



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:18 AM GMT

PDB ID : 3LIB  
Title : Crystal Structure of the extracellular domain of the putative histidine kinase  
mmHK1S-Z3  
Authors : Zhang, Z.; Hendrickson, W.A.  
Deposited on : 2010-01-24  
Resolution : 2.99 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

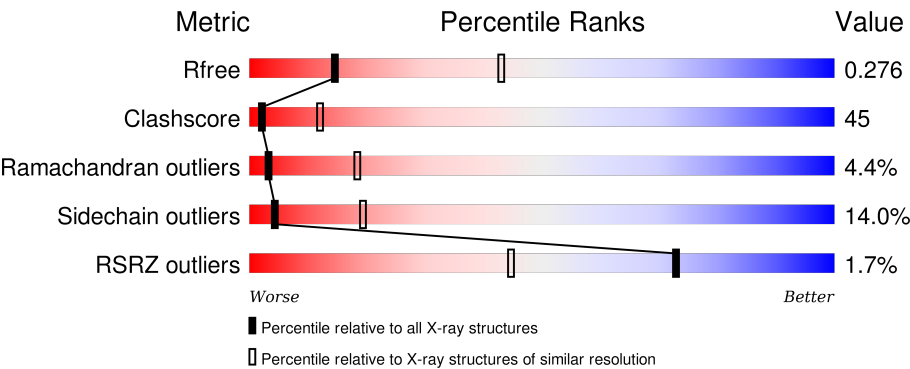
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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>	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	290	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>41%42%10%7%</div></div>
1	B	290	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>37%45%11%7%</div></div>
1	C	290	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>34%44%12%8%</div></div>
1	D	290	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>39%44%10%7%</div></div>
1	E	290	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>46%37%9%8%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	290	<div><div><div></div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>51%34%9%7%</div></div>
1	G	290	<div><div><div></div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>47%33%12%7%</div></div>
1	H	290	<div><div><div></div><div></div><div></div><div></div></div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>39%41%11%8%</div></div>
1	I	290	<div><div><div></div><div></div><div></div><div></div></div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>45%38%10%7%</div></div>
1	J	290	<div><div><div></div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>43%40%8%7%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21176 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 Hypothetical sensory transduction histidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2122	1352	335	427	8			
1	B	271	Total	C	N	O	S	0	0	0
			2122	1352	335	427	8			
1	C	268	Total	C	N	O	S	0	0	0
			2092	1333	329	422	8			
1	D	271	Total	C	N	O	S	0	0	0
			2122	1352	335	427	8			
1	E	268	Total	C	N	O	S	0	0	0
			2094	1335	329	422	8			
1	F	271	Total	C	N	O	S	0	0	0
			2122	1352	335	427	8			
1	G	270	Total	C	N	O	S	0	0	0
			2113	1347	334	424	8			
1	H	267	Total	C	N	O	S	0	0	0
			2086	1331	328	419	8			
1	I	271	Total	C	N	O	S	0	0	0
			2122	1352	335	427	8			
1	J	271	Total	C	N	O	S	0	0	0
			2122	1352	335	427	8			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
A	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
A	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
A	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
A	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
A	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
A	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
A	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
A	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
B	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
B	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
B	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
B	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
B	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
B	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
B	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
B	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
C	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
C	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
C	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
C	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
C	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
C	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
C	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
C	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
C	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
D	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
D	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
D	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
D	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
D	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
D	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
D	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
D	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
D	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
E	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
E	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
E	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
E	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
E	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
E	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
E	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
E	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
E	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
F	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
F	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
F	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
F	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
F	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
F	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
F	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
F	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
G	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
G	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
G	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
G	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
G	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
G	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
G	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
G	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
G	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
H	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
H	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
H	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
H	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
H	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
H	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
H	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
H	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
H	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
I	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
I	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
I	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
I	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
I	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
I	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
I	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
I	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
I	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1
J	30	MET	-	EXPRESSION TAG	UNP Q8PSW1
J	31	GLU	-	EXPRESSION TAG	UNP Q8PSW1
J	313	GLU	-	EXPRESSION TAG	UNP Q8PSW1
J	314	HIS	-	EXPRESSION TAG	UNP Q8PSW1
J	315	HIS	-	EXPRESSION TAG	UNP Q8PSW1
J	316	HIS	-	EXPRESSION TAG	UNP Q8PSW1
J	317	HIS	-	EXPRESSION TAG	UNP Q8PSW1
J	318	HIS	-	EXPRESSION TAG	UNP Q8PSW1
J	319	HIS	-	EXPRESSION TAG	UNP Q8PSW1

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total K 1 1	0	0
2	J	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0
2	E	1	Total K 1 1	0	0
2	H	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0
2	I	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	A	1	Total K 1 1	0	0
2	F	1	Total K 1 1	0	0

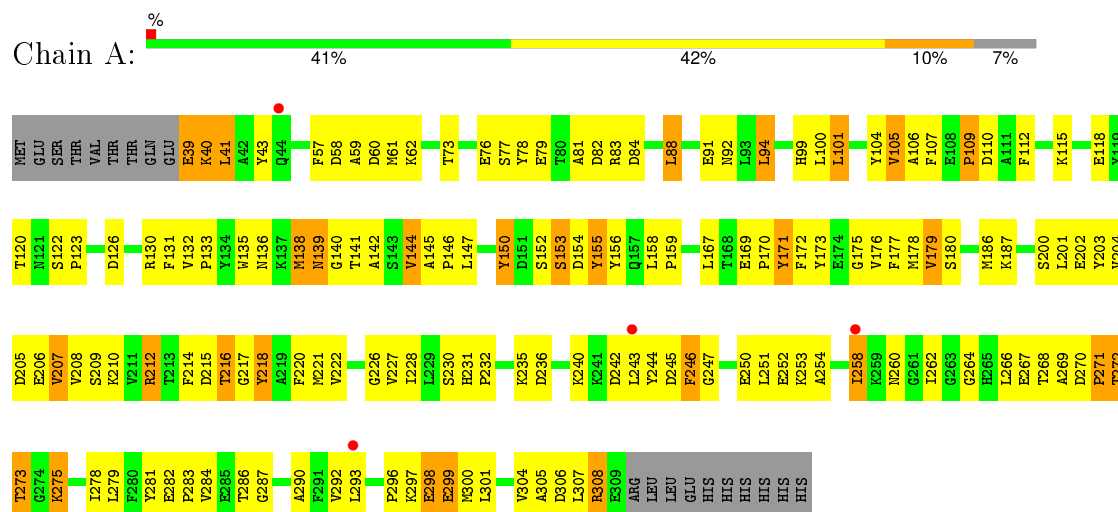
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	C	7	Total O 7 7	0	0
3	D	7	Total O 7 7	0	0
3	E	6	Total O 6 6	0	0
3	F	8	Total O 8 8	0	0
3	G	3	Total O 3 3	0	0
3	H	3	Total O 3 3	0	0
3	I	2	Total O 2 2	0	0
3	J	8	Total O 8 8	0	0

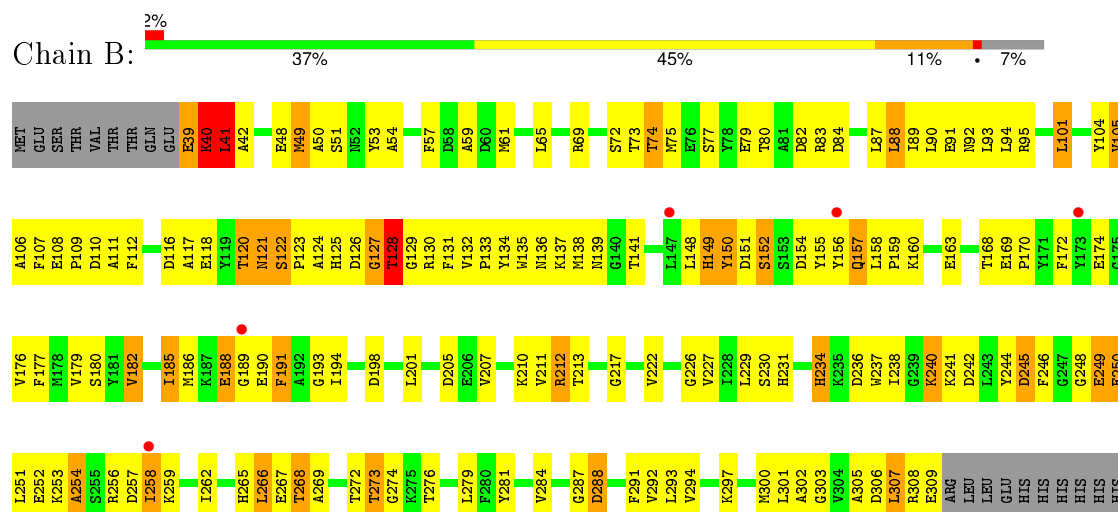
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Hypothetical sensory transduction histidine kinase



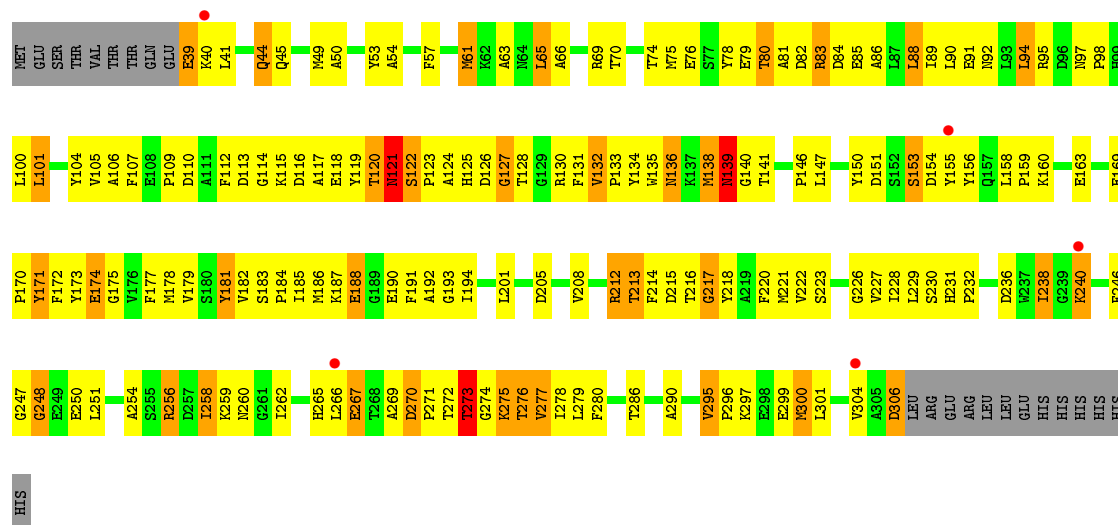
- Molecule 1: Hypothetical sensory transduction histidine kinase



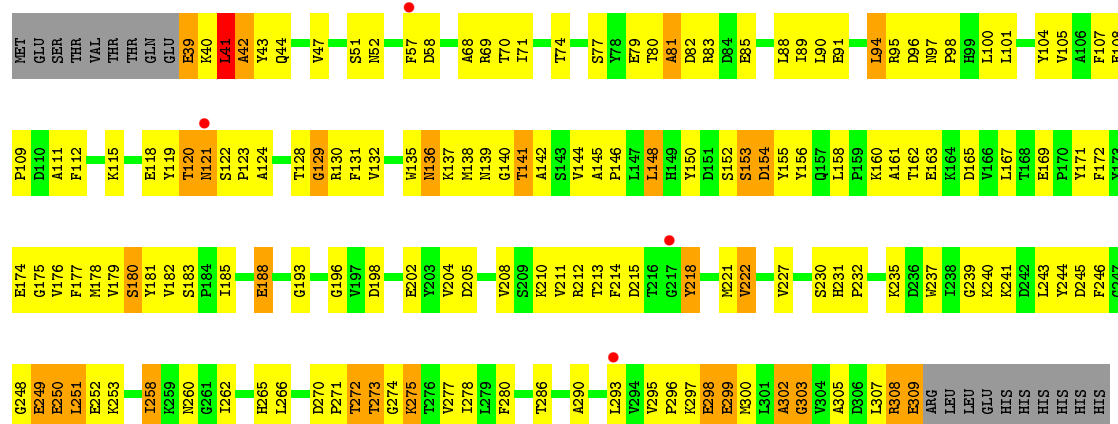
- Molecule 1: Hypothetical sensory transduction histidine kinase



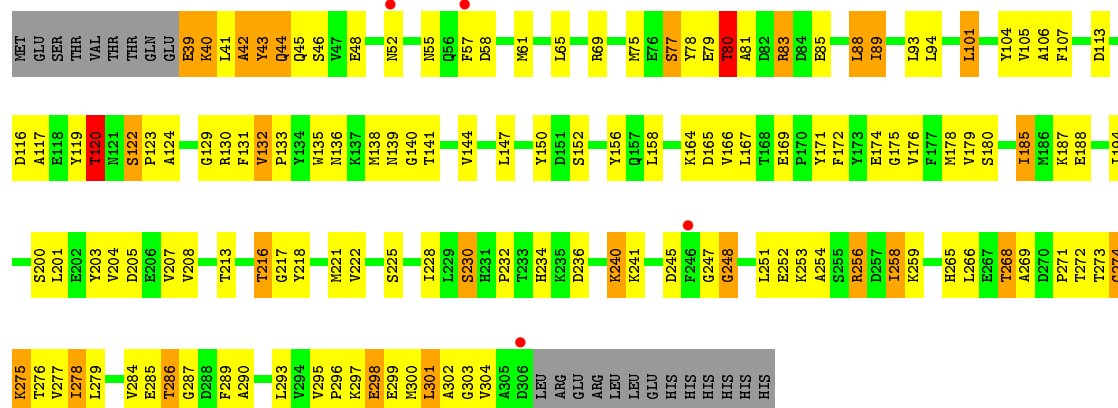




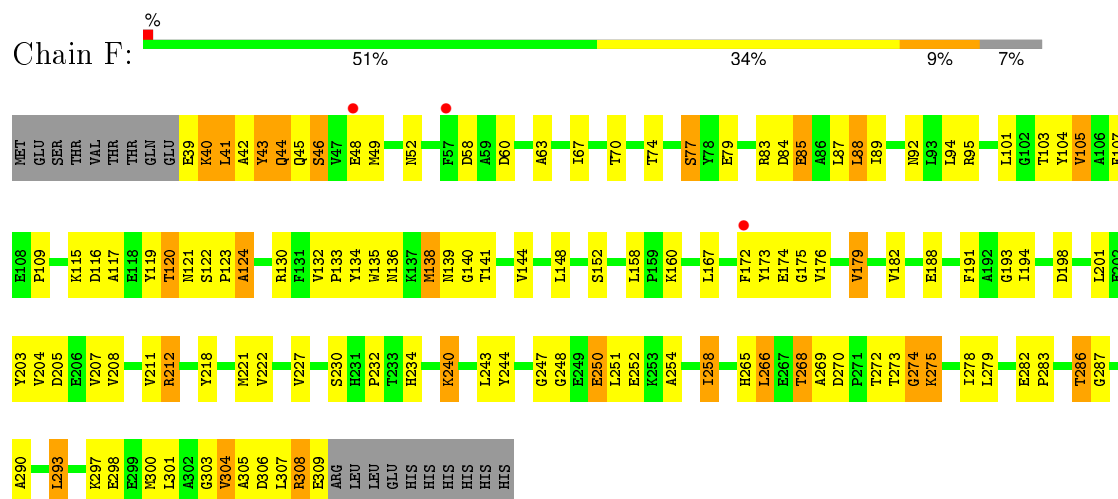
• Molecule 1: Hypothetical sensory transduction histidine kinase



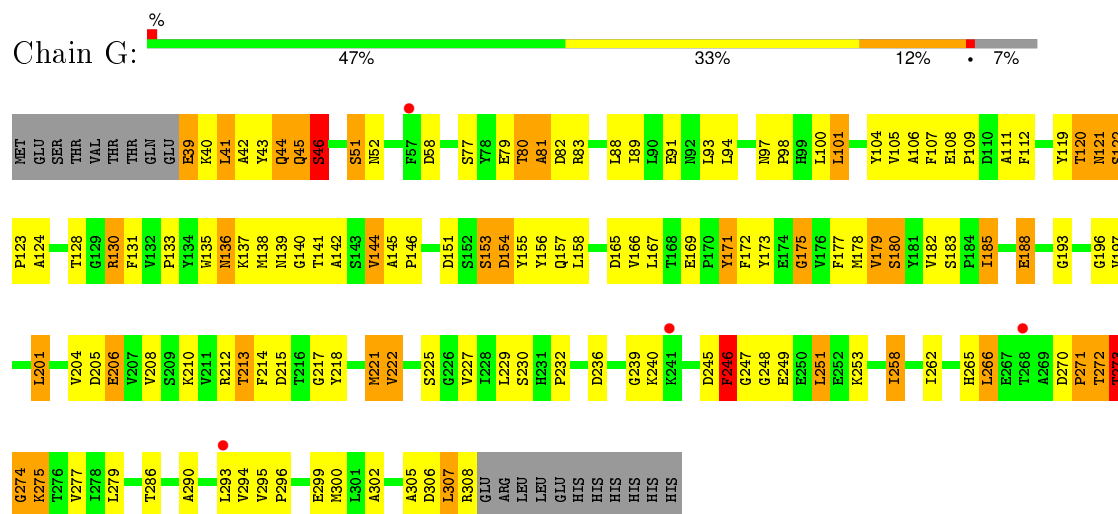
• Molecule 1: Hypothetical sensory transduction histidine kinase



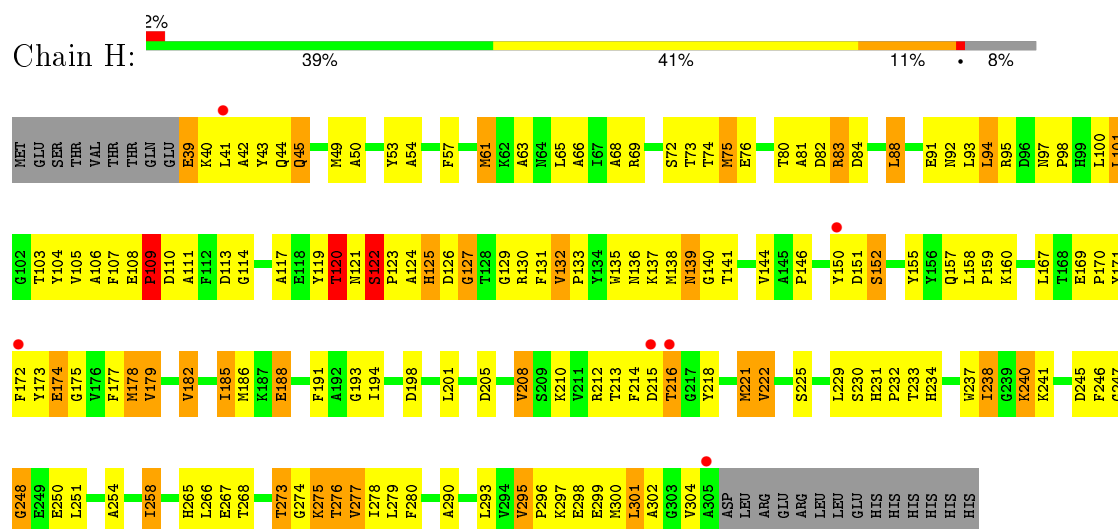
• Molecule 1: Hypothetical sensory transduction histidine kinase



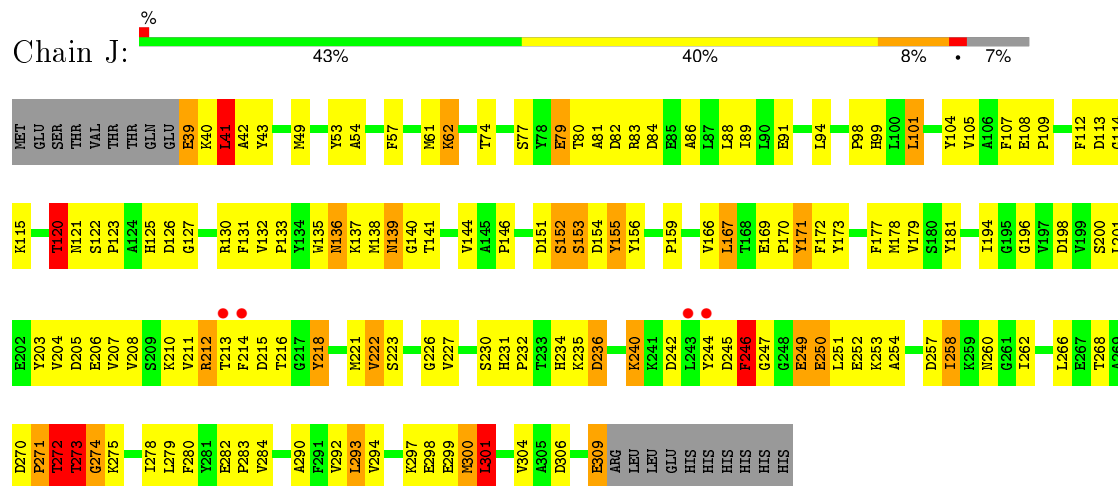
- Molecule 1: Hypothetical sensory transduction histidine kinase



- Molecule 1: Hypothetical sensory transduction histidine kinase



- Molecule 1: Hypothetical sensory transduction histidine kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.52Å 129.52Å 404.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.72 – 2.99 46.12 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.72-2.99) 99.3 (46.12-2.99)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.197 , 0.272 0.202 , 0.276	Depositor DCC
$R_{free}$ test set	3839 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.4	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.4	EDS
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 76427 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21176	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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, 0.375 respectively for untwinned datasets, and 0.333, 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:  
K

