:LEU:H	1:E:307:LEU:CD1	2.29	0.45
1:E:376:GLN:O	1:E:380:VAL:HG23	2.17	0.45
1:E:90:PRO:O	1:E:93:VAL:N	2.50	0.45
1:F:175:LYS:HZ3	1:F:175:LYS:CB	2.30	0.45
1:F:275:GLY:CA	1:F:278:LYS:HG3	2.43	0.45
1:F:337:ASN:C	1:F:339:ILE:N	2.69	0.45
1:F:357:TRP:CZ3	1:F:439:ASN:ND2	2.85	0.45
1:F:375:GLY:O	1:F:377:GLN:N	2.50	0.45
1:F:444:PHE:N	1:F:444:PHE:CD1	2.85	0.45
1:F:492:TYR:CE2	1:F:574:VAL:HG21	2.52	0.45
1:F:581:GLN:HB3	1:F:627:TYR:HE1	1.82	0.45
2:Q:97:ASN:ND2	2:Q:99:TYR:H	2.14	0.45
2:S:97:ASN:ND2	2:S:97:ASN:N	2.60	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PRO:HG2	1:A:139:SER:OG	2.17	0.45
1:A:278:LYS:O	1:A:281:GLU:N	2.50	0.45
1:A:376:GLN:O	1:A:380:VAL:HG23	2.17	0.45
1:A:580:GLU:O	1:A:583:ASN:HB2	2.17	0.45
1:B:141:PHE:HD1	1:B:141:PHE:N	2.14	0.45
1:B:296:LEU:O	1:B:301:ALA:HB2	2.17	0.45
1:B:395:GLU:OE1	1:B:395:GLU:O	2.35	0.45
1:B:552:TRP:O	1:B:553:GLN:C	2.53	0.45
1:B:611:THR:HG22	1:B:615:ILE:HD11	1.99	0.45
1:B:622:LYS:HD3	1:B:622:LYS:HA	1.51	0.45
1:B:697:ILE:O	1:B:699:GLY:N	2.47	0.45
1:C:636:ALA:HA	1:C:637:PRO:HD3	1.85	0.45
1:C:746:LYS:HG2	1:C:750:GLN:HE21	1.82	0.45
1:D:186:LYS:O	1:D:186:LYS:HG2	2.17	0.45
1:D:279:ILE:HG22	1:D:283:LEU:HD13	1.98	0.45
1:D:357:TRP:HZ3	1:D:439:ASN:HB2	1.82	0.45
1:D:391:ILE:CG1	1:D:399:GLY:HA2	2.40	0.45
1:D:759:GLN:NE2	1:D:762:LEU:HD23	2.32	0.45
1:E:238:GLN:O	1:E:240:ALA:N	2.50	0.45
1:F:403:LEU:CD2	1:F:474:ILE:HG21	2.46	0.45
1:F:660:SER:O	1:F:663:PHE:HB3	2.16	0.45
2:O:65:PHE:CB	2:O:66:PRO:HD3	2.38	0.45
2:P:49:GLN:O	2:P:53:ASN:N	2.43	0.45
2:P:3:GLN:N	2:P:77:LYS:HD3	2.32	0.45
2:Q:69:LEU:O	2:Q:69:LEU:HD12	2.17	0.45
2:R:39:LEU:HA	2:R:39:LEU:HD23	1.74	0.45
2:R:97:ASN:ND2	2:R:99:TYR:H	2.15	0.45
1:A:697:ILE:C	1:A:699:GLY:N	2.67	0.44
1:B:165:GLN:C	1:B:167:LYS:N	2.70	0.44
1:B:227:ILE:HG22	1:B:227:ILE:O	2.16	0.44
1:B:234:LEU:N	1:B:234:LEU:HD23	2.31	0.44
1:B:376:GLN:O	1:B:378:LEU:N	2.50	0.44
1:B:93:VAL:HG23	1:B:179:LEU:CD1	2.40	0.44
1:C:296:LEU:O	1:C:301:ALA:HB2	2.16	0.44
1:C:76:LEU:N	1:C:76:LEU:CD2	2.80	0.44
1:C:90:PRO:O	1:C:93:VAL:N	2.50	0.44
1:D:182:ILE:HD13	1:D:182:ILE:O	2.17	0.44
1:D:227:ILE:HG22	1:D:227:ILE:O	2.15	0.44
1:D:375:GLY:O	1:D:377:GLN:N	2.50	0.44
1:D:443:GLU:HG3	1:D:458:LYS:HZ2	1.83	0.44
1:D:772:GLU:O	1:D:773:PHE:C	2.55	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:509:PRO:HG2	1:E:512:GLU:HG3	1.99	0.44
1:E:772:GLU:O	1:E:773:PHE:C	2.56	0.44
1:F:154:ILE:CG1	1:F:171:TYR:CE1	2.88	0.44
1:F:186:LYS:O	1:F:186:LYS:HG2	2.17	0.44
1:F:622:LYS:HD3	1:F:622:LYS:HA	1.51	0.44
1:F:629:ASN:HB3	1:F:632:TYR:CE1	2.52	0.44
1:A:135:VAL:N	1:A:136:PRO:CD	2.81	0.44
1:A:297:LYS:NZ	1:A:297:LYS:HB3	2.32	0.44
1:A:447:SER:OG	1:A:448:ASP:N	2.49	0.44
1:B:307:LEU:CD1	1:B:307:LEU:H	2.29	0.44
1:B:424:LYS:HB3	1:B:424:LYS:NZ	2.32	0.44
1:B:772:GLU:O	1:B:773:PHE:C	2.56	0.44
1:C:345:THR:O	1:C:479:LYS:HE2	2.16	0.44
1:C:552:TRP:HA	1:C:555:GLN:HG2	1.99	0.44
1:D:172:GLU:O	1:D:176:GLY:N	2.34	0.44
1:D:252:ASP:OD2	1:D:253:HIS:CD2	2.70	0.44
1:D:444:PHE:CD1	1:D:444:PHE:N	2.85	0.44
1:D:325:TYR:CD1	1:D:598:PRO:HD3	2.52	0.44
1:E:148:GLU:CG	1:E:149:THR:N	2.75	0.44
1:E:318:ILE:HG23	1:E:322:LEU:HD12	1.98	0.44
1:E:376:GLN:O	1:E:378:LEU:N	2.50	0.44
1:E:529:VAL:O	1:E:532:LEU:HB2	2.17	0.44
1:E:785:ASN:OD1	1:E:785:ASN:O	2.35	0.44
1:F:234:LEU:HD23	1:F:234:LEU:N	2.32	0.44
1:F:307:LEU:CD1	1:F:307:LEU:H	2.30	0.44
1:F:318:ILE:H	1:F:318:ILE:CD1	2.27	0.44
1:F:509:PRO:HD2	1:F:536:TYR:CE2	2.52	0.44
1:F:709:ASN:O	1:F:717:LYS:HE3	2.17	0.44
1:F:90:PRO:O	1:F:93:VAL:N	2.51	0.44
2:Q:105:LEU:HD21	2:Q:124:MSE:SE	2.67	0.44
2:Q:3:GLN:N	2:Q:77:LYS:HD3	2.32	0.44
2:R:102:ALA:HB1	2:R:121:VAL:CG1	2.44	0.44
2:S:138:TYR:CZ	2:S:142:VAL:HG21	2.53	0.44
2:S:28:THR:OG1	2:S:30:LYS:HE2	2.17	0.44
1:A:234:LEU:HD23	1:A:234:LEU:N	2.32	0.44
1:A:635:ILE:CD1	1:A:635:ILE:N	2.71	0.44
1:A:90:PRO:O	1:A:93:VAL:N	2.49	0.44
1:B:697:ILE:HG12	1:B:732:ILE:HD13	1.98	0.44
1:C:333:LYS:HA	1:C:336:THR:OG1	2.17	0.44
1:C:444:PHE:N	1:C:444:PHE:CD1	2.86	0.44
1:C:552:TRP:O	1:C:553:GLN:C	2.53	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:LEU:HD22	1:C:606:LYS:HE2	1.99	0.44
1:C:794:GLN:O	1:C:797:ILE:HG12	2.18	0.44
1:D:323:ASN:C	1:D:324:THR:CG2	2.85	0.44
1:D:376:GLN:O	1:D:380:VAL:HG23	2.17	0.44
1:D:509:PRO:HD2	1:D:536:TYR:CE2	2.52	0.44
1:E:697:ILE:O	1:E:699:GLY:N	2.48	0.44
1:F:135:VAL:N	1:F:136:PRO:CD	2.80	0.44
1:F:345:THR:O	1:F:479:LYS:HE2	2.17	0.44
1:F:478:ALA:CB	1:F:486:LYS:O	2.61	0.44
2:O:69:LEU:O	2:O:69:LEU:HD12	2.17	0.44
2:P:88:ALA:O	2:P:91:VAL:HB	2.17	0.44
2:R:109:MSE:HG3	2:R:116:LEU:CD1	2.45	0.44
2:S:141:PHE:CZ	2:S:145:MSE:HE3	2.51	0.44
1:A:408:LEU:HD12	1:A:408:LEU:N	2.04	0.44
1:A:700:TYR:HD1	1:A:728:ALA:N	2.16	0.44
1:A:78:LYS:HD2	1:A:156:ILE:HD13	1.99	0.44
1:A:97:TYR:OH	1:A:150:PRO:HB2	2.17	0.44
1:B:629:ASN:HB3	1:B:632:TYR:CE1	2.53	0.44
1:C:357:TRP:CZ3	1:C:439:ASN:ND2	2.84	0.44
1:C:357:TRP:CZ3	1:C:439:ASN:HB2	2.51	0.44
1:C:629:ASN:HB3	1:C:632:TYR:CE1	2.52	0.44
1:D:216:GLU:HA	1:D:219:GLU:OE2	2.17	0.44
1:D:296:LEU:O	1:D:301:ALA:HB2	2.17	0.44
1:D:345:THR:O	1:D:479:LYS:HE2	2.17	0.44
1:D:794:GLN:O	1:D:797:ILE:HG12	2.18	0.44
1:E:127:SER:O	1:E:133:GLU:CD	2.48	0.44
1:E:424:LYS:NZ	1:E:424:LYS:HB3	2.32	0.44
1:E:76:LEU:O	1:E:77:ASP:C	2.56	0.44
1:F:325:TYR:CD1	1:F:598:PRO:HD3	2.52	0.44
1:F:357:TRP:CZ3	1:F:439:ASN:HB2	2.52	0.44
1:F:580:GLU:O	1:F:583:ASN:HB2	2.17	0.44
1:F:697:ILE:O	1:F:699:GLY:N	2.49	0.44
1:F:794:GLN:O	1:F:797:ILE:HG12	2.17	0.44
1:A:533:LEU:HD12	2:O:112:LEU:HD11	1.99	0.44
2:P:105:LEU:HD21	2:P:124:MSE:SE	2.68	0.44
2:R:46:ALA:HA	2:R:49:GLN:NE2	2.33	0.44
2:R:76:MSE:HA	2:R:79:THR:HG22	2.00	0.44
2:T:141:PHE:CZ	2:T:145:MSE:HE3	2.52	0.44
1:A:100:LEU:HD13	1:A:182:ILE:HG21	1.99	0.44
1:A:238:GLN:C	1:A:240:ALA:H	2.20	0.44
1:A:376:GLN:O	1:A:378:LEU:N	2.51	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:LYS:HA	1:A:622:LYS:HD3	1.51	0.44
1:A:746:LYS:HG2	1:A:750:GLN:HE21	1.82	0.44
1:B:357:TRP:CH2	1:B:439:ASN:ND2	2.85	0.44
1:C:375:GLY:O	1:C:377:GLN:N	2.50	0.44
1:C:697:ILE:HG12	1:C:732:ILE:HD13	2.00	0.44
1:C:736:LEU:HD11	1:C:750:GLN:HE21	1.80	0.44
1:C:93:VAL:HG23	1:C:179:LEU:CD1	2.43	0.44
1:D:136:PRO:HG2	1:D:139:SER:OG	2.17	0.44
1:D:540:ARG:NH1	1:D:627:TYR:CE1	2.86	0.44
1:D:718:ARG:O	1:D:722:ILE:HG13	2.17	0.44
1:E:375:GLY:O	1:E:377:GLN:N	2.51	0.44
1:E:444:PHE:N	1:E:444:PHE:CD1	2.86	0.44
1:E:447:SER:OG	1:E:448:ASP:N	2.49	0.44
1:E:794:GLN:O	1:E:797:ILE:HG12	2.18	0.44
1:F:136:PRO:HG2	1:F:139:SER:OG	2.18	0.44
1:F:581:GLN:O	1:F:629:ASN:HA	2.17	0.44
2:O:105:LEU:HD21	2:O:124:MSE:SE	2.67	0.44
2:O:97:ASN:ND2	2:O:99:TYR:H	2.16	0.44
2:P:117:THR:C	2:P:119:GLU:N	2.71	0.44
1:B:523:LEU:HD22	2:P:127:GLU:HG2	2.00	0.44
2:Q:13:LYS:O	2:Q:14:GLU:C	2.55	0.44
2:S:62:THR:HB	2:S:62:THR:CG2	2.19	0.44
2:T:102:ALA:HB1	2:T:121:VAL:CG1	2.46	0.44
2:T:42:ASN:HA	2:T:43:PRO:HD2	1.89	0.44
1:A:318:ILE:HG23	1:A:322:LEU:HD12	1.98	0.44
1:A:540:ARG:NH1	1:A:627:TYR:CE1	2.85	0.44
1:B:444:PHE:CD1	1:B:444:PHE:N	2.86	0.44
1:C:115:LYS:HB3	1:C:115:LYS:HZ3	1.80	0.44
1:C:238:GLN:O	1:C:240:ALA:N	2.50	0.44
1:C:275:GLY:O	1:C:278:LYS:HB2	2.18	0.44
1:C:622:LYS:HA	1:C:622:LYS:HD3	1.52	0.44
1:C:759:GLN:NE2	1:C:762:LEU:HD23	2.32	0.44
1:C:772:GLU:O	1:C:773:PHE:C	2.55	0.44
1:D:135:VAL:N	1:D:136:PRO:CD	2.81	0.44
1:D:78:LYS:HD2	1:D:156:ILE:HD13	1.99	0.44
1:D:285:LYS:C	1:D:287:GLY:H	2.21	0.44
1:D:447:SER:OG	1:D:448:ASP:N	2.49	0.44
1:D:793:PHE:O	1:D:794:GLN:C	2.56	0.44
1:D:792:VAL:O	1:D:795:LYS:HB2	2.18	0.44
1:E:398:ILE:HD13	1:E:479:LYS:HA	2.00	0.44
1:E:660:SER:O	1:E:663:PHE:HB3	2.18	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:GLU:HA	1:F:302:LEU:HB3	1.99	0.44
2:O:24:ASP:CG	2:O:25:GLY:H	2.20	0.44
2:P:46:ALA:HA	2:P:49:GLN:NE2	2.33	0.44
2:R:138:TYR:CZ	2:R:142:VAL:HG21	2.53	0.44
2:T:55:VAL:CB	2:T:67:GLU:OE2	2.60	0.44
1:A:325:TYR:CD1	1:A:598:PRO:HD3	2.53	0.44
1:A:444:PHE:N	1:A:444:PHE:CD1	2.85	0.44
1:B:135:VAL:N	1:B:136:PRO:CD	2.80	0.44
1:B:252:ASP:OD2	1:B:253:HIS:CD2	2.70	0.44
1:B:297:LYS:HB3	1:B:297:LYS:NZ	2.33	0.44
1:B:99:GLU:C	1:B:101:GLY:H	2.19	0.44
1:C:135:VAL:N	1:C:136:PRO:CD	2.80	0.44
1:C:97:TYR:OH	1:C:150:PRO:HB2	2.18	0.44
1:C:311:HIS:O	1:C:314:ALA:N	2.50	0.44
1:D:238:GLN:C	1:D:240:ALA:H	2.20	0.44
1:D:275:GLY:O	1:D:278:LYS:HB2	2.18	0.44
1:D:288:VAL:CG2	1:D:289:GLU:N	2.78	0.44
1:D:297:LYS:NZ	1:D:297:LYS:HB3	2.32	0.44
1:D:403:LEU:CG	1:D:405:LEU:CD1	2.95	0.44
1:D:636:ALA:HA	1:D:637:PRO:HD3	1.86	0.44
1:D:746:LYS:HG2	1:D:750:GLN:HE21	1.82	0.44
1:E:182:ILE:O	1:E:182:ILE:HD13	2.18	0.44
1:E:234:LEU:N	1:E:234:LEU:HD23	2.32	0.44
1:E:700:TYR:HD1	1:E:728:ALA:N	2.16	0.44
1:F:281:GLU:C	1:F:283:LEU:N	2.69	0.44
1:F:357:TRP:HZ3	1:F:439:ASN:HB2	1.83	0.44
1:F:533:LEU:HD12	2:T:112:LEU:HD11	1.99	0.44
1:F:772:GLU:O	1:F:773:PHE:C	2.55	0.44
2:P:138:TYR:CZ	2:P:142:VAL:HG21	2.52	0.44
2:T:24:ASP:CG	2:T:25:GLY:H	2.21	0.44
2:T:69:LEU:O	2:T:69:LEU:HD12	2.18	0.44
2:T:3:GLN:N	2:T:77:LYS:HD3	2.32	0.44
1:A:165:GLN:HG2	1:A:251:PRO:HG2	2.00	0.44
1:A:660:SER:O	1:A:663:PHE:HB3	2.18	0.44
1:B:104:ILE:HG23	1:B:152:LEU:CD2	2.48	0.44
1:B:180:ASP:CG	1:B:181:ILE:H	2.18	0.44
1:B:333:LYS:HA	1:B:336:THR:OG1	2.18	0.44
1:B:373:LYS:O	1:B:380:VAL:CG2	2.66	0.44
1:B:666:ASN:HB2	1:B:748:TYR:OH	2.17	0.44
1:C:152:LEU:HD21	1:C:154:ILE:HD11	1.99	0.44
1:C:165:GLN:HG2	1:C:251:PRO:HG2	1.99	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:LYS:NZ	1:C:297:LYS:HB3	2.32	0.44
1:D:173:ILE:O	1:D:174:GLY:C	2.54	0.44
1:D:234:LEU:HD23	1:D:234:LEU:N	2.33	0.44
1:D:579:THR:C	1:D:581:GLN:N	2.71	0.44
1:D:736:LEU:HD11	1:D:750:GLN:HE21	1.80	0.44
1:E:122:GLU:HG3	1:E:147:ARG:H	1.83	0.44