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	0.75	0/2172	0.83	0/2950
1	B	0.70	0/2172	0.77	0/2950
1	C	0.83	1/2142 (0.0%)	0.86	1/2910 (0.0%)
1	D	0.75	0/2172	0.84	1/2950 (0.0%)
1	E	0.77	1/2144 (0.0%)	0.85	0/2913
1	F	0.74	0/2172	0.83	1/2950 (0.0%)
1	G	0.73	0/2163	0.84	1/2938 (0.0%)
1	H	0.80	0/2136	0.84	2/2902 (0.1%)
1	I	0.68	0/2172	0.74	0/2950
1	J	0.77	0/2172	0.84	0/2950
All	All	0.75	2/21617 (0.0%)	0.83	6/29363 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	52	ASN	CG-OD1	5.32	1.35	1.24
1	C	139	ASN	CG-OD1	5.01	1.34	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	45	GLN	N-CA-C	6.15	127.61	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	83	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	H	178	MET	CB-CG-SD	-5.24	96.67	112.40
1	F	274	GLY	N-CA-C	-5.24	100.00	113.10
1	H	75	MET	CG-SD-CE	-5.12	92.00	100.20
1	D	303	GLY	N-CA-C	-5.03	100.52	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	297	LYS	Peptide
1	D	298	GLU	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	2122	0	2022	192	0
1	B	2122	0	2022	200	0
1	C	2092	0	1985	235	0
1	D	2122	0	2022	197	0
1	E	2094	0	1991	158	0
1	F	2122	0	2022	142	0
1	G	2113	0	2016	193	0
1	H	2086	0	1988	215	0
1	I	2122	0	2022	172	0
1	J	2122	0	2022	222	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	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	A	5	0	0	1	0
3	C	7	0	0	4	0
3	D	7	0	0	0	0
3	E	6	0	0	0	0
3	F	8	0	0	1	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	2	0	0	0	0
3	J	8	0	0	0	0
All	All	21176	0	20112	1852	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (1852) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:LEU:CD2	1:D:42:ALA:H	1.17	1.56
1:D:39:GLU:N	1:D:40:LYS:CG	1.71	1.50
1:C:270:ASP:CB	1:C:271:PRO:HA	1.32	1.44
1:E:39:GLU:N	1:E:40:LYS:HB3	1.31	1.42
1:D:41:LEU:CD2	1:D:42:ALA:N	1.77	1.41
1:A:39:GLU:HA	1:A:40:LYS:CB	1.41	1.39
1:D:41:LEU:HD22	1:D:42:ALA:N	1.05	1.35
1:F:39:GLU:CA	1:F:40:LYS:HB2	1.60	1.32
1:F:39:GLU:HA	1:F:40:LYS:CB	1.54	1.31
1:H:231:HIS:ND1	1:H:232:PRO:HD2	1.48	1.28
1:C:270:ASP:CB	1:C:271:PRO:CA	2.14	1.26
1:C:39:GLU:HB3	1:C:40:LYS:CB	1.64	1.25
1:D:41:LEU:O	1:D:43:TYR:N	1.70	1.23
1:C:91:GLU:HG3	1:C:135:TRP:CE2	1.75	1.21
1:A:39:GLU:OE2	1:A:40:LYS:HD3	1.07	1.21
1:B:307:LEU:CD2	1:B:307:LEU:N	2.05	1.19
1:E:273:THR:HG23	1:E:274:GLY:N	1.41	1.19
1:E:273:THR:CG2	1:E:274:GLY:H	1.50	1.18
1:G:136:ASN:OD1	1:G:138:MET:HB2	1.43	1.18
1:C:91:GLU:HG3	1:C:135:TRP:CZ2	1.78	1.18
1:A:39:GLU:CA	1:A:40:LYS:HB2	1.72	1.17
1:J:214:PHE:CD2	1:J:299:GLU:HB3	1.79	1.17
1:G:43:TYR:CE1	1:G:300:MET:HE2	1.79	1.17
1:D:298:GLU:N	1:D:299:GLU:HB2	1.60	1.16

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:273:THR:HG23	1:F:274:GLY:N	1.59	1.16
1:E:273:THR:HG21	1:E:275:LYS:CG	1.76	1.15
1:I:39:GLU:N	1:I:40:LYS:HB2	1.62	1.14
1:J:273:THR:OG1	1:J:274:GLY:N	1.70	1.14
1:H:39:GLU:HA	1:H:41:LEU:H	1.02	1.14
1:C:277:VAL:HG12	1:C:296:PRO:HA	1.21	1.14
1:E:273:THR:HG21	1:E:275:LYS:HG3	1.29	1.13
1:E:273:THR:HG21	1:E:275:LYS:CD	1.78	1.13
1:E:43:TYR:O	1:E:45:GLN:N	1.82	1.12
1:J:249:GLU:HB2	1:J:252:GLU:N	1.64	1.12
1:C:270:ASP:HB3	1:C:271:PRO:HA	1.16	1.12
1:A:308:ARG:HH11	1:A:308:ARG:HG2	1.00	1.12
1:C:39:GLU:HB3	1:C:40:LYS:HB3	1.25	1.11
1:J:245:ASP:O	1:J:247:GLY:N	1.82	1.11
1:A:173:TYR:HB3	1:A:178:MET:HE3	1.23	1.11
1:E:273:THR:HG21	1:E:275:LYS:HD2	1.32	1.11
1:C:270:ASP:HB2	1:C:271:PRO:CA	1.80	1.10
1:B:307:LEU:HD22	1:B:307:LEU:N	1.63	1.10
1:E:77:SER:HB3	1:F:88:LEU:HD13	1.15	1.10
1:B:249:GLU:O	1:B:251:LEU:N	1.85	1.10
1:D:39:GLU:N	1:D:40:LYS:HG3	0.77	1.10
1:G:270:ASP:OD2	1:G:273:THR:HG23	1.48	1.09
1:J:249:GLU:CG	1:J:252:GLU:HB2	1.82	1.09
1:D:298:GLU:H	1:D:299:GLU:HB2	0.94	1.07
1:C:272:THR:O	1:C:273:THR:HB	1.53	1.07
1:I:270:ASP:OD2	1:I:273:THR:HG23	1.51	1.07
1:A:298:GLU:OE1	1:H:121:ASN:HB3	1.54	1.07
1:A:39:GLU:OE2	1:A:40:LYS:CD	2.02	1.07
1:J:249:GLU:CB	1:J:252:GLU:H	1.65	1.07
1:C:120:THR:O	1:C:121:ASN:HB2	1.51	1.07
1:J:173:TYR:HB3	1:J:178:MET:CE	1.82	1.06
1:J:309:GLU:OE2	1:J:309:GLU:N	1.88	1.06
1:H:39:GLU:OE2	1:H:39:GLU:N	1.88	1.06
1:A:260:ASN:HB2	1:A:262:ILE:HD12	1.36	1.06
1:I:222:VAL:HG13	1:I:226:GLY:HA2	1.33	1.06
1:F:273:THR:HG21	1:F:275:LYS:HB3	1.37	1.06
1:J:249:GLU:HA	1:J:250:GLU:HG3	1.36	1.06
1:F:273:THR:CG2	1:F:274:GLY:H	1.64	1.06
1:H:39:GLU:N	1:H:40:LYS:HB2	1.71	1.06
1:J:298:GLU:HA	1:J:301:LEU:CD2	1.86	1.05
1:F:273:THR:HG23	1:F:275:LYS:N	1.71	1.05

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:40:LYS:O	1:J:42:ALA:N	1.89	1.05
1:B:240:LYS:HA	1:B:240:LYS:HE2	1.35	1.05
1:J:249:GLU:CA	1:J:250:GLU:HG3	1.87	1.04
1:H:91:GLU:HG3	1:H:135:TRP:CE2	1.92	1.04
1:F:273:THR:HG23	1:F:275:LYS:H	1.16	1.04
1:J:249:GLU:HG3	1:J:252:GLU:HB2	1.10	1.03
1:J:251:LEU:HD23	1:J:266:LEU:CD1	1.88	1.03
1:H:250:GLU:HB3	1:H:266:LEU:CD2	1.89	1.03
1:F:301:LEU:HA	1:F:304:VAL:CG2	1.88	1.03
1:C:273:THR:CG2	1:C:275:LYS:HG3	1.88	1.02
1:B:222:VAL:HG13	1:B:226:GLY:HA2	1.39	1.02
1:I:306:ASP:O	1:I:308:ARG:N	1.93	1.02
1:H:91:GLU:HG3	1:H:135:TRP:CZ2	1.94	1.02
1:G:40:LYS:HA	1:G:42:ALA:H	1.24	1.02
1:A:308:ARG:HH11	1:A:308:ARG:CG	1.73	1.02
1:G:272:THR:HG22	1:G:273:THR:H	1.19	1.02
1:B:307:LEU:H	1:B:307:LEU:HD23	1.24	1.02
1:D:41:LEU:HD22	1:D:42:ALA:CA	1.90	1.01
1:J:214:PHE:HB3	1:J:299:GLU:HG2	1.40	1.01
1:D:270:ASP:OD1	1:D:277:VAL:CG2	2.07	1.01
1:D:135:TRP:CE2	1:D:144:VAL:HG23	1.94	1.01
1:C:270:ASP:OD2	1:C:274:GLY:HA2	1.59	1.01
1:H:231:HIS:ND1	1:H:232:PRO:CD	2.22	1.01
1:D:39:GLU:N	1:D:39:GLU:OE1	1.93	1.01
1:H:39:GLU:CD	1:H:39:GLU:N	2.14	1.01
1:D:298:GLU:HG3	1:D:299:GLU:CG	1.91	1.00
1:F:273:THR:HG23	1:F:274:GLY:H	0.85	1.00
1:J:91:GLU:HB2	1:J:135:TRP:CE2	1.96	1.00
1:C:270:ASP:HB2	1:C:271:PRO:HA	1.01	1.00
1:E:273:THR:CG2	1:E:275:LYS:HD2	1.92	1.00
1:J:297:LYS:C	1:J:301:LEU:HD22	1.83	0.99
1:J:173:TYR:HB3	1:J:178:MET:HE2	1.41	0.99
1:B:120:THR:O	1:B:121:ASN:HB2	1.61	0.99
1:E:278:ILE:HD12	1:E:278:ILE:N	1.77	0.99
1:H:231:HIS:CE1	1:H:232:PRO:HD2	1.98	0.98
1:J:249:GLU:HB2	1:J:252:GLU:H	0.82	0.98
1:H:136:ASN:OD1	1:H:138:MET:HB2	1.63	0.98
1:I:122:SER:HB2	1:I:123:PRO:HD2	1.41	0.98
1:G:135:TRP:CD2	1:G:144:VAL:HG23	1.99	0.98
1:G:43:TYR:CD1	1:G:300:MET:CE	2.47	0.98
1:J:298:GLU:HA	1:J:301:LEU:HD23	1.45	0.98

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:300:MET:O	1:F:304:VAL:HG22	1.61	0.98
1:B:39:GLU:N	1:B:39:GLU:OE2	1.97	0.98
1:E:39:GLU:N	1:E:40:LYS:CB	2.27	0.97
1:C:270:ASP:HB3	1:C:271:PRO:CA	1.83	0.97
1:D:270:ASP:OD1	1:D:277:VAL:HG21	1.62	0.97
1:A:173:TYR:HB3	1:A:178:MET:CE	1.95	0.97
1:G:272:THR:HG22	1:G:273:THR:N	1.77	0.96
1:A:231:HIS:ND1	1:A:232:PRO:HD2	1.79	0.96
1:I:75:MET:HE2	1:I:75:MET:HA	1.44	0.96
1:B:191:PHE:O	1:B:191:PHE:HD2	1.49	0.96
1:A:39:GLU:HA	1:A:40:LYS:CG	1.95	0.95
1:D:273:THR:OG1	1:D:274:GLY:HA2	1.64	0.95
1:C:39:GLU:HB3	1:C:40:LYS:HB2	1.46	0.95
1:I:205:ASP:HA	1:I:230:SER:HB2	1.47	0.95
1:A:91:GLU:HG3	1:A:135:TRP:CZ2	2.00	0.95
1:G:273:THR:HG21	1:G:275:LYS:HE3	1.48	0.94
1:A:39:GLU:CA	1:A:40:LYS:CB	2.33	0.94
1:E:273:THR:HG23	1:E:275:LYS:H	1.28	0.94
1:J:300:MET:CA	1:J:301:LEU:HB2	1.97	0.94
1:G:135:TRP:CE2	1:G:144:VAL:HG23	2.00	0.94
1:I:191:PHE:O	1:I:191:PHE:HD2	1.49	0.94
1:D:39:GLU:CA	1:D:40:LYS:HG3	1.97	0.94
1:J:240:LYS:HA	1:J:240:LYS:HE2	1.49	0.94
1:C:160:LYS:HG3	1:C:191:PHE:CE2	2.02	0.94
1:C:132:VAL:O	1:C:132:VAL:HG23	1.65	0.94
1:F:303:GLY:O	1:F:307:LEU:HG	1.68	0.93
1:C:39:GLU:CB	1:C:40:LYS:HB3	1.96	0.93
1:H:39:GLU:HA	1:H:41:LEU:N	1.82	0.93
1:J:298:GLU:CA	1:J:301:LEU:CD2	2.47	0.93
1:B:48:GLU:O	1:B:51:SER:HB3	1.69	0.93
1:B:163:GLU:HB3	1:B:186:MET:HE1	1.49	0.93
1:J:231:HIS:ND1	1:J:232:PRO:HD2	1.82	0.93
1:I:309:GLU:C	1:I:309:GLU:OE1	2.07	0.93
1:J:260:ASN:HB2	1:J:262:ILE:HD12	1.49	0.92
1:I:307:LEU:HD11	1:J:41:LEU:HD21	1.50	0.92
1:I:191:PHE:O	1:I:191:PHE:CD2	2.23	0.92
1:E:188:GLU:O	1:E:188:GLU:HG3	1.69	0.92
1:F:234:HIS:CE1	1:F:272:THR:HG23	2.04	0.92
1:C:277:VAL:HG12	1:C:296:PRO:CA	1.98	0.92
1:F:222:VAL:HG12	1:F:290:ALA:HB3	1.50	0.92
1:F:41:LEU:HD12	1:F:41:LEU:C	1.91	0.92

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:271:PRO:O	1:J:273:THR:N	2.02	0.91
1:D:277:VAL:HG12	1:D:296:PRO:HA	1.50	0.91
1:H:250:GLU:HB3	1:H:266:LEU:HD21	1.52	0.91
1:B:69:ARG:HH11	1:B:69:ARG:HG2	1.31	0.91
1:D:39:GLU:HA	1:D:40:LYS:HB2	1.53	0.91
1:H:250:GLU:C	1:H:266:LEU:HD11	1.91	0.91
1:C:163:GLU:HB3	1:E:259:LYS:NZ	1.85	0.91
1:J:298:GLU:CA	1:J:301:LEU:HD22	2.00	0.90
1:G:39:GLU:CA	1:G:40:LYS:HB2	1.99	0.90
1:J:297:LYS:O	1:J:301:LEU:HD22	1.71	0.90
1:A:58:ASP:OD2	1:A:286:THR:HG23	1.71	0.90
1:I:39:GLU:N	1:I:39:GLU:OE2	2.03	0.90
1:D:309:GLU:HA	1:D:309:GLU:OE1	1.72	0.90
1:E:204:VAL:O	1:E:208:VAL:HG23	1.72	0.90
1:J:79:GLU:OE2	1:J:79:GLU:HA	1.70	0.90
1:D:265:HIS:O	1:D:266:LEU:HD23	1.72	0.90
1:E:77:SER:CB	1:F:88:LEU:HD13	2.02	0.89
1:F:41:LEU:CD1	1:F:41:LEU:C	2.40	0.89
1:E:273:THR:HG23	1:E:275:LYS:N	1.86	0.89
1:J:298:GLU:N	1:J:301:LEU:HD22	1.87	0.89
1:G:122:SER:HB2	1:G:123:PRO:HD2	1.52	0.89
1:J:300:MET:N	1:J:301:LEU:HB2	1.88	0.88
1:E:247:GLY:O	1:E:248:GLY:O	1.91	0.88
1:D:296:PRO:O	1:D:299:GLU:HB3	1.73	0.88
1:A:43:TYR:HE1	1:A:300:MET:HE1	1.37	0.88
1:E:302:ALA:N	1:E:303:GLY:HA3	1.87	0.88
1:G:205:ASP:HA	1:G:230:SER:HB2	1.56	0.88
1:J:249:GLU:HA	1:J:251:LEU:H	1.38	0.88
1:C:273:THR:HG21	1:C:275:LYS:HG3	1.53	0.88
1:H:273:THR:OG1	1:H:275:LYS:HG2	1.74	0.88
1:E:117:ALA:O	1:E:120:THR:HG22	1.74	0.88
1:E:39:GLU:CA	1:E:40:LYS:HB3	2.03	0.88
1:H:117:ALA:O	1:H:120:THR:HG22	1.74	0.87
1:G:245:ASP:O	1:G:247:GLY:N	2.07	0.87
1:G:39:GLU:N	1:G:40:LYS:HB2	1.90	0.87
1:D:58:ASP:OD2	1:D:286:THR:HG23	1.73	0.87
1:G:218:TYR:CD2	1:G:232:PRO:HG2	2.10	0.87
1:F:139:ASN:O	1:F:141:THR:N	2.07	0.87
1:B:191:PHE:O	1:B:191:PHE:CD2	2.27	0.87
1:C:231:HIS:ND1	1:C:232:PRO:HD2	1.90	0.86
1:D:177:PHE:CZ	1:D:240:LYS:HD2	2.10	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:GLY:O	1:B:249:GLU:HB2	1.73	0.86
1:H:275:LYS:HB3	1:H:275:LYS:NZ	1.90	0.86
1:A:305:ALA:HA	1:A:308:ARG:HH12	1.40	0.86
1:G:77:SER:OG	1:H:92:ASN:OD1	1.92	0.86
1:G:43:TYR:CE1	1:G:300:MET:CE	2.57	0.86
1:E:48:GLU:HG3	1:F:48:GLU:HG3	1.57	0.86
1:C:120:THR:O	1:C:121:ASN:CB	2.24	0.86
1:A:308:ARG:HG2	1:A:308:ARG:NH1	1.83	0.86
1:B:177:PHE:HB3	1:B:201:LEU:HD12	1.56	0.86
1:I:136:ASN:OD1	1:I:138:MET:HB2	1.76	0.86
1:D:41:LEU:HD23	1:D:42:ALA:N	1.91	0.86
1:E:58:ASP:OD1	1:E:286:THR:HG23	1.74	0.86
1:F:234:HIS:HE1	1:F:272:THR:HG23	1.41	0.85
1:E:172:PHE:CZ	1:E:175:GLY:HA2	2.09	0.85
1:A:296:PRO:HB2	1:A:299:GLU:HG3	1.56	0.85
1:H:247:GLY:O	1:H:248:GLY:O	1.94	0.85
1:E:273:THR:CG2	1:E:275:LYS:HG3	2.05	0.85
1:I:39:GLU:CA	1:I:40:LYS:HB2	2.06	0.85
1:A:231:HIS:CE1	1:A:232:PRO:HD2	2.10	0.85
1:B:128:THR:OG1	1:B:130:ARG:HG3	1.77	0.85
1:D:135:TRP:CD2	1:D:144:VAL:HG23	2.11	0.85
1:B:104:TYR:HE2	1:B:198:ASP:OD2	1.60	0.84
1:G:58:ASP:OD2	1:G:286:THR:HG23	1.76	0.84
1:H:39:GLU:CA	1:H:41:LEU:H	1.88	0.84
1:F:273:THR:CG2	1:F:275:LYS:H	1.89	0.84
1:A:260:ASN:CB	1:A:262:ILE:HD12	2.07	0.84
1:C:273:THR:HG23	1:C:275:LYS:HG3	1.59	0.84
1:H:214:PHE:HE2	1:H:300:MET:HA	1.43	0.84
1:B:83:ARG:O	1:B:87:LEU:HD12	1.77	0.84
1:J:249:GLU:HG3	1:J:252:GLU:CB	2.03	0.83
1:C:277:VAL:CG1	1:C:296:PRO:HA	2.06	0.83
1:C:273:THR:HG23	1:C:275:LYS:CG	2.08	0.83
1:G:120:THR:O	1:G:121:ASN:HB2	1.77	0.83
1:E:88:LEU:HD13	1:F:77:SER:HB3	1.57	0.83
1:J:156:TYR:O	1:J:159:PRO:HD2	1.77	0.83
1:C:278:ILE:HG22	1:C:280:PHE:CE1	2.12	0.83
1:I:222:VAL:CG1	1:I:226:GLY:HA2	2.08	0.83
1:A:43:TYR:CE1	1:A:300:MET:HE1	2.12	0.83
1:F:204:VAL:O	1:F:208:VAL:HG23	1.77	0.83
1:E:273:THR:HG23	1:E:274:GLY:H	0.68	0.83
1:H:188:GLU:O	1:H:188:GLU:HG2	1.76	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:272:THR:HG22	1:G:273:THR:HG22	1.58	0.83
1:F:41:LEU:HD12	1:F:42:ALA:N	1.94	0.83
1:A:39:GLU:HA	1:A:40:LYS:HB2	0.84	0.82
1:D:39:GLU:CA	1:D:40:LYS:CB	2.57	0.82
1:G:43:TYR:CD1	1:G:300:MET:HE2	2.10	0.82
1:A:136:ASN:HD22	1:A:138:MET:HB2	1.42	0.82
1:J:245:ASP:C	1:J:247:GLY:N	2.32	0.82
1:I:120:THR:O	1:I:120:THR:HG23	1.78	0.82
1:A:77:SER:OG	1:B:92:ASN:OD1	1.97	0.82
1:D:270:ASP:O	1:D:274:GLY:HA3	1.80	0.82
1:I:191:PHE:C	1:I:191:PHE:CD2	2.53	0.82
1:F:122:SER:HB2	1:F:123:PRO:HD2	1.62	0.82
1:E:273:THR:CG2	1:E:275:LYS:H	1.92	0.82
1:J:139:ASN:O	1:J:141:THR:HG22	1.78	0.82
1:B:163:GLU:HB3	1:B:186:MET:CE	2.09	0.82
1:C:273:THR:CG2	1:C:275:LYS:CG	2.57	0.81
1:C:136:ASN:OD1	1:C:138:MET:HB2	1.79	0.81
1:D:136:ASN:OD1	1:D:138:MET:HB2	1.79	0.81
1:D:298:GLU:HG3	1:D:299:GLU:HG2	1.62	0.81
1:G:273:THR:HG21	1:G:275:LYS:CE	2.09	0.81
1:I:75:MET:CE	1:I:75:MET:HA	2.10	0.81
1:H:240:LYS:CE	1:H:240:LYS:HA	2.11	0.81
1:G:273:THR:OG1	1:G:274:GLY:N	2.08	0.81
1:G:213:THR:O	1:G:217:GLY:HA3	1.81	0.81
1:C:91:GLU:HG3	1:C:135:TRP:CH2	2.15	0.81
1:H:39:GLU:N	1:H:40:LYS:HD2	1.95	0.81
1:D:91:GLU:OE1	1:D:135:TRP:CZ2	2.34	0.81
1:B:39:GLU:HB3	1:B:40:LYS:O	1.80	0.81
1:J:260:ASN:CB	1:J:262:ILE:HD12	2.10	0.81
1:J:122:SER:HB2	1:J:123:PRO:HD2	1.61	0.81
1:D:270:ASP:OD1	1:D:277:VAL:HG22	1.79	0.81
1:A:173:TYR:CB	1:A:178:MET:HE3	2.07	0.81
1:C:205:ASP:HA	1:C:230:SER:HB2	1.62	0.81
1:C:121:ASN:O	1:C:122:SER:HB2	1.79	0.81
1:B:191:PHE:CD2	1:B:191:PHE:C	2.54	0.81
1:C:218:TYR:CD2	1:C:232:PRO:HG2	2.16	0.81
1:H:174:GLU:HA	1:H:174:GLU:OE2	1.77	0.81
1:B:257:ASP:HB3	1:B:262:ILE:O	1.81	0.80
1:B:39:GLU:CB	1:B:40:LYS:O	2.30	0.80
1:I:120:THR:O	1:I:121:ASN:HB2	1.80	0.80
1:C:91:GLU:CG	1:C:135:TRP:CZ2	2.62	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LEU:HD11	1:B:307:LEU:CD1	2.11	0.80
1:G:43:TYR:CD1	1:G:300:MET:HE1	2.14	0.80
1:B:246:PHE:O	1:B:251:LEU:HD13	1.82	0.80
1:C:119:TYR:O	1:C:121:ASN:N	2.14	0.80
1:H:214:PHE:CE2	1:H:300:MET:HA	2.17	0.80
1:H:39:GLU:N	1:H:40:LYS:CB	2.45	0.80
1:J:298:GLU:O	1:J:301:LEU:HB3	1.80	0.80
1:D:107:PHE:O	1:D:130:ARG:HD2	1.82	0.80
1:I:43:TYR:O	1:I:47:VAL:HG23	1.80	0.80
1:E:273:THR:CG2	1:E:274:GLY:N	2.17	0.80
1:E:278:ILE:CD1	1:E:278:ILE:N	2.44	0.80
1:D:208:VAL:O	1:D:211:VAL:HG23	1.81	0.80
1:I:258:ILE:HG13	1:I:259:LYS:N	1.95	0.80
1:J:300:MET:CB	1:J:301:LEU:HB2	2.12	0.79
1:H:246:PHE:O	1:H:251:LEU:HD12	1.83	0.79
1:B:120:THR:O	1:B:120:THR:HG23	1.82	0.79
1:B:101:LEU:O	1:B:101:LEU:HD22	1.81	0.79
1:D:296:PRO:HB2	1:D:299:GLU:HG3	1.64	0.79
1:J:249:GLU:N	1:J:249:GLU:OE1	2.14	0.79
1:F:222:VAL:CG1	1:F:290:ALA:HB3	2.11	0.79
1:I:306:ASP:C	1:I:308:ARG:H	1.85	0.79
1:H:83:ARG:NH1	1:H:113:ASP:OD2	2.16	0.79
1:A:298:GLU:O	1:A:300:MET:N	2.16	0.79
1:H:91:GLU:HG3	1:H:135:TRP:CH2	2.18	0.79
1:F:203:TYR:O	1:F:207:VAL:HG23	1.83	0.79
1:A:203:TYR:O	1:A:207:VAL:HG23	1.83	0.79
1:H:95:ARG:NH1	1:J:253:LYS:HG3	1.98	0.79
1:E:234:HIS:NE2	1:E:272:THR:HG23	1.97	0.78
1:C:91:GLU:HG3	1:C:135:TRP:CD2	2.18	0.78
1:I:270:ASP:OD2	1:I:273:THR:CG2	2.31	0.78
1:A:91:GLU:HG3	1:A:135:TRP:CE2	2.18	0.78
1:C:174:GLU:OE2	1:C:174:GLU:HA	1.84	0.78
1:A:244:TYR:CE2	1:A:252:GLU:HG2	2.19	0.78
1:H:278:ILE:HG21	1:H:280:PHE:CE1	2.19	0.78
1:B:95:ARG:CZ	1:D:253:LYS:HB3	2.13	0.78
1:C:177:PHE:HB3	1:C:201:LEU:HD12	1.64	0.78
1:E:203:TYR:O	1:E:207:VAL:HG23	1.83	0.78
1:D:39:GLU:HA	1:D:40:LYS:CB	2.13	0.78
1:A:39:GLU:OE2	1:A:39:GLU:N	2.17	0.78
1:C:174:GLU:CA	1:C:174:GLU:OE2	2.32	0.78
1:D:39:GLU:CD	1:D:39:GLU:N	2.36	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:277:VAL:HG12	1:H:296:PRO:HA	1.64	0.78
1:D:270:ASP:HB3	1:D:272:THR:HG22	1.67	0.77
1:J:177:PHE:HB3	1:J:201:LEU:HD12	1.66	0.77
1:J:215:ASP:HB2	1:J:299:GLU:OE2	1.84	0.77
1:H:278:ILE:CG2	1:H:280:PHE:CE1	2.67	0.77
1:I:83:ARG:NH1	1:I:125:HIS:CD2	2.52	0.77
1:G:89:ILE:HD13	1:H:74:THR:HG23	1.66	0.77
1:E:278:ILE:HD11	1:E:297:LYS:HD3	1.66	0.77
1:C:278:ILE:HD12	1:C:300:MET:HE1	1.67	0.77
1:F:139:ASN:O	1:F:141:THR:HG22	1.85	0.77
1:E:85:GLU:OE1	1:F:79:GLU:HB2	1.83	0.77
1:G:277:VAL:HG12	1:G:296:PRO:HA	1.67	0.77
1:J:91:GLU:HB2	1:J:135:TRP:NE1	1.99	0.76
1:H:132:VAL:HG23	1:H:132:VAL:O	1.81	0.76
1:A:79:GLU:OE2	1:A:79:GLU:HA	1.84	0.76
1:G:135:TRP:CE2	1:G:144:VAL:CG2	2.67	0.76
1:D:80:THR:HG22	1:D:80:THR:O	1.85	0.76
1:H:130:ARG:O	1:H:132:VAL:HG13	1.86	0.76
1:I:39:GLU:N	1:I:39:GLU:CD	2.32	0.76
1:B:246:PHE:O	1:B:251:LEU:CD1	2.34	0.76
1:G:39:GLU:HA	1:G:40:LYS:HB2	1.67	0.76
1:E:132:VAL:HG23	1:E:147:LEU:H	1.51	0.76
1:H:57:PHE:O	1:H:61:MET:HG3	1.85	0.76
1:C:213:THR:HG21	1:C:295:VAL:HG23	1.67	0.76
1:I:256:ARG:HG3	1:I:256:ARG:HH11	1.50	0.76
1:H:277:VAL:CG1	1:H:296:PRO:HA	2.16	0.75
1:F:107:PHE:O	1:F:130:ARG:HD2	1.86	0.75
1:F:298:GLU:CD	1:F:298:GLU:H	1.90	0.75
1:C:125:HIS:O	1:C:146:PRO:HG2	1.86	0.75
1:A:231:HIS:ND1	1:A:232:PRO:CD	2.49	0.75
1:F:43:TYR:O	1:F:45:GLN:N	2.20	0.75
1:H:122:SER:HB2	1:H:123:PRO:HD2	1.69	0.75
1:E:188:GLU:CG	1:E:188:GLU:O	2.33	0.75
1:G:120:THR:HG23	1:G:120:THR:O	1.86	0.75
1:B:222:VAL:CG1	1:B:226:GLY:HA2	2.16	0.75
1:D:94:LEU:HD13	1:D:137:LYS:HE3	1.69	0.75
1:D:260:ASN:HB2	1:D:262:ILE:HD12	1.69	0.75
1:F:273:THR:HG21	1:F:275:LYS:CE	2.16	0.75
1:E:132:VAL:O	1:E:132:VAL:HG23	1.86	0.75
1:J:250:GLU:O	1:J:253:LYS:HB2	1.85	0.74
1:H:160:LYS:HG3	1:H:191:PHE:CE2	2.22	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:188:GLU:CG	1:H:188:GLU:O	2.33	0.74
1:A:136:ASN:ND2	1:A:138:MET:HB2	2.01	0.74
1:H:91:GLU:HG3	1:H:135:TRP:CD2	2.23	0.74
1:A:305:ALA:HA	1:A:308:ARG:NH1	2.02	0.74
1:F:41:LEU:O	1:F:41:LEU:HD13	1.87	0.74
1:H:105:VAL:HG13	1:H:107:PHE:HE1	1.52	0.74
1:H:95:ARG:CZ	1:J:253:LYS:HG3	2.17	0.74
1:C:91:GLU:CG	1:C:135:TRP:CE2	2.66	0.74
1:D:39:GLU:N	1:D:40:LYS:CB	2.51	0.74
1:A:91:GLU:HG3	1:A:135:TRP:CH2	2.23	0.74
1:H:80:THR:HG22	1:H:82:ASP:H	1.51	0.74
1:C:92:ASN:OD1	1:D:77:SER:OG	2.06	0.74
1:A:246:PHE:HB3	1:A:251:LEU:HD12	1.69	0.74
1:E:167:LEU:HD23	1:E:287:GLY:HA3	1.70	0.74
1:B:148:LEU:O	1:B:149:HIS:HB2	1.86	0.74
1:D:214:PHE:CD1	1:D:295:VAL:HG13	2.23	0.74
1:J:231:HIS:CE1	1:J:232:PRO:HD2	2.23	0.74
1:J:120:THR:O	1:J:120:THR:HG23	1.87	0.74
1:G:218:TYR:HD2	1:G:232:PRO:HG2	1.53	0.73
1:F:306:ASP:O	1:F:309:GLU:OE2	2.06	0.73
1:C:231:HIS:ND1	1:C:232:PRO:CD	2.51	0.73
1:G:100:LEU:HD22	1:G:197:VAL:HB	1.70	0.73
1:J:300:MET:N	1:J:301:LEU:CB	2.51	0.73
1:J:249:GLU:CG	1:J:252:GLU:CB	2.63	0.73
1:E:83:ARG:HD2	1:E:113:ASP:OD1	1.88	0.73
1:C:278:ILE:CG2	1:C:280:PHE:CE1	2.72	0.73
1:B:61:MET:CE	1:B:284:VAL:HG11	2.19	0.73
1:D:273:THR:OG1	1:D:274:GLY:CA	2.37	0.73
1:F:273:THR:HG21	1:F:275:LYS:CB	2.17	0.73
1:A:246:PHE:HB3	1:A:251:LEU:CD1	2.18	0.73
1:A:139:ASN:O	1:A:141:THR:HG22	1.89	0.73
1:J:251:LEU:CD2	1:J:266:LEU:CD1	2.67	0.73
1:D:296:PRO:O	1:D:299:GLU:CB	2.36	0.73
1:B:107:PHE:O	1:B:130:ARG:HD2	1.88	0.73
1:F:273:THR:HG21	1:F:275:LYS:HE2	1.70	0.72
1:A:298:GLU:OE1	1:H:121:ASN:CB	2.35	0.72
1:J:231:HIS:ND1	1:J:232:PRO:CD	2.52	0.72
1:J:122:SER:HB2	1:J:123:PRO:CD	2.19	0.72
1:J:251:LEU:HD23	1:J:266:LEU:HD11	1.69	0.72
1:J:57:PHE:O	1:J:61:MET:HG3	1.88	0.72
1:C:250:GLU:O	1:C:266:LEU:HD11	1.88	0.72