1:E:405:LEU:CD1	1:E:405:LEU:H	2.27	0.44
1:E:756:ILE:H	1:E:756:ILE:HG12	1.63	0.44
1:F:173:ILE:C	1:F:175:LYS:N	2.67	0.44
1:F:252:ASP:OD2	1:F:253:HIS:CD2	2.70	0.44
1:F:376:GLN:O	1:F:380:VAL:HG23	2.18	0.44
2:Q:117:THR:C	2:Q:119:GLU:N	2.71	0.44
2:Q:138:TYR:CZ	2:Q:142:VAL:HG21	2.53	0.44
2:R:13:LYS:NZ	2:R:65:PHE:CB	2.61	0.44
2:R:69:LEU:O	2:R:69:LEU:HD12	2.18	0.44
2:R:75:LYS:O	2:R:79:THR:HG22	2.18	0.44
2:T:138:TYR:CZ	2:T:142:VAL:HG21	2.53	0.44
1:A:173:ILE:O	1:A:174:GLY:C	2.54	0.44
1:A:333:LYS:HA	1:A:336:THR:OG1	2.18	0.44
1:A:764:LEU:HA	1:A:764:LEU:HD23	1.86	0.44
1:B:148:GLU:CG	1:B:149:THR:N	2.75	0.44
1:B:152:LEU:HD21	1:B:154:ILE:HD11	1.99	0.44
1:B:275:GLY:CA	1:B:278:LYS:HE3	2.36	0.44
1:B:325:TYR:CD1	1:B:598:PRO:HD3	2.52	0.44
1:C:123:GLU:CG	1:C:124:GLU:N	2.79	0.44
1:C:99:GLU:C	1:C:101:GLY:H	2.21	0.44
1:D:208:LEU:HD12	1:D:208:LEU:N	2.33	0.44
1:D:579:THR:C	1:D:581:GLN:H	2.20	0.44
1:E:123:GLU:CG	1:E:124:GLU:N	2.80	0.44
1:E:135:VAL:N	1:E:136:PRO:CD	2.80	0.44
1:E:395:GLU:O	1:E:395:GLU:OE1	2.36	0.44
1:E:580:GLU:O	1:E:583:ASN:HB2	2.18	0.44
1:F:305:SER:O	1:F:331:VAL:HG23	2.18	0.44
1:F:376:GLN:O	1:F:378:LEU:N	2.50	0.44
1:F:697:ILE:HG12	1:F:732:ILE:CD1	2.48	0.44
2:R:65:PHE:CB	2:R:66:PRO:HD3	2.38	0.44
2:T:46:ALA:HA	2:T:49:GLN:NE2	2.33	0.44
1:A:122:GLU:HG3	1:A:147:ARG:H	1.82	0.43
1:A:186:LYS:HG2	1:A:186:LYS:O	2.17	0.43
1:A:278:LYS:HB2	1:A:279:ILE:CD1	2.48	0.43
1:A:278:LYS:CB	1:A:279:ILE:HD13	2.48	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:HD22	1:A:606:LYS:HE2	1.99	0.43
1:A:697:ILE:HD13	1:A:732:ILE:HD13	2.00	0.43
1:A:772:GLU:O	1:A:773:PHE:C	2.55	0.43
1:B:136:PRO:HG2	1:B:139:SER:OG	2.18	0.43
1:B:186:LYS:HG2	1:B:186:LYS:O	2.18	0.43
1:B:238:GLN:C	1:B:240:ALA:H	2.20	0.43
1:B:165:GLN:HG2	1:B:251:PRO:HG2	1.99	0.43
1:B:279:ILE:HG22	1:B:283:LEU:HD13	1.99	0.43
1:B:357:TRP:CZ3	1:B:439:ASN:ND2	2.85	0.43
1:B:375:GLY:O	1:B:377:GLN:N	2.50	0.43
1:B:357:TRP:HZ3	1:B:439:ASN:HB2	1.83	0.43
1:B:580:GLU:O	1:B:583:ASN:HB2	2.18	0.43
1:C:136:PRO:HG2	1:C:139:SER:OG	2.17	0.43
1:C:325:TYR:CD1	1:C:598:PRO:HD3	2.53	0.43
1:C:677:GLY:HA2	1:C:745:TYR:OH	2.18	0.43
1:D:357:TRP:CZ3	1:D:439:ASN:ND2	2.85	0.43
1:D:671:ARG:NH1	1:D:671:ARG:HG3	2.33	0.43
1:D:756:ILE:HG12	1:D:756:ILE:H	1.62	0.43
1:E:197:LYS:HZ3	1:E:197:LYS:C	2.20	0.43
1:E:285:LYS:C	1:E:287:GLY:H	2.21	0.43
1:E:318:ILE:H	1:E:318:ILE:CD1	2.28	0.43
1:E:333:LYS:HA	1:E:336:THR:OG1	2.18	0.43
1:E:333:LYS:HA	1:E:336:THR:HG1	1.83	0.43
1:F:122:GLU:HG3	1:F:147:ARG:H	1.83	0.43
1:F:165:GLN:HG2	1:F:251:PRO:HG2	1.99	0.43
1:F:278:LYS:O	1:F:281:GLU:N	2.49	0.43
1:F:793:PHE:O	1:F:794:GLN:C	2.56	0.43
2:O:65:PHE:O	2:O:68:PHE:HB3	2.18	0.43
2:P:109:MSE:HG3	2:P:116:LEU:CD1	2.44	0.43
2:Q:133:ASP:OD2	2:Q:135:GLN:HG3	2.18	0.43
2:S:97:ASN:ND2	2:S:99:TYR:H	2.16	0.43
1:A:148:GLU:CG	1:A:149:THR:N	2.75	0.43
1:A:182:ILE:O	1:A:182:ILE:HD13	2.18	0.43
1:A:443:GLU:O	1:A:455:TYR:HA	2.18	0.43
1:A:736:LEU:HD11	1:A:750:GLN:HE21	1.79	0.43
1:B:123:GLU:CG	1:B:124:GLU:N	2.79	0.43
1:C:611:THR:HG22	1:C:615:ILE:HD11	1.99	0.43
1:C:718:ARG:O	1:C:722:ILE:HG13	2.18	0.43
1:D:122:GLU:HG3	1:D:147:ARG:H	1.82	0.43
1:D:296:LEU:HD22	1:D:606:LYS:HE2	1.99	0.43
1:D:700:TYR:HD1	1:D:728:ALA:N	2.16	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:697:ILE:HD13	1:D:732:ILE:HD13	2.01	0.43
1:E:345:THR:OG1	1:E:573:ASP:O	2.36	0.43
1:E:581:GLN:HB3	1:E:627:TYR:HE1	1.81	0.43
1:E:694:VAL:CG2	2:S:18:LEU:HD21	2.48	0.43
1:E:697:ILE:HD13	1:E:732:ILE:HD13	2.00	0.43
1:F:173:ILE:HD12	1:F:243:LEU:HD21	2.00	0.43
1:F:285:LYS:C	1:F:287:GLY:H	2.21	0.43
1:F:414:LYS:HA	1:F:414:LYS:HZ3	1.83	0.43
2:P:36:MSE:HE3	2:P:43:PRO:CG	2.38	0.43
2:P:65:PHE:CB	2:P:66:PRO:HD3	2.38	0.43
1:C:523:LEU:HD22	2:Q:127:GLU:HG2	2.00	0.43
2:Q:13:LYS:NZ	2:Q:65:PHE:CB	2.62	0.43
2:Q:75:LYS:O	2:Q:79:THR:HG22	2.18	0.43
2:R:13:LYS:O	2:R:14:GLU:C	2.55	0.43
2:R:3:GLN:N	2:R:77:LYS:HD3	2.33	0.43
2:S:6:GLU:O	2:S:9:ILE:N	2.47	0.43
1:A:446:ILE:HD11	1:A:451:ASN:CB	2.41	0.43
1:A:523:LEU:HD22	2:O:127:GLU:HG2	2.00	0.43
1:B:85:LEU:HD12	1:B:168:GLU:OE1	2.18	0.43
1:C:376:GLN:O	1:C:380:VAL:HG23	2.18	0.43
1:C:395:GLU:OE1	1:C:395:GLU:O	2.36	0.43
1:C:457:THR:HG21	1:C:468:LYS:HA	2.01	0.43
1:D:376:GLN:CB	1:D:379:ALA:HB3	2.48	0.43
1:D:512:GLU:O	1:D:516:VAL:HG23	2.19	0.43
1:E:97:TYR:OH	1:E:150:PRO:HB2	2.18	0.43
1:E:216:GLU:HA	1:E:219:GLU:OE2	2.19	0.43
1:F:424:LYS:HB3	1:F:424:LYS:NZ	2.31	0.43
1:F:792:VAL:O	1:F:795:LYS:HB2	2.18	0.43
2:O:46:ALA:HA	2:O:49:GLN:NE2	2.33	0.43
2:O:76:MSE:HA	2:O:79:THR:HG22	2.01	0.43
2:S:65:PHE:CB	2:S:66:PRO:HD3	2.38	0.43
2:T:105:LEU:HD21	2:T:124:MSE:SE	2.68	0.43
1:A:133:GLU:OE1	1:A:134:LYS:N	2.52	0.43
1:A:208:LEU:N	1:A:208:LEU:HD12	2.33	0.43
1:A:252:ASP:OD2	1:A:253:HIS:CD2	2.72	0.43
1:A:288:VAL:CG2	1:A:289:GLU:N	2.79	0.43
1:A:311:HIS:O	1:A:314:ALA:N	2.51	0.43
1:A:521:ASN:HB3	1:A:524:GLU:HB3	2.01	0.43
1:B:133:GLU:OE1	1:B:134:LYS:N	2.52	0.43
1:B:199:LEU:O	1:B:201:ASP:N	2.51	0.43
1:B:311:HIS:O	1:B:314:ALA:N	2.52	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:LEU:HD23	1:B:532:LEU:HA	1.76	0.43
1:B:71:PHE:CD2	1:B:73:ASN:HB2	2.53	0.43
1:B:677:GLY:HA2	1:B:745:TYR:OH	2.18	0.43
1:B:794:GLN:O	1:B:797:ILE:HG12	2.17	0.43
1:C:398:ILE:HD13	1:C:479:LYS:HA	2.00	0.43
1:C:509:PRO:HD2	1:C:536:TYR:CE2	2.53	0.43
1:C:792:VAL:O	1:C:795:LYS:HB2	2.19	0.43
1:C:88:LYS:HZ3	1:C:172:GLU:CD	2.21	0.43
1:D:199:LEU:O	1:D:201:ASP:N	2.51	0.43
1:D:376:GLN:O	1:D:378:LEU:N	2.51	0.43
1:E:170:TYR:HA	1:E:173:ILE:CG2	2.49	0.43
1:E:173:ILE:HD12	1:E:243:LEU:HD21	2.01	0.43
1:E:173:ILE:C	1:E:175:LYS:N	2.66	0.43
1:E:165:GLN:HG2	1:E:251:PRO:HG2	1.99	0.43
1:E:697:ILE:HG12	1:E:732:ILE:HD13	2.00	0.43
1:F:611:THR:HG22	1:F:615:ILE:HD11	2.00	0.43
1:F:700:TYR:HD1	1:F:728:ALA:N	2.16	0.43
1:F:76:LEU:O	1:F:77:ASP:C	2.57	0.43
2:O:81:SER:C	2:O:83:GLU:N	2.72	0.43
1:A:184:LYS:CE	1:A:191:GLU:HB2	2.49	0.43
1:A:281:GLU:C	1:A:283:LEU:H	2.22	0.43
1:A:373:LYS:O	1:A:380:VAL:CG2	2.67	0.43
1:A:76:LEU:O	1:A:77:ASP:C	2.57	0.43
1:B:182:ILE:O	1:B:182:ILE:HD13	2.18	0.43
1:B:285:LYS:C	1:B:287:GLY:H	2.21	0.43
1:B:697:ILE:HD13	1:B:732:ILE:HD13	2.00	0.43
1:C:285:LYS:C	1:C:287:GLY:H	2.21	0.43
1:C:376:GLN:O	1:C:378:LEU:N	2.51	0.43
1:C:376:GLN:CB	1:C:379:ALA:HB3	2.48	0.43
1:C:581:GLN:HB3	1:C:627:TYR:HE1	1.82	0.43
1:C:755:ARG:O	1:C:756:ILE:C	2.57	0.43
1:D:462:ILE:CG1	1:D:463:THR:N	2.80	0.43
1:D:478:ALA:CB	1:D:486:LYS:O	2.63	0.43
1:D:543:ASP:OD1	1:D:544:SER:N	2.52	0.43
1:D:552:TRP:HA	1:D:555:GLN:HG2	1.99	0.43
1:D:785:ASN:O	1:D:785:ASN:OD1	2.36	0.43
1:E:137:PHE:O	1:E:140:ARG:N	2.51	0.43
1:F:254:ARG:HD2	1:F:254:ARG:N	2.34	0.43
1:F:515:LYS:HZ1	1:F:516:VAL:CG2	2.30	0.43
1:F:527:LYS:HB3	1:F:527:LYS:HE2	1.87	0.43
1:F:71:PHE:CD2	1:F:73:ASN:HB2	2.53	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:785:ASN:OD1	1:F:785:ASN:O	2.36	0.43
2:O:39:LEU:HA	2:O:39:LEU:HD23	1.75	0.43
2:P:55:VAL:CG2	2:P:67:GLU:CD	2.87	0.43
2:S:106:ARG:NH2	2:S:118:ASP:OD2	2.52	0.43
2:T:117:THR:C	2:T:119:GLU:N	2.71	0.43
1:A:254:ARG:HD2	1:A:254:ARG:N	2.34	0.43
1:A:424:LYS:NZ	1:A:424:LYS:HB3	2.32	0.43
1:A:697:ILE:HG12	1:A:732:ILE:CD1	2.49	0.43
1:B:216:GLU:HA	1:B:219:GLU:OE2	2.19	0.43
1:B:512:GLU:O	1:B:516:VAL:HG23	2.19	0.43
1:C:122:GLU:HG3	1:C:147:ARG:H	1.82	0.43
1:C:278:LYS:HB2	1:C:279:ILE:CD1	2.49	0.43
1:C:660:SER:O	1:C:663:PHE:HB3	2.18	0.43
1:C:785:ASN:O	1:C:785:ASN:OD1	2.36	0.43
1:D:165:GLN:HG2	1:D:251:PRO:HG2	2.00	0.43
1:D:398:ILE:HD13	1:D:479:LYS:HA	1.99	0.43
1:E:104:ILE:HG23	1:E:152:LEU:CD2	2.48	0.43
1:E:152:LEU:HD21	1:E:154:ILE:HD11	2.01	0.43
1:E:792:VAL:O	1:E:795:LYS:HB2	2.18	0.43
1:F:182:ILE:O	1:F:182:ILE:HD13	2.18	0.43
1:F:395:GLU:O	1:F:395:GLU:OE1	2.36	0.43
2:O:117:THR:C	2:O:119:GLU:N	2.70	0.43
2:O:75:LYS:O	2:O:79:THR:HG22	2.19	0.43
2:P:141:PHE:CZ	2:P:145:MSE:HE3	2.53	0.43
2:P:75:LYS:O	2:P:79:THR:HG22	2.19	0.43
2:T:76:MSE:HA	2:T:79:THR:HG22	2.01	0.43
1:A:199:LEU:O	1:A:201:ASP:N	2.52	0.43
1:B:403:LEU:CG	1:B:405:LEU:CD1	2.96	0.43
1:B:521:ASN:HB3	1:B:524:GLU:HB3	2.01	0.43
1:B:598:PRO:HG3	1:B:624:TYR:OH	2.18	0.43
1:B:700:TYR:HD1	1:B:728:ALA:N	2.16	0.43
1:B:697:ILE:HG12	1:B:732:ILE:CD1	2.49	0.43
1:B:739:LYS:HG2	1:B:740:GLN:N	2.30	0.43
1:C:182:ILE:O	1:C:182:ILE:HD13	2.18	0.43
1:C:186:LYS:HG2	1:C:186:LYS:O	2.18	0.43
1:C:443:GLU:O	1:C:455:TYR:HA	2.19	0.43
1:C:598:PRO:HG3	1:C:624:TYR:OH	2.18	0.43
1:C:700:TYR:HD1	1:C:728:ALA:N	2.15	0.43
1:D:457:THR:HG21	1:D:468:LYS:HA	2.01	0.43
1:D:71:PHE:CD2	1:D:73:ASN:HB2	2.53	0.43
1:E:133:GLU:OE1	1:E:134:LYS:N	2.52	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:PRO:HG2	1:E:139:SER:OG	2.18	0.43
1:E:186:LYS:HG2	1:E:186:LYS:O	2.18	0.43
1:F:104:ILE:HG23	1:F:152:LEU:CD2	2.49	0.43
1:F:671:ARG:HG3	1:F:671:ARG:NH1	2.34	0.43
2:Q:76:MSE:HA	2:Q:79:THR:HG22	2.01	0.43
2:S:46:ALA:HA	2:S:49:GLN:NE2	2.33	0.43
2:S:55:VAL:CB	2:S:67:GLU:OE2	2.59	0.43
2:S:65:PHE:O	2:S:68:PHE:HB3	2.19	0.43
2:S:76:MSE:HA	2:S:79:THR:HG22	2.00	0.43
2:S:76:MSE:HE3	2:S:76:MSE:HB2	1.65	0.43
2:T:77:LYS:HG3	2:T:77:LYS:O	2.19	0.43
1:A:216:GLU:HA	1:A:219:GLU:OE2	2.18	0.43
1:A:279:ILE:HG22	1:A:283:LEU:HD13	1.99	0.43
1:A:286:GLU:HG2	1:A:286:GLU:O	2.18	0.43
1:A:71:PHE:CD2	1:A:73:ASN:HB2	2.54	0.43
1:A:794:GLN:O	1:A:797:ILE:HG12	2.18	0.43
1:B:709:ASN:O	1:B:717:LYS:HE3	2.18	0.43
1:C:183:SER:HB3	1:C:184:LYS:H	1.51	0.43
1:D:133:GLU:OE1	1:D:134:LYS:N	2.52	0.43
1:D:137:PHE:O	1:D:140:ARG:N	2.52	0.43
1:D:181:ILE:HD12	1:D:238:GLN:OE1	2.19	0.43
1:D:173:ILE:HD12	1:D:243:LEU:HD21	2.00	0.43
1:D:311:HIS:O	1:D:314:ALA:N	2.52	0.43
1:D:333:LYS:HA	1:D:336:THR:OG1	2.18	0.43