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:GLU:HB2	1:D:135:TRP:NE1	2.04	0.72
1:I:104:TYR:HD2	1:I:134:TYR:CE2	2.08	0.72
1:J:156:TYR:C	1:J:159:PRO:HD2	2.10	0.72
1:F:301:LEU:HA	1:F:304:VAL:HG23	1.70	0.72
1:C:178:MET:HE1	3:C:8:HOH:O	1.88	0.72
1:H:240:LYS:HE2	1:H:240:LYS:HA	1.72	0.72
1:E:136:ASN:OD1	1:E:138:MET:HB2	1.88	0.72
1:C:267:GLU:OE1	1:C:297:LYS:NZ	2.19	0.72
1:J:300:MET:HB2	1:J:301:LEU:HB2	1.70	0.72
1:H:91:GLU:CG	1:H:135:TRP:CZ2	2.72	0.72
1:B:69:ARG:HG2	1:B:69:ARG:NH1	2.04	0.72
1:F:122:SER:CB	1:F:123:PRO:HD2	2.19	0.72
1:H:82:ASP:OD1	1:H:84:ASP:HB2	1.90	0.72
1:A:154:ASP:O	1:A:156:TYR:N	2.23	0.72
1:H:240:LYS:HE2	1:H:240:LYS:CA	2.19	0.72
1:D:39:GLU:CA	1:D:40:LYS:CG	2.60	0.71
1:C:273:THR:HG23	1:C:275:LYS:H	1.53	0.71
1:J:240:LYS:HA	1:J:240:LYS:CE	2.19	0.71
1:B:104:TYR:CE2	1:B:198:ASP:OD2	2.43	0.71
1:B:185:ILE:HG13	1:B:194:ILE:N	2.05	0.71
1:B:205:ASP:HA	1:B:230:SER:HB2	1.71	0.71
1:G:271:PRO:O	1:G:272:THR:C	2.29	0.71
1:J:171:TYR:N	1:J:171:TYR:CD1	2.57	0.71
1:B:39:GLU:CA	1:B:40:LYS:O	2.39	0.71
1:J:249:GLU:HA	1:J:251:LEU:N	2.05	0.71
1:J:173:TYR:CB	1:J:178:MET:CE	2.67	0.71
1:D:250:GLU:HG3	1:D:266:LEU:HD13	1.73	0.71
1:D:41:LEU:CG	1:D:42:ALA:H	2.02	0.71
1:A:298:GLU:O	1:A:301:LEU:N	2.23	0.71
1:H:275:LYS:HB3	1:H:275:LYS:HZ3	1.54	0.71
1:C:231:HIS:CE1	1:C:232:PRO:HD2	2.26	0.71
1:G:204:VAL:O	1:G:208:VAL:HG23	1.90	0.71
1:H:136:ASN:OD1	1:H:138:MET:CB	2.39	0.71
1:B:148:LEU:O	1:B:149:HIS:CB	2.38	0.71
1:C:75:MET:CE	1:C:105:VAL:HG21	2.21	0.71
1:J:171:TYR:HD1	1:J:171:TYR:N	1.89	0.70
1:I:168:THR:HG23	1:I:180:SER:O	1.91	0.70
1:A:218:TYR:N	1:A:218:TYR:CD1	2.57	0.70
1:H:238:ILE:HG22	1:H:238:ILE:O	1.92	0.70
1:J:214:PHE:HD2	1:J:299:GLU:HB3	1.47	0.70
1:J:139:ASN:O	1:J:141:THR:N	2.23	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:124:ALA:O	1:H:146:PRO:HB3	1.91	0.70
1:H:109:PRO:CD	1:H:130:ARG:HD3	2.22	0.70
1:G:80:THR:HG22	1:G:80:THR:O	1.88	0.70
1:J:245:ASP:C	1:J:247:GLY:H	1.94	0.70
1:D:218:TYR:CD2	1:D:232:PRO:HG2	2.27	0.70
1:G:222:VAL:HG12	1:G:290:ALA:HB3	1.74	0.70
1:A:39:GLU:CA	1:A:40:LYS:CG	2.66	0.70
1:H:174:GLU:CA	1:H:174:GLU:OE2	2.39	0.70
1:J:120:THR:O	1:J:120:THR:CG2	2.38	0.70
1:C:270:ASP:HB3	1:C:271:PRO:C	2.12	0.70
1:G:272:THR:CG2	1:G:273:THR:H	1.98	0.70
1:H:139:ASN:O	1:H:141:THR:N	2.18	0.70
1:J:278:ILE:HG22	1:J:280:PHE:CE1	2.26	0.70
1:E:277:VAL:C	1:E:278:ILE:HD12	2.11	0.70
1:C:139:ASN:O	1:C:141:THR:N	2.23	0.70
1:D:95:ARG:CZ	1:E:253:LYS:HD2	2.22	0.70
1:B:250:GLU:HA	1:B:253:LYS:HE2	1.72	0.70
1:J:240:LYS:CA	1:J:240:LYS:HE2	2.21	0.70
1:J:154:ASP:O	1:J:156:TYR:N	2.25	0.70
1:H:277:VAL:HG12	1:H:296:PRO:CA	2.21	0.70
1:D:205:ASP:HA	1:D:230:SER:HB2	1.74	0.70
1:F:301:LEU:HA	1:F:304:VAL:HG22	1.72	0.69
1:I:149:HIS:C	1:I:151:ASP:H	1.96	0.69
1:F:109:PRO:N	1:F:130:ARG:HD3	2.07	0.69
1:B:272:THR:O	1:B:272:THR:HG22	1.92	0.69
1:A:107:PHE:O	1:A:130:ARG:NH1	2.25	0.69
1:D:298:GLU:HG3	1:D:299:GLU:HG3	1.72	0.69
1:J:214:PHE:CD2	1:J:299:GLU:CB	2.70	0.69
1:E:41:LEU:O	1:E:42:ALA:C	2.31	0.69
1:H:120:THR:O	1:H:121:ASN:HB2	1.93	0.69
1:A:205:ASP:HA	1:A:230:SER:HB2	1.75	0.69
1:D:139:ASN:C	1:D:141:THR:H	1.95	0.69
1:F:218:TYR:CD2	1:F:232:PRO:HG2	2.27	0.69
1:B:74:THR:O	1:B:77:SER:N	2.25	0.69
1:C:39:GLU:CB	1:C:40:LYS:CB	2.56	0.69
1:H:250:GLU:CB	1:H:266:LEU:CD1	2.70	0.69
1:H:109:PRO:HD3	1:H:130:ARG:HD3	1.74	0.69
1:C:82:ASP:OD1	1:C:84:ASP:HB2	1.92	0.69
1:H:43:TYR:HA	1:H:300:MET:HE1	1.73	0.69
1:F:273:THR:CG2	1:F:275:LYS:HB3	2.19	0.69
1:D:91:GLU:HB2	1:D:135:TRP:CE2	2.28	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ARG:NH1	1:B:125:HIS:CD2	2.61	0.69
1:E:116:ASP:OD2	1:E:130:ARG:HG2	1.92	0.69
1:C:188:GLU:HB3	1:E:252:GLU:OE2	1.93	0.69
1:B:83:ARG:HH11	1:B:125:HIS:CD2	2.11	0.69
1:A:250:GLU:HB2	1:A:266:LEU:HD22	1.75	0.69
1:E:222:VAL:CG2	1:E:290:ALA:HB3	2.22	0.69
1:J:249:GLU:HA	1:J:250:GLU:CG	2.17	0.68
1:C:132:VAL:CG2	1:C:132:VAL:O	2.41	0.68
1:D:248:GLY:O	1:D:251:LEU:HB2	1.93	0.68
1:I:83:ARG:HH11	1:I:125:HIS:CD2	2.09	0.68
1:I:65:LEU:O	1:I:69:ARG:HG3	1.94	0.68
1:C:272:THR:O	1:C:272:THR:HG23	1.93	0.68
1:H:65:LEU:O	1:H:69:ARG:HG3	1.93	0.68
1:G:273:THR:CG2	1:G:275:LYS:HE3	2.21	0.68
1:G:305:ALA:O	1:G:308:ARG:HG3	1.93	0.68
1:H:301:LEU:O	1:H:304:VAL:HG23	1.93	0.68
1:G:43:TYR:HD1	1:G:300:MET:HE1	1.59	0.68
1:C:278:ILE:HD12	1:C:300:MET:CE	2.23	0.68
1:C:214:PHE:CE2	1:C:300:MET:HA	2.29	0.68
1:B:39:GLU:HA	1:B:40:LYS:CB	2.24	0.68
1:J:254:ALA:O	1:J:258:ILE:HG23	1.94	0.68
1:C:267:GLU:HG2	1:C:278:ILE:HG12	1.76	0.67
1:H:105:VAL:HG13	1:H:107:PHE:CE1	2.30	0.67
1:J:222:VAL:HA	1:J:227:VAL:O	1.94	0.67
1:D:174:GLU:OE2	1:D:174:GLU:HA	1.94	0.67
1:G:45:GLN:H	1:G:46:SER:HB2	1.59	0.67
1:D:302:ALA:O	1:D:305:ALA:HB3	1.94	0.67
1:F:278:ILE:CD1	1:F:300:MET:HG3	2.24	0.67
1:H:231:HIS:CD2	1:H:237:TRP:HE3	2.13	0.67
1:A:218:TYR:CD2	1:A:232:PRO:HG2	2.29	0.67
1:A:43:TYR:HE1	1:A:300:MET:CE	2.05	0.67
1:D:139:ASN:O	1:D:141:THR:N	2.27	0.67
1:C:222:VAL:HG22	1:C:226:GLY:HA2	1.77	0.67
1:J:167:LEU:HD22	1:J:181:TYR:CE2	2.29	0.67
1:J:101:LEU:HD22	1:J:101:LEU:O	1.94	0.67
1:G:272:THR:CG2	1:G:273:THR:N	2.49	0.67
1:A:214:PHE:HB3	1:A:299:GLU:OE1	1.94	0.67
1:I:74:THR:O	1:I:77:SER:N	2.26	0.67
1:C:131:PHE:CE1	1:C:133:PRO:HG3	2.29	0.67
1:H:105:VAL:CG1	1:H:107:PHE:HE1	2.08	0.67
1:D:132:VAL:O	1:D:132:VAL:HG23	1.93	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:ASN:C	1:C:141:THR:H	1.99	0.67
1:H:151:ASP:O	1:H:152:SER:HB3	1.93	0.67
1:F:58:ASP:OD1	1:F:286:THR:HG23	1.95	0.67
1:D:165:ASP:OD1	1:D:183:SER:OG	2.09	0.67
1:E:43:TYR:O	1:E:44:GLN:C	2.34	0.66
1:J:173:TYR:HB3	1:J:178:MET:HE3	1.75	0.66
1:J:218:TYR:N	1:J:218:TYR:CD1	2.62	0.66
1:G:122:SER:HB2	1:G:123:PRO:CD	2.25	0.66
1:G:135:TRP:HZ3	1:G:142:ALA:O	1.78	0.66
1:I:265:HIS:O	1:I:266:LEU:HD23	1.96	0.66
1:F:123:PRO:O	1:F:124:ALA:HB3	1.95	0.66
1:I:105:VAL:HG12	1:I:133:PRO:HD2	1.77	0.66
1:J:213:THR:HG21	1:J:293:LEU:HD21	1.77	0.66
1:F:41:LEU:O	1:F:41:LEU:CD1	2.44	0.66
1:G:214:PHE:CD1	1:G:295:VAL:HG13	2.31	0.66
1:B:157:GLN:HE21	1:B:157:GLN:HA	1.59	0.66
1:C:75:MET:HE2	1:C:105:VAL:HG21	1.78	0.66
1:D:120:THR:HG23	1:D:120:THR:O	1.96	0.66
1:J:105:VAL:CG1	1:J:107:PHE:CE1	2.79	0.66
1:C:74:THR:HG23	1:D:89:ILE:HG12	1.78	0.66
1:I:57:PHE:HE2	1:I:207:VAL:CG1	2.09	0.66
1:D:41:LEU:CD2	1:D:42:ALA:CA	2.62	0.65
1:E:222:VAL:HG23	1:E:290:ALA:HB3	1.78	0.65
1:F:244:TYR:CE2	1:F:252:GLU:HG3	2.31	0.65
1:D:120:THR:O	1:D:121:ASN:HB2	1.94	0.65
1:B:40:LYS:O	1:B:42:ALA:N	2.24	0.65
1:G:245:ASP:C	1:G:247:GLY:N	2.48	0.65
1:I:107:PHE:O	1:I:130:ARG:HD2	1.96	0.65
1:I:155:TYR:O	1:I:159:PRO:HG2	1.96	0.65
1:I:307:LEU:HD11	1:J:41:LEU:CD2	2.23	0.65
1:H:109:PRO:HD3	1:H:130:ARG:CD	2.26	0.65
1:G:80:THR:O	1:G:82:ASP:N	2.29	0.65
1:G:182:VAL:HG12	1:G:183:SER:N	2.10	0.65
1:I:39:GLU:N	1:I:40:LYS:CB	2.52	0.65
1:D:177:PHE:CE1	1:D:240:LYS:HD2	2.32	0.65
1:F:205:ASP:HA	1:F:230:SER:HB2	1.79	0.65
1:C:178:MET:CE	3:C:8:HOH:O	2.44	0.65
1:H:158:LEU:HB2	1:H:159:PRO:HD3	1.79	0.65
1:J:297:LYS:HD2	1:J:301:LEU:HD13	1.78	0.65
1:I:131:PHE:CE1	1:I:133:PRO:HG3	2.32	0.65
1:J:105:VAL:HG11	1:J:107:PHE:HE1	1.61	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:136:ASN:OD1	1:J:138:MET:HB2	1.96	0.65
1:H:185:ILE:HG13	1:H:193:GLY:O	1.97	0.65
1:A:39:GLU:N	1:A:40:LYS:HD3	2.12	0.64
1:C:273:THR:HG21	1:C:275:LYS:CG	2.25	0.64
1:J:113:ASP:O	1:J:115:LYS:HG3	1.97	0.64
1:B:259:LYS:HG2	1:B:259:LYS:O	1.96	0.64
1:D:135:TRP:CE2	1:D:144:VAL:CG2	2.78	0.64
1:G:248:GLY:O	1:G:251:LEU:HB2	1.97	0.64
1:C:41:LEU:HD23	1:C:44:GLN:OE1	1.97	0.64
1:D:300:MET:O	1:D:303:GLY:HA3	1.98	0.64
1:A:308:ARG:CG	1:A:308:ARG:NH1	2.42	0.64
1:E:276:THR:O	1:E:297:LYS:CB	2.46	0.64
1:J:204:VAL:O	1:J:208:VAL:HG23	1.98	0.64
1:F:83:ARG:O	1:F:87:LEU:HD12	1.97	0.64
1:F:270:ASP:OD2	1:F:272:THR:HB	1.98	0.64
1:D:237:TRP:CD1	1:D:241:LYS:HD2	2.33	0.64
1:J:249:GLU:CA	1:J:250:GLU:CG	2.73	0.64
1:H:250:GLU:HB3	1:H:266:LEU:HD22	1.78	0.64
1:D:96:ASP:HB2	1:E:256:ARG:HH22	1.62	0.64
1:E:298:GLU:O	1:E:301:LEU:HB3	1.98	0.64
1:J:249:GLU:CA	1:J:251:LEU:H	2.10	0.64
1:B:39:GLU:N	1:B:39:GLU:CD	2.51	0.64
1:F:244:TYR:HE2	1:F:252:GLU:HG3	1.63	0.64
1:B:110:ASP:H	1:B:116:ASP:CG	2.01	0.64
1:B:306:ASP:C	1:B:307:LEU:HD22	2.18	0.64
1:H:250:GLU:CB	1:H:266:LEU:HD11	2.28	0.64
1:J:105:VAL:CG1	1:J:107:PHE:HE1	2.11	0.64
1:A:43:TYR:CE1	1:A:300:MET:CE	2.81	0.64
1:H:278:ILE:HG21	1:H:280:PHE:CZ	2.33	0.64
1:I:257:ASP:HB3	1:I:262:ILE:O	1.98	0.64
1:A:169:GLU:HB3	1:A:170:PRO:HD2	1.79	0.63
1:D:158:LEU:O	1:D:162:THR:HG23	1.97	0.63
1:B:122:SER:HB2	1:B:123:PRO:HD2	1.80	0.63
1:B:82:ASP:OD1	1:B:82:ASP:C	2.36	0.63
1:A:244:TYR:CD2	1:A:252:GLU:HG2	2.34	0.63
1:B:136:ASN:OD1	1:B:138:MET:HB2	1.98	0.63
1:C:163:GLU:HG2	1:C:186:MET:HE1	1.80	0.63
1:B:267:GLU:OE1	1:B:297:LYS:HE3	1.97	0.63
1:J:39:GLU:HG2	1:J:40:LYS:N	2.14	0.63
1:I:75:MET:CE	1:I:75:MET:CA	2.76	0.63
1:E:136:ASN:OD1	1:E:138:MET:CB	2.46	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ASP:OD1	1:B:116:ASP:HB2	1.98	0.63
1:J:83:ARG:HG3	1:J:112:PHE:HE1	1.64	0.63
1:J:298:GLU:CA	1:J:301:LEU:HD23	2.18	0.63
1:G:40:LYS:N	1:G:41:LEU:HB3	2.14	0.63
1:G:253:LYS:HB3	1:I:95:ARG:CZ	2.29	0.63
1:H:250:GLU:HB2	1:H:266:LEU:HD13	1.81	0.63
1:G:139:ASN:C	1:G:141:THR:H	2.00	0.63
1:I:309:GLU:C	1:I:309:GLU:CD	2.56	0.63
1:G:279:LEU:CD2	1:G:294:VAL:HG22	2.28	0.63
1:A:139:ASN:O	1:A:141:THR:N	2.30	0.63
1:G:173:TYR:HB3	1:G:178:MET:HE3	1.79	0.63
1:C:260:ASN:CB	1:C:262:ILE:HD12	2.29	0.63
1:B:307:LEU:N	1:B:307:LEU:HD23	1.85	0.63
1:A:222:VAL:HG22	1:A:226:GLY:HA2	1.81	0.63
1:J:177:PHE:HB3	1:J:201:LEU:CD1	2.28	0.63
1:E:43:TYR:C	1:E:45:GLN:N	2.52	0.62
1:H:250:GLU:HB3	1:H:266:LEU:CD1	2.29	0.62
1:D:299:GLU:O	1:D:302:ALA:CB	2.46	0.62
1:I:160:LYS:HG2	1:I:160:LYS:O	2.00	0.62
1:I:135:TRP:CZ3	1:I:143:SER:HA	2.34	0.62
1:E:300:MET:O	1:E:304:VAL:HG23	1.98	0.62
1:I:259:LYS:HG2	1:I:259:LYS:O	1.99	0.62
1:A:244:TYR:HE2	1:A:252:GLU:HG2	1.63	0.62
1:H:83:ARG:HH11	1:H:113:ASP:CG	2.02	0.62
1:E:40:LYS:O	1:E:40:LYS:HD2	1.99	0.62
1:D:298:GLU:CA	1:D:299:GLU:HB2	2.28	0.62
1:C:121:ASN:O	1:C:122:SER:CB	2.46	0.62
1:C:124:ALA:C	1:C:146:PRO:HG3	2.19	0.62
1:B:120:THR:O	1:B:121:ASN:CB	2.43	0.62
1:A:62:LYS:HD3	1:B:59:ALA:HB1	1.81	0.62
1:D:222:VAL:CG1	1:D:258:ILE:HD13	2.30	0.62
1:I:267:GLU:C	1:I:268:THR:HG22	2.20	0.62
1:F:172:PHE:CZ	1:F:175:GLY:HA2	2.35	0.62
1:C:269:ALA:HA	1:C:276:THR:HA	1.82	0.62
1:G:40:LYS:HA	1:G:42:ALA:N	2.07	0.62
1:I:91:GLU:HB2	1:I:135:TRP:NE1	2.15	0.62
1:I:105:VAL:HG12	1:I:133:PRO:CD	2.30	0.62
1:C:213:THR:HG22	1:C:217:GLY:HA3	1.82	0.62
1:G:120:THR:O	1:G:120:THR:CG2	2.47	0.62
1:E:254:ALA:O	1:E:258:ILE:HG23	2.00	0.62
1:E:164:LYS:O	1:E:166:VAL:HG23	1.99	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ARG:NH1	1:C:212:ARG:NH2	2.47	0.62
1:B:248:GLY:O	1:B:249:GLU:CB	2.45	0.61
1:I:91:GLU:HB2	1:I:135:TRP:CE2	2.35	0.61
1:C:256:ARG:HD3	3:C:321:HOH:O	2.00	0.61
1:E:79:GLU:O	1:E:81:ALA:N	2.33	0.61
1:C:213:THR:HG21	1:C:295:VAL:CG2	2.30	0.61
1:G:218:TYR:HD2	1:G:232:PRO:CG	2.13	0.61
1:E:48:GLU:CG	1:F:48:GLU:HG3	2.30	0.61
1:E:172:PHE:CE2	1:E:175:GLY:HA2	2.34	0.61
1:G:306:ASP:O	1:G:308:ARG:N	2.33	0.61
1:D:222:VAL:HG12	1:D:290:ALA:HB3	1.81	0.61
1:C:306:ASP:OD1	1:C:306:ASP:N	2.34	0.61
1:D:249:GLU:HG3	1:D:249:GLU:O	2.00	0.61
1:H:275:LYS:HB3	1:H:275:LYS:HZ2	1.64	0.61
1:D:85:GLU:O	1:D:89:ILE:HD12	2.00	0.61
1:J:245:ASP:O	1:J:246:PHE:C	2.38	0.61
1:H:231:HIS:CD2	1:H:237:TRP:CE3	2.88	0.61
1:B:84:ASP:HA	1:B:87:LEU:HD12	1.83	0.61
1:I:265:HIS:HA	1:I:279:LEU:O	2.00	0.61
1:B:105:VAL:HG12	1:B:133:PRO:HD2	1.81	0.61
1:A:57:PHE:O	1:A:61:MET:HG3	2.01	0.61
1:F:254:ALA:O	1:F:258:ILE:HG23	2.00	0.61
1:J:120:THR:OG1	1:J:127:GLY:O	2.17	0.61
1:I:234:HIS:CE1	1:I:272:THR:HG23	2.36	0.61
1:I:108:GLU:O	1:I:111:ALA:CB	2.49	0.61
1:E:41:LEU:O	1:E:43:TYR:N	2.34	0.60
1:A:214:PHE:HE2	1:A:299:GLU:O	1.83	0.60
1:I:57:PHE:HE2	1:I:207:VAL:HG12	1.65	0.60
1:C:110:ASP:OD1	1:C:114:GLY:C	2.39	0.60
1:H:216:THR:OG1	1:H:299:GLU:OE2	2.20	0.60
1:G:135:TRP:CD2	1:G:144:VAL:CG2	2.81	0.60
1:I:104:TYR:HD2	1:I:134:TYR:HE2	1.49	0.60
1:A:105:VAL:CG1	1:A:107:PHE:HE1	2.13	0.60
1:C:115:LYS:O	1:C:116:ASP:C	2.39	0.60
1:J:300:MET:CA	1:J:301:LEU:CB	2.78	0.60
1:B:177:PHE:CZ	1:B:240:LYS:HD2	2.37	0.60
1:E:228:ILE:HD12	1:E:241:LYS:O	2.01	0.60
1:H:275:LYS:CB	1:H:275:LYS:NZ	2.60	0.60
1:F:79:GLU:OE2	1:F:79:GLU:HA	2.01	0.60
1:H:186:MET:HE2	1:H:191:PHE:HD1	1.67	0.60
1:G:165:ASP:C	1:G:166:VAL:HG23	2.21	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:TYR:HB3	1:F:134:TYR:HD2	1.66	0.60
1:H:91:GLU:CG	1:H:135:TRP:CE2	2.80	0.60
1:F:139:ASN:C	1:F:141:THR:H	2.01	0.60
1:G:185:ILE:HG13	1:G:193:GLY:C	2.21	0.60
1:C:172:PHE:CZ	1:C:175:GLY:HA2	2.36	0.60
1:F:211:VAL:HG12	1:F:212:ARG:N	2.15	0.60
1:G:43:TYR:HE1	1:G:300:MET:HE2	1.57	0.60
1:G:271:PRO:O	1:G:272:THR:O	2.20	0.60
1:F:250:GLU:O	1:F:266:LEU:HD11	2.02	0.60
1:C:163:GLU:HB3	1:E:259:LYS:HZ3	1.64	0.60
1:H:43:TYR:HA	1:H:300:MET:CE	2.32	0.60
1:D:105:VAL:HG13	1:D:107:PHE:HE1	1.65	0.60
1:G:307:LEU:HD23	1:G:307:LEU:N	2.17	0.60
1:C:150:TYR:HB3	1:C:155:TYR:OH	2.01	0.60
1:E:117:ALA:O	1:E:120:THR:CG2	2.49	0.60
1:F:117:ALA:O	1:F:120:THR:HG22	2.01	0.60
1:I:106:ALA:HB3	1:I:194:ILE:HG12	1.84	0.60
1:H:273:THR:OG1	1:H:274:GLY:N	2.34	0.60
1:H:278:ILE:HG22	1:H:280:PHE:CE1	2.37	0.60
1:I:120:THR:O	1:I:121:ASN:CB	2.50	0.60
1:H:130:ARG:NH2	1:H:150:TYR:HE1	2.00	0.60
1:D:94:LEU:HD11	1:D:137:LYS:HG3	1.84	0.60
1:A:105:VAL:HG11	1:A:107:PHE:HE1	1.67	0.60
1:A:171:TYR:N	1:A:171:TYR:CD1	2.70	0.59
1:J:278:ILE:CG2	1:J:280:PHE:CE1	2.85	0.59
1:E:276:THR:O	1:E:297:LYS:HB3	2.02	0.59
1:J:54:ALA:O	1:J:284:VAL:HG22	2.02	0.59
1:C:247:GLY:O	1:C:248:GLY:O	2.19	0.59
1:I:59:ALA:HB1	1:J:62:LYS:HD2	1.84	0.59
1:G:104:TYR:OH	1:G:180:SER:HB3	2.01	0.59
1:D:250:GLU:CG	1:D:266:LEU:HD13	2.32	0.59
1:F:172:PHE:CE2	1:F:175:GLY:HA2	2.37	0.59
1:H:106:ALA:HB3	1:H:194:ILE:HG12	1.84	0.59
1:I:110:ASP:H	1:I:116:ASP:CG	2.05	0.59
1:C:185:ILE:HD11	1:C:194:ILE:O	2.01	0.59
1:B:281:TYR:HB3	1:B:292:VAL:HG22	1.84	0.59
1:G:101:LEU:O	1:G:101:LEU:HD23	2.02	0.59
1:A:101:LEU:HD22	1:A:101:LEU:O	2.01	0.59
1:J:270:ASP:OD2	1:J:273:THR:HG23	2.03	0.59
1:J:249:GLU:HB2	1:J:251:LEU:N	2.17	0.59
1:D:105:VAL:HG13	1:D:107:PHE:CE1	2.37	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:VAL:CG1	1:D:107:PHE:HE1	2.15	0.59
1:C:130:ARG:O	1:C:132:VAL:HG13	2.02	0.59
1:H:130:ARG:C	1:H:132:VAL:HG13	2.22	0.59
1:I:256:ARG:HG3	1:I:256:ARG:NH1	2.14	0.59
1:F:116:ASP:OD2	1:F:130:ARG:HG2	2.02	0.59
1:D:245:ASP:O	1:D:246:PHE:HD2	1.85	0.59
1:D:80:THR:O	1:D:81:ALA:C	2.40	0.59
1:I:147:LEU:O	1:I:150:TYR:CE2	2.56	0.59
1:A:245:ASP:C	1:A:247:GLY:N	2.56	0.59
1:H:212:ARG:NH1	1:I:232:PRO:O	2.36	0.59
1:G:253:LYS:HD3	1:I:95:ARG:NH1	2.18	0.59
1:B:168:THR:HG23	1:B:180:SER:O	2.01	0.59
1:H:167:LEU:HD11	1:H:179:VAL:HG13	1.84	0.59
1:J:169:GLU:HB3	1:J:170:PRO:HD2	1.84	0.59
1:H:205:ASP:HA	1:H:230:SER:HB2	1.85	0.59
1:G:45:GLN:N	1:G:46:SER:HB2	2.17	0.59
1:G:41:LEU:O	1:G:41:LEU:HD13	2.03	0.59
1:A:91:GLU:CG	1:A:135:TRP:CZ2	2.82	0.59
1:C:131:PHE:CD1	1:C:133:PRO:HD3	2.38	0.59
1:C:101:LEU:HD22	1:C:101:LEU:O	2.01	0.59
1:E:43:TYR:O	1:E:46:SER:N	2.36	0.59
1:G:270:ASP:OD2	1:G:273:THR:CG2	2.37	0.59
1:E:48:GLU:HG3	1:F:48:GLU:CG	2.32	0.59
1:J:249:GLU:CA	1:J:251:LEU:N	2.65	0.59
1:F:136:ASN:OD1	1:F:138:MET:HB2	2.03	0.58
1:G:249:GLU:O	1:G:249:GLU:HG2	2.02	0.58
1:I:85:GLU:O	1:I:86:ALA:C	2.41	0.58
1:H:208:VAL:HG11	1:H:230:SER:OG	2.03	0.58
1:B:117:ALA:O	1:B:120:THR:HG22	2.03	0.58
1:J:177:PHE:CZ	1:J:240:LYS:HD2	2.38	0.58
1:C:265:HIS:HA	1:C:279:LEU:O	2.03	0.58
1:C:297:LYS:HE2	1:C:301:LEU:HD11	1.84	0.58
1:B:158:LEU:HB2	1:B:159:PRO:HD3	1.86	0.58
1:H:126:ASP:O	1:H:127:GLY:C	2.41	0.58
1:A:270:ASP:HB3	1:A:273:THR:O	2.04	0.58
1:H:110:ASP:OD1	1:H:114:GLY:C	2.42	0.58
1:A:82:ASP:OD1	1:A:84:ASP:N	2.33	0.58
1:D:231:HIS:ND1	1:D:232:PRO:HD2	2.19	0.58
1:F:270:ASP:HB3	1:F:273:THR:HG22	1.86	0.58
1:G:270:ASP:OD1	1:G:271:PRO:N	2.37	0.58
1:I:308:ARG:HA	1:I:309:GLU:C	2.24	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:305:ALA:HA	1:G:308:ARG:NH1	2.19	0.58
1:G:43:TYR:HD1	1:G:300:MET:CE	2.09	0.58
1:C:125:HIS:O	1:C:146:PRO:CG	2.52	0.58
1:B:39:GLU:HA	1:B:40:LYS:O	2.04	0.58
1:B:185:ILE:HG13	1:B:193:GLY:C	2.23	0.58
1:I:48:GLU:O	1:I:51:SER:HB3	2.04	0.58
1:B:120:THR:CG2	1:B:120:THR:O	2.52	0.58
1:B:108:GLU:O	1:B:111:ALA:CB	2.52	0.58
1:A:254:ALA:O	1:A:258:ILE:HG23	2.04	0.58
1:J:173:TYR:CB	1:J:178:MET:HE3	2.31	0.58
1:B:177:PHE:HZ	1:B:240:LYS:HD2	1.68	0.58
1:A:218:TYR:N	1:A:218:TYR:HD1	1.99	0.57
1:C:250:GLU:CD	1:C:250:GLU:H	2.07	0.57
1:A:104:TYR:OH	1:A:180:SER:HB3	2.03	0.57
1:G:136:ASN:HD22	1:G:136:ASN:H	1.51	0.57
1:C:214:PHE:HE2	1:C:300:MET:HA	1.69	0.57
1:A:262:ILE:CD1	1:C:98:PRO:HG3	2.34	0.57
1:A:222:VAL:HG23	1:A:227:VAL:O	2.03	0.57
1:F:211:VAL:CG1	1:F:212:ARG:N	2.67	0.57
1:D:41:LEU:CD2	1:D:41:LEU:C	2.67	0.57
1:C:91:GLU:CG	1:C:135:TRP:CH2	2.86	0.57
1:G:43:TYR:C	1:G:45:GLN:H	2.08	0.57
1:B:155:TYR:O	1:B:159:PRO:HG2	2.04	0.57
1:I:120:THR:CG2	1:I:120:THR:O	2.49	0.57
1:B:149:HIS:C	1:B:151:ASP:H	2.05	0.57
1:F:306:ASP:O	1:F:309:GLU:HG3	2.03	0.57
1:D:39:GLU:CA	1:D:40:LYS:HB2	2.22	0.57
1:E:83:ARG:HD3	1:E:119:TYR:CZ	2.39	0.57
1:H:109:PRO:HD3	1:H:130:ARG:NH1	2.20	0.57
1:J:171:TYR:H	1:J:171:TYR:HD1	1.53	0.57
1:B:306:ASP:C	1:B:308:ARG:H	2.08	0.57
1:D:177:PHE:HZ	1:D:240:LYS:HD2	1.64	0.57
1:B:53:TYR:O	1:B:54:ALA:C	2.42	0.57
1:J:271:PRO:C	1:J:273:THR:H	2.02	0.57
1:B:149:HIS:C	1:B:151:ASP:N	2.58	0.57
1:A:145:ALA:HB1	1:A:146:PRO:HD2	1.85	0.57
1:E:122:SER:CB	1:E:123:PRO:HD2	2.34	0.57
1:B:302:ALA:O	1:B:305:ALA:HB3	2.05	0.57
1:A:262:ILE:HG12	1:C:98:PRO:HG3	1.85	0.57
1:B:108:GLU:O	1:B:111:ALA:HB3	2.05	0.57
1:A:105:VAL:CG1	1:A:107:PHE:CE1	2.88	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:108:GLU:HB2	1:I:111:ALA:HB2	1.86	0.57
1:H:39:GLU:N	1:H:40:LYS:CD	2.68	0.57
1:J:105:VAL:HG13	1:J:107:PHE:CE1	2.40	0.57
1:G:80:THR:O	1:G:81:ALA:C	2.43	0.57
1:C:260:ASN:HB2	1:C:262:ILE:HD12	1.87	0.57
1:E:123:PRO:O	1:E:124:ALA:HB3	2.05	0.57
1:B:188:GLU:C	1:B:190:GLU:H	2.08	0.57
1:C:240:LYS:HE2	1:C:240:LYS:HA	1.85	0.57
1:D:41:LEU:C	1:D:43:TYR:H	2.03	0.56
1:E:39:GLU:CA	1:E:40:LYS:CB	2.82	0.56
1:E:274:GLY:O	1:E:275:LYS:C	2.44	0.56
1:A:214:PHE:HD2	1:A:299:GLU:HB3	1.68	0.56
1:I:185:ILE:HG13	1:I:193:GLY:C	2.26	0.56
1:J:203:TYR:O	1:J:207:VAL:HG23	2.05	0.56
1:H:157:GLN:HA	1:H:157:GLN:OE1	2.05	0.56
1:C:295:VAL:HG11	1:C:300:MET:HG3	1.87	0.56
1:E:41:LEU:C	1:E:43:TYR:N	2.58	0.56
1:H:250:GLU:HB2	1:H:266:LEU:CD1	2.34	0.56
1:G:185:ILE:HG13	1:G:193:GLY:O	2.05	0.56
1:G:104:TYR:CZ	1:G:196:GLY:HA3	2.39	0.56
1:F:273:THR:CG2	1:F:275:LYS:N	2.53	0.56
1:F:273:THR:HG21	1:F:275:LYS:CD	2.35	0.56
1:J:249:GLU:N	1:J:250:GLU:HG3	2.21	0.56
1:J:249:GLU:CB	1:J:251:LEU:N	2.68	0.56
1:H:123:PRO:O	1:H:124:ALA:HB3	2.05	0.56
1:F:43:TYR:O	1:F:44:GLN:C	2.44	0.56
1:D:122:SER:HB3	1:D:123:PRO:HD2	1.85	0.56
1:B:108:GLU:HA	1:B:130:ARG:NH1	2.20	0.56
1:I:105:VAL:O	1:I:133:PRO:HD2	2.05	0.56
1:H:57:PHE:O	1:H:61:MET:CG	2.52	0.56
1:G:306:ASP:C	1:G:308:ARG:H	2.08	0.56
1:G:165:ASP:C	1:G:166:VAL:CG2	2.73	0.56
1:I:106:ALA:O	1:I:193:GLY:HA3	2.05	0.56
1:G:151:ASP:HA	1:G:157:GLN:OE1	2.06	0.56
1:J:205:ASP:HA	1:J:230:SER:HB2	1.86	0.56
1:A:122:SER:HB2	1:A:123:PRO:HD2	1.85	0.56
1:I:108:GLU:O	1:I:111:ALA:HB3	2.05	0.56
1:D:302:ALA:HB3	1:D:303:GLY:CA	2.36	0.56
1:I:104:TYR:CD2	1:I:134:TYR:CE2	2.93	0.56
1:B:234:HIS:CE1	1:B:272:THR:HG23	2.40	0.56
1:F:160:LYS:HG3	1:F:191:PHE:CE2	2.41	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:THR:HG23	1:A:120:THR:O	2.06	0.56
1:J:172:PHE:HB2	1:J:177:PHE:CE2	2.40	0.56
1:J:260:ASN:CB	1:J:262:ILE:CD1	2.83	0.56
1:E:89:ILE:HD13	1:F:74:THR:HG23	1.88	0.56
1:E:132:VAL:O	1:E:132:VAL:CG2	2.54	0.56
1:D:95:ARG:NE	1:E:253:LYS:HD2	2.21	0.56
1:G:253:LYS:HD3	1:I:95:ARG:HH12	1.71	0.56
1:I:153:SER:O	1:I:157:GLN:HG2	2.06	0.56
1:G:43:TYR:O	1:G:45:GLN:N	2.39	0.56
1:C:273:THR:HG23	1:C:275:LYS:HG2	1.87	0.56
1:E:122:SER:CB	1:E:123:PRO:CD	2.84	0.56
1:E:65:LEU:O	1:E:69:ARG:HG3	2.06	0.56
1:H:234:HIS:HB2	1:H:237:TRP:CE3	2.41	0.56
1:E:43:TYR:C	1:E:45:GLN:H	2.10	0.56
1:J:251:LEU:CD2	1:J:266:LEU:HD12	2.36	0.56
1:E:296:PRO:HB2	1:E:299:GLU:HG3	1.88	0.56
1:A:245:ASP:C	1:A:247:GLY:H	2.07	0.56
1:A:41:LEU:CD1	1:B:307:LEU:CD1	2.84	0.56
1:J:246:PHE:HB3	1:J:251:LEU:CD1	2.36	0.56
1:C:163:GLU:HB3	1:E:259:LYS:HZ1	1.68	0.56
1:G:246:PHE:HB3	1:G:251:LEU:CD1	2.35	0.56
1:A:222:VAL:HA	1:A:227:VAL:O	2.06	0.56
1:E:169:GLU:OE2	1:E:225:SER:OG	2.24	0.56
1:E:41:LEU:HD22	1:E:44:GLN:OE1	2.06	0.56
1:J:249:GLU:C	1:J:250:GLU:CG	2.74	0.56
1:C:186:MET:CE	1:C:191:PHE:HD1	2.19	0.56
1:G:101:LEU:CD2	1:G:101:LEU:O	2.54	0.56
1:A:39:GLU:CA	1:A:39:GLU:OE2	2.54	0.55
1:J:245:ASP:O	1:J:247:GLY:CA	2.54	0.55
1:C:132:VAL:HG23	1:C:147:LEU:H	1.71	0.55
1:B:57:PHE:HE2	1:B:207:VAL:CG1	2.19	0.55
1:D:104:TYR:OH	1:D:180:SER:HB3	2.06	0.55
1:H:185:ILE:HG13	1:H:193:GLY:C	2.26	0.55
1:F:176:VAL:HA	3:F:6:HOH:O	2.05	0.55
1:G:91:GLU:HB2	1:G:135:TRP:NE1	2.21	0.55
1:H:80:THR:HG22	1:H:82:ASP:N	2.21	0.55
1:J:167:LEU:C	1:J:167:LEU:HD12	2.26	0.55
1:C:105:VAL:HG13	1:C:107:PHE:CE1	2.41	0.55
1:C:158:LEU:HB2	1:C:159:PRO:HD3	1.87	0.55
1:J:104:TYR:CZ	1:J:196:GLY:HA3	2.41	0.55
1:H:250:GLU:O	1:H:266:LEU:HD11	2.06	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:CE1	1:A:133:PRO:HG3	2.41	0.55
1:G:139:ASN:O	1:G:141:THR:N	2.28	0.55
1:D:83:ARG:HG2	1:D:112:PHE:HE1	1.70	0.55
1:H:122:SER:HB2	1:H:123:PRO:CD	2.36	0.55
1:D:124:ALA:HB2	1:D:144:VAL:HG11	1.89	0.55
1:E:83:ARG:HD3	1:E:119:TYR:CE1	2.41	0.55
1:H:42:ALA:C	1:H:300:MET:CE	2.75	0.55
1:I:258:ILE:CG1	1:I:259:LYS:N	2.68	0.55
1:I:156:TYR:O	1:I:159:PRO:HD2	2.06	0.55
1:A:39:GLU:N	1:A:40:LYS:CD	2.70	0.55
1:G:41:LEU:CD1	1:G:41:LEU:O	2.54	0.55
1:J:82:ASP:OD1	1:J:82:ASP:C	2.45	0.55
1:E:273:THR:CG2	1:E:275:LYS:CG	2.66	0.55
1:D:299:GLU:O	1:D:302:ALA:HB2	2.07	0.55
1:F:123:PRO:O	1:F:124:ALA:CB	2.55	0.55
1:A:297:LYS:HD2	1:A:297:LYS:O	2.06	0.55
1:A:260:ASN:CB	1:A:262:ILE:CD1	2.82	0.55
1:E:301:LEU:C	1:E:301:LEU:HD23	2.26	0.55
1:H:222:VAL:HG12	1:H:290:ALA:HB3	1.89	0.55
1:D:273:THR:CB	1:D:274:GLY:HA2	2.37	0.54
1:J:297:LYS:O	1:J:301:LEU:CD2	2.51	0.54
1:J:154:ASP:O	1:J:155:TYR:C	2.46	0.54
1:H:185:ILE:HD11	1:H:194:ILE:O	2.07	0.54
1:C:57:PHE:O	1:C:61:MET:CG	2.55	0.54
1:F:182:VAL:HG11	1:F:194:ILE:HD12	1.89	0.54
1:D:265:HIS:C	1:D:266:LEU:HD23	2.27	0.54
1:J:153:SER:HB3	1:J:155:TYR:CD1	2.42	0.54
1:A:250:GLU:H	1:A:250:GLU:CD	2.09	0.54
1:F:167:LEU:HD23	1:F:287:GLY:HA3	1.88	0.54
1:G:266:LEU:HD23	1:G:266:LEU:H	1.72	0.54
1:E:273:THR:HG22	1:E:275:LYS:HD2	1.86	0.54
1:A:215:ASP:N	1:A:299:GLU:OE1	2.36	0.54
1:I:306:ASP:C	1:I:308:ARG:N	2.50	0.54
1:E:130:ARG:NH2	1:E:150:TYR:HE1	2.04	0.54
1:E:273:THR:CG2	1:E:275:LYS:CD	2.63	0.54
1:D:296:PRO:HB2	1:D:299:GLU:CG	2.36	0.54
1:D:298:GLU:N	1:D:299:GLU:CB	2.52	0.54
1:B:240:LYS:HE2	1:B:240:LYS:CA	2.18	0.54
1:D:104:TYR:CZ	1:D:196:GLY:HA3	2.42	0.54
1:I:242:ASP:OD2	1:I:245:ASP:OD2	2.26	0.54
1:J:249:GLU:CB	1:J:252:GLU:N	2.42	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:122:SER:HB2	1:I:123:PRO:CD	2.26	0.54
1:J:177:PHE:CB	1:J:201:LEU:HD12	2.35	0.54
1:C:187:LYS:HG3	1:C:192:ALA:HB2	1.89	0.54
1:F:301:LEU:HD23	1:F:304:VAL:HG21	1.90	0.54
1:F:42:ALA:HB3	1:F:300:MET:HE1	1.89	0.54
1:E:79:GLU:O	1:E:80:THR:C	2.45	0.54
1:B:188:GLU:O	1:B:190:GLU:N	2.39	0.54
1:C:254:ALA:O	1:C:258:ILE:HG23	2.08	0.54
1:G:93:LEU:HD23	1:H:73:THR:HG21	1.89	0.54
1:G:45:GLN:CA	1:G:46:SER:HB2	2.38	0.54
1:E:187:LYS:O	1:E:188:GLU:HG2	2.08	0.54
1:C:248:GLY:HA3	1:C:250:GLU:OE2	2.08	0.54
1:B:213:THR:CG2	1:B:217:GLY:HA3	2.38	0.54
1:C:109:PRO:HD3	1:C:130:ARG:NH1	2.23	0.54
1:A:250:GLU:N	1:A:250:GLU:OE1	2.30	0.54
1:A:167:LEU:HD23	1:A:287:GLY:HA3	1.90	0.54
1:C:222:VAL:CG2	1:C:226:GLY:HA2	2.38	0.54
1:I:108:GLU:HB2	1:I:111:ALA:CB	2.38	0.54
1:G:137:LYS:HA	1:G:141:THR:O	2.08	0.54
1:G:266:LEU:HD23	1:G:266:LEU:N	2.22	0.54
1:E:139:ASN:O	1:E:141:THR:N	2.33	0.54
1:F:43:TYR:HD1	1:F:300:MET:HE1	1.73	0.53
1:D:90:LEU:HD11	1:D:105:VAL:HB	1.90	0.53
1:I:258:ILE:C	1:I:258:ILE:HD12	2.29	0.53
1:F:120:THR:O	1:F:121:ASN:HB2	2.08	0.53
1:A:270:ASP:OD1	1:A:271:PRO:N	2.41	0.53
1:G:107:PHE:O	1:G:130:ARG:HD2	2.08	0.53
1:C:79:GLU:OE2	1:C:79:GLU:HA	2.09	0.53
1:H:109:PRO:HD3	1:H:130:ARG:CZ	2.38	0.53
1:H:185:ILE:N	1:H:193:GLY:O	2.33	0.53
1:C:126:ASP:O	1:C:127:GLY:C	2.45	0.53
1:G:273:THR:CG2	1:G:275:LYS:CE	2.83	0.53
1:C:75:MET:HE3	1:C:105:VAL:HG21	1.88	0.53
1:I:213:THR:HG21	1:I:293:LEU:HD21	1.91	0.53
1:A:275:LYS:HB3	1:H:122:SER:HB3	1.91	0.53
1:D:94:LEU:CD1	1:D:137:LYS:HE3	2.36	0.53
1:C:115:LYS:O	1:C:117:ALA:N	2.42	0.53
1:B:265:HIS:HA	1:B:279:LEU:O	2.09	0.53
1:E:273:THR:CG2	1:E:275:LYS:N	2.62	0.53
1:J:214:PHE:HD2	1:J:299:GLU:CB	2.18	0.53
1:B:230:SER:HA	1:B:238:ILE:HG12	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:VAL:HG13	1:C:290:ALA:HB3	1.89	0.53
1:C:61:MET:HB2	1:C:286:THR:OG1	2.09	0.53
1:D:273:THR:HG1	1:D:274:GLY:HA2	1.70	0.53
1:B:104:TYR:HB3	1:B:134:TYR:HD2	1.74	0.53
1:G:213:THR:O	1:G:217:GLY:CA	2.53	0.53
1:I:157:GLN:HA	1:I:157:GLN:OE1	2.09	0.53
1:C:277:VAL:HA	1:C:297:LYS:H	1.72	0.53
1:J:249:GLU:C	1:J:250:GLU:HG3	2.29	0.53
1:B:108:GLU:HA	1:B:130:ARG:HH11	1.73	0.53
1:H:105:VAL:CG1	1:H:107:PHE:CE1	2.89	0.53
1:J:120:THR:O	1:J:121:ASN:HB2	2.09	0.53
1:E:122:SER:OG	1:E:123:PRO:HD2	2.09	0.53
1:J:249:GLU:O	1:J:249:GLU:CD	2.48	0.53
1:E:83:ARG:NH2	1:E:129:GLY:O	2.42	0.53
1:A:281:TYR:N	1:A:281:TYR:CD2	2.77	0.53
1:F:63:ALA:O	1:F:67:ILE:HG13	2.09	0.53
1:G:145:ALA:HB1	1:G:146:PRO:HD2	1.91	0.53
1:H:131:PHE:C	1:H:132:VAL:CG1	2.77	0.53