1:D:395:GLU:O	1:D:395:GLU:OE1	2.36	0.43
1:D:408:LEU:N	1:D:408:LEU:HD12	2.05	0.43
1:D:637:PRO:O	1:D:638:GLY:C	2.57	0.43
1:D:755:ARG:O	1:D:756:ILE:C	2.57	0.43
1:D:778:LYS:HE3	1:D:778:LYS:HB3	1.74	0.43
1:E:671:ARG:NH1	1:E:671:ARG:HG3	2.34	0.43
1:E:759:GLN:NE2	1:E:762:LEU:HD23	2.34	0.43
1:F:99:GLU:C	1:F:101:GLY:H	2.21	0.43
1:F:199:LEU:O	1:F:201:ASP:N	2.51	0.43
2:O:3:GLN:N	2:O:77:LYS:HD3	2.33	0.43
2:S:133:ASP:OD2	2:S:135:GLN:HG3	2.19	0.43
1:A:112:VAL:CG1	1:A:113:GLU:N	2.77	0.43
1:A:398:ILE:HD13	1:A:479:LYS:HA	2.00	0.43
1:A:794:GLN:HE22	1:A:795:LYS:CG	2.31	0.43
1:B:281:GLU:C	1:B:283:LEU:N	2.70	0.43
1:B:286:GLU:HG2	1:B:286:GLU:O	2.19	0.43
1:B:292:ARG:NE	1:B:617:LYS:HE3	2.34	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ILE:HD13	1:B:479:LYS:HA	2.00	0.43
1:C:133:GLU:OE1	1:C:134:LYS:N	2.52	0.43
1:C:397:GLU:O	1:C:480:ASN:N	2.50	0.43
1:C:512:GLU:O	1:C:516:VAL:HG23	2.18	0.43
1:C:793:PHE:O	1:C:794:GLN:C	2.56	0.43
1:D:278:LYS:HB2	1:D:279:ILE:CD1	2.49	0.43
1:D:281:GLU:C	1:D:283:LEU:H	2.21	0.43
1:D:338:LEU:O	1:D:343:VAL:CG2	2.66	0.43
1:D:373:LYS:O	1:D:380:VAL:CG2	2.67	0.43
1:E:81:GLN:OE1	1:E:156:ILE:HG21	2.18	0.43
1:E:278:LYS:CB	1:E:279:ILE:HD13	2.49	0.43
1:E:305:SER:O	1:E:331:VAL:HG23	2.19	0.43
1:F:133:GLU:OE1	1:F:134:LYS:N	2.52	0.43
1:F:271:LEU:HA	1:F:271:LEU:HD23	1.86	0.43
1:F:755:ARG:O	1:F:756:ILE:C	2.57	0.43
2:Q:81:SER:C	2:Q:83:GLU:N	2.72	0.43
2:R:42:ASN:HA	2:R:43:PRO:HD2	1.88	0.43
2:T:76:MSE:HE3	2:T:76:MSE:HB2	1.64	0.43
1:A:376:GLN:CB	1:A:379:ALA:HB3	2.49	0.43
1:B:208:LEU:N	1:B:208:LEU:HD12	2.34	0.43
1:B:318:ILE:H	1:B:318:ILE:CD1	2.26	0.43
1:B:597:ASN:HD21	1:B:601:GLU:CB	2.10	0.43
1:C:334:LEU:HD23	1:C:356:ASP:HA	2.01	0.43
1:C:71:PHE:CD2	1:C:73:ASN:HB2	2.53	0.43
1:D:305:SER:O	1:D:331:VAL:HG23	2.19	0.43
1:D:345:THR:OG1	1:D:573:ASP:O	2.37	0.43
1:D:581:GLN:O	1:D:629:ASN:HA	2.19	0.43
1:D:74:GLU:C	1:D:75:THR:O	2.57	0.43
1:D:99:GLU:C	1:D:101:GLY:H	2.21	0.43
1:E:181:ILE:HD12	1:E:238:GLN:OE1	2.19	0.43
1:E:373:LYS:O	1:E:380:VAL:CG2	2.67	0.43
1:E:794:GLN:HE22	1:E:795:LYS:CG	2.31	0.43
1:F:170:TYR:HA	1:F:173:ILE:CG2	2.49	0.43
1:F:373:LYS:O	1:F:380:VAL:CG2	2.67	0.43
1:F:391:ILE:CG1	1:F:399:GLY:HA2	2.41	0.43
2:O:138:TYR:O	2:O:141:PHE:HB3	2.19	0.43
2:R:54:GLU:O	2:R:55:VAL:HG22	2.19	0.43
2:R:77:LYS:HG3	2:R:77:LYS:O	2.19	0.43
2:T:65:PHE:O	2:T:68:PHE:HB3	2.19	0.43
1:A:285:LYS:C	1:A:287:GLY:H	2.22	0.42
1:A:307:LEU:HD12	1:A:307:LEU:N	2.34	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:ARG:NH1	1:A:671:ARG:HG3	2.34	0.42
1:A:671:ARG:O	1:A:675:ASN:HA	2.19	0.42
1:B:170:TYR:HA	1:B:173:ILE:CG2	2.49	0.42
1:B:443:GLU:O	1:B:455:TYR:HA	2.19	0.42
1:B:76:LEU:O	1:B:77:ASP:C	2.57	0.42
1:C:100:LEU:HD13	1:C:182:ILE:HG21	2.01	0.42
1:C:286:GLU:HG2	1:C:286:GLU:O	2.19	0.42
1:C:373:LYS:O	1:C:380:VAL:CG2	2.67	0.42
1:C:671:ARG:HG3	1:C:671:ARG:NH1	2.34	0.42
1:C:671:ARG:O	1:C:675:ASN:HA	2.19	0.42
1:D:161:ILE:CG2	1:D:161:ILE:O	2.67	0.42
1:E:208:LEU:N	1:E:208:LEU:HD12	2.33	0.42
1:E:443:GLU:O	1:E:455:TYR:HA	2.19	0.42
1:E:71:PHE:CD2	1:E:73:ASN:HB2	2.53	0.42
1:F:128:MET:HE3	1:F:239:HIS:NE2	2.34	0.42
1:F:677:GLY:HA2	1:F:745:TYR:OH	2.19	0.42
1:F:759:GLN:NE2	1:F:762:LEU:HD23	2.33	0.42
1:F:764:LEU:HD23	1:F:764:LEU:HA	1.85	0.42
2:O:13:LYS:NZ	2:O:65:PHE:CB	2.62	0.42
2:P:42:ASN:HA	2:P:43:PRO:HD2	1.88	0.42
2:P:44:THR:H	2:P:47:GLU:HB3	1.84	0.42
1:A:173:ILE:HD12	1:A:243:LEU:HD21	2.00	0.42
1:A:532:LEU:HA	1:A:532:LEU:HD23	1.78	0.42
1:B:184:LYS:CE	1:B:191:GLU:HB2	2.49	0.42
1:B:275:GLY:O	1:B:278:LYS:HB2	2.19	0.42
1:B:376:GLN:O	1:B:380:VAL:HG23	2.19	0.42
1:B:579:THR:O	1:B:581:GLN:N	2.52	0.42
1:B:785:ASN:OD1	1:B:785:ASN:O	2.36	0.42
1:C:318:ILE:CD1	1:C:318:ILE:H	2.28	0.42
1:D:186:LYS:CE	1:D:234:LEU:HB2	2.49	0.42
1:D:275:GLY:CA	1:D:278:LYS:HE3	2.36	0.42
1:D:463:THR:HG22	1:D:465:LEU:H	1.84	0.42
1:D:580:GLU:O	1:D:583:ASN:HB2	2.19	0.42
1:E:275:GLY:O	1:E:278:LYS:HB2	2.18	0.42
1:E:515:LYS:HZ1	1:E:516:VAL:CG2	2.30	0.42
1:E:85:LEU:HD12	1:E:168:GLU:OE1	2.19	0.42
1:F:333:LYS:HA	1:F:336:THR:HG1	1.83	0.42
2:O:42:ASN:HA	2:O:43:PRO:HD2	1.88	0.42
2:P:106:ARG:NH2	2:P:118:ASP:OD2	2.52	0.42
2:S:44:THR:H	2:S:47:GLU:HB3	1.84	0.42
2:S:49:GLN:O	2:S:53:ASN:N	2.44	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:GLN:HE21	1:A:794:GLN:HB3	1.66	0.42
1:A:85:LEU:HD12	1:A:168:GLU:OE1	2.19	0.42
1:B:540:ARG:NH1	1:B:627:TYR:CE1	2.87	0.42
1:B:792:VAL:O	1:B:795:LYS:HB2	2.18	0.42
1:B:794:GLN:HB3	1:B:794:GLN:HE21	1.66	0.42
1:B:794:GLN:HE22	1:B:795:LYS:CG	2.31	0.42
1:B:90:PRO:O	1:B:93:VAL:N	2.51	0.42
1:C:137:PHE:O	1:C:140:ARG:N	2.53	0.42
1:C:208:LEU:HD12	1:C:208:LEU:N	2.34	0.42
1:C:216:GLU:HA	1:C:219:GLU:OE2	2.19	0.42
1:C:532:LEU:HD23	1:C:532:LEU:HA	1.78	0.42
1:C:581:GLN:O	1:C:629:ASN:HA	2.19	0.42
1:C:637:PRO:O	1:C:638:GLY:C	2.58	0.42
1:D:97:TYR:OH	1:D:150:PRO:HB2	2.19	0.42
1:D:334:LEU:HD23	1:D:356:ASP:HA	2.02	0.42
1:E:99:GLU:C	1:E:101:GLY:H	2.22	0.42
1:E:88:LYS:HZ3	1:E:172:GLU:CD	2.21	0.42
1:F:286:GLU:HG2	1:F:286:GLU:O	2.19	0.42
1:F:457:THR:HG21	1:F:468:LYS:HA	2.02	0.42
1:F:736:LEU:HD11	1:F:750:GLN:HE21	1.81	0.42
1:F:85:LEU:O	1:F:88:LYS:HE3	2.20	0.42
2:O:77:LYS:O	2:O:77:LYS:HG3	2.19	0.42
2:P:77:LYS:HG3	2:P:77:LYS:O	2.19	0.42
2:R:106:ARG:NH2	2:R:118:ASP:OD2	2.53	0.42
2:R:133:ASP:OD2	2:R:135:GLN:HG3	2.18	0.42
2:T:54:GLU:O	2:T:55:VAL:HG22	2.19	0.42
1:A:100:LEU:CD1	1:A:182:ILE:HG21	2.49	0.42
1:A:137:PHE:O	1:A:140:ARG:N	2.52	0.42
1:A:305:SER:O	1:A:331:VAL:HG23	2.19	0.42
1:A:403:LEU:CG	1:A:405:LEU:CD1	2.96	0.42
1:A:792:VAL:O	1:A:795:LYS:HB2	2.19	0.42
1:B:186:LYS:HE3	1:B:234:LEU:HB2	2.02	0.42
1:B:278:LYS:HB2	1:B:279:ILE:CD1	2.48	0.42
1:B:579:THR:C	1:B:581:GLN:N	2.72	0.42
1:B:671:ARG:HG3	1:B:671:ARG:NH1	2.34	0.42
1:C:85:LEU:O	1:C:88:LYS:HE3	2.20	0.42
1:D:527:LYS:HE2	1:D:527:LYS:HB3	1.86	0.42
1:D:697:ILE:HG12	1:D:732:ILE:CD1	2.49	0.42
1:D:677:GLY:HA2	1:D:745:TYR:OH	2.19	0.42
1:D:76:LEU:O	1:D:77:ASP:C	2.57	0.42
1:E:306:GLY:O	1:E:307:LEU:C	2.58	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:376:GLN:CB	1:E:379:ALA:HB3	2.49	0.42
1:E:598:PRO:HG3	1:E:624:TYR:OH	2.20	0.42
1:F:115:LYS:HB3	1:F:115:LYS:HZ3	1.83	0.42
1:F:97:TYR:OH	1:F:150:PRO:HB2	2.19	0.42
1:F:512:GLU:O	1:F:516:VAL:HG23	2.19	0.42
1:F:694:VAL:CG2	2:T:18:LEU:HD21	2.50	0.42
2:O:106:ARG:NH2	2:O:118:ASP:OD2	2.52	0.42
2:P:138:TYR:O	2:P:141:PHE:HB3	2.19	0.42
2:P:5:THR:O	2:P:8:GLN:HB3	2.20	0.42
2:Q:18:LEU:HB3	2:Q:19:PHE:CE1	2.54	0.42
2:R:18:LEU:HB3	2:R:19:PHE:CE1	2.54	0.42
2:S:42:ASN:HA	2:S:43:PRO:HD2	1.88	0.42
2:T:81:SER:C	2:T:83:GLU:N	2.72	0.42
1:A:170:TYR:HA	1:A:173:ILE:CG2	2.49	0.42
1:A:333:LYS:H	1:A:333:LYS:HD2	1.85	0.42
1:A:667:LEU:O	1:A:668:SER:C	2.57	0.42
1:A:785:ASN:OD1	1:A:785:ASN:O	2.36	0.42
1:A:85:LEU:O	1:A:88:LYS:HE3	2.19	0.42
1:A:90:PRO:O	1:A:92:ASP:N	2.52	0.42
1:B:543:ASP:OD1	1:B:544:SER:N	2.53	0.42
1:C:181:ILE:HD12	1:C:238:GLN:OE1	2.20	0.42
1:C:218:LEU:C	1:C:220:LEU:H	2.15	0.42
1:C:391:ILE:CG1	1:C:399:GLY:HA2	2.40	0.42
1:D:81:GLN:OE1	1:D:156:ILE:HG21	2.19	0.42
1:D:254:ARG:HD2	1:D:254:ARG:N	2.35	0.42
1:D:671:ARG:O	1:D:675:ASN:HA	2.20	0.42
1:D:90:PRO:O	1:D:93:VAL:N	2.52	0.42
1:E:286:GLU:HG2	1:E:286:GLU:O	2.19	0.42
1:E:521:ASN:HB3	1:E:524:GLU:HB3	2.02	0.42
1:F:208:LEU:N	1:F:208:LEU:HD12	2.33	0.42
1:F:216:GLU:HA	1:F:219:GLU:OE2	2.19	0.42
1:F:281:GLU:C	1:F:283:LEU:H	2.22	0.42
1:F:446:ILE:HD11	1:F:451:ASN:CB	2.41	0.42
1:F:521:ASN:HB3	1:F:524:GLU:HB3	2.01	0.42
1:F:345:THR:OG1	1:F:573:ASP:O	2.36	0.42
2:Q:44:THR:H	2:Q:47:GLU:HB3	1.84	0.42
2:S:117:THR:C	2:S:119:GLU:N	2.71	0.42
1:A:81:GLN:OE1	1:A:156:ILE:HG21	2.19	0.42
1:A:334:LEU:HD23	1:A:356:ASP:HA	2.01	0.42
1:B:376:GLN:CB	1:B:379:ALA:HB3	2.49	0.42
1:B:585:GLU:HA	1:B:585:GLU:OE1	2.18	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LYS:HZ3	1:B:172:GLU:CD	2.23	0.42
1:C:170:TYR:HA	1:C:173:ILE:CG2	2.50	0.42
1:C:414:LYS:C	1:C:416:ASN:H	2.23	0.42
1:C:462:ILE:CG1	1:C:463:THR:N	2.80	0.42
1:C:521:ASN:HB3	1:C:524:GLU:HB3	2.01	0.42
1:C:680:LYS:O	1:C:687:GLU:HG2	2.19	0.42
1:C:76:LEU:O	1:C:77:ASP:C	2.58	0.42
1:D:186:LYS:HE3	1:D:234:LEU:HB2	2.01	0.42
1:D:278:LYS:CB	1:D:279:ILE:HD13	2.49	0.42
1:D:286:GLU:HG2	1:D:286:GLU:O	2.19	0.42
1:D:412:GLU:O	1:D:416:ASN:HB2	2.20	0.42
1:E:184:LYS:CE	1:E:191:GLU:HB2	2.48	0.42
1:E:462:ILE:CG1	1:E:463:THR:N	2.80	0.42
1:F:443:GLU:O	1:F:455:TYR:HA	2.19	0.42
1:F:292:ARG:NE	1:F:617:LYS:HE3	2.35	0.42
2:P:18:LEU:HA	2:P:18:LEU:HD23	1.83	0.42
2:Q:106:ARG:NH2	2:Q:118:ASP:OD2	2.53	0.42
2:Q:77:LYS:HG3	2:Q:77:LYS:O	2.19	0.42
1:A:186:LYS:HE3	1:A:234:LEU:HB2	2.02	0.42
1:A:186:LYS:CE	1:A:234:LEU:HB2	2.50	0.42
1:A:333:LYS:HA	1:A:336:THR:HG1	1.84	0.42
1:A:457:THR:HG21	1:A:468:LYS:HA	2.01	0.42
1:A:598:PRO:HG3	1:A:624:TYR:OH	2.20	0.42
1:A:739:LYS:CG	1:A:740:GLN:H	2.26	0.42
1:B:81:GLN:OE1	1:B:156:ILE:HG21	2.19	0.42
1:B:172:GLU:O	1:B:175:LYS:HB3	2.20	0.42
1:C:254:ARG:N	1:C:254:ARG:HD2	2.34	0.42
1:C:550:SER:HB2	1:C:553:GLN:HG3	1.98	0.42
1:D:115:LYS:N	1:D:118:GLN:HB2	2.34	0.42
1:D:170:TYR:HA	1:D:173:ILE:CG2	2.49	0.42
1:D:521:ASN:HB3	1:D:524:GLU:HB3	2.02	0.42
1:D:636:ALA:O	1:D:640:LYS:CA	2.68	0.42
1:D:680:LYS:O	1:D:687:GLU:HG2	2.19	0.42
1:E:254:ARG:N	1:E:254:ARG:HD2	2.35	0.42
1:E:463:THR:HG22	1:E:465:LEU:H	1.85	0.42
1:E:543:ASP:OD1	1:E:544:SER:N	2.53	0.42
1:E:579:THR:C	1:E:581:GLN:N	2.72	0.42
1:E:579:THR:C	1:E:581:GLN:H	2.23	0.42
1:F:137:PHE:O	1:F:140:ARG:N	2.53	0.42
1:F:579:THR:C	1:F:581:GLN:N	2.73	0.42
1:F:718:ARG:O	1:F:722:ILE:HG13	2.19	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:776:LEU:C	1:F:776:LEU:CD2	2.88	0.42
2:S:54:GLU:O	2:S:55:VAL:HG13	2.20	0.42