1:J:207:VAL:O	1:J:210:LYS:CG	2.56	0.53
1:J:94:LEU:HD11	1:J:137:LYS:HG3	1.91	0.53
1:F:42:ALA:HB3	1:F:300:MET:CE	2.39	0.52
1:B:69:ARG:CG	1:B:69:ARG:NH1	2.70	0.52
1:B:104:TYR:HE2	1:B:198:ASP:CG	2.12	0.52
1:C:88:LEU:HD22	1:C:92:ASN:OD1	2.10	0.52
1:E:297:LYS:O	1:E:300:MET:HB2	2.08	0.52
1:A:205:ASP:OD2	1:A:209:SER:OG	2.25	0.52
1:H:173:TYR:O	1:H:174:GLU:C	2.48	0.52
1:D:80:THR:O	1:D:80:THR:CG2	2.55	0.52
1:F:268:THR:HG23	1:F:269:ALA:N	2.24	0.52
1:D:97:ASN:HB2	1:D:100:LEU:HD12	1.92	0.52
1:C:163:GLU:CB	1:E:259:LYS:NZ	2.68	0.52
1:I:104:TYR:HE2	1:I:198:ASP:CG	2.12	0.52
1:I:159:PRO:O	1:I:163:GLU:N	2.40	0.52
1:B:127:GLY:O	1:B:129:GLY:N	2.43	0.52
1:H:177:PHE:HB3	1:H:201:LEU:HD12	1.89	0.52
1:D:178:MET:CE	1:D:198:ASP:OD1	2.58	0.52
1:B:159:PRO:O	1:B:163:GLU:N	2.42	0.52
1:H:278:ILE:HG22	1:H:280:PHE:CD1	2.45	0.52
1:F:308:ARG:O	1:F:309:GLU:C	2.48	0.52
1:D:169:GLU:HA	1:D:169:GLU:OE2	2.08	0.52
1:A:41:LEU:CD1	1:B:307:LEU:HD11	2.39	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:GLU:HB2	1:G:135:TRP:CE2	2.44	0.52
1:I:104:TYR:HB3	1:I:134:TYR:HD2	1.74	0.52
1:A:59:ALA:HA	1:B:59:ALA:HA	1.91	0.52
1:G:272:THR:HG22	1:G:273:THR:CG2	2.34	0.52
1:J:39:GLU:O	1:J:304:VAL:HG21	2.10	0.52
1:B:240:LYS:HA	1:B:240:LYS:CE	2.21	0.52
1:A:218:TYR:HD1	1:A:218:TYR:H	1.56	0.52
1:B:186:MET:SD	1:B:191:PHE:HB2	2.50	0.52
1:D:80:THR:O	1:D:82:ASP:N	2.42	0.52
1:D:139:ASN:C	1:D:141:THR:N	2.61	0.52
1:C:248:GLY:CA	1:C:250:GLU:OE2	2.58	0.52
1:J:107:PHE:O	1:J:130:ARG:NH1	2.40	0.52
1:G:139:ASN:C	1:G:141:THR:N	2.63	0.52
1:G:101:LEU:CD2	1:G:101:LEU:C	2.78	0.52
1:I:247:GLY:O	1:I:248:GLY:O	2.27	0.52
1:I:149:HIS:C	1:I:151:ASP:N	2.59	0.52
1:C:185:ILE:N	1:C:193:GLY:O	2.39	0.52
1:H:170:PRO:HG3	1:H:229:LEU:HD21	1.90	0.52
1:G:188:GLU:HG3	1:G:188:GLU:O	2.10	0.52
1:B:95:ARG:NH1	1:D:253:LYS:HB3	2.25	0.52
1:C:105:VAL:HG13	1:C:107:PHE:HE1	1.74	0.52
1:I:150:TYR:H	1:I:150:TYR:HD2	1.48	0.52
1:J:99:HIS:HD1	1:J:203:TYR:HE1	1.57	0.52
1:D:215:ASP:HB2	1:D:299:GLU:OE2	2.09	0.52
1:D:299:GLU:O	1:D:302:ALA:HB3	2.09	0.52
1:H:125:HIS:N	1:H:125:HIS:HD1	2.07	0.52
1:D:214:PHE:HD1	1:D:295:VAL:HG13	1.71	0.52
1:H:139:ASN:OD1	1:H:139:ASN:N	2.43	0.52
1:H:119:TYR:O	1:H:120:THR:C	2.48	0.51
1:J:298:GLU:O	1:J:301:LEU:HD23	2.10	0.51
1:B:272:THR:CG2	1:B:272:THR:O	2.57	0.51
1:A:105:VAL:O	1:A:133:PRO:HD2	2.11	0.51
1:I:158:LEU:N	1:I:159:PRO:CD	2.72	0.51
1:D:115:LYS:HD3	1:D:118:GLU:OE2	2.10	0.51
1:D:41:LEU:O	1:D:43:TYR:HB2	2.11	0.51
1:B:39:GLU:HA	1:B:40:LYS:HB3	1.92	0.51
1:B:90:LEU:HD13	1:B:104:TYR:HA	1.90	0.51
1:I:258:ILE:HG13	1:I:259:LYS:H	1.71	0.51
1:A:264:GLY:C	1:A:281:TYR:CE2	2.84	0.51
1:F:148:LEU:HD12	1:F:174:GLU:OE2	2.10	0.51
1:D:153:SER:HB2	1:D:155:TYR:CD1	2.45	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:83:ARG:HG2	1:G:112:PHE:HE1	1.74	0.51
1:A:214:PHE:CE2	1:A:299:GLU:O	2.61	0.51
1:A:156:TYR:O	1:A:159:PRO:HD2	2.10	0.51
1:B:265:HIS:O	1:B:266:LEU:HD23	2.10	0.51
1:B:268:THR:HG23	1:B:269:ALA:O	2.11	0.51
1:G:206:GLU:C	1:G:206:GLU:OE1	2.48	0.51
1:D:271:PRO:CD	1:D:272:THR:H	2.24	0.51
1:D:272:THR:HG22	1:D:273:THR:HG23	1.93	0.51
1:C:273:THR:HG23	1:C:275:LYS:N	2.22	0.51
1:F:43:TYR:CD1	1:F:300:MET:HE1	2.45	0.51
1:E:300:MET:O	1:E:304:VAL:N	2.43	0.51
1:G:123:PRO:O	1:G:124:ALA:HB3	2.11	0.51
1:J:154:ASP:C	1:J:156:TYR:N	2.62	0.51
1:A:278:ILE:HD11	1:A:297:LYS:HD3	1.93	0.51
1:C:296:PRO:O	1:C:297:LYS:C	2.48	0.51
1:B:251:LEU:C	1:B:254:ALA:HB3	2.30	0.51
1:C:174:GLU:OE2	1:C:174:GLU:N	2.42	0.51
1:D:119:TYR:O	1:D:121:ASN:N	2.43	0.51
1:F:265:HIS:HA	1:F:279:LEU:O	2.10	0.51
1:H:72:SER:O	1:H:76:GLU:HG3	2.10	0.51
1:D:41:LEU:CD2	1:D:42:ALA:HA	2.40	0.51
1:G:43:TYR:C	1:G:45:GLN:N	2.63	0.51
1:G:218:TYR:CD2	1:G:232:PRO:CG	2.88	0.51
1:G:177:PHE:HZ	1:G:240:LYS:HD2	1.76	0.51
1:J:49:MET:CE	1:J:53:TYR:HE1	2.24	0.51
1:C:270:ASP:OD2	1:C:274:GLY:CA	2.46	0.51
1:G:136:ASN:OD1	1:G:138:MET:CE	2.59	0.51
1:I:309:GLU:O	1:I:309:GLU:OE1	2.29	0.51
1:A:267:GLU:OE1	1:A:297:LYS:NZ	2.44	0.51
1:H:91:GLU:CG	1:H:135:TRP:CH2	2.91	0.51
1:H:91:GLU:HG3	1:H:135:TRP:CZ3	2.45	0.51
1:I:117:ALA:O	1:I:120:THR:HG22	2.10	0.51
1:F:105:VAL:O	1:F:133:PRO:HD2	2.10	0.51
1:E:205:ASP:HA	1:E:230:SER:HB2	1.92	0.51
1:A:39:GLU:CB	1:A:40:LYS:HB2	2.38	0.51
1:B:82:ASP:OD1	1:B:83:ARG:N	2.44	0.51
1:A:203:TYR:CE2	1:A:207:VAL:HG21	2.46	0.51
1:C:169:GLU:HB3	1:C:170:PRO:CD	2.40	0.51
1:D:41:LEU:O	1:D:43:TYR:CA	2.55	0.51
1:J:40:LYS:C	1:J:42:ALA:N	2.63	0.51
1:F:266:LEU:O	1:F:278:ILE:HG23	2.11	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:TYR:O	1:F:46:SER:N	2.42	0.51
1:D:91:GLU:OE1	1:D:135:TRP:HZ2	1.93	0.51
1:B:83:ARG:O	1:B:87:LEU:CD1	2.53	0.51
1:C:139:ASN:OD1	1:C:139:ASN:N	2.43	0.51
1:A:105:VAL:HG13	1:A:107:PHE:CE1	2.46	0.51
1:A:83:ARG:HG2	1:A:112:PHE:HE1	1.76	0.51
1:E:165:ASP:C	1:E:166:VAL:HG23	2.31	0.51
1:C:76:GLU:HG3	1:C:185:ILE:HG23	1.93	0.51
1:A:279:LEU:HD22	1:A:292:VAL:HG11	1.93	0.51
1:J:272:THR:O	1:J:273:THR:HG22	2.10	0.50
1:J:246:PHE:HB3	1:J:251:LEU:HD12	1.93	0.50
1:G:270:ASP:C	1:G:270:ASP:OD1	2.49	0.50
1:B:157:GLN:O	1:B:160:LYS:N	2.44	0.50
1:A:156:TYR:C	1:A:159:PRO:HD2	2.31	0.50
1:D:154:ASP:N	1:D:154:ASP:OD1	2.44	0.50
1:J:74:THR:O	1:J:77:SER:N	2.44	0.50
1:D:136:ASN:HD22	1:D:136:ASN:H	1.59	0.50
1:E:269:ALA:O	1:E:271:PRO:HD3	2.11	0.50
1:J:218:TYR:N	1:J:218:TYR:HD1	2.07	0.50
1:B:230:SER:O	1:B:231:HIS:HB2	2.11	0.50
1:E:106:ALA:HB3	1:E:194:ILE:HG12	1.93	0.50
1:D:272:THR:CG2	1:D:273:THR:HG23	2.41	0.50
1:J:40:LYS:C	1:J:42:ALA:H	2.14	0.50
1:A:218:TYR:CD2	1:A:232:PRO:CG	2.95	0.50
1:I:110:ASP:N	1:I:116:ASP:OD2	2.37	0.50
1:J:82:ASP:OD1	1:J:84:ASP:N	2.44	0.50
1:A:106:ALA:HB2	1:A:147:LEU:HD12	1.93	0.50
1:J:279:LEU:HD23	1:J:294:VAL:HG22	1.93	0.50
1:A:109:PRO:HA	1:A:130:ARG:HD3	1.92	0.50
1:G:188:GLU:O	1:G:188:GLU:CG	2.59	0.50
1:H:241:LYS:HA	1:H:245:ASP:OD2	2.10	0.50
1:G:122:SER:CB	1:G:123:PRO:CD	2.90	0.50
1:I:104:TYR:HE2	1:I:198:ASP:OD2	1.95	0.50
1:G:165:ASP:O	1:G:166:VAL:HG22	2.11	0.50
1:B:249:GLU:C	1:B:251:LEU:N	2.61	0.50
1:D:204:VAL:O	1:D:208:VAL:HG23	2.12	0.50
1:B:75:MET:HE2	1:B:75:MET:HA	1.93	0.50
1:D:107:PHE:O	1:D:130:ARG:CD	2.57	0.50
1:J:109:PRO:HA	1:J:130:ARG:HD3	1.94	0.50
1:D:172:PHE:CZ	1:D:175:GLY:HA2	2.47	0.50
1:C:123:PRO:O	1:C:124:ALA:HB3	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:213:THR:O	1:H:214:PHE:HB2	2.10	0.50
1:H:131:PHE:CE1	1:H:133:PRO:HG3	2.47	0.50
1:I:282:GLU:OE2	1:I:283:PRO:HD2	2.11	0.50
1:D:124:ALA:HB2	1:D:144:VAL:CG1	2.42	0.49
1:G:122:SER:CB	1:G:123:PRO:HD2	2.34	0.49
1:F:278:ILE:HD11	1:F:300:MET:HG3	1.93	0.49
1:F:45:GLN:O	1:F:45:GLN:HG2	2.12	0.49
1:C:170:PRO:HG3	1:C:229:LEU:HD21	1.94	0.49
1:C:139:ASN:C	1:C:141:THR:N	2.65	0.49
1:J:108:GLU:HA	1:J:130:ARG:NH1	2.27	0.49
1:G:136:ASN:OD1	1:G:138:MET:CB	2.37	0.49
1:I:123:PRO:O	1:I:124:ALA:HB3	2.12	0.49
1:C:86:ALA:CB	1:C:131:PHE:CZ	2.95	0.49
1:B:48:GLU:O	1:B:51:SER:CB	2.51	0.49
1:B:108:GLU:HB2	1:B:111:ALA:HB2	1.94	0.49
1:F:49:MET:CE	1:F:293:LEU:HD11	2.42	0.49
1:G:262:ILE:CD1	1:I:98:PRO:HG3	2.41	0.49
1:G:221:MET:HE3	1:G:229:LEU:HD12	1.94	0.49
1:D:41:LEU:HD22	1:D:42:ALA:H	0.38	0.49
1:J:270:ASP:OD1	1:J:271:PRO:N	2.45	0.49
1:H:98:PRO:HG3	1:J:262:ILE:CD1	2.43	0.49
1:G:246:PHE:HB3	1:G:251:LEU:HD12	1.94	0.49
1:I:104:TYR:HD2	1:I:134:TYR:CD2	2.30	0.49
1:C:260:ASN:HB3	1:C:262:ILE:HD12	1.94	0.49
1:C:65:LEU:O	1:C:69:ARG:HG3	2.12	0.49
1:B:65:LEU:HD12	1:B:65:LEU:O	2.13	0.49
1:C:295:VAL:HG12	1:C:295:VAL:O	2.12	0.49
1:C:78:TYR:OH	1:C:85:GLU:HB3	2.13	0.49
1:H:277:VAL:HG12	1:H:296:PRO:N	2.27	0.49
1:A:305:ALA:C	1:A:307:LEU:H	2.16	0.49
1:H:267:GLU:OE1	1:H:297:LYS:HD3	2.13	0.49
1:C:222:VAL:CG1	1:C:290:ALA:HB3	2.43	0.49
1:G:165:ASP:O	1:G:166:VAL:CG2	2.60	0.49
1:G:172:PHE:CE2	1:G:175:GLY:HA2	2.47	0.49
1:B:50:ALA:HA	1:B:293:LEU:HD12	1.94	0.49
1:F:270:ASP:C	1:F:272:THR:H	2.14	0.49
1:C:275:LYS:CB	1:C:275:LYS:NZ	2.76	0.49
1:B:39:GLU:OE2	1:B:39:GLU:CA	2.60	0.49
1:C:80:THR:O	1:C:81:ALA:C	2.51	0.49
1:C:208:VAL:HG11	1:C:220:PHE:HA	1.93	0.49
1:H:277:VAL:HG12	1:H:295:VAL:C	2.32	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:112:PHE:CD1	1:I:131:PHE:CD2	3.00	0.49
1:C:115:LYS:C	1:C:117:ALA:N	2.63	0.49
1:H:254:ALA:O	1:H:258:ILE:HG23	2.13	0.49
1:G:39:GLU:CA	1:G:40:LYS:CB	2.75	0.49
1:C:80:THR:O	1:C:80:THR:HG22	2.10	0.49
1:E:130:ARG:NH2	1:E:150:TYR:CE1	2.80	0.49
1:H:186:MET:CE	1:H:191:PHE:HD1	2.25	0.49
1:I:267:GLU:O	1:I:268:THR:HG22	2.11	0.49
1:D:154:ASP:O	1:D:156:TYR:N	2.45	0.49
1:B:49:MET:HG2	1:B:293:LEU:HD11	1.95	0.49
1:G:273:THR:OG1	1:G:275:LYS:HD2	2.13	0.49
1:C:86:ALA:CB	1:C:131:PHE:HZ	2.25	0.49
1:G:77:SER:CB	1:H:88:LEU:HD13	2.43	0.49
1:I:120:THR:HA	1:I:129:GLY:HA3	1.94	0.49
1:B:297:LYS:O	1:B:301:LEU:HG	2.13	0.49
1:E:75:MET:HB2	1:E:185:ILE:HD13	1.95	0.49
1:J:125:HIS:O	1:J:146:PRO:HG3	2.12	0.49
1:D:185:ILE:HG13	1:D:193:GLY:O	2.13	0.49
1:J:309:GLU:OE2	1:J:309:GLU:CA	2.59	0.49
1:D:177:PHE:CE2	1:D:239:GLY:O	2.66	0.49
1:G:302:ALA:O	1:G:305:ALA:HB3	2.13	0.49
1:G:177:PHE:HB3	1:G:201:LEU:HD22	1.94	0.49
1:E:55:ASN:ND2	1:F:52:ASN:OD1	2.42	0.49
1:H:49:MET:O	1:H:50:ALA:C	2.50	0.49
1:A:115:LYS:HD3	1:A:118:GLU:OE2	2.11	0.49
1:D:298:GLU:HG3	1:D:299:GLU:CB	2.42	0.48
1:J:298:GLU:C	1:J:301:LEU:CD2	2.82	0.48
1:B:148:LEU:O	1:B:149:HIS:CG	2.66	0.48
1:I:234:HIS:HB3	1:I:237:TRP:CD1	2.47	0.48
1:I:185:ILE:HG13	1:I:194:ILE:CA	2.43	0.48
1:H:169:GLU:HB3	1:H:170:PRO:HD2	1.93	0.48
1:A:200:SER:O	1:A:204:VAL:HG23	2.12	0.48
1:H:122:SER:CB	1:H:123:PRO:HD2	2.40	0.48
1:J:309:GLU:CD	1:J:309:GLU:H	2.15	0.48
1:J:300:MET:HB2	1:J:301:LEU:HD13	1.95	0.48
1:B:40:LYS:C	1:B:42:ALA:H	2.12	0.48
1:E:48:GLU:CG	1:F:48:GLU:CG	2.91	0.48
1:D:137:LYS:HA	1:D:141:THR:O	2.13	0.48
1:A:109:PRO:O	1:A:110:ASP:HB2	2.12	0.48
1:I:150:TYR:CD2	1:I:150:TYR:N	2.68	0.48
1:G:173:TYR:CD2	1:G:178:MET:HE3	2.48	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:TYR:N	1:A:171:TYR:HD1	2.08	0.48
1:C:130:ARG:NH2	1:C:150:TYR:HE1	2.12	0.48
1:C:171:TYR:OH	1:C:178:MET:HE3	2.13	0.48
1:A:154:ASP:O	1:A:155:TYR:C	2.52	0.48
1:C:57:PHE:O	1:C:61:MET:HG2	2.13	0.48
1:C:187:LYS:HG3	1:C:192:ALA:CB	2.43	0.48
1:H:171:TYR:OH	1:H:178:MET:HE3	2.13	0.48
1:J:260:ASN:HB3	1:J:262:ILE:CD1	2.43	0.48
1:E:302:ALA:N	1:E:303:GLY:CA	2.69	0.48
1:H:130:ARG:NH2	1:H:150:TYR:CE1	2.81	0.48
1:I:57:PHE:CE2	1:I:207:VAL:HG12	2.48	0.48
1:C:49:MET:O	1:C:50:ALA:C	2.50	0.48
1:I:254:ALA:O	1:I:258:ILE:HG23	2.14	0.48
1:D:214:PHE:CD1	1:D:295:VAL:CG1	2.94	0.48
1:I:108:GLU:OE2	1:I:160:LYS:HE3	2.14	0.48
1:I:185:ILE:HG13	1:I:194:ILE:N	2.29	0.48
1:E:213:THR:HG22	1:E:217:GLY:HA3	1.94	0.48
1:D:182:VAL:HG12	1:D:183:SER:N	2.27	0.48
1:E:79:GLU:C	1:E:81:ALA:N	2.63	0.48
1:C:115:LYS:HB3	1:C:118:GLU:HG3	1.96	0.48
1:J:151:ASP:O	1:J:152:SER:HB3	2.13	0.48
1:I:39:GLU:HA	1:I:40:LYS:HB2	1.93	0.48
1:H:98:PRO:HG3	1:J:262:ILE:HD11	1.94	0.48
1:H:273:THR:HG1	1:H:275:LYS:HG2	1.73	0.48
1:H:42:ALA:O	1:H:300:MET:HE3	2.13	0.48
1:A:154:ASP:C	1:A:156:TYR:N	2.66	0.48
1:C:256:ARG:HH22	1:F:92:ASN:CG	2.17	0.48
1:C:258:ILE:HG13	1:C:259:LYS:N	2.22	0.48
1:F:122:SER:CB	1:F:123:PRO:CD	2.88	0.48
1:J:105:VAL:HG11	1:J:107:PHE:CE1	2.44	0.48
1:C:70:THR:HB	1:D:70:THR:HG21	1.95	0.48
1:F:158:LEU:HD23	1:F:158:LEU:HA	1.56	0.48
1:H:91:GLU:HG3	1:H:135:TRP:CE3	2.49	0.48
1:J:61:MET:SD	1:J:284:VAL:HG11	2.54	0.48
1:A:83:ARG:HG2	1:A:112:PHE:CE1	2.49	0.48
1:F:182:VAL:CG1	1:F:194:ILE:HD12	2.43	0.48
1:D:188:GLU:CG	1:D:188:GLU:O	2.61	0.48
1:F:132:VAL:O	1:F:132:VAL:HG23	2.14	0.48
1:J:173:TYR:CG	1:J:178:MET:HE3	2.49	0.48
1:B:237:TRP:CE2	1:B:241:LYS:NZ	2.82	0.48
1:G:306:ASP:C	1:G:308:ARG:N	2.67	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:208:VAL:HG21	1:H:221:MET:HG3	1.95	0.48
1:D:145:ALA:HB1	1:D:146:PRO:HD2	1.94	0.48
1:A:41:LEU:HD11	1:B:307:LEU:HD11	1.94	0.47
1:J:251:LEU:HD23	1:J:266:LEU:HD13	1.85	0.47
1:G:272:THR:CG2	1:G:273:THR:HG22	2.37	0.47
1:E:295:VAL:CG1	1:E:300:MET:HG2	2.44	0.47
1:B:104:TYR:HD2	1:B:134:TYR:CE2	2.32	0.47
1:A:132:VAL:N	1:A:133:PRO:HD3	2.28	0.47
1:H:125:HIS:O	1:H:146:PRO:HG3	2.13	0.47
1:C:218:TYR:CD2	1:C:232:PRO:CG	2.94	0.47
1:H:43:TYR:N	1:H:300:MET:HE2	2.29	0.47
1:J:222:VAL:HG22	1:J:226:GLY:C	2.35	0.47
1:B:279:LEU:CD2	1:B:294:VAL:HG22	2.45	0.47
1:E:265:HIS:HA	1:E:279:LEU:O	2.14	0.47
1:C:112:PHE:CG	1:C:131:PHE:HD2	2.33	0.47
1:C:169:GLU:HB3	1:C:170:PRO:HD2	1.97	0.47
1:G:79:GLU:C	1:G:81:ALA:H	2.17	0.47
1:F:49:MET:HE1	1:F:293:LEU:HD11	1.95	0.47
1:I:150:TYR:HB2	1:I:156:TYR:CD1	2.49	0.47
1:I:154:ASP:OD2	1:I:158:LEU:HD11	2.14	0.47
1:C:256:ARG:CD	3:C:321:HOH:O	2.61	0.47
1:A:135:TRP:HZ3	1:A:142:ALA:O	1.97	0.47
1:J:113:ASP:O	1:J:115:LYS:N	2.47	0.47
1:H:182:VAL:HG11	1:H:194:ILE:HD12	1.97	0.47
1:J:200:SER:O	1:J:204:VAL:HG23	2.14	0.47
1:C:273:THR:CG2	1:C:275:LYS:HG2	2.43	0.47
1:D:214:PHE:CE1	1:D:295:VAL:HG11	2.49	0.47