2:S:75:LYS:O	2:S:79:THR:HG22	2.20	0.42
2:T:133:ASP:OD2	2:T:135:GLN:HG3	2.19	0.42
2:T:138:TYR:O	2:T:141:PHE:HB3	2.19	0.42
2:T:16:PHE:CE1	2:T:27:ILE:HG12	2.55	0.42
1:A:152:LEU:HD21	1:A:154:ILE:HD11	2.01	0.42
1:A:483:GLY:C	1:A:484:VAL:CG2	2.88	0.42
1:B:106:PHE:CZ	1:B:171:TYR:OH	2.64	0.42
1:B:333:LYS:HA	1:B:336:THR:HG1	1.84	0.42
1:B:635:ILE:CD1	1:B:635:ILE:N	2.71	0.42
1:C:463:THR:HG22	1:C:465:LEU:H	1.85	0.42
1:C:697:ILE:HG12	1:C:732:ILE:CD1	2.50	0.42
1:D:136:PRO:O	1:D:137:PHE:C	2.58	0.42
1:D:443:GLU:O	1:D:455:TYR:HA	2.19	0.42
1:D:557:LEU:HD11	1:D:575:VAL:CG1	2.50	0.42
1:E:186:LYS:CE	1:E:234:LEU:HB2	2.49	0.42
1:E:278:LYS:HB2	1:E:279:ILE:CD1	2.49	0.42
1:F:462:ILE:CG1	1:F:463:THR:N	2.80	0.42
2:O:5:THR:O	2:O:8:GLN:HB3	2.20	0.42
2:P:65:PHE:O	2:P:68:PHE:HB3	2.20	0.42
2:P:81:SER:C	2:P:83:GLU:N	2.73	0.42
2:Q:21:LYS:O	2:Q:23:GLY:N	2.49	0.42
2:Q:28:THR:CG2	2:Q:30:LYS:HZ1	2.33	0.42
2:R:54:GLU:O	2:R:55:VAL:HG13	2.20	0.42
2:R:5:THR:O	2:R:8:GLN:HB3	2.20	0.42
2:S:39:LEU:HA	2:S:39:LEU:HD23	1.74	0.42
2:T:61:GLY:C	2:T:62:THR:HG22	2.40	0.42
1:A:181:ILE:HD12	1:A:238:GLN:OE1	2.20	0.42
1:A:318:ILE:H	1:A:318:ILE:CD1	2.26	0.42
1:A:338:LEU:HD21	1:A:409:ARG:HD3	2.02	0.42
1:A:579:THR:C	1:A:581:GLN:N	2.73	0.42
1:A:73:ASN:HB3	1:A:74:GLU:OE2	2.20	0.42
1:A:793:PHE:O	1:A:794:GLN:C	2.57	0.42
1:B:306:GLY:O	1:B:307:LEU:C	2.58	0.42
1:B:462:ILE:CG1	1:B:463:THR:N	2.81	0.42
1:B:483:GLY:C	1:B:484:VAL:CG2	2.89	0.42
1:B:515:LYS:HZ1	1:B:516:VAL:CG2	2.31	0.42
1:C:172:GLU:O	1:C:175:LYS:HB3	2.19	0.42
1:C:333:LYS:HD2	1:C:333:LYS:H	1.85	0.42
1:C:527:LYS:HB3	1:C:527:LYS:HE2	1.87	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:794:GLN:HE22	1:C:795:LYS:CG	2.31	0.42
1:D:279:ILE:HG22	1:D:283:LEU:CD1	2.50	0.42
1:D:292:ARG:NE	1:D:617:LYS:HE3	2.34	0.42
1:D:73:ASN:HB3	1:D:74:GLU:OE2	2.20	0.42
1:E:100:LEU:HD13	1:E:182:ILE:HG21	2.02	0.42
1:E:136:PRO:O	1:E:137:PHE:C	2.59	0.42
1:E:90:PRO:O	1:E:92:ASP:N	2.53	0.42
1:F:333:LYS:H	1:F:333:LYS:HD2	1.85	0.42
1:F:376:GLN:CB	1:F:379:ALA:HB3	2.49	0.42
1:F:543:ASP:OD1	1:F:544:SER:N	2.52	0.42
1:F:671:ARG:O	1:F:675:ASN:HA	2.19	0.42
1:F:693:SER:OG	1:F:731:GLU:OE1	2.38	0.42
1:F:697:ILE:HD13	1:F:732:ILE:HD13	2.02	0.42
2:Q:44:THR:OG1	2:Q:47:GLU:CB	2.68	0.42
2:Q:6:GLU:O	2:Q:9:ILE:HB	2.20	0.42
2:R:27:ILE:HA	2:R:31:GLU:OE2	2.20	0.42
2:R:44:THR:H	2:R:47:GLU:HB3	1.85	0.42
2:R:56:ASP:CG	2:R:60:ASN:HA	2.38	0.42
2:S:5:THR:O	2:S:8:GLN:HB3	2.20	0.42
2:T:44:THR:OG1	2:T:47:GLU:CB	2.68	0.42
1:A:503:GLU:HA	1:A:503:GLU:OE1	2.20	0.42
1:A:739:LYS:HG2	1:A:740:GLN:N	2.30	0.42
1:B:115:LYS:N	1:B:118:GLN:HB2	2.35	0.42
1:B:136:PRO:O	1:B:137:PHE:C	2.59	0.42
1:B:338:LEU:O	1:B:343:VAL:CG2	2.68	0.42
1:B:522:SER:O	2:P:124:MSE:HE2	2.20	0.42
1:B:793:PHE:O	1:B:794:GLN:C	2.56	0.42
1:B:83:GLN:O	1:B:84:ASP:C	2.58	0.42
1:C:161:ILE:CG2	1:C:161:ILE:O	2.68	0.42
1:C:173:ILE:HD12	1:C:243:LEU:HD21	2.01	0.42
1:C:292:ARG:NE	1:C:617:LYS:HE3	2.35	0.42
1:C:579:THR:O	1:C:581:GLN:N	2.53	0.42
1:C:636:ALA:O	1:C:640:LYS:CA	2.68	0.42
1:C:776:LEU:CD2	1:C:776:LEU:C	2.88	0.42
1:D:503:GLU:HA	1:D:503:GLU:OE1	2.20	0.42
1:D:776:LEU:CD2	1:D:776:LEU:C	2.88	0.42
1:D:794:GLN:HB3	1:D:794:GLN:HE21	1.66	0.42
1:E:134:LYS:C	1:E:136:PRO:HD3	2.40	0.42
1:E:191:GLU:O	1:E:192:PHE:C	2.59	0.42
1:E:210:PHE:CD1	1:E:210:PHE:C	2.94	0.42
1:E:281:GLU:C	1:E:283:LEU:H	2.22	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:680:LYS:O	1:E:687:GLU:HG2	2.19	0.42
1:E:755:ARG:O	1:E:756:ILE:C	2.59	0.42
1:F:311:HIS:O	1:F:314:ALA:N	2.53	0.42
1:F:334:LEU:HD23	1:F:356:ASP:HA	2.01	0.42
2:P:133:ASP:OD2	2:P:135:GLN:HG3	2.20	0.42
2:P:18:LEU:HB3	2:P:19:PHE:CE1	2.55	0.42
2:Q:65:PHE:CB	2:Q:66:PRO:HD3	2.38	0.42
2:S:18:LEU:HB3	2:S:19:PHE:CE1	2.55	0.42
2:T:106:ARG:NH2	2:T:118:ASP:OD2	2.53	0.42
1:A:512:GLU:O	1:A:516:VAL:HG23	2.20	0.41
1:A:550:SER:HB3	1:A:553:GLN:CG	2.39	0.41
1:A:585:GLU:OE1	1:A:585:GLU:HA	2.20	0.41
1:A:755:ARG:O	1:A:756:ILE:C	2.57	0.41
1:B:97:TYR:OH	1:B:150:PRO:HB2	2.19	0.41
1:B:278:LYS:CB	1:B:279:ILE:HD13	2.49	0.41
1:B:736:LEU:HD11	1:B:750:GLN:HE21	1.80	0.41
1:C:281:GLU:C	1:C:283:LEU:H	2.23	0.41
1:C:306:GLY:O	1:C:307:LEU:C	2.57	0.41
1:C:557:LEU:HD11	1:C:575:VAL:CG1	2.50	0.41
1:C:579:THR:C	1:C:581:GLN:H	2.23	0.41
1:C:656:THR:HG22	1:C:657:ILE:O	2.20	0.41
1:D:414:LYS:C	1:D:416:ASN:H	2.23	0.41
1:D:739:LYS:HG2	1:D:740:GLN:N	2.30	0.41
1:E:117:LEU:HD12	1:E:145:LYS:HZ3	1.85	0.41
1:E:128:MET:HE3	1:E:239:HIS:NE2	2.35	0.41
1:E:186:LYS:HE3	1:E:234:LEU:HB2	2.02	0.41
1:E:457:THR:HG21	1:E:468:LYS:HA	2.01	0.41
1:E:462:ILE:HD11	1:E:466:GLY:CA	2.49	0.41
1:E:637:PRO:O	1:E:638:GLY:C	2.58	0.41
1:E:671:ARG:O	1:E:675:ASN:HA	2.19	0.41
1:F:318:ILE:O	1:F:319:ALA:C	2.59	0.41
1:F:338:LEU:O	1:F:343:VAL:CG2	2.67	0.41
1:F:414:LYS:C	1:F:416:ASN:H	2.23	0.41
1:F:74:GLU:C	1:F:75:THR:O	2.57	0.41
1:F:81:GLN:OE1	1:F:156:ILE:HG21	2.20	0.41
2:O:18:LEU:HB3	2:O:19:PHE:CE1	2.54	0.41
2:O:44:THR:H	2:O:47:GLU:HB3	1.85	0.41
2:P:117:THR:O	2:P:118:ASP:C	2.58	0.41
2:P:44:THR:OG1	2:P:47:GLU:CB	2.68	0.41
1:C:694:VAL:CG2	2:Q:18:LEU:HD21	2.50	0.41
2:S:21:LYS:O	2:S:23:GLY:N	2.49	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:44:THR:H	2:T:47:GLU:HB3	1.85	0.41
1:A:543:ASP:OD1	1:A:544:SER:N	2.53	0.41
1:A:581:GLN:O	1:A:629:ASN:HA	2.20	0.41
1:A:776:LEU:C	1:A:776:LEU:CD2	2.88	0.41
1:B:191:GLU:O	1:B:192:PHE:C	2.59	0.41
1:B:318:ILE:O	1:B:319:ALA:C	2.58	0.41
1:B:423:LYS:HE2	1:B:425:GLU:OE1	2.20	0.41
1:B:671:ARG:O	1:B:675:ASN:HA	2.20	0.41
1:B:776:LEU:CD2	1:B:776:LEU:C	2.88	0.41
1:C:136:PRO:O	1:C:137:PHE:C	2.58	0.41
1:C:318:ILE:CG2	1:C:322:LEU:HD12	2.50	0.41
1:C:345:THR:OG1	1:C:573:ASP:O	2.37	0.41
1:C:368:GLN:HG3	1:C:383:GLY:C	2.41	0.41
1:D:100:LEU:HD13	1:D:182:ILE:HG21	2.01	0.41
1:D:210:PHE:C	1:D:210:PHE:CD1	2.93	0.41
1:D:307:LEU:HD12	1:D:307:LEU:N	2.34	0.41
1:D:515:LYS:O	1:D:515:LYS:HG2	2.20	0.41
1:D:629:ASN:HB3	1:D:632:TYR:CZ	2.55	0.41
1:D:660:SER:O	1:D:663:PHE:HB3	2.20	0.41
1:D:66:LEU:HD11	1:D:97:TYR:HD2	1.85	0.41
1:E:333:LYS:HD2	1:E:333:LYS:H	1.85	0.41
1:E:581:GLN:O	1:E:629:ASN:HA	2.19	0.41
1:E:736:LEU:HD11	1:E:750:GLN:HE21	1.80	0.41
1:F:134:LYS:C	1:F:136:PRO:HD3	2.41	0.41
1:F:175:LYS:HB2	1:F:175:LYS:HZ2	1.83	0.41
2:P:76:MSE:HA	2:P:79:THR:HG22	2.02	0.41
2:Q:16:PHE:CE1	2:Q:27:ILE:HG12	2.55	0.41
2:Q:54:GLU:O	2:Q:55:VAL:HG22	2.20	0.41
2:R:65:PHE:O	2:R:68:PHE:HB3	2.20	0.41
2:R:6:GLU:O	2:R:9:ILE:HB	2.21	0.41
2:S:138:TYR:O	2:S:141:PHE:HB3	2.19	0.41
2:T:27:ILE:HA	2:T:31:GLU:OE2	2.20	0.41
1:A:257:LEU:O	1:A:261:ALA:O	2.38	0.41
1:A:522:SER:O	2:O:124:MSE:HE2	2.20	0.41
1:B:231:LYS:HB2	1:B:231:LYS:HE3	1.85	0.41
1:B:333:LYS:HD2	1:B:333:LYS:H	1.85	0.41
1:B:457:THR:HG21	1:B:468:LYS:HA	2.02	0.41
1:B:755:ARG:O	1:B:756:ILE:C	2.58	0.41
1:B:90:PRO:O	1:B:92:ASP:N	2.53	0.41
1:C:106:PHE:CZ	1:C:171:TYR:OH	2.65	0.41
1:C:70:GLU:CB	1:C:107:THR:HG22	2.44	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:LYS:N	1:C:118:GLN:HB2	2.34	0.41
1:C:217:LYS:HB2	1:C:236:GLU:CG	2.50	0.41
1:C:186:LYS:CE	1:C:234:LEU:HB2	2.49	0.41
1:C:275:GLY:O	1:C:278:LYS:HD2	2.20	0.41
1:C:278:LYS:CB	1:C:279:ILE:HD13	2.50	0.41
1:C:74:GLU:C	1:C:75:THR:O	2.58	0.41
1:C:764:LEU:HA	1:C:764:LEU:HD23	1.84	0.41
1:D:318:ILE:CD1	1:D:318:ILE:H	2.28	0.41
1:D:423:LYS:HE2	1:D:425:GLU:OE1	2.21	0.41
1:D:93:VAL:HG23	1:D:179:LEU:CD1	2.41	0.41
1:E:217:LYS:HB2	1:E:236:GLU:CG	2.51	0.41
1:E:579:THR:O	1:E:581:GLN:N	2.53	0.41
1:E:693:SER:OG	1:E:731:GLU:OE1	2.38	0.41
1:E:70:GLU:HB3	1:E:71:PHE:H	1.75	0.41
1:E:793:PHE:O	1:E:794:GLN:C	2.56	0.41
1:F:181:ILE:HD12	1:F:238:GLN:OE1	2.20	0.41
1:F:184:LYS:CE	1:F:191:GLU:HB2	2.49	0.41
1:F:210:PHE:CD1	1:F:210:PHE:C	2.94	0.41
1:F:338:LEU:HD21	1:F:409:ARG:HD3	2.01	0.41
1:F:412:GLU:O	1:F:416:ASN:HB2	2.20	0.41
1:F:579:THR:C	1:F:581:GLN:H	2.24	0.41
1:F:579:THR:O	1:F:581:GLN:N	2.53	0.41
2:O:133:ASP:OD2	2:O:135:GLN:HG3	2.20	0.41
2:O:36:MSE:O	2:O:37:ARG:C	2.59	0.41
2:P:4:LEU:CB	2:P:8:GLN:HE21	2.33	0.41
2:R:117:THR:C	2:R:119:GLU:N	2.71	0.41
2:R:6:GLU:O	2:R:9:ILE:N	2.48	0.41
1:A:106:PHE:CZ	1:A:171:TYR:OH	2.63	0.41
1:A:338:LEU:O	1:A:343:VAL:CG2	2.68	0.41
1:A:407:HIS:N	1:A:407:HIS:ND1	2.69	0.41
1:A:462:ILE:CG1	1:A:463:THR:N	2.80	0.41
1:A:463:THR:HG22	1:A:465:LEU:H	1.85	0.41
1:B:210:PHE:C	1:B:210:PHE:CD1	2.94	0.41
1:B:186:LYS:CE	1:B:234:LEU:HB2	2.49	0.41
1:B:254:ARG:HG2	1:B:255:THR:N	2.35	0.41
1:B:73:ASN:HB3	1:B:74:GLU:OE2	2.20	0.41
1:C:333:LYS:HA	1:C:336:THR:HG1	1.84	0.41
1:C:349:ASN:HD22	1:C:350:VAL:HG23	1.86	0.41
1:C:424:LYS:HB3	1:C:424:LYS:NZ	2.31	0.41
1:C:522:SER:O	2:Q:124:MSE:HE2	2.20	0.41
1:C:543:ASP:OD1	1:C:544:SER:N	2.53	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:LEU:HD12	1:D:168:GLU:OE1	2.20	0.41
1:E:161:ILE:O	1:E:161:ILE:CG2	2.68	0.41
1:E:318:ILE:O	1:E:319:ALA:C	2.59	0.41
1:E:324:THR:CG2	1:E:499:PRO:HA	2.51	0.41
1:E:292:ARG:NE	1:E:617:LYS:HE3	2.35	0.41
1:E:655:ASN:ND2	1:E:655:ASN:N	2.68	0.41
1:E:697:ILE:HG12	1:E:732:ILE:CD1	2.50	0.41
1:F:106:PHE:CZ	1:F:171:TYR:OH	2.65	0.41
1:F:172:GLU:O	1:F:176:GLY:N	2.35	0.41
1:F:794:GLN:HE22	1:F:795:LYS:CG	2.32	0.41
1:F:85:LEU:HD12	1:F:168:GLU:OE1	2.20	0.41
1:F:90:PRO:O	1:F:92:ASP:N	2.54	0.41
2:O:6:GLU:O	2:O:9:ILE:HB	2.20	0.41
2:T:18:LEU:HB3	2:T:19:PHE:HD1	1.83	0.41
2:T:65:PHE:CB	2:T:66:PRO:HD3	2.38	0.41
2:T:6:GLU:O	2:T:9:ILE:HB	2.20	0.41
1:A:324:THR:CG2	1:A:499:PRO:HA	2.51	0.41
1:A:66:LEU:HD11	1:A:97:TYR:HD2	1.86	0.41
1:A:680:LYS:O	1:A:687:GLU:HG2	2.21	0.41
1:B:137:PHE:O	1:B:140:ARG:N	2.52	0.41
1:B:181:ILE:HD12	1:B:238:GLN:OE1	2.20	0.41
1:B:217:LYS:HB2	1:B:236:GLU:CG	2.50	0.41
1:B:607:ASN:HB3	1:B:609:GLU:OE2	2.20	0.41
1:B:637:PRO:O	1:B:638:GLY:C	2.59	0.41
1:B:655:ASN:ND2	1:B:655:ASN:N	2.68	0.41
1:B:694:VAL:CG2	2:P:18:LEU:HD21	2.50	0.41
1:B:66:LEU:HD11	1:B:97:TYR:CD2	2.55	0.41
1:C:131:ARG:CB	1:C:170:TYR:OH	2.69	0.41
1:C:191:GLU:O	1:C:192:PHE:C	2.59	0.41
1:C:199:LEU:O	1:C:201:ASP:N	2.52	0.41
1:C:412:GLU:O	1:C:416:ASN:HB2	2.21	0.41
1:C:73:ASN:HB3	1:C:74:GLU:OE2	2.21	0.41
1:D:217:LYS:HB2	1:D:236:GLU:CG	2.51	0.41
1:D:217:LYS:HG3	1:D:236:GLU:HG3	2.03	0.41
1:D:333:LYS:HA	1:D:336:THR:HG1	1.85	0.41
1:D:666:ASN:HB2	1:D:748:TYR:CZ	2.56	0.41
1:E:115:LYS:N	1:E:118:GLN:HB2	2.35	0.41
1:E:172:GLU:O	1:E:175:LYS:HB3	2.21	0.41
1:E:199:LEU:O	1:E:201:ASP:N	2.52	0.41
1:E:414:LYS:C	1:E:416:ASN:H	2.23	0.41
1:F:70:GLU:CB	1:F:107:THR:HG22	2.44	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:PRO:O	1:F:137:PHE:C	2.59	0.41
1:F:161:ILE:O	1:F:161:ILE:CG2	2.68	0.41
1:F:463:THR:HG22	1:F:465:LEU:H	1.85	0.41
1:F:667:LEU:HD13	1:F:678:VAL:HG21	2.01	0.41
2:P:117:THR:HG23	2:P:120:GLU:CG	2.50	0.41
2:P:54:GLU:O	2:P:55:VAL:HG22	2.21	0.41
2:Q:138:TYR:O	2:Q:141:PHE:HB3	2.20	0.41
2:S:44:THR:OG1	2:S:47:GLU:CB	2.68	0.41
2:S:81:SER:C	2:S:83:GLU:N	2.73	0.41
2:S:4:LEU:CB	2:S:8:GLN:HE21	2.34	0.41
1:A:557:LEU:HD11	1:A:575:VAL:CG1	2.51	0.41
1:A:637:PRO:O	1:A:638:GLY:C	2.59	0.41
1:B:183:SER:HB3	1:B:184:LYS:H	1.50	0.41
1:B:173:ILE:HD12	1:B:243:LEU:HD21	2.02	0.41
1:B:281:GLU:C	1:B:283:LEU:H	2.23	0.41
1:B:463:THR:HG22	1:B:465:LEU:H	1.85	0.41
1:B:527:LYS:HB3	1:B:527:LYS:HE2	1.88	0.41
1:C:515:LYS:O	1:C:515:LYS:HG2	2.21	0.41
1:C:540:ARG:HD3	1:C:627:TYR:OH	2.20	0.41
1:D:134:LYS:HZ2	1:D:136:PRO:HG3	1.85	0.41
1:D:131:ARG:CB	1:D:170:TYR:OH	2.67	0.41
1:D:306:GLY:O	1:D:307:LEU:C	2.58	0.41
1:D:368:GLN:HG3	1:D:383:GLY:C	2.41	0.41
1:D:74:GLU:O	1:D:75:THR:O	2.39	0.41
1:E:231:LYS:HE3	1:E:231:LYS:HB2	1.86	0.41
1:E:508:ILE:HG12	1:E:536:TYR:CD2	2.55	0.41
1:E:585:GLU:HA	1:E:585:GLU:OE1	2.18	0.41
1:E:667:LEU:O	1:E:668:SER:C	2.59	0.41
1:E:66:LEU:HD11	1:E:97:TYR:HD2	1.86	0.41
1:E:73:ASN:HB3	1:E:74:GLU:OE2	2.20	0.41
1:E:776:LEU:CD2	1:E:776:LEU:C	2.89	0.41
1:F:279:ILE:HG22	1:F:283:LEU:CD1	2.51	0.41
1:F:743:PRO:HA	1:F:746:LYS:HE3	2.03	0.41
1:F:66:LEU:HD11	1:F:97:TYR:CD2	2.55	0.41
2:O:44:THR:OG1	2:O:47:GLU:CB	2.68	0.41
2:Q:117:THR:O	2:Q:118:ASP:C	2.59	0.41
2:S:117:THR:HG23	2:S:120:GLU:CG	2.51	0.41
2:S:16:PHE:CE1	2:S:27:ILE:HG12	2.56	0.41
2:S:77:LYS:O	2:S:77:LYS:HG3	2.20	0.41
2:T:54:GLU:O	2:T:55:VAL:HG13	2.20	0.41
1:A:217:LYS:HB2	1:A:236:GLU:CG	2.51	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LYS:HB2	1:A:231:LYS:HE3	1.85	0.41
1:A:423:LYS:HE2	1:A:425:GLU:OE1	2.20	0.41
1:A:559:ARG:O	1:A:563:ALA:HB2	2.21	0.41
1:B:254:ARG:HD2	1:B:254:ARG:N	2.34	0.41
1:B:305:SER:O	1:B:331:VAL:HG23	2.20	0.41
1:B:414:LYS:C	1:B:416:ASN:H	2.23	0.41
1:B:579:THR:C	1:B:581:GLN:H	2.24	0.41
1:B:636:ALA:O	1:B:640:LYS:CA	2.68	0.41
1:B:779:GLN:OE1	1:B:796:ILE:HD12	2.21	0.41
1:B:85:LEU:O	1:B:88:LYS:HE3	2.20	0.41
1:B:66:LEU:HD11	1:B:97:TYR:HD2	1.85	0.41
1:C:161:ILE:HG21	1:C:168:GLU:OE2	2.21	0.41
1:C:503:GLU:OE1	1:C:503:GLU:HA	2.21	0.41
1:C:579:THR:C	1:C:581:GLN:N	2.73	0.41
1:D:403:LEU:CG	1:D:405:LEU:HD11	2.51	0.41
1:D:407:HIS:ND1	1:D:407:HIS:N	2.69	0.41
1:D:522:SER:O	2:R:124:MSE:HE2	2.21	0.41
1:D:655:ASN:N	1:D:655:ASN:ND2	2.69	0.41
1:D:70:GLU:HB3	1:D:71:PHE:H	1.74	0.41
1:E:622:LYS:HA	1:E:622:LYS:HD3	1.52	0.41
1:F:483:GLY:C	1:F:484:VAL:CG2	2.89	0.41
1:F:83:GLN:O	1:F:84:ASP:C	2.59	0.41
2:P:6:GLU:O	2:P:9:ILE:HB	2.20	0.41
2:R:140:GLU:O	2:R:143:GLN:HB2	2.21	0.41
2:S:117:THR:O	2:S:118:ASP:C	2.59	0.41
2:S:27:ILE:HA	2:S:31:GLU:OE2	2.21	0.41
2:S:55:VAL:CG2	2:S:67:GLU:CD	2.88	0.41
2:S:6:GLU:O	2:S:9:ILE:HB	2.19	0.41
2:T:58:ASP:C	2:T:59:GLY:O	2.54	0.41
2:T:5:THR:O	2:T:8:GLN:HB3	2.20	0.41
2:T:4:LEU:CB	2:T:8:GLN:HE21	2.33	0.41
1:A:115:LYS:N	1:A:118:GLN:HB2	2.35	0.41
1:A:136:PRO:O	1:A:137:PHE:C	2.59	0.41
1:A:210:PHE:CD1	1:A:210:PHE:C	2.94	0.41
1:A:412:GLU:O	1:A:416:ASN:HB2	2.20	0.41
1:A:607:ASN:HB3	1:A:609:GLU:OE2	2.21	0.41
1:A:667:LEU:HD13	1:A:678:VAL:HG21	2.02	0.41
1:B:134:LYS:C	1:B:136:PRO:HD3	2.41	0.41
1:B:407:HIS:ND1	1:B:407:HIS:N	2.68	0.41
1:B:670:ILE:O	1:B:671:ARG:C	2.59	0.41
1:C:85:LEU:HD12	1:C:168:GLU:OE1	2.21	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:585:GLU:HA	1:C:585:GLU:OE1	2.20	0.41
1:C:90:PRO:O	1:C:92:ASP:N	2.53	0.41
1:D:148:GLU:CG	1:D:149:THR:N	2.75	0.41
1:D:333:LYS:HD2	1:D:333:LYS:H	1.86	0.41
1:D:585:GLU:OE1	1:D:585:GLU:HA	2.21	0.41
1:D:667:LEU:O	1:D:668:SER:C	2.59	0.41
1:E:338:LEU:HD21	1:E:409:ARG:HD3	2.02	0.41
1:E:334:LEU:HD23	1:E:356:ASP:HA	2.02	0.41
1:F:131:ARG:CB	1:F:170:TYR:OH	2.69	0.41
1:F:186:LYS:CE	1:F:234:LEU:HB2	2.50	0.41
1:F:275:GLY:O	1:F:278:LYS:HD2	2.21	0.41
1:F:431:LYS:O	1:F:432:TYR:CD2	2.74	0.41
1:F:503:GLU:OE1	1:F:503:GLU:HA	2.21	0.41
1:F:585:GLU:HA	1:F:585:GLU:OE1	2.20	0.41
1:F:636:ALA:O	1:F:640:LYS:CA	2.69	0.41
2:P:59:GLY:O	2:P:62:THR:HG22	2.19	0.41
2:Q:65:PHE:O	2:Q:68:PHE:HB3	2.20	0.41
2:R:138:TYR:O	2:R:141:PHE:HB3	2.21	0.41
1:D:694:VAL:CG2	2:R:18:LEU:HD21	2.50	0.41
2:T:18:LEU:HB3	2:T:19:PHE:CE1	2.54	0.41
2:T:52:ILE:CG2	2:T:53:ASN:H	2.34	0.41
2:T:75:LYS:O	2:T:79:THR:HG22	2.20	0.41
1:A:117:LEU:HD12	1:A:145:LYS:HZ3	1.86	0.41
1:A:306:GLY:O	1:A:307:LEU:C	2.57	0.41
1:A:508:ILE:HG12	1:A:536:TYR:CD2	2.56	0.41
1:A:292:ARG:NE	1:A:617:LYS:HE3	2.35	0.41
1:A:670:ILE:O	1:A:671:ARG:C	2.59	0.41
1:A:694:VAL:CG2	2:O:18:LEU:HD21	2.50	0.41
1:B:100:LEU:CD1	1:B:182:ILE:HG21	2.51	0.41
1:B:338:LEU:HD21	1:B:409:ARG:HD3	2.02	0.41
1:B:558:ASP:O	1:B:559:ARG:C	2.60	0.41
1:B:574:VAL:HG13	1:B:575:VAL:HG23	2.03	0.41
1:B:581:GLN:O	1:B:629:ASN:HA	2.20	0.41
1:C:186:LYS:HE3	1:C:234:LEU:HB2	2.02	0.41
1:C:307:LEU:N	1:C:307:LEU:HD12	2.34	0.41
1:C:629:ASN:HB3	1:C:632:TYR:CZ	2.56	0.41
1:C:74:GLU:O	1:C:75:THR:O	2.39	0.41
1:C:83:GLN:O	1:C:84:ASP:C	2.58	0.41
1:D:184:LYS:CE	1:D:191:GLU:HB2	2.50	0.41
1:D:338:LEU:HD21	1:D:409:ARG:HD3	2.02	0.41
1:D:483:GLY:C	1:D:484:VAL:CG2	2.89	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:784:GLU:HG3	1:D:785:ASN:N	2.36	0.41
1:E:184:LYS:NZ	1:E:191:GLU:HB2	2.36	0.41
1:E:279:ILE:HG22	1:E:283:LEU:CD1	2.51	0.41
1:E:412:GLU:O	1:E:416:ASN:HB2	2.21	0.41
1:E:636:ALA:O	1:E:640:LYS:CA	2.69	0.41
1:E:685:LYS:HA	1:E:685:LYS:HD3	1.90	0.41
1:E:767:GLN:HB3	1:E:768:LYS:H	1.55	0.41
1:E:778:LYS:HE3	1:E:778:LYS:HB3	1.75	0.41
1:E:93:VAL:HG23	1:E:179:LEU:CD1	2.42	0.41
1:F:100:LEU:HD13	1:F:182:ILE:HG21	2.01	0.41
1:F:557:LEU:HD11	1:F:575:VAL:CG1	2.51	0.41
1:F:559:ARG:O	1:F:563:ALA:HB2	2.21	0.41
1:F:66:LEU:HD11	1:F:97:TYR:HD2	1.86	0.41
2:T:140:GLU:O	2:T:143:GLN:HB2	2.20	0.41
1:A:172:GLU:O	1:A:175:LYS:HB3	2.21	0.41
1:A:191:GLU:O	1:A:192:PHE:C	2.59	0.41
1:A:431:LYS:O	1:A:432:TYR:CD2	2.74	0.41
1:A:521:ASN:HB3	1:A:524:GLU:CB	2.51	0.41
1:B:270:LYS:HA	1:B:273:LYS:CG	2.51	0.41
1:B:412:GLU:O	1:B:416:ASN:HB2	2.21	0.41
1:C:134:LYS:C	1:C:136:PRO:HD3	2.41	0.41
1:C:210:PHE:C	1:C:210:PHE:CD1	2.94	0.41
1:C:257:LEU:O	1:C:261:ALA:O	2.38	0.41
1:C:279:ILE:HG22	1:C:283:LEU:CD1	2.51	0.41
1:C:338:LEU:O	1:C:343:VAL:CG2	2.67	0.41
1:C:403:LEU:CG	1:C:405:LEU:HD11	2.51	0.41
1:C:423:LYS:HE2	1:C:425:GLU:OE1	2.21	0.41
1:C:431:LYS:O	1:C:432:TYR:CD2	2.74	0.41
1:C:741:ILE:O	1:C:741:ILE:HG13	2.21	0.41
1:C:743:PRO:HA	1:C:746:LYS:HE3	2.03	0.41
1:D:462:ILE:HD11	1:D:466:GLY:CA	2.48	0.41
1:D:779:GLN:OE1	1:D:796:ILE:HD12	2.21	0.41
1:D:85:LEU:O	1:D:88:LYS:HE3	2.21	0.41
1:F:115:LYS:N	1:F:118:GLN:HB2	2.35	0.41
1:F:127:SER:O	1:F:133:GLU:CD	2.48	0.41
1:F:217:LYS:HB2	1:F:236:GLU:CG	2.51	0.41
1:F:278:LYS:O	1:F:281:GLU:HB2	2.21	0.41
1:F:637:PRO:O	1:F:638:GLY:C	2.59	0.41
1:F:680:LYS:O	1:F:687:GLU:HG2	2.20	0.41
2:O:111:ASN:C	2:O:113:GLY:H	2.24	0.41
2:Q:117:THR:HG23	2:Q:120:GLU:CG	2.51	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:52:ILE:CG2	2:Q:53:ASN:N	2.84	0.41
2:Q:55:VAL:CG2	2:Q:67:GLU:CD	2.88	0.41
2:Q:4:LEU:CB	2:Q:8:GLN:HE21	2.33	0.41
2:R:16:PHE:CE1	2:R:27:ILE:HG12	2.56	0.41
2:S:148:LYS:HE3	2:S:148:LYS:HB3	1.96	0.41
2:S:36:MSE:O	2:S:37:ARG:C	2.59	0.41
2:S:54:GLU:O	2:S:55:VAL:HG22	2.21	0.41
2:S:61:GLY:C	2:S:62:THR:HG22	2.41	0.41
2:S:59:GLY:O	2:S:62:THR:HG22	2.19	0.41
2:T:111:ASN:C	2:T:113:GLY:H	2.25	0.41
2:T:117:THR:HG23	2:T:120:GLU:CG	2.50	0.41
1:A:677:GLY:HA2	1:A:745:TYR:OH	2.20	0.41
1:B:161:ILE:HG21	1:B:168:GLU:OE2	2.21	0.41
1:B:515:LYS:O	1:B:515:LYS:HG2	2.21	0.41
1:B:74:GLU:C	1:B:75:THR:O	2.57	0.41
1:C:184:LYS:CE	1:C:191:GLU:HB2	2.49	0.41
1:D:161:ILE:HG21	1:D:168:GLU:OE2	2.20	0.41
1:D:492:TYR:HB2	1:D:575:VAL:HG22	2.03	0.41
1:D:66:LEU:HD11	1:D:97:TYR:CD2	2.55	0.41
1:D:670:ILE:O	1:D:671:ARG:C	2.59	0.41
1:D:794:GLN:HE22	1:D:795:LYS:CG	2.32	0.41
1:E:483:GLY:C	1:E:484:VAL:CG2	2.90	0.41
1:F:257:LEU:O	1:F:261:ALA:O	2.39	0.41
1:F:306:GLY:O	1:F:307:LEU:C	2.57	0.41
2:O:27:ILE:HA	2:O:31:GLU:OE2	2.21	0.41
2:P:54:GLU:O	2:P:55:VAL:HG13	2.21	0.41
2:R:117:THR:O	2:R:118:ASP:C	2.59	0.41
2:R:117:THR:HG23	2:R:120:GLU:CG	2.51	0.41
2:R:36:MSE:O	2:R:37:ARG:C	2.59	0.41
2:R:44:THR:OG1	2:R:47:GLU:CB	2.68	0.41
2:T:56:ASP:CG	2:T:60:ASN:CG	2.80	0.41
1:A:128:MET:HE3	1:A:239:HIS:NE2	2.36	0.40
1:A:172:GLU:HB3	1:A:246:SER:CA	2.46	0.40
1:A:349:ASN:HD22	1:A:350:VAL:HG23	1.85	0.40
1:A:585:GLU:HB3	1:A:586:PHE:CD1	2.56	0.40
1:A:700:TYR:CD1	1:A:727:GLN:C	2.94	0.40
1:A:779:GLN:OE1	1:A:796:ILE:HD12	2.21	0.40
1:B:334:LEU:HD23	1:B:356:ASP:HA	2.02	0.40
1:B:680:LYS:O	1:B:687:GLU:HG2	2.20	0.40
1:C:270:LYS:HA	1:C:273:LYS:CG	2.51	0.40
1:C:338:LEU:HD21	1:C:409:ARG:HD3	2.02	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:LEU:O	1:D:261:ALA:O	2.39	0.40