1:G:172:PHE:CZ	1:G:175:GLY:HA2	2.50	0.47
1:E:83:ARG:HH11	1:E:113:ASP:CG	2.15	0.47
1:C:105:VAL:CG1	1:C:107:PHE:HE1	2.27	0.47
1:B:279:LEU:HD22	1:B:294:VAL:HG22	1.97	0.47
1:A:39:GLU:CA	1:A:40:LYS:HG3	2.42	0.47
1:H:250:GLU:CB	1:H:266:LEU:HD13	2.42	0.47
1:E:295:VAL:HG11	1:E:300:MET:HG2	1.96	0.47
1:C:186:MET:HE2	1:C:191:PHE:HD1	1.80	0.47
1:H:302:ALA:C	1:H:304:VAL:H	2.18	0.47
1:G:182:VAL:CG1	1:G:183:SER:N	2.76	0.47
1:B:131:PHE:CE1	1:B:133:PRO:HG3	2.49	0.47
1:A:61:MET:SD	1:A:284:VAL:HG11	2.55	0.47
1:D:172:PHE:CE2	1:D:175:GLY:HA2	2.50	0.47
1:B:91:GLU:HB2	1:B:135:TRP:CE2	2.50	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:LEU:CD2	1:F:70:THR:HG23	2.45	0.47
1:E:93:LEU:HD21	1:F:70:THR:HG23	1.96	0.47
1:D:71:ILE:O	1:D:74:THR:HB	2.15	0.47
1:J:234:HIS:O	1:J:236:ASP:N	2.48	0.47
1:F:240:LYS:HE3	1:F:240:LYS:HB3	1.61	0.47
1:B:89:ILE:O	1:B:90:LEU:C	2.51	0.47
1:A:251:LEU:HD23	1:A:266:LEU:CD1	2.45	0.47
1:I:104:TYR:CD2	1:I:134:TYR:HE2	2.29	0.47
1:F:85:GLU:O	1:F:89:ILE:HG13	2.15	0.47
1:D:249:GLU:CG	1:D:249:GLU:O	2.62	0.47
1:G:249:GLU:O	1:G:249:GLU:CG	2.63	0.47
1:G:128:THR:C	1:G:130:ARG:H	2.18	0.47
1:G:154:ASP:OD1	1:G:154:ASP:N	2.47	0.47
1:G:273:THR:HG21	1:G:275:LYS:HE2	1.94	0.47
1:B:160:LYS:HA	1:B:191:PHE:CE1	2.50	0.47
1:B:130:ARG:NH2	1:B:150:TYR:CD1	2.83	0.47
1:I:88:LEU:HD13	1:J:77:SER:HB3	1.97	0.47
1:B:50:ALA:CA	1:B:293:LEU:HD12	2.45	0.47
1:J:278:ILE:HD11	1:J:297:LYS:HD3	1.97	0.47
1:D:136:ASN:HD22	1:D:136:ASN:N	2.12	0.47
1:I:107:PHE:HB3	1:I:111:ALA:HB3	1.97	0.47
1:C:301:LEU:HA	1:C:304:VAL:HG23	1.96	0.46
1:B:39:GLU:HA	1:B:40:LYS:C	2.35	0.46
1:A:99:HIS:ND1	1:A:203:TYR:CE1	2.83	0.46
1:E:107:PHE:O	1:E:130:ARG:HD2	2.15	0.46
1:A:250:GLU:N	1:A:250:GLU:CD	2.67	0.46
1:I:156:TYR:C	1:I:159:PRO:HD2	2.35	0.46
1:B:122:SER:CB	1:B:123:PRO:HD2	2.45	0.46
1:J:169:GLU:CB	1:J:170:PRO:HD2	2.43	0.46
1:H:126:ASP:O	1:H:129:GLY:N	2.47	0.46
1:D:188:GLU:O	1:D:188:GLU:HG3	2.14	0.46
1:H:101:LEU:HD22	1:H:101:LEU:O	2.15	0.46
1:G:45:GLN:H	1:G:46:SER:CB	2.26	0.46
1:B:39:GLU:CA	1:B:40:LYS:CB	2.92	0.46
1:C:80:THR:CG2	1:C:80:THR:O	2.60	0.46
1:G:245:ASP:O	1:G:246:PHE:C	2.51	0.46
1:F:298:GLU:CD	1:F:298:GLU:N	2.65	0.46
1:H:215:ASP:HB2	1:H:299:GLU:OE1	2.15	0.46
1:F:193:GLY:O	1:F:194:ILE:HG22	2.15	0.46
1:F:273:THR:CG2	1:F:274:GLY:N	2.33	0.46
1:A:262:ILE:CG1	1:C:98:PRO:HG3	2.44	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:222:VAL:HG13	1:I:226:GLY:CA	2.25	0.46
1:H:231:HIS:HD2	1:H:237:TRP:HE3	1.62	0.46
1:C:278:ILE:HG22	1:C:280:PHE:CD1	2.49	0.46
1:A:300:MET:O	1:A:304:VAL:HG23	2.16	0.46
1:D:108:GLU:O	1:D:111:ALA:CB	2.63	0.46
1:H:277:VAL:HG13	1:H:296:PRO:HA	1.96	0.46
1:E:85:GLU:O	1:E:89:ILE:HG13	2.15	0.46
1:B:106:ALA:HB3	1:B:194:ILE:HG12	1.96	0.46
1:C:97:ASN:HB2	1:C:100:LEU:HD12	1.97	0.46
1:D:272:THR:HG23	1:D:273:THR:HG22	1.97	0.46
1:C:213:THR:O	1:C:217:GLY:HA3	2.15	0.46
1:D:136:ASN:OD1	1:D:138:MET:CB	2.58	0.46
1:G:80:THR:CG2	1:G:80:THR:O	2.59	0.46
1:B:138:MET:CE	1:B:174:GLU:HG2	2.45	0.46
1:J:83:ARG:HG3	1:J:112:PHE:CE1	2.46	0.46
1:J:98:PRO:HA	1:J:137:LYS:NZ	2.31	0.46
1:F:247:GLY:HA3	1:F:251:LEU:HD12	1.98	0.46
1:A:73:THR:HG21	1:B:93:LEU:HD23	1.97	0.46
1:A:187:LYS:NZ	3:A:7:HOH:O	2.48	0.46
1:C:85:GLU:O	1:C:86:ALA:C	2.54	0.46
1:A:201:LEU:O	1:A:204:VAL:N	2.49	0.46
1:H:39:GLU:N	1:H:40:LYS:CG	2.79	0.46
1:C:85:GLU:O	1:C:89:ILE:HG13	2.15	0.46
1:A:79:GLU:OE2	1:A:79:GLU:CA	2.60	0.46
1:A:222:VAL:HG12	1:A:290:ALA:O	2.15	0.46
1:C:57:PHE:O	1:C:61:MET:HG3	2.15	0.46
1:J:249:GLU:N	1:J:249:GLU:CD	2.68	0.46
1:A:298:GLU:C	1:A:300:MET:N	2.69	0.46
1:D:109:PRO:N	1:D:130:ARG:HD3	2.31	0.46
1:A:242:ASP:O	1:A:244:TYR:N	2.49	0.46
1:E:78:TYR:OH	1:E:85:GLU:HB3	2.16	0.46
1:D:231:HIS:O	1:D:235:LYS:HD3	2.15	0.46
1:B:213:THR:HG23	1:B:217:GLY:HA3	1.98	0.46
1:D:178:MET:HE3	1:D:198:ASP:OD1	2.15	0.46
1:A:41:LEU:HD11	1:B:307:LEU:HD12	1.95	0.46
1:H:135:TRP:CD2	1:H:144:VAL:HB	2.51	0.46
1:G:77:SER:HB3	1:H:88:LEU:HD13	1.96	0.46
1:I:171:TYR:N	1:I:171:TYR:CD1	2.84	0.46
1:E:80:THR:O	1:E:81:ALA:C	2.53	0.46
1:E:131:PHE:CE1	1:E:133:PRO:HG3	2.51	0.46
1:C:91:GLU:HG3	1:C:135:TRP:CZ3	2.50	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:THR:HG23	1:C:120:THR:O	2.16	0.46
1:F:43:TYR:C	1:F:45:GLN:N	2.70	0.46
1:J:80:THR:O	1:J:81:ALA:HB3	2.16	0.46
1:C:208:VAL:HG21	1:C:221:MET:HG3	1.98	0.46
1:I:147:LEU:O	1:I:150:TYR:CD2	2.69	0.46
1:B:109:PRO:HA	1:B:116:ASP:OD2	2.16	0.46
1:B:57:PHE:HE2	1:B:207:VAL:HG11	1.80	0.46
1:C:83:ARG:NH2	1:C:113:ASP:OD2	2.34	0.46
1:G:273:THR:OG1	1:G:275:LYS:HE2	2.15	0.45
1:A:99:HIS:ND1	1:A:203:TYR:HE1	2.14	0.45
1:I:57:PHE:HE2	1:I:207:VAL:HG11	1.80	0.45
1:H:182:VAL:HG12	1:H:194:ILE:HB	1.98	0.45
1:B:126:ASP:O	1:B:127:GLY:C	2.54	0.45
1:B:287:GLY:O	1:B:288:ASP:C	2.54	0.45
1:G:265:HIS:ND1	1:G:265:HIS:O	2.48	0.45
1:J:215:ASP:H	1:J:299:GLU:HG2	1.81	0.45
1:F:270:ASP:C	1:F:272:THR:N	2.70	0.45
1:H:98:PRO:HG3	1:J:262:ILE:HG12	1.97	0.45
1:I:131:PHE:C	1:I:132:VAL:HG13	2.36	0.45
1:E:132:VAL:HG23	1:E:147:LEU:HB2	1.98	0.45
1:A:88:LEU:HD22	1:A:92:ASN:OD1	2.16	0.45
1:J:214:PHE:HE2	1:J:299:GLU:O	1.98	0.45
1:G:41:LEU:C	1:G:41:LEU:CD1	2.85	0.45
1:G:135:TRP:CE3	1:G:144:VAL:HG23	2.50	0.45
1:C:134:TYR:O	1:C:136:ASN:ND2	2.46	0.45
1:G:177:PHE:CZ	1:G:240:LYS:HD2	2.51	0.45
1:I:250:GLU:OE1	1:I:250:GLU:HA	2.15	0.45
1:B:308:ARG:O	1:B:309:GLU:HB2	2.17	0.45
1:H:120:THR:O	1:H:121:ASN:CB	2.62	0.45
1:H:246:PHE:O	1:H:251:LEU:CD1	2.60	0.45
1:B:117:ALA:O	1:B:120:THR:CG2	2.64	0.45
1:E:83:ARG:CD	1:E:119:TYR:CE1	2.99	0.45
1:A:258:ILE:HG22	1:A:281:TYR:CD1	2.51	0.45
1:B:91:GLU:HB2	1:B:135:TRP:NE1	2.32	0.45
1:H:117:ALA:O	1:H:120:THR:CG2	2.56	0.45
1:I:307:LEU:C	1:I:308:ARG:HG3	2.30	0.45
1:I:136:ASN:OD1	1:I:138:MET:CB	2.57	0.45
1:J:156:TYR:CD1	1:J:194:ILE:HD13	2.52	0.45
1:A:82:ASP:OD1	1:A:82:ASP:C	2.55	0.45
1:G:154:ASP:O	1:G:156:TYR:N	2.49	0.45
1:I:302:ALA:O	1:I:305:ALA:HB3	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:244:TYR:C	1:I:246:PHE:H	2.19	0.45
1:C:213:THR:CG2	1:C:295:VAL:CG2	2.95	0.45
1:J:246:PHE:CD1	1:J:251:LEU:HD11	2.51	0.45
1:B:130:ARG:NH2	1:B:150:TYR:HD1	2.15	0.45
1:A:251:LEU:HA	1:A:251:LEU:HD23	1.72	0.45
1:C:182:VAL:HG12	1:C:194:ILE:HB	1.99	0.45
1:J:104:TYR:CE1	1:J:196:GLY:HA3	2.50	0.45
1:D:272:THR:HG23	1:D:273:THR:CG2	2.47	0.45
1:B:182:VAL:HG11	1:B:194:ILE:HD12	1.97	0.45
1:B:112:PHE:CE1	1:B:131:PHE:CD2	3.04	0.45
1:C:126:ASP:O	1:C:128:THR:N	2.50	0.45
1:E:218:TYR:CD2	1:E:232:PRO:HG2	2.52	0.45
1:D:160:LYS:O	1:D:161:ALA:C	2.54	0.45
1:J:282:GLU:OE2	1:J:282:GLU:HA	2.17	0.45
1:E:298:GLU:HG2	1:E:299:GLU:N	2.31	0.45
1:C:110:ASP:OD1	1:C:114:GLY:O	2.34	0.45
1:H:178:MET:HE3	1:H:198:ASP:OD1	2.16	0.45
1:A:240:LYS:HA	1:A:240:LYS:HE2	1.98	0.45
1:A:150:TYR:CD1	1:A:150:TYR:C	2.90	0.45
1:B:172:PHE:O	1:B:172:PHE:CG	2.69	0.45
1:G:275:LYS:HD2	1:G:275:LYS:N	2.31	0.45
1:G:279:LEU:HD21	1:G:294:VAL:HG22	1.99	0.45
1:E:88:LEU:HD23	1:E:88:LEU:HA	1.57	0.45
1:D:95:ARG:CZ	1:E:253:LYS:CD	2.93	0.45
1:J:213:THR:HG21	1:J:293:LEU:CD2	2.44	0.45
1:A:169:GLU:CB	1:A:170:PRO:HD2	2.46	0.45
1:B:105:VAL:O	1:B:133:PRO:HD2	2.17	0.45
1:D:83:ARG:HD3	1:D:131:PHE:CD1	2.52	0.45
1:I:264:GLY:HA3	1:I:281:TYR:CZ	2.52	0.45
1:A:126:ASP:N	1:A:126:ASP:OD2	2.50	0.45
1:F:270:ASP:O	1:F:272:THR:N	2.50	0.45
1:G:273:THR:OG1	1:G:275:LYS:CE	2.65	0.45
1:E:130:ARG:HH21	1:E:150:TYR:HE1	1.65	0.45
1:F:84:ASP:HA	1:F:87:LEU:HD12	1.99	0.45
1:C:256:ARG:NH2	1:F:92:ASN:CG	2.71	0.45
1:A:282:GLU:OE2	1:A:283:PRO:HD2	2.16	0.45
1:E:275:LYS:HG3	1:E:275:LYS:H	1.55	0.44
1:B:254:ALA:O	1:B:258:ILE:HG23	2.17	0.44
1:B:159:PRO:O	1:B:163:GLU:HA	2.17	0.44
1:H:275:LYS:CB	1:H:275:LYS:HZ2	2.28	0.44
1:I:86:ALA:CB	1:I:131:PHE:HE2	2.30	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:ARG:HA	1:D:308:ARG:HE	1.81	0.44
1:A:94:LEU:HD21	1:A:100:LEU:O	2.17	0.44
1:F:88:LEU:HD23	1:F:88:LEU:HA	1.67	0.44
1:B:40:LYS:C	1:B:42:ALA:N	2.71	0.44
1:C:205:ASP:HB2	1:C:238:ILE:HD13	2.00	0.44
1:C:201:LEU:HD21	1:C:229:LEU:HD22	1.99	0.44
1:H:139:ASN:C	1:H:141:THR:N	2.71	0.44
1:B:123:PRO:O	1:B:124:ALA:HB3	2.17	0.44
1:H:212:ARG:HH22	1:I:235:LYS:NZ	2.15	0.44
1:D:185:ILE:HG13	1:D:193:GLY:C	2.38	0.44
1:G:215:ASP:HB2	1:G:299:GLU:CD	2.38	0.44
1:B:169:GLU:HB3	1:B:170:PRO:HD2	2.00	0.44
1:A:208:VAL:HG11	1:A:220:PHE:HA	1.99	0.44
1:J:212:ARG:HA	1:J:212:ARG:HD3	1.71	0.44
1:G:270:ASP:OD1	1:G:272:THR:HB	2.17	0.44
1:C:273:THR:O	1:C:275:LYS:N	2.47	0.44
1:H:150:TYR:HB3	1:H:155:TYR:OH	2.17	0.44
1:I:104:TYR:CE2	1:I:198:ASP:OD2	2.70	0.44
1:H:167:LEU:CD1	1:H:179:VAL:HG13	2.45	0.44
1:C:154:ASP:O	1:C:156:TYR:N	2.50	0.44
1:H:125:HIS:N	1:H:125:HIS:ND1	2.63	0.44
1:G:39:GLU:HA	1:G:40:LYS:CB	2.34	0.44
1:H:276:THR:OG1	1:H:297:LYS:HB3	2.18	0.44
1:H:132:VAL:N	1:H:133:PRO:HD3	2.32	0.44
1:D:120:THR:O	1:D:120:THR:CG2	2.65	0.44
1:D:104:TYR:CE2	1:D:196:GLY:C	2.91	0.44
1:F:193:GLY:C	1:F:194:ILE:CG2	2.85	0.44
1:A:177:PHE:HB3	1:A:201:LEU:HD12	1.99	0.44
1:E:135:TRP:CE2	1:E:144:VAL:HB	2.53	0.44
1:G:108:GLU:HB2	1:G:111:ALA:HB2	2.00	0.44
1:G:136:ASN:OD1	1:G:138:MET:HE2	2.17	0.44
1:J:91:GLU:OE1	1:J:135:TRP:CZ2	2.71	0.44
1:C:94:LEU:HD11	1:C:136:ASN:HA	1.99	0.44
1:B:105:VAL:HG12	1:B:133:PRO:CD	2.45	0.44
1:C:240:LYS:HA	1:C:240:LYS:CE	2.48	0.44
1:J:203:TYR:O	1:J:206:GLU:HB3	2.18	0.44
1:E:61:MET:SD	1:E:284:VAL:HG11	2.58	0.44
1:D:213:THR:HG21	1:D:293:LEU:HD22	2.00	0.44
1:I:167:LEU:HD12	1:I:167:LEU:C	2.38	0.44
1:G:43:TYR:O	1:G:46:SER:HB3	2.18	0.44
1:G:275:LYS:HD2	1:G:275:LYS:H	1.83	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ILE:HD11	1:C:98:PRO:HG3	2.00	0.44
1:J:213:THR:CG2	1:J:293:LEU:HD21	2.46	0.44
1:H:97:ASN:CB	1:H:100:LEU:HD12	2.47	0.44
1:G:158:LEU:HD23	1:G:158:LEU:HA	1.80	0.44
1:H:108:GLU:O	1:H:111:ALA:HB3	2.17	0.44
1:H:108:GLU:O	1:H:111:ALA:CB	2.65	0.44
1:C:215:ASP:HB2	1:C:299:GLU:OE1	2.18	0.44
1:A:216:THR:OG1	1:A:299:GLU:OE2	2.28	0.44
1:C:86:ALA:HB3	1:C:131:PHE:HZ	1.82	0.44
1:C:78:TYR:CE1	1:C:80:THR:HB	2.53	0.44
1:F:305:ALA:O	1:F:308:ARG:CB	2.66	0.44
1:I:272:THR:O	1:I:272:THR:HG22	2.18	0.44
1:B:53:TYR:HB3	1:B:291:PHE:CE1	2.52	0.44
1:J:203:TYR:CE2	1:J:207:VAL:HG21	2.52	0.44
1:H:293:LEU:HD23	1:H:293:LEU:HA	1.83	0.44
1:F:39:GLU:HA	1:F:40:LYS:HB2	0.64	0.44
1:J:39:GLU:HG2	1:J:40:LYS:H	1.82	0.44
1:D:266:LEU:O	1:D:278:ILE:HA	2.18	0.44
1:G:245:ASP:C	1:G:247:GLY:H	2.20	0.44
1:B:101:LEU:O	1:B:101:LEU:CD2	2.60	0.44
1:B:211:VAL:CG1	1:B:212:ARG:N	2.80	0.44
1:A:269:ALA:O	1:A:270:ASP:C	2.55	0.44
1:G:221:MET:CE	1:G:229:LEU:HD12	2.48	0.44
1:G:44:GLN:NE2	1:H:45:GLN:OE1	2.50	0.44
1:D:299:GLU:HA	1:D:299:GLU:OE1	2.17	0.44
1:B:244:TYR:C	1:B:246:PHE:H	2.22	0.44
1:A:209:SER:HB3	1:A:232:PRO:HA	1.99	0.44
1:J:218:TYR:CD2	1:J:232:PRO:HG2	2.53	0.44
1:F:222:VAL:CG1	1:F:258:ILE:HD12	2.48	0.44
1:D:57:PHE:CE2	1:D:208:VAL:HG22	2.53	0.44
1:B:61:MET:SD	1:B:284:VAL:HG11	2.58	0.44
1:I:207:VAL:O	1:I:210:LYS:HB2	2.17	0.44
1:B:57:PHE:HE2	1:B:207:VAL:HG12	1.83	0.44
1:F:193:GLY:C	1:F:194:ILE:HG23	2.39	0.44
1:I:98:PRO:HA	1:I:137:LYS:NZ	2.33	0.44
1:C:53:TYR:O	1:C:54:ALA:C	2.57	0.44
1:D:273:THR:OG1	1:D:275:LYS:N	2.50	0.43
1:C:173:TYR:CD2	1:C:178:MET:HE1	2.53	0.43
1:E:122:SER:HB2	1:E:123:PRO:HD2	2.00	0.43
1:G:105:VAL:HG13	1:G:107:PHE:CE1	2.52	0.43
1:J:282:GLU:OE2	1:J:283:PRO:HD2	2.17	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:PHE:O	1:E:61:MET:HG3	2.18	0.43
1:C:181:TYR:CD1	1:C:181:TYR:N	2.86	0.43
1:I:148:LEU:HD12	1:I:174:GLU:OE2	2.17	0.43
1:J:242:ASP:OD2	1:J:242:ASP:C	2.56	0.43
1:C:295:VAL:CG1	1:C:300:MET:HG3	2.48	0.43
1:J:244:TYR:HE2	1:J:252:GLU:HG2	1.83	0.43
1:C:272:THR:O	1:C:272:THR:CG2	2.64	0.43
1:J:231:HIS:ND1	1:J:232:PRO:N	2.65	0.43
1:G:119:TYR:O	1:G:121:ASN:N	2.49	0.43
1:H:132:VAL:O	1:H:132:VAL:CG2	2.56	0.43
1:B:148:LEU:C	1:B:149:HIS:CG	2.91	0.43
1:C:250:GLU:HB2	1:C:266:LEU:HD13	2.00	0.43
1:I:171:TYR:OH	1:I:180:SER:OG	2.30	0.43
1:H:68:ALA:O	1:H:69:ARG:C	2.56	0.43
1:J:166:VAL:HG12	1:J:167:LEU:N	2.33	0.43
1:J:207:VAL:O	1:J:210:LYS:HG3	2.17	0.43
1:J:279:LEU:HD22	1:J:292:VAL:HG11	1.99	0.43
1:A:253:LYS:HD3	1:C:95:ARG:NH2	2.34	0.43
1:B:79:GLU:O	1:B:80:THR:C	2.57	0.43
1:B:250:GLU:C	1:B:252:GLU:H	2.22	0.43
1:J:300:MET:N	1:J:301:LEU:HB3	2.33	0.43
1:A:135:TRP:CD2	1:A:144:VAL:HB	2.53	0.43
1:I:186:MET:SD	1:I:191:PHE:HB2	2.58	0.43
1:C:238:ILE:O	1:C:238:ILE:HG22	2.18	0.43
1:I:81:ALA:HA	1:I:112:PHE:CE2	2.54	0.43
1:H:131:PHE:CD1	1:H:133:PRO:HD3	2.53	0.43
1:F:148:LEU:HD12	1:F:174:GLU:CD	2.39	0.43
1:H:178:MET:CE	1:H:198:ASP:OD1	2.66	0.43
1:H:265:HIS:HA	1:H:279:LEU:O	2.18	0.43
1:C:273:THR:C	1:C:275:LYS:H	2.21	0.43
1:J:40:LYS:CG	1:J:41:LEU:H	2.32	0.43
1:B:201:LEU:HA	1:B:201:LEU:HD23	1.65	0.43
1:G:40:LYS:H	1:G:41:LEU:HB3	1.81	0.43
1:G:218:TYR:CE1	1:G:294:VAL:HG11	2.54	0.43
1:F:105:VAL:HG13	1:F:107:PHE:CE1	2.54	0.43
1:A:222:VAL:HG22	1:A:226:GLY:CA	2.47	0.43