1:D:700:TYR:CD1	1:D:727:GLN:C	2.95	0.40
1:D:693:SER:OG	1:D:731:GLU:OE1	2.39	0.40
1:E:338:LEU:O	1:E:343:VAL:CG2	2.67	0.40
1:E:515:LYS:HG2	1:E:515:LYS:O	2.21	0.40
1:E:512:GLU:O	1:E:516:VAL:HG23	2.20	0.40
1:E:527:LYS:HE2	1:E:527:LYS:HB3	1.86	0.40
1:E:693:SER:O	1:E:696:LYS:HB2	2.21	0.40
1:F:521:ASN:HB3	1:F:524:GLU:CB	2.51	0.40
2:O:16:PHE:CE1	2:O:27:ILE:HG12	2.55	0.40
2:P:52:ILE:CG2	2:P:53:ASN:N	2.84	0.40
2:Q:27:ILE:HA	2:Q:31:GLU:OE2	2.21	0.40
2:Q:54:GLU:O	2:Q:55:VAL:HG13	2.21	0.40
2:Q:61:GLY:C	2:Q:62:THR:HG22	2.40	0.40
1:A:338:LEU:HD21	1:A:409:ARG:NE	2.37	0.40
1:A:368:GLN:HG3	1:A:383:GLY:C	2.42	0.40
1:A:345:THR:OG1	1:A:573:ASP:O	2.37	0.40
1:A:632:TYR:O	1:A:633:ASN:HB2	2.20	0.40
1:A:784:GLU:HG3	1:A:785:ASN:N	2.36	0.40
1:B:175:LYS:HZ2	1:B:175:LYS:CB	2.34	0.40
1:B:184:LYS:NZ	1:B:191:GLU:HB2	2.37	0.40
1:B:275:GLY:O	1:B:278:LYS:HD2	2.21	0.40
1:B:403:LEU:CG	1:B:405:LEU:HD11	2.52	0.40
1:B:338:LEU:HD21	1:B:409:ARG:NE	2.37	0.40
1:C:666:ASN:HB2	1:C:748:TYR:CZ	2.57	0.40
1:C:670:ILE:O	1:C:671:ARG:C	2.58	0.40
1:D:191:GLU:O	1:D:192:PHE:C	2.58	0.40
1:D:585:GLU:HB3	1:D:586:PHE:CD1	2.56	0.40
1:D:743:PRO:HA	1:D:746:LYS:HB3	2.03	0.40
1:D:764:LEU:HA	1:D:764:LEU:HD23	1.85	0.40
1:E:257:LEU:O	1:E:261:ALA:O	2.38	0.40
1:E:368:GLN:HG3	1:E:383:GLY:C	2.41	0.40
1:E:407:HIS:N	1:E:407:HIS:ND1	2.69	0.40
1:E:503:GLU:HA	1:E:503:GLU:OE1	2.21	0.40
1:E:574:VAL:HG13	1:E:575:VAL:HG23	2.03	0.40
1:F:197:LYS:HE3	1:F:264:MET:SD	2.61	0.40
1:F:318:ILE:CG2	1:F:322:LEU:HD12	2.51	0.40
1:F:423:LYS:HE2	1:F:425:GLU:OE1	2.20	0.40
1:F:629:ASN:HB3	1:F:632:TYR:CZ	2.56	0.40
2:P:27:ILE:HA	2:P:31:GLU:OE2	2.20	0.40
2:R:66:PRO:C	2:R:68:PHE:H	2.24	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:117:THR:O	2:T:118:ASP:C	2.59	0.40
1:A:271:LEU:HD23	1:A:271:LEU:HA	1.87	0.40
1:A:278:LYS:O	1:A:281:GLU:HB2	2.21	0.40
1:A:414:LYS:C	1:A:416:ASN:H	2.23	0.40
1:A:666:ASN:HB2	1:A:748:TYR:CZ	2.57	0.40
1:A:66:LEU:HD11	1:A:97:TYR:CD2	2.56	0.40
1:A:74:GLU:C	1:A:75:THR:O	2.58	0.40
1:B:128:MET:HG2	1:B:128:MET:H	1.77	0.40
1:B:515:LYS:HZ3	1:B:516:VAL:CG2	2.34	0.40
1:B:636:ALA:HA	1:B:637:PRO:HD3	1.86	0.40
1:C:159:TYR:CD1	1:C:159:TYR:N	2.90	0.40
1:C:217:LYS:HG3	1:C:236:GLU:HG3	2.03	0.40
1:C:165:GLN:HG2	1:C:251:PRO:CG	2.51	0.40
1:C:504:ILE:H	1:C:504:ILE:CD1	2.32	0.40
1:C:559:ARG:O	1:C:563:ALA:HB2	2.21	0.40
1:C:779:GLN:OE1	1:C:796:ILE:HD12	2.21	0.40
1:C:81:GLN:OE1	1:C:156:ILE:HG21	2.21	0.40
1:D:152:LEU:HD21	1:D:154:ILE:HD11	2.02	0.40
1:D:278:LYS:HB2	1:D:279:ILE:H	1.64	0.40
1:D:658:PRO:HD3	1:D:755:ARG:HH11	1.86	0.40
1:D:88:LYS:HZ3	1:D:172:GLU:CD	2.25	0.40
1:E:423:LYS:HE2	1:E:425:GLU:OE1	2.21	0.40
1:E:607:ASN:HB3	1:E:609:GLU:OE2	2.22	0.40
1:F:191:GLU:O	1:F:192:PHE:C	2.59	0.40
1:F:368:GLN:HG3	1:F:383:GLY:C	2.42	0.40
1:F:508:ILE:HG12	1:F:536:TYR:CD2	2.56	0.40
1:F:492:TYR:HB2	1:F:575:VAL:HG22	2.04	0.40
1:F:598:PRO:HG3	1:F:624:TYR:OH	2.20	0.40
2:O:117:THR:HG23	2:O:120:GLU:CG	2.51	0.40
2:O:55:VAL:CG2	2:O:67:GLU:CD	2.89	0.40
2:P:66:PRO:C	2:P:68:PHE:H	2.25	0.40
2:R:111:ASN:C	2:R:113:GLY:H	2.24	0.40
2:R:52:ILE:CG2	2:R:53:ASN:N	2.84	0.40
1:A:743:PRO:HA	1:A:746:LYS:HE3	2.03	0.40
1:B:217:LYS:HG3	1:B:236:GLU:HG3	2.03	0.40
1:B:285:LYS:C	1:B:287:GLY:N	2.75	0.40
1:B:412:GLU:C	1:B:414:LYS:N	2.75	0.40
1:B:431:LYS:O	1:B:432:TYR:CD2	2.74	0.40
1:B:540:ARG:HD3	1:B:627:TYR:OH	2.21	0.40
1:B:585:GLU:HB3	1:B:586:PHE:CD1	2.56	0.40
1:B:667:LEU:HD13	1:B:678:VAL:HG21	2.03	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741:ILE:HG13	1:B:741:ILE:O	2.21	0.40
1:B:784:GLU:HG3	1:B:785:ASN:H	1.87	0.40
1:B:784:GLU:HG3	1:B:785:ASN:N	2.36	0.40
1:B:88:LYS:NZ	1:B:172:GLU:CD	2.75	0.40
1:C:199:LEU:C	1:C:201:ASP:N	2.67	0.40
1:C:700:TYR:CD1	1:C:727:GLN:C	2.95	0.40
1:C:784:GLU:HG3	1:C:785:ASN:N	2.36	0.40
1:C:66:LEU:HD11	1:C:97:TYR:HD2	1.86	0.40
1:D:134:LYS:C	1:D:136:PRO:HD3	2.41	0.40
1:D:767:GLN:HB3	1:D:768:LYS:H	1.55	0.40
1:E:504:ILE:CD1	1:E:504:ILE:H	2.32	0.40
1:E:522:SER:O	2:S:124:MSE:HE2	2.22	0.40
1:E:784:GLU:HG3	1:E:785:ASN:N	2.36	0.40
1:F:338:LEU:HD21	1:F:409:ARG:NE	2.36	0.40
1:F:73:ASN:HB3	1:F:74:GLU:OE2	2.21	0.40
1:F:756:ILE:HG12	1:F:756:ILE:H	1.63	0.40
2:P:61:GLY:C	2:P:62:THR:HG22	2.41	0.40
2:R:56:ASP:OD2	2:R:60:ASN:C	2.59	0.40
2:S:66:PRO:C	2:S:68:PHE:H	2.25	0.40
1:A:264:MET:SD	1:A:267:TYR:HD2	2.45	0.40
1:A:318:ILE:CG2	1:A:322:LEU:HD12	2.52	0.40
1:A:403:LEU:CG	1:A:405:LEU:HD11	2.52	0.40
1:A:579:THR:C	1:A:581:GLN:H	2.24	0.40
1:A:636:ALA:O	1:A:640:LYS:CA	2.68	0.40
1:A:74:GLU:O	1:A:75:THR:O	2.39	0.40
1:B:318:ILE:CG2	1:B:322:LEU:HD12	2.51	0.40
1:B:690:LYS:HD3	1:B:741:ILE:HG23	2.04	0.40
1:B:764:LEU:HD23	1:B:764:LEU:HA	1.85	0.40
1:C:483:GLY:C	1:C:484:VAL:CG2	2.89	0.40
1:C:585:GLU:HB3	1:C:586:PHE:CD1	2.56	0.40
1:C:656:THR:O	1:C:755:ARG:NH1	2.55	0.40
1:C:66:LEU:HD11	1:C:97:TYR:CD2	2.56	0.40
1:D:275:GLY:O	1:D:278:LYS:HD2	2.21	0.40
1:D:532:LEU:HD23	1:D:532:LEU:HA	1.77	0.40
1:D:558:ASP:O	1:D:559:ARG:C	2.60	0.40
1:E:70:GLU:CB	1:E:107:THR:HG22	2.43	0.40
1:E:275:GLY:O	1:E:278:LYS:HD2	2.21	0.40
1:E:585:GLU:HB3	1:E:586:PHE:CD1	2.57	0.40
1:E:743:PRO:HA	1:E:746:LYS:HE3	2.04	0.40
1:E:677:GLY:HA2	1:E:745:TYR:OH	2.22	0.40
1:F:172:GLU:O	1:F:175:LYS:HB3	2.21	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:231:LYS:HB2	1:F:231:LYS:HE3	1.85	0.40
1:F:585:GLU:HB3	1:F:586:PHE:CD1	2.56	0.40
1:F:784:GLU:HG3	1:F:785:ASN:N	2.36	0.40
1:F:88:LYS:NZ	1:F:172:GLU:CD	2.75	0.40
2:O:18:LEU:HB3	2:O:19:PHE:HD1	1.83	0.40
2:O:66:PRO:C	2:O:68:PHE:H	2.25	0.40
2:P:30:LYS:HD3	2:P:30:LYS:N	2.11	0.40
2:Q:102:ALA:CA	2:Q:125:ILE:HG13	2.51	0.40
2:Q:18:LEU:HB3	2:Q:19:PHE:HD1	1.82	0.40
2:R:18:LEU:HB3	2:R:19:PHE:HD1	1.83	0.40
2:R:76:MSE:HB2	2:R:76:MSE:HE3	1.65	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:SER:O	1:B:682:SER:O[2_555]	2.16	0.04
1:C:682:SER:O	1:F:682:SER:O[4_556]	2.18	0.02

## 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	733/777 (94%)	526 (72%)	161 (22%)	46 (6%)	1	12
1	B	733/777 (94%)	525 (72%)	159 (22%)	49 (7%)	1	10
1	C	733/777 (94%)	526 (72%)	159 (22%)	48 (6%)	1	11
1	D	733/777 (94%)	523 (71%)	162 (22%)	48 (6%)	1	11
1	E	733/777 (94%)	522 (71%)	164 (22%)	47 (6%)	1	11
1	F	733/777 (94%)	526 (72%)	158 (22%)	49 (7%)	1	10
2	O	144/149 (97%)	110 (76%)	21 (15%)	13 (9%)	1	5

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	144/149 (97%)	108 (75%)	22 (15%)	14 (10%)	1	4
2	Q	144/149 (97%)	109 (76%)	23 (16%)	12 (8%)	1	6
2	R	144/149 (97%)	108 (75%)	24 (17%)	12 (8%)	1	6
2	S	144/149 (97%)	109 (76%)	23 (16%)	12 (8%)	1	6
2	T	144/149 (97%)	110 (76%)	22 (15%)	12 (8%)	1	6
All	All	5262/5556 (95%)	3802 (72%)	1098 (21%)	362 (7%)	1	9

All (362) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	THR
1	A	80	GLN
1	A	135	VAL
1	A	137	PHE
1	A	180	ASP
1	A	181	ILE
1	A	278	LYS
1	A	438	ASN
1	A	510	GLN
1	A	675	ASN
1	A	787	THR
1	B	75	THR
1	B	80	GLN
1	B	135	VAL
1	B	137	PHE
1	B	180	ASP
1	B	181	ILE
1	B	278	LYS
1	B	438	ASN
1	B	510	GLN
1	B	675	ASN
1	B	787	THR
1	C	75	THR
1	C	80	GLN
1	C	135	VAL
1	C	137	PHE
1	C	180	ASP
1	C	181	ILE
1	C	278	LYS
1	C	438	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	510	GLN
1	C	675	ASN
1	C	787	THR
1	D	75	THR
1	D	80	GLN
1	D	135	VAL
1	D	137	PHE
1	D	180	ASP
1	D	181	ILE
1	D	278	LYS
1	D	438	ASN
1	D	510	GLN
1	D	675	ASN
1	D	787	THR
1	E	75	THR
1	E	80	GLN
1	E	135	VAL
1	E	137	PHE
1	E	180	ASP
1	E	181	ILE
1	E	278	LYS
1	E	438	ASN
1	E	510	GLN
1	E	675	ASN
1	E	787	THR
1	F	75	THR
1	F	80	GLN
1	F	135	VAL
1	F	137	PHE
1	F	180	ASP
1	F	181	ILE
1	F	278	LYS
1	F	438	ASN
1	F	510	GLN
1	F	675	ASN
1	F	787	THR
2	O	23	GLY
2	O	60	ASN
2	P	23	GLY
2	Q	23	GLY
2	R	23	GLY
2	S	23	GLY

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	T	23	GLY
1	A	109	ILE
1	A	120	LEU
1	A	138	ALA
1	A	176	GLY
1	A	192	PHE
1	A	290	LYS
1	A	302	LEU
1	A	559	ARG
1	B	109	ILE
1	B	120	LEU
1	B	138	ALA
1	B	176	GLY
1	B	192	PHE
1	B	290	LYS
1	B	302	LEU
1	B	559	ARG
1	C	109	ILE
1	C	120	LEU
1	C	138	ALA
1	C	176	GLY
1	C	192	PHE
1	C	290	LYS
1	C	302	LEU
1	C	559	ARG
1	D	109	ILE
1	D	120	LEU
1	D	138	ALA
1	D	176	GLY
1	D	192	PHE
1	D	290	LYS
1	D	302	LEU
1	D	559	ARG
1	E	109	ILE
1	E	120	LEU
1	E	138	ALA
1	E	176	GLY
1	E	192	PHE
1	E	290	LYS
1	E	302	LEU
1	E	559	ARG
1	F	109	ILE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	F	120	LEU
1	F	138	ALA
1	F	176	GLY
1	F	192	PHE
1	F	290	LYS
1	F	302	LEU
1	F	559	ARG
2	O	24	ASP
2	O	50	ASP
2	O	67	GLU
2	P	24	ASP
2	P	50	ASP
2	P	67	GLU
2	Q	24	ASP
2	Q	50	ASP
2	Q	67	GLU
2	R	24	ASP
2	R	50	ASP
2	R	67	GLU
2	S	24	ASP
2	S	50	ASP
2	S	67	GLU
2	T	24	ASP
2	T	50	ASP
2	T	67	GLU
1	A	70	GLU
1	A	91	LYS
1	A	113	GLU
1	A	200	SER
1	A	232	GLU
1	A	377	GLN
1	A	638	GLY
1	A	698	ALA
1	A	779	GLN
1	B	70	GLU
1	B	91	LYS
1	B	113	GLU
1	B	200	SER
1	B	232	GLU
1	B	376	GLN
1	B	377	GLN
1	B	638	GLY

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	698	ALA
1	B	779	GLN
1	C	70	GLU
1	C	91	LYS
1	C	113	GLU
1	C	200	SER
1	C	232	GLU
1	C	376	GLN
1	C	377	GLN
1	C	638	GLY
1	C	698	ALA
1	C	779	GLN
1	D	70	GLU
1	D	113	GLU
1	D	200	SER
1	D	232	GLU
1	D	376	GLN
1	D	638	GLY
1	D	698	ALA
1	D	779	GLN
1	E	70	GLU
1	E	91	LYS
1	E	113	GLU
1	E	200	SER
1	E	232	GLU
1	E	376	GLN
1	E	638	GLY
1	E	698	ALA
1	E	779	GLN
1	F	70	GLU
1	F	91	LYS
1	F	113	GLU
1	F	200	SER
1	F	232	GLU
1	F	376	GLN
1	F	638	GLY
1	F	698	ALA
1	F	779	GLN
2	O	25	GLY
2	O	74	ARG
2	O	82	GLU
2	O	118	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	O	120	GLU
2	P	60	ASN
2	P	74	ARG
2	P	82	GLU
2	P	118	ASP
2	P	120	GLU
2	Q	74	ARG
2	Q	82	GLU
2	Q	118	ASP
2	Q	120	GLU
2	R	74	ARG
2	R	82	GLU
2	R	118	ASP
2	R	120	GLU
2	S	74	ARG
2	S	118	ASP
2	S	120	GLU
2	T	25	GLY
2	T	74	ARG
2	T	82	GLU
2	T	118	ASP
2	T	120	GLU
1	A	108	ASP
1	A	307	LEU
1	A	376	GLN
1	A	452	GLU
1	A	471	TRP
1	B	108	ASP
1	B	471	TRP
1	B	537	GLY
1	C	108	ASP
1	C	307	LEU
1	C	471	TRP
1	C	672	ARG
1	D	91	LYS
1	D	108	ASP
1	D	307	LEU
1	D	377	GLN
1	D	452	GLU
1	D	471	TRP
1	D	672	ARG
1	E	108	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	E	294	ASP
1	E	307	LEU
1	E	377	GLN
1	E	471	TRP
1	E	672	ARG
1	F	108	ASP
1	F	307	LEU
1	F	377	GLN
1	F	471	TRP
2	O	12	PHE
2	P	12	PHE
2	P	25	GLY
2	Q	12	PHE
2	Q	22	ASP
2	Q	25	GLY
2	R	12	PHE
2	R	25	GLY
2	S	12	PHE
2	S	25	GLY
2	S	82	GLU
2	T	12	PHE
1	A	177	ILE
1	A	274	GLY
1	A	294	ASP
1	A	334	LEU
1	A	537	GLY
1	A	672	ARG
1	B	274	GLY
1	B	294	ASP
1	B	307	LEU
1	B	334	LEU
1	B	452	GLU
1	B	672	ARG
1	B	775	LEU
1	C	274	GLY
1	C	294	ASP
1	C	334	LEU
1	C	452	GLU
1	C	537	GLY
1	D	274	GLY
1	D	294	ASP
1	D	334	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	537	GLY
1	D	580	GLU
1	D	775	LEU
1	E	274	GLY
1	E	334	LEU
1	E	452	GLU
1	E	537	GLY
1	E	775	LEU
1	F	274	GLY
1	F	294	ASP
1	F	334	LEU
1	F	452	GLU
1	F	537	GLY
1	F	580	GLU
1	F	672	ARG
1	F	775	LEU
2	O	21	LYS
2	O	22	ASP
2	P	21	LYS
2	P	22	ASP
2	Q	21	LYS
2	R	21	LYS
2	R	22	ASP
2	S	21	LYS
2	S	22	ASP
2	T	21	LYS
2	T	22	ASP
1	A	775	LEU
1	B	65	ASN
1	B	177	ILE
1	B	580	GLU
1	B	585	GLU
1	C	177	ILE
1	C	580	GLU
1	C	669	SER
1	C	775	LEU
1	D	177	ILE
1	D	669	SER
1	E	177	ILE
1	E	580	GLU
1	F	177	ILE
1	F	423	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	F	669	SER
2	P	61	GLY
1	A	112	VAL
1	A	711	ILE
1	B	112	VAL
1	B	711	ILE
1	C	112	VAL
1	D	112	VAL
1	E	112	VAL
1	E	711	ILE
1	F	112	VAL
1	F	711	ILE
1	A	484	VAL
1	B	484	VAL
1	C	484	VAL
1	C	711	ILE
1	D	484	VAL
1	D	711	ILE
1	F	481	VAL
1	F	484	VAL
1	A	182	ILE
1	A	441	VAL
1	A	481	VAL
1	B	182	ILE
1	B	441	VAL
1	B	481	VAL
1	C	182	ILE
1	C	441	VAL
1	C	481	VAL
1	D	182	ILE
1	D	441	VAL
1	D	481	VAL
1	E	182	ILE
1	E	441	VAL
1	E	481	VAL
1	E	484	VAL
1	F	182	ILE
1	F	441	VAL



### 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	664/705 (94%)	585 (88%)	79 (12%)	6	26
1	B	664/705 (94%)	585 (88%)	79 (12%)	6	26
1	C	664/705 (94%)	585 (88%)	79 (12%)	6	26
1	D	664/705 (94%)	584 (88%)	80 (12%)	6	26
1	E	664/705 (94%)	585 (88%)	79 (12%)	6	26
1	F	664/705 (94%)	585 (88%)	79 (12%)	6	26
2	O	123/117 (105%)	103 (84%)	20 (16%)	3	13
2	P	123/117 (105%)	104 (85%)	19 (15%)	3	15
2	Q	123/117 (105%)	103 (84%)	20 (16%)	3	13
2	R	123/117 (105%)	104 (85%)	19 (15%)	3	15
2	S	123/117 (105%)	103 (84%)	20 (16%)	3	13
2	T	123/117 (105%)	103 (84%)	20 (16%)	3	13
All	All	4722/4932 (96%)	4129 (87%)	593 (13%)	5	24

All (593) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	VAL
1	A	69	THR
1	A	71	PHE
1	A	78	LYS
1	A	88	LYS
1	A	114	HIS
1	A	115	LYS
1	A	118	GLN
1	A	120	LEU
1	A	122	GLU
1	A	129	ASN
1	A	133	GLU
1	A	137	PHE
1	A	140	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	141	PHE
1	A	147	ARG
1	A	149	THR
1	A	156	ILE
1	A	158	ASP
1	A	172	GLU
1	A	179	LEU
1	A	180	ASP
1	A	182	ILE
1	A	188	LEU
1	A	197	LYS
1	A	210	PHE
1	A	212	GLN
1	A	213	LYS
1	A	229	PHE
1	A	236	GLU
1	A	254	ARG
1	A	255	THR
1	A	260	TYR
1	A	279	ILE
1	A	284	LYS
1	A	292	ARG
1	A	296	LEU
1	A	320	ARG
1	A	323	ASN
1	A	324	THR
1	A	349	ASN
1	A	376	GLN
1	A	377	GLN
1	A	395	GLU
1	A	397	GLU
1	A	400	LYS
1	A	408	LEU
1	A	414	LYS
1	A	415	GLU
1	A	427	ASP
1	A	434	LEU
1	A	438	ASN
1	A	455	TYR
1	A	469	PHE
1	A	473	ASN
1	A	479	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	480	ASN
1	A	484	VAL
1	A	515	LYS
1	A	562	GLU
1	A	567	THR
1	A	581	GLN
1	A	583	ASN
1	A	629	ASN
1	A	635	ILE
1	A	639	ASN
1	A	644	GLU
1	A	646	THR
1	A	665	LYS
1	A	669	SER
1	A	672	ARG
1	A	678	VAL
1	A	688	PHE
1	A	709	ASN
1	A	714	GLN
1	A	744	GLU
1	A	755	ARG
1	A	766	HIS
1	A	794	GLN
1	B	67	VAL
1	B	69	THR
1	B	71	PHE
1	B	78	LYS
1	B	88	LYS
1	B	114	HIS
1	B	115	LYS
1	B	118	GLN
1	B	120	LEU
1	B	122	GLU
1	B	129	ASN
1	B	133	GLU
1	B	137	PHE
1	B	140	ARG
1	B	141	PHE
1	B	147	ARG
1	B	149	THR
1	B	156	ILE
1	B	158	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	172	GLU
1	B	179	LEU
1	B	180	ASP
1	B	182	ILE
1	B	188	LEU
1	B	197	LYS
1	B	210	PHE
1	B	212	GLN
1	B	213	LYS
1	B	229	PHE
1	B	236	GLU
1	B	254	ARG
1	B	255	THR
1	B	260	TYR
1	B	279	ILE
1	B	284	LYS
1	B	292	ARG
1	B	296	LEU
1	B	320	ARG
1	B	323	ASN
1	B	324	THR
1	B	349	ASN
1	B	376	GLN
1	B	377	GLN
1	B	395	GLU
1	B	397	GLU
1	B	400	LYS
1	B	408	LEU
1	B	414	LYS
1	B	415	GLU
1	B	427	ASP
1	B	434	LEU
1	B	438	ASN
1	B	455	TYR
1	B	469	PHE
1	B	473	ASN
1	B	479	LYS
1	B	480	ASN
1	B	484	VAL
1	B	515	LYS
1	B	562	GLU
1	B	567	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	581	GLN
1	B	583	ASN
1	B	629	ASN
1	B	635	ILE
1	B	639	ASN
1	B	644	GLU
1	B	646	THR
1	B	665	LYS
1	B	669	SER
1	B	672	ARG
1	B	678	VAL
1	B	688	PHE
1	B	709	ASN
1	B	714	GLN
1	B	744	GLU
1	B	755	ARG
1	B	766	HIS
1	B	794	GLN
1	C	67	VAL
1	C	69	THR
1	C	71	PHE
1	C	78	LYS
1	C	88	LYS
1	C	114	HIS
1	C	115	LYS
1	C	118	GLN
1	C	120	LEU
1	C	122	GLU
1	C	129	ASN
1	C	133	GLU
1	C	137	PHE
1	C	140	ARG
1	C	141	PHE
1	C	147	ARG
1	C	149	THR
1	C	156	ILE
1	C	158	ASP
1	C	172	GLU
1	C	179	LEU
1	C	180	ASP
1	C	182	ILE
1	C	188	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	197	LYS
1	C	210	PHE
1	C	212	GLN
1	C	213	LYS
1	C	229	PHE
1	C	236	GLU
1	C	254	ARG
1	C	255	THR
1	C	260	TYR
1	C	279	ILE
1	C	284	LYS
1	C	292	ARG
1	C	296	LEU
1	C	320	ARG
1	C	323	ASN
1	C	324	THR
1	C	349	ASN
1	C	376	GLN
1	C	377	GLN
1	C	395	GLU
1	C	397	GLU
1	C	400	LYS
1	C	408	LEU
1	C	414	LYS
1	C	415	GLU
1	C	427	ASP
1	C	434	LEU
1	C	438	ASN
1	C	455	TYR
1	C	469	PHE
1	C	473	ASN
1	C	479	LYS
1	C	480	ASN
1	C	484	VAL
1	C	515	LYS
1	C	562	GLU
1	C	567	THR
1	C	581	GLN
1	C	583	ASN
1	C	629	ASN
1	C	635	ILE
1	C	639	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	644	GLU
1	C	646	THR
1	C	665	LYS
1	C	669	SER
1	C	672	ARG
1	C	678	VAL
1	C	688	PHE
1	C	709	ASN
1	C	714	GLN
1	C	744	GLU
1	C	755	ARG
1	C	766	HIS
1	C	794	GLN
1	D	67	VAL
1	D	69	THR
1	D	71	PHE
1	D	78	LYS
1	D	88	LYS
1	D	114	HIS
1	D	115	LYS
1	D	118	GLN
1	D	120	LEU
1	D	122	GLU
1	D	129	ASN
1	D	133	GLU
1	D	137	PHE
1	D	140	ARG
1	D	141	PHE
1	D	147	ARG
1	D	149	THR
1	D	156	ILE
1	D	158	ASP
1	D	172	GLU
1	D	179	LEU
1	D	180	ASP
1	D	182	ILE
1	D	188	LEU
1	D	197	LYS
1	D	210	PHE
1	D	212	GLN
1	D	213	LYS
1	D	229	PHE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	236	GLU
1	D	254	ARG
1	D	255	THR
1	D	260	TYR
1	D	279	ILE
1	D	284	LYS
1	D	292	ARG
1	D	296	LEU
1	D	320	ARG
1	D	323	ASN
1	D	324	THR
1	D	349	ASN
1	D	376	GLN
1	D	377	GLN
1	D	395	GLU
1	D	397	GLU
1	D	400	LYS
1	D	408	LEU
1	D	414	LYS
1	D	415	GLU
1	D	427	ASP
1	D	434	LEU
1	D	438	ASN
1	D	455	TYR
1	D	469	PHE
1	D	473	ASN
1	D	479	LYS
1	D	480	ASN
1	D	484	VAL
1	D	515	LYS
1	D	562	GLU
1	D	567	THR
1	D	581	GLN
1	D	583	ASN
1	D	622	LYS
1	D	629	ASN
1	D	635	ILE
1	D	639	ASN
1	D	644	GLU
1	D	646	THR
1	D	665	LYS
1	D	669	SER

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	672	ARG
1	D	678	VAL
1	D	688	PHE
1	D	709	ASN
1	D	714	GLN
1	D	744	GLU
1	D	755	ARG
1	D	766	HIS
1	D	794	GLN
1	E	67	VAL
1	E	69	THR
1	E	71	PHE
1	E	78	LYS
1	E	88	LYS
1	E	114	HIS
1	E	115	LYS
1	E	118	GLN
1	E	120	LEU
1	E	122	GLU
1	E	129	ASN
1	E	133	GLU
1	E	137	PHE
1	E	140	ARG
1	E	141	PHE
1	E	147	ARG
1	E	149	THR
1	E	156	ILE
1	E	158	ASP
1	E	172	GLU
1	E	179	LEU
1	E	180	ASP
1	E	182	ILE
1	E	188	LEU
1	E	197	LYS
1	E	210	PHE
1	E	212	GLN
1	E	213	LYS
1	E	229	PHE
1	E	236	GLU
1	E	254	ARG
1	E	255	THR
1	E	260	TYR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	E	279	ILE
1	E	284	LYS
1	E	292	ARG
1	E	296	LEU
1	E	320	ARG
1	E	323	ASN
1	E	324	THR
1	E	349	ASN
1	E	376	GLN
1	E	377	GLN
1	E	395	GLU
1	E	397	GLU
1	E	400	LYS
1	E	408	LEU
1	E	414	LYS
1	E	415	GLU
1	E	427	ASP
1	E	434	LEU
1	E	438	ASN
1	E	455	TYR
1	E	469	PHE
1	E	473	ASN
1	E	479	LYS
1	E	480	ASN
1	E	484	VAL
1	E	515	LYS
1	E	562	GLU
1	E	567	THR
1	E	581	GLN
1	E	583	ASN
1	E	629	ASN
1	E	635	ILE
1	E	639	ASN
1	E	644	GLU
1	E	646	THR
1	E	665	LYS
1	E	669	SER
1	E	672	ARG
1	E	678	VAL
1	E	688	PHE
1	E	709	ASN
1	E	714	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	E	744	GLU
1	E	755	ARG
1	E	766	HIS
1	E	794	GLN
1	F	67	VAL
1	F	69	THR
1	F	71	PHE
1	F	78	LYS
1	F	88	LYS
1	F	114	HIS
1	F	115	LYS
1	F	118	GLN
1	F	120	LEU
1	F	122	GLU
1	F	129	ASN
1	F	133	GLU
1	F	137	PHE
1	F	140	ARG
1	F	141	PHE
1	F	147	ARG
1	F	149	THR
1	F	156	ILE
1	F	158	ASP
1	F	172	GLU
1	F	179	LEU
1	F	180	ASP
1	F	182	ILE
1	F	188	LEU
1	F	197	LYS
1	F	210	PHE
1	F	212	GLN
1	F	213	LYS
1	F	229	PHE
1	F	236	GLU
1	F	254	ARG
1	F	255	THR
1	F	260	TYR
1	F	279	ILE
1	F	284	LYS
1	F	292	ARG
1	F	296	LEU
1	F	320	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	F	323	ASN
1	F	324	THR
1	F	349	ASN
1	F	376	GLN
1	F	377	GLN
1	F	395	GLU
1	F	397	GLU
1	F	400	LYS
1	F	408	LEU
1	F	414	LYS
1	F	415	GLU
1	F	427	ASP
1	F	434	LEU
1	F	438	ASN
1	F	455	TYR
1	F	469	PHE
1	F	473	ASN
1	F	479	LYS
1	F	480	ASN
1	F	484	VAL
1	F	515	LYS
1	F	562	GLU
1	F	567	THR
1	F	581	GLN
1	F	583	ASN
1	F	629	ASN
1	F	635	ILE
1	F	639	ASN
1	F	644	GLU
1	F	646	THR
1	F	665	LYS
1	F	669	SER
1	F	672	ARG
1	F	678	VAL
1	F	688	PHE
1	F	709	ASN
1	F	714	GLN
1	F	744	GLU
1	F	755	ARG
1	F	766	HIS
1	F	794	GLN
2	O	5	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	O	13	LYS
2	O	14	GLU
2	O	18	LEU
2	O	21	LYS
2	O	30	LYS
2	O	49	GLN
2	O	50	ASP
2	O	54	GLU
2	O	55	VAL
2	O	56	ASP
2	O	58	ASP
2	O	62	THR
2	O	64	ASP
2	O	65	PHE
2	O	69	LEU
2	O	76	MSE
2	O	97	ASN
2	O	117	THR
2	O	123	GLN
2	P	5	THR
2	P	13	LYS
2	P	14	GLU
2	P	18	LEU
2	P	21	LYS
2	P	30	LYS
2	P	49	GLN
2	P	50	ASP
2	P	54	GLU
2	P	55	VAL
2	P	56	ASP
2	P	58	ASP
2	P	64	ASP
2	P	65	PHE
2	P	69	LEU
2	P	76	MSE
2	P	97	ASN
2	P	117	THR
2	P	123	GLN
2	Q	5	THR
2	Q	13	LYS
2	Q	14	GLU
2	Q	18	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	Q	21	LYS
2	Q	30	LYS
2	Q	49	GLN
2	Q	50	ASP
2	Q	54	GLU
2	Q	55	VAL
2	Q	56	ASP
2	Q	58	ASP
2	Q	62	THR
2	Q	64	ASP
2	Q	65	PHE
2	Q	69	LEU
2	Q	76	MSE
2	Q	97	ASN
2	Q	117	THR
2	Q	123	GLN
2	R	5	THR
2	R	13	LYS
2	R	14	GLU
2	R	18	LEU
2	R	21	LYS
2	R	30	LYS
2	R	49	GLN
2	R	50	ASP
2	R	54	GLU
2	R	55	VAL
2	R	56	ASP
2	R	58	ASP
2	R	64	ASP
2	R	65	PHE
2	R	69	LEU
2	R	76	MSE
2	R	97	ASN
2	R	117	THR
2	R	123	GLN
2	S	5	THR
2	S	13	LYS
2	S	14	GLU
2	S	18	LEU
2	S	21	LYS
2	S	30	LYS
2	S	49	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	S	50	ASP
2	S	54	GLU
2	S	55	VAL
2	S	56	ASP
2	S	58	ASP
2	S	62	THR
2	S	64	ASP
2	S	65	PHE
2	S	69	LEU
2	S	76	MSE
2	S	97	ASN
2	S	117	THR
2	S	123	GLN
2	T	5	THR
2	T	13	LYS
2	T	14	GLU
2	T	18	LEU
2	T	21	LYS
2	T	30	LYS
2	T	49	GLN
2	T	50	ASP
2	T	54	GLU
2	T	55	VAL
2	T	56	ASP
2	T	58	ASP
2	T	62	THR
2	T	64	ASP
2	T	65	PHE
2	T	69	LEU
2	T	76	MSE
2	T	97	ASN
2	T	117	THR
2	T	123	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (229) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	129	ASN
1	A	165	GLN
1	A	212	GLN
1	A	323	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	349	ASN
1	A	368	GLN
1	A	377	GLN
1	A	387	ASN
1	A	438	ASN
1	A	451	ASN
1	A	480	ASN
1	A	507	GLN
1	A	510	GLN
1	A	518	ASN
1	A	551	ASN
1	A	553	GLN
1	A	576	ASN
1	A	581	GLN
1	A	618	ASN
1	A	629	ASN
1	A	639	ASN
1	A	655	ASN
1	A	666	ASN
1	A	709	ASN
1	A	730	ASN
1	A	747	ASN
1	A	750	GLN
1	A	758	ASN
1	A	767	GLN
1	A	770	ASN
1	A	781	ASN
1	A	785	ASN
1	A	794	GLN
1	B	64	ASN
1	B	80	GLN
1	B	81	GLN
1	B	129	ASN
1	B	165	GLN
1	B	212	GLN
1	B	323	ASN
1	B	349	ASN
1	B	368	GLN
1	B	377	GLN
1	B	387	ASN
1	B	438	ASN
1	B	451	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	480	ASN
1	B	507	GLN
1	B	510	GLN
1	B	518	ASN
1	B	551	ASN
1	B	553	GLN
1	B	576	ASN
1	B	581	GLN
1	B	618	ASN
1	B	629	ASN
1	B	639	ASN
1	B	655	ASN
1	B	666	ASN
1	B	709	ASN
1	B	730	ASN
1	B	747	ASN
1	B	750	GLN
1	B	758	ASN
1	B	767	GLN
1	B	770	ASN
1	B	781	ASN
1	B	785	ASN
1	B	794	GLN
1	C	80	GLN
1	C	81	GLN
1	C	129	ASN
1	C	165	GLN
1	C	212	GLN
1	C	323	ASN
1	C	349	ASN
1	C	368	GLN
1	C	377	GLN
1	C	387	ASN
1	C	438	ASN
1	C	451	ASN
1	C	480	ASN
1	C	507	GLN
1	C	510	GLN
1	C	518	ASN
1	C	551	ASN
1	C	553	GLN
1	C	576	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	581	GLN
1	C	618	ASN
1	C	629	ASN
1	C	639	ASN
1	C	655	ASN
1	C	666	ASN
1	C	709	ASN
1	C	730	ASN
1	C	747	ASN
1	C	750	GLN
1	C	758	ASN
1	C	767	GLN
1	C	770	ASN
1	C	781	ASN
1	C	785	ASN
1	C	794	GLN
1	D	64	ASN
1	D	80	GLN
1	D	81	GLN
1	D	129	ASN
1	D	165	GLN
1	D	212	GLN
1	D	323	ASN
1	D	349	ASN
1	D	368	GLN
1	D	377	GLN
1	D	387	ASN
1	D	438	ASN
1	D	451	ASN
1	D	480	ASN
1	D	507	GLN
1	D	510	GLN
1	D	518	ASN
1	D	551	ASN
1	D	553	GLN
1	D	576	ASN
1	D	581	GLN
1	D	618	ASN
1	D	629	ASN
1	D	639	ASN
1	D	655	ASN
1	D	666	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	709	ASN
1	D	730	ASN
1	D	747	ASN
1	D	750	GLN
1	D	758	ASN
1	D	767	GLN
1	D	770	ASN
1	D	781	ASN
1	D	785	ASN
1	D	794	GLN
1	E	80	GLN
1	E	129	ASN
1	E	165	GLN
1	E	212	GLN
1	E	323	ASN
1	E	349	ASN
1	E	368	GLN
1	E	377	GLN
1	E	387	ASN
1	E	438	ASN
1	E	451	ASN
1	E	480	ASN
1	E	507	GLN
1	E	510	GLN
1	E	518	ASN
1	E	551	ASN
1	E	553	GLN
1	E	576	ASN
1	E	581	GLN
1	E	618	ASN
1	E	629	ASN
1	E	639	ASN
1	E	655	ASN
1	E	666	ASN
1	E	709	ASN
1	E	730	ASN
1	E	747	ASN
1	E	750	GLN
1	E	758	ASN
1	E	767	GLN
1	E	770	ASN
1	E	781	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	E	785	ASN
1	E	794	GLN
1	F	64	ASN
1	F	80	GLN
1	F	81	GLN
1	F	129	ASN
1	F	165	GLN
1	F	212	GLN
1	F	323	ASN
1	F	349	ASN
1	F	368	GLN
1	F	377	GLN
1	F	387	ASN
1	F	438	ASN
1	F	451	ASN
1	F	480	ASN
1	F	507	GLN
1	F	510	GLN
1	F	518	ASN
1	F	551	ASN
1	F	553	GLN
1	F	576	ASN
1	F	581	GLN
1	F	618	ASN
1	F	629	ASN
1	F	639	ASN
1	F	655	ASN
1	F	666	ASN
1	F	709	ASN
1	F	730	ASN
1	F	747	ASN
1	F	750	GLN
1	F	758	ASN
1	F	767	GLN
1	F	770	ASN
1	F	781	ASN
1	F	785	ASN
1	F	794	GLN
2	O	8	GLN
2	O	49	GLN
2	O	111	ASN
2	P	8	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	P	49	GLN
2	P	111	ASN
2	Q	8	GLN
2	Q	49	GLN
2	Q	111	ASN
2	R	8	GLN
2	R	49	GLN
2	R	111	ASN
2	S	8	GLN
2	S	49	GLN
2	S	111	ASN
2	T	8	GLN
2	T	49	GLN
2	T	111	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 30 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 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	735/777 (94%)	-0.00	31 (4%) 37 24	34, 87, 140, 151	0
1	B	735/777 (94%)	0.01	23 (3%) 49 33	35, 87, 141, 153	0
1	C	735/777 (94%)	0.03	25 (3%) 46 30	34, 87, 141, 153	0
1	D	735/777 (94%)	0.01	28 (3%) 41 27	35, 87, 140, 152	0
1	E	735/777 (94%)	0.01	25 (3%) 46 30	34, 87, 140, 153	0
1	F	735/777 (94%)	-0.03	28 (3%) 41 27	34, 87, 140, 153	0
2	O	137/149 (91%)	-0.21	1 (0%) 87 80	27, 74, 124, 135	0
2	P	137/149 (91%)	-0.17	2 (1%) 74 61	28, 74, 124, 135	0
2	Q	137/149 (91%)	-0.18	1 (0%) 87 80	29, 74, 124, 135	0
2	R	137/149 (91%)	-0.24	1 (0%) 87 80	28, 74, 125, 135	0
2	S	137/149 (91%)	-0.24	1 (0%) 87 80	29, 74, 125, 135	0
2	T	137/149 (91%)	-0.24	1 (0%) 87 80	29, 73, 124, 135	0
All	All	5232/5556 (94%)	-0.03	167 (3%) 48 32	27, 83, 140, 153	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	204	ASP	8.7
1	C	126	ASN	7.6
1	E	204	ASP	6.9
1	B	126	ASN	6.5
1	F	162	ASN	6.1
1	A	225	ILE	6.0
1	A	204	ASP	5.9
1	D	230	ILE	5.8
1	F	204	ASP	5.7
1	B	205	SER	5.7
1	E	212	GLN	5.7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	126	ASN	5.7
1	E	126	ASN	5.6
1	A	206	SER	5.5
1	A	230	ILE	5.5
1	D	162	ASN	5.4
1	F	226	ASP	5.4
1	F	260	TYR	5.4
1	C	206	SER	5.3
1	F	225	ILE	5.3
1	D	225	ILE	5.3
1	D	260	TYR	5.2
1	D	204	ASP	5.2
1	B	162	ASN	5.2
1	C	162	ASN	5.0
1	D	212	GLN	5.0
1	F	205	SER	4.9
1	C	204	ASP	4.9
1	C	225	ILE	4.9
1	A	126	ASN	4.8
1	E	162	ASN	4.6
1	B	230	ILE	4.6
1	F	206	SER	4.5
1	A	162	ASN	4.5
1	D	206	SER	4.5
1	B	225	ILE	4.5
1	E	260	TYR	4.4
1	A	260	TYR	4.4
1	C	205	SER	4.4
1	E	171	TYR	4.3
1	E	206	SER	4.3
1	D	229	PHE	4.3
1	D	420	LEU	4.3
1	C	260	TYR	4.3
1	B	203	SER	4.2
1	B	226	ASP	4.2
1	B	420	LEU	4.2
1	A	226	ASP	4.2
1	C	230	ILE	4.1
1	B	260	TYR	4.1
1	A	113	GLU	4.1
1	A	229	PHE	4.1
1	A	171	TYR	4.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	212	GLN	4.0
1	E	230	ILE	4.0
1	D	226	ASP	3.9
1	D	203	SER	3.8
1	E	207	ASP	3.8
1	E	225	ILE	3.8
1	F	131	ARG	3.8
1	F	126	ASN	3.8
1	A	421	LYS	3.7
1	C	212	GLN	3.7
1	C	192	PHE	3.6
1	C	226	ASP	3.6
1	F	203	SER	3.6
1	F	230	ILE	3.6
1	A	131	ARG	3.5
1	D	171	TYR	3.5
1	C	229	PHE	3.5
1	E	163	SER	3.4
1	E	127	SER	3.4
1	B	171	TYR	3.4
1	D	127	SER	3.4
1	D	222	ASN	3.4
1	A	222	ASN	3.3
1	B	212	GLN	3.3
1	C	127	SER	3.3
1	A	205	SER	3.3
1	A	72	THR	3.3
1	E	226	ASP	3.3
1	B	192	PHE	3.3
1	A	207	ASP	3.2
2	P	78	ASP	3.2
1	F	171	TYR	3.1
1	F	207	ASP	3.1
1	D	205	SER	3.1
1	F	72	THR	3.1
1	C	468	LYS	3.0
2	R	78	ASP	3.0
1	D	163	SER	3.0
1	F	192	PHE	3.0
1	E	202	ASP	3.0
1	A	212	GLN	3.0
1	E	221	ASN	2.9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	205	SER	2.9
1	B	206	SER	2.9
1	F	420	LEU	2.9
1	C	227	ILE	2.9
1	C	203	SER	2.9
1	F	460	GLY	2.9
1	D	207	ASP	2.9
1	E	229	PHE	2.9
1	C	420	LEU	2.9
1	B	229	PHE	2.9
1	B	127	SER	2.8
2	S	78	ASP	2.8
1	D	125	LYS	2.8
1	C	131	ARG	2.8
1	E	420	LEU	2.8
1	F	222	ASN	2.8
1	A	420	LEU	2.8
1	E	421	LYS	2.7
1	B	158	ASP	2.7
1	C	171	TYR	2.7
1	E	228	ASN	2.7
1	F	229	PHE	2.7
1	D	769	SER	2.6
1	F	113	GLU	2.6
1	A	433	TYR	2.6
2	Q	78	ASP	2.6
1	E	125	LYS	2.5
1	D	192	PHE	2.5
1	E	113	GLU	2.5
1	F	158	ASP	2.5
1	F	227	ILE	2.5
1	B	257	LEU	2.5
1	F	213	LYS	2.4
1	C	163	SER	2.4
1	D	131	ARG	2.4
1	A	221	ASN	2.4
1	F	127	SER	2.4
1	F	214	PHE	2.4
1	C	185	ASP	2.4
1	A	192	PHE	2.4
1	A	469	PHE	2.4
1	D	72	THR	2.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	113	GLU	2.3
2	T	78	ASP	2.3
2	P	52	ILE	2.3
1	A	158	ASP	2.3
1	B	468	LYS	2.3
1	C	160	ALA	2.3
1	D	221	ASN	2.3
1	A	127	SER	2.3
1	A	405	LEU	2.3
1	A	159	TYR	2.3
1	F	245	PHE	2.3
1	F	221	ASN	2.2
1	A	186	LYS	2.2
1	C	159	TYR	2.2
1	B	227	ILE	2.2
1	D	237	PHE	2.2
1	E	203	SER	2.2
1	E	192	PHE	2.2
1	B	131	ARG	2.2
1	A	160	ALA	2.2
2	O	78	ASP	2.2
1	C	296	LEU	2.2
1	E	216	GLU	2.1
1	A	203	SER	2.1
1	D	185	ASP	2.1
1	D	181	ILE	2.1
1	C	469	PHE	2.1
1	A	163	SER	2.0
1	B	237	PHE	2.0
1	B	228	ASN	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	CA	S	709	1/1	0.97	0.19	0.70	83,83,83,83	0
4	CA	T	711	1/1	0.96	0.16	0.19	84,84,84,84	0
4	CA	O	801	1/1	0.99	0.17	0.13	36,36,36,36	0
4	CA	O	802	1/1	0.97	0.20	-0.02	44,44,44,44	0
4	CA	T	812	1/1	0.96	0.18	-0.04	48,48,48,48	0
4	CA	P	803	1/1	0.99	0.18	-0.11	36,36,36,36	0
4	CA	P	703	1/1	0.96	0.15	-0.22	88,88,88,88	0
4	CA	Q	806	1/1	0.95	0.20	-0.23	46,46,46,46	0
4	CA	R	808	1/1	0.99	0.18	-0.28	44,44,44,44	0
4	CA	S	810	1/1	0.94	0.18	-0.38	44,44,44,44	0
4	CA	S	809	1/1	0.99	0.16	-0.39	37,37,37,37	0
4	CA	R	807	1/1	0.98	0.16	-0.44	38,38,38,38	0
4	CA	O	701	1/1	0.95	0.14	-0.53	83,83,83,83	0
4	CA	Q	705	1/1	0.90	0.13	-0.56	86,86,86,86	0
4	CA	R	707	1/1	0.93	0.13	-0.62	85,85,85,85	0
4	CA	P	804	1/1	0.94	0.17	-0.65	46,46,46,46	0
4	CA	Q	805	1/1	0.99	0.16	-0.68	38,38,38,38	0
4	CA	R	708	1/1	0.77	0.14	-0.79	85,85,85,85	0
4	CA	T	811	1/1	0.99	0.15	-0.91	43,43,43,43	0
4	CA	O	702	1/1	0.63	0.09	-1.27	84,84,84,84	0
4	CA	T	712	1/1	0.65	0.11	-1.47	85,85,85,85	0
4	CA	S	710	1/1	0.38	0.11	-1.57	87,87,87,87	0
4	CA	Q	706	1/1	0.45	0.07	-1.65	84,84,84,84	0
4	CA	P	704	1/1	0.43	0.07	-2.02	82,82,82,82	0
3	MG	D	903	1/1	0.95	0.18	-	27,27,27,27	0
3	MG	E	904	1/1	0.95	0.22	-	23,23,23,23	0
3	MG	C	902	1/1	0.98	0.23	-	23,23,23,23	0
3	MG	A	900	1/1	0.95	0.19	-	28,28,28,28	0
3	MG	F	905	1/1	0.94	0.21	-	22,22,22,22	0
3	MG	B	901	1/1	0.95	0.27	-	28,28,28,28	0

## 6.5 Other polymers

There are no such residues in this entry.