1:J:298:GLU:C	1:J:301:LEU:HD23	2.38	0.43
1:E:119:TYR:O	1:E:120:THR:C	2.57	0.43
1:B:101:LEU:HD23	1:B:101:LEU:HA	1.57	0.43
1:I:86:ALA:CB	1:I:131:PHE:CE2	3.01	0.43
1:I:149:HIS:O	1:I:151:ASP:N	2.51	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:214:PHE:CE1	1:G:295:VAL:CG1	3.02	0.43
1:C:158:LEU:HB2	1:C:159:PRO:CD	2.49	0.43
1:F:167:LEU:HD11	1:F:179:VAL:HG13	1.99	0.43
1:I:88:LEU:HA	1:I:88:LEU:HD23	1.76	0.43
1:J:131:PHE:CD1	1:J:133:PRO:HD3	2.53	0.43
1:B:258:ILE:HG13	1:B:259:LYS:N	2.33	0.43
1:B:156:TYR:C	1:B:159:PRO:HD2	2.38	0.43
1:B:61:MET:HE1	1:B:284:VAL:HG11	2.00	0.43
1:D:307:LEU:O	1:D:308:ARG:C	2.56	0.43
1:B:139:ASN:C	1:B:141:THR:H	2.21	0.43
1:D:68:ALA:O	1:D:69:ARG:C	2.57	0.43
1:D:41:LEU:C	1:D:43:TYR:N	2.54	0.43
1:F:39:GLU:CA	1:F:40:LYS:CB	2.46	0.43
1:C:276:THR:O	1:C:297:LYS:HB3	2.19	0.43
1:H:250:GLU:HB3	1:H:266:LEU:HD11	1.99	0.43
1:J:177:PHE:HZ	1:J:240:LYS:HD2	1.80	0.43
1:C:208:VAL:HG11	1:C:230:SER:OG	2.18	0.43
1:C:170:PRO:HG2	1:C:227:VAL:HG11	2.00	0.43
1:I:148:LEU:O	1:I:149:HIS:HB2	2.19	0.43
1:H:110:ASP:OD1	1:H:114:GLY:HA2	2.19	0.43
1:A:212:ARG:HG3	1:A:217:GLY:O	2.18	0.43
1:D:296:PRO:O	1:D:299:GLU:HB2	2.19	0.43
1:C:130:ARG:HH21	1:C:150:TYR:HE1	1.66	0.43
1:I:83:ARG:HH12	1:I:125:HIS:CD2	2.36	0.43
1:D:79:GLU:C	1:D:81:ALA:H	2.21	0.43
1:H:75:MET:CE	1:H:105:VAL:HG21	2.48	0.43
1:B:110:ASP:N	1:B:116:ASP:OD2	2.49	0.43
1:G:253:LYS:HB3	1:I:95:ARG:NH1	2.32	0.43
1:I:169:GLU:HB3	1:I:170:PRO:HD2	2.01	0.43
1:D:148:LEU:HD12	1:D:148:LEU:HA	1.73	0.43
1:C:216:THR:OG1	1:C:299:GLU:OE2	2.26	0.43
1:A:171:TYR:CE2	1:A:173:TYR:HB2	2.53	0.43
1:B:249:GLU:HB2	1:B:250:GLU:OE2	2.18	0.43
1:G:77:SER:HB3	1:H:88:LEU:HB3	2.01	0.43
1:J:122:SER:CB	1:J:123:PRO:CD	2.91	0.43
1:B:151:ASP:O	1:B:152:SER:HB3	2.18	0.43
1:A:169:GLU:OE2	1:A:170:PRO:HD2	2.18	0.43
1:F:173:TYR:O	1:F:174:GLU:C	2.57	0.43
1:H:103:THR:C	1:H:104:TYR:CD2	2.93	0.43
1:C:132:VAL:N	1:C:133:PRO:HD3	2.34	0.42
1:E:245:ASP:C	1:E:247:GLY:H	2.23	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LEU:HD22	1:B:101:LEU:C	2.40	0.42
1:D:218:TYR:N	1:D:218:TYR:CD1	2.86	0.42
1:B:227:VAL:HA	1:B:242:ASP:HB3	2.01	0.42
1:B:94:LEU:HD13	1:B:137:LYS:HE3	2.01	0.42
1:A:206:GLU:O	1:A:210:LYS:HG2	2.19	0.42
1:I:101:LEU:HD23	1:I:101:LEU:HA	1.78	0.42
1:C:91:GLU:HG3	1:C:135:TRP:CE3	2.53	0.42
1:C:278:ILE:HG21	1:C:280:PHE:CE1	2.53	0.42
1:C:112:PHE:CD2	1:C:131:PHE:HD2	2.36	0.42
1:E:216:THR:OG1	1:E:299:GLU:OE2	2.36	0.42
1:F:120:THR:HG23	1:F:120:THR:O	2.19	0.42
1:A:78:TYR:CE2	1:A:81:ALA:N	2.87	0.42
1:H:41:LEU:HA	1:H:41:LEU:HD23	1.80	0.42
1:C:295:VAL:HA	1:C:296:PRO:HD3	1.79	0.42
1:C:153:SER:HB3	1:C:155:TYR:CD1	2.54	0.42
1:I:109:PRO:CA	1:I:130:ARG:HD3	2.49	0.42
1:A:104:TYR:HH	1:A:180:SER:HB3	1.84	0.42
1:J:234:HIS:O	1:J:235:LYS:C	2.57	0.42
1:B:72:SER:O	1:B:73:THR:C	2.57	0.42
1:G:245:ASP:O	1:G:247:GLY:CA	2.68	0.42
1:H:295:VAL:HA	1:H:296:PRO:HD3	1.83	0.42
1:C:246:PHE:HB2	1:C:251:LEU:HD13	2.01	0.42
1:E:240:LYS:HE2	1:E:240:LYS:CA	2.50	0.42
1:C:296:PRO:HB2	1:C:299:GLU:HG3	2.01	0.42
1:A:218:TYR:HD2	1:A:232:PRO:CG	2.32	0.42
1:A:231:HIS:HA	1:A:232:PRO:HD3	1.89	0.42
1:C:160:LYS:HG3	1:C:191:PHE:CD2	2.53	0.42
1:E:245:ASP:C	1:E:247:GLY:N	2.73	0.42
1:E:248:GLY:N	1:E:251:LEU:HD12	2.34	0.42
1:D:107:PHE:HB3	1:D:111:ALA:HB3	2.00	0.42
1:I:112:PHE:CE1	1:I:131:PHE:CD2	3.07	0.42
1:A:227:VAL:CG1	1:A:228:ILE:N	2.82	0.42
1:J:169:GLU:OE2	1:J:223:SER:OG	2.24	0.42
1:A:212:ARG:HB2	1:A:212:ARG:HE	1.53	0.42
1:G:171:TYR:N	1:G:171:TYR:CD1	2.88	0.42
1:D:167:LEU:HD13	1:D:181:TYR:CD2	2.54	0.42
1:D:298:GLU:CG	1:D:299:GLU:HB2	2.48	0.42
1:G:97:ASN:HB2	1:G:100:LEU:HD12	2.01	0.42
1:C:105:VAL:CG1	1:C:107:PHE:CE1	3.03	0.42
1:I:268:THR:OG1	1:I:269:ALA:N	2.53	0.42
1:F:104:TYR:HE1	1:F:198:ASP:OD2	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:PHE:CE1	1:A:175:GLY:O	2.72	0.42
1:C:90:LEU:HD13	1:C:104:TYR:HA	2.02	0.42
1:H:120:THR:O	1:H:120:THR:HG23	2.19	0.42
1:E:203:TYR:CE2	1:E:207:VAL:HG21	2.55	0.42
1:I:65:LEU:HG	1:I:69:ARG:HD2	2.02	0.42
1:I:130:ARG:NH2	1:I:150:TYR:CD1	2.88	0.42
1:J:104:TYR:N	1:J:104:TYR:CD2	2.87	0.42
1:B:213:THR:HG22	1:B:217:GLY:HA3	2.02	0.42
1:E:240:LYS:HA	1:E:240:LYS:CE	2.48	0.42
1:G:273:THR:OG1	1:G:275:LYS:CD	2.67	0.42
1:B:201:LEU:HD21	1:B:229:LEU:HD22	2.01	0.42
1:A:246:PHE:CD1	1:A:251:LEU:HD11	2.55	0.42
1:E:165:ASP:C	1:E:166:VAL:CG2	2.88	0.42
1:E:79:GLU:HB2	1:F:85:GLU:OE1	2.19	0.42
1:G:105:VAL:CG1	1:G:107:PHE:HE1	2.33	0.42
1:H:241:LYS:HD2	1:H:245:ASP:OD2	2.20	0.42
1:H:93:LEU:O	1:H:94:LEU:C	2.57	0.42
1:B:273:THR:HB	1:B:274:GLY:H	1.77	0.42
1:E:158:LEU:HA	1:E:158:LEU:HD23	1.35	0.42
1:I:139:ASN:N	1:I:139:ASN:OD1	2.52	0.42
1:I:241:LYS:HD3	1:I:241:LYS:HA	1.89	0.42
1:H:218:TYR:CD2	1:H:232:PRO:CG	3.03	0.42
1:B:306:ASP:C	1:B:308:ARG:N	2.72	0.42
1:J:40:LYS:O	1:J:43:TYR:N	2.46	0.42
1:A:222:VAL:CG2	1:A:227:VAL:O	2.66	0.42
1:I:115:LYS:O	1:I:116:ASP:C	2.57	0.42
1:J:86:ALA:O	1:J:89:ILE:HB	2.20	0.42
1:B:88:LEU:HA	1:B:88:LEU:HD23	1.68	0.42
1:B:245:ASP:N	1:B:245:ASP:OD2	2.52	0.42
1:E:201:LEU:HD23	1:E:201:LEU:HA	1.61	0.42
1:E:40:LYS:O	1:E:40:LYS:CD	2.67	0.42
1:H:233:THR:OG1	1:H:234:HIS:HD2	2.02	0.42
1:H:119:TYR:HB3	1:H:125:HIS:CD2	2.55	0.42
1:C:119:TYR:O	1:C:120:THR:C	2.58	0.42
1:G:89:ILE:CD1	1:H:74:THR:HG23	2.42	0.42
1:C:88:LEU:HD13	1:D:77:SER:HB3	2.02	0.42
1:F:305:ALA:O	1:F:308:ARG:HB3	2.20	0.42
1:I:130:ARG:NH2	1:I:150:TYR:HD1	2.17	0.42
1:G:128:THR:C	1:G:130:ARG:N	2.72	0.42
1:G:131:PHE:CD1	1:G:133:PRO:HD3	2.55	0.42
1:I:80:THR:O	1:I:82:ASP:N	2.53	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:TYR:CD1	1:E:171:TYR:N	2.88	0.42
1:D:251:LEU:HD23	1:D:266:LEU:HD12	2.01	0.41
1:C:231:HIS:ND1	1:C:232:PRO:N	2.68	0.41
1:E:130:ARG:O	1:E:132:VAL:HG13	2.20	0.41
1:H:75:MET:HE3	1:H:105:VAL:HG21	2.02	0.41
1:G:214:PHE:CE1	1:G:295:VAL:HG13	2.55	0.41
1:A:104:TYR:CD2	1:A:104:TYR:N	2.87	0.41
1:H:53:TYR:O	1:H:54:ALA:C	2.58	0.41
1:F:243:LEU:HA	1:F:243:LEU:HD23	1.82	0.41
1:E:285:GLU:O	1:E:285:GLU:HG2	2.19	0.41
1:E:156:TYR:CD2	1:E:156:TYR:C	2.93	0.41
1:J:298:GLU:N	1:J:301:LEU:CD2	2.70	0.41
1:B:156:TYR:O	1:B:159:PRO:HD2	2.21	0.41
1:H:42:ALA:C	1:H:300:MET:HE2	2.40	0.41
1:F:115:LYS:O	1:F:116:ASP:C	2.58	0.41
1:B:234:HIS:HB3	1:B:237:TRP:CD1	2.55	0.41
1:J:135:TRP:CE2	1:J:144:VAL:HB	2.56	0.41
1:E:276:THR:O	1:E:297:LYS:HB2	2.19	0.41
1:A:231:HIS:CG	1:A:232:PRO:CD	3.03	0.41
1:H:278:ILE:HD12	1:H:300:MET:SD	2.60	0.41
1:J:141:THR:O	1:J:141:THR:HG23	2.19	0.41
1:H:296:PRO:O	1:H:297:LYS:C	2.57	0.41
1:I:83:ARG:HG2	1:I:112:PHE:HE1	1.85	0.41
1:G:97:ASN:HA	1:G:98:PRO:HD2	1.69	0.41
1:I:168:THR:CG2	1:I:180:SER:HB2	2.50	0.41
1:B:131:PHE:C	1:B:132:VAL:HG13	2.40	0.41
1:G:104:TYR:N	1:G:104:TYR:CD2	2.88	0.41
1:E:123:PRO:O	1:E:124:ALA:CB	2.68	0.41
1:J:104:TYR:CE2	1:J:198:ASP:OD2	2.73	0.41
1:D:83:ARG:HG2	1:D:112:PHE:CE1	2.54	0.41
1:I:293:LEU:HD23	1:I:294:VAL:N	2.35	0.41
1:G:262:ILE:HD13	1:I:98:PRO:HG3	2.02	0.41
1:A:158:LEU:HA	1:A:158:LEU:HD23	1.80	0.41
1:B:249:GLU:C	1:B:251:LEU:H	2.18	0.41
1:D:123:PRO:O	1:D:124:ALA:HB3	2.20	0.41
1:H:138:MET:HB3	1:H:138:MET:HE3	1.83	0.41
1:D:171:TYR:OH	1:D:178:MET:HE3	2.20	0.41
1:G:108:GLU:O	1:G:111:ALA:CB	2.67	0.41
1:G:258:ILE:HG21	1:G:258:ILE:HD13	1.62	0.41
1:D:135:TRP:NE1	1:D:144:VAL:CG2	2.84	0.41
1:D:91:GLU:HB2	1:D:135:TRP:CD1	2.55	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:THR:HG23	1:B:269:ALA:N	2.35	0.41
1:G:154:ASP:O	1:G:155:TYR:C	2.58	0.41
1:H:97:ASN:HB2	1:H:100:LEU:HD12	2.03	0.41
1:E:156:TYR:CD2	1:E:156:TYR:O	2.73	0.41
1:E:104:TYR:OH	1:E:180:SER:HB3	2.20	0.41
1:D:244:TYR:CE2	1:D:252:GLU:HG2	2.55	0.41
1:A:298:GLU:O	1:A:299:GLU:C	2.59	0.41
1:A:244:TYR:CD2	1:A:252:GLU:CG	3.03	0.41
1:H:80:THR:O	1:H:81:ALA:C	2.57	0.41
1:C:250:GLU:HG2	1:C:251:LEU:N	2.35	0.41
1:G:106:ALA:O	1:G:193:GLY:HA3	2.21	0.41
1:A:122:SER:CB	1:A:123:PRO:HD2	2.50	0.41
1:E:101:LEU:CD1	1:E:178:MET:HE2	2.51	0.41
1:F:135:TRP:CE2	1:F:144:VAL:HB	2.55	0.41
1:C:122:SER:HA	1:C:123:PRO:HA	1.81	0.41
1:J:278:ILE:CD1	1:J:297:LYS:HD3	2.51	0.41
1:B:61:MET:HE2	1:B:284:VAL:HG11	2.01	0.41
1:A:112:PHE:CD1	1:A:131:PHE:CD2	3.09	0.41
1:I:237:TRP:O	1:I:238:ILE:C	2.57	0.41
1:A:101:LEU:O	1:A:101:LEU:CD2	2.67	0.41
1:C:223:SER:O	1:C:258:ILE:HD11	2.20	0.41
1:G:177:PHE:CE2	1:G:239:GLY:O	2.74	0.41
1:J:126:ASP:OD2	1:J:126:ASP:N	2.54	0.41
1:J:132:VAL:O	1:J:132:VAL:HG23	2.21	0.41
1:F:201:LEU:HD23	1:F:201:LEU:HA	1.65	0.41
1:H:132:VAL:N	1:H:133:PRO:CD	2.84	0.41
1:A:153:SER:HB3	1:A:155:TYR:CD1	2.56	0.41
1:D:231:HIS:NE2	1:D:237:TRP:HZ3	2.19	0.41
1:D:222:VAL:HG22	1:D:227:VAL:O	2.21	0.41
1:C:256:ARG:HG3	1:C:256:ARG:NH1	2.35	0.41
1:J:49:MET:HE2	1:J:53:TYR:HE1	1.85	0.41
1:C:270:ASP:HA	1:C:274:GLY:N	2.36	0.41
1:D:272:THR:CG2	1:D:273:THR:N	2.83	0.41
1:H:251:LEU:HD23	1:H:266:LEU:HD12	2.03	0.41
1:C:130:ARG:C	1:C:132:VAL:HG13	2.41	0.41
1:J:79:GLU:O	1:J:80:THR:C	2.58	0.41
1:D:231:HIS:CD2	1:D:237:TRP:CE3	3.09	0.41
1:H:298:GLU:HA	1:H:301:LEU:HB2	2.02	0.41
1:I:135:TRP:HZ3	1:I:142:ALA:O	2.03	0.41
1:F:103:THR:O	1:F:104:TYR:HB3	2.20	0.41
1:G:101:LEU:C	1:G:101:LEU:HD23	2.42	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:THR:C	1:A:273:THR:HG22	2.40	0.41
1:B:213:THR:HG22	1:B:217:GLY:C	2.41	0.41
1:A:167:LEU:HD11	1:A:179:VAL:CG1	2.50	0.41
1:H:172:PHE:CD1	1:H:177:PHE:CE2	3.08	0.41
1:E:268:THR:HG23	1:E:269:ALA:N	2.35	0.41
1:G:108:GLU:O	1:G:109:PRO:C	2.58	0.41
1:J:214:PHE:CE2	1:J:299:GLU:O	2.74	0.41
1:D:135:TRP:HZ3	1:D:142:ALA:O	2.04	0.41
1:J:81:ALA:HB1	1:J:113:ASP:HB3	2.02	0.41
1:G:222:VAL:HG22	1:G:227:VAL:O	2.21	0.41
1:C:240:LYS:HE2	1:C:240:LYS:CA	2.47	0.41
1:D:97:ASN:HA	1:D:98:PRO:HD2	1.84	0.41
1:C:63:ALA:O	1:C:66:ALA:HB3	2.20	0.41
1:I:172:PHE:O	1:I:172:PHE:CG	2.74	0.41
1:A:308:ARG:HA	1:A:308:ARG:HD3	1.60	0.40
1:B:40:LYS:O	1:B:41:LEU:HG	2.20	0.40
1:I:75:MET:N	1:I:75:MET:HE3	2.36	0.40
1:B:158:LEU:CB	1:B:159:PRO:HD3	2.51	0.40
1:C:106:ALA:HB2	1:C:147:LEU:HD12	2.03	0.40
1:D:231:HIS:ND1	1:D:232:PRO:CD	2.84	0.40
1:J:222:VAL:HG12	1:J:290:ALA:HB3	2.03	0.40
1:F:119:TYR:O	1:F:120:THR:C	2.60	0.40
1:H:222:VAL:CG1	1:H:290:ALA:HB3	2.51	0.40
1:G:128:THR:O	1:G:130:ARG:N	2.53	0.40
1:I:236:ASP:O	1:I:240:LYS:HG2	2.21	0.40
1:A:235:LYS:H	1:A:235:LYS:HG2	1.53	0.40
1:C:91:GLU:CD	1:C:135:TRP:CZ2	2.94	0.40
1:J:249:GLU:O	1:J:249:GLU:OE2	2.39	0.40
1:E:241:LYS:HD2	1:E:245:ASP:OD2	2.21	0.40
1:H:173:TYR:O	1:H:175:GLY:N	2.54	0.40
1:A:132:VAL:N	1:A:133:PRO:CD	2.85	0.40
1:I:185:ILE:HD11	1:I:194:ILE:C	2.42	0.40
1:G:112:PHE:CD1	1:G:131:PHE:CD2	3.10	0.40
1:G:153:SER:HB2	1:G:155:TYR:CD2	2.56	0.40
1:I:82:ASP:OD1	1:I:82:ASP:C	2.58	0.40
1:D:47:VAL:HG23	1:D:280:PHE:HE2	1.85	0.40
1:C:184:PRO:HB2	1:C:186:MET:CE	2.51	0.40
1:F:222:VAL:HG23	1:F:227:VAL:O	2.21	0.40
1:C:201:LEU:CD2	1:C:229:LEU:HD22	2.52	0.40
1:D:128:THR:O	1:D:129:GLY:C	2.59	0.40
1:D:243:LEU:HD23	1:D:243:LEU:HA	1.81	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:GLY:O	1:B:306:ASP:HB2	2.21	0.40
1:F:278:ILE:HD11	1:F:297:LYS:HD2	2.03	0.40
1:J:113:ASP:C	1:J:115:LYS:H	2.24	0.40
1:F:218:TYR:O	1:F:293:LEU:HD23	2.21	0.40
1:B:211:VAL:HG12	1:B:212:ARG:N	2.35	0.40
1:J:207:VAL:O	1:J:210:LYS:HG2	2.21	0.40
1:D:154:ASP:O	1:D:155:TYR:C	2.60	0.40
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.73	0.40
1:I:126:ASP:O	1:I:127:GLY:C	2.59	0.40
1:G:167:LEU:HD11	1:G:179:VAL:HG13	2.02	0.40
1:A:76:GLU:HG2	1:A:186:MET:O	2.21	0.40
1:H:63:ALA:O	1:H:66:ALA:HB3	2.21	0.40
1:D:302:ALA:CB	1:D:303:GLY:CA	2.98	0.40
1:H:123:PRO:O	1:H:124:ALA:CB	2.70	0.40
1:I:138:MET:HB3	1:I:138:MET:HE3	1.80	0.40
1:C:134:TYR:CE1	1:C:173:TYR:HE2	2.40	0.40
1:I:86:ALA:HB3	1:I:131:PHE:CZ	2.57	0.40
1:F:193:GLY:O	1:F:194:ILE:CG2	2.68	0.40
1:H:172:PHE:HD1	1:H:177:PHE:CD2	2.38	0.40
1:A:177:PHE:HB3	1:A:201:LEU:CD1	2.52	0.40
1:A:73:THR:CG2	1:B:93:LEU:HD23	2.52	0.40
1:E:101:LEU:HG	1:E:200:SER:HB3	2.04	0.40
1:G:169:GLU:OE2	1:G:225:SER:OG	2.38	0.40
1:F:282:GLU:HA	1:F:283:PRO:HD3	1.94	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	269/290 (93%)	230 (86%)	29 (11%)	10 (4%)	<b>4</b> <b>23</b>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	269/290 (93%)	209 (78%)	46 (17%)	14 (5%)	2	15
1	C	266/290 (92%)	221 (83%)	33 (12%)	12 (4%)	3	18
1	D	269/290 (93%)	224 (83%)	34 (13%)	11 (4%)	3	20
1	E	266/290 (92%)	221 (83%)	34 (13%)	11 (4%)	3	20
1	F	269/290 (93%)	231 (86%)	30 (11%)	8 (3%)	5	29
1	G	268/290 (92%)	225 (84%)	28 (10%)	15 (6%)	2	13
1	H	265/290 (91%)	219 (83%)	37 (14%)	9 (3%)	5	25
1	I	269/290 (93%)	217 (81%)	38 (14%)	14 (5%)	2	15
1	J	269/290 (93%)	222 (82%)	32 (12%)	15 (6%)	2	13
All	All	2679/2900 (92%)	2219 (83%)	341 (13%)	119 (4%)	3	18

All (119) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	GLU
1	A	299	GLU
1	B	120	THR
1	B	149	HIS
1	B	188	GLU
1	B	250	GLU
1	C	120	THR
1	C	121	ASN
1	C	248	GLY
1	C	270	ASP
1	C	273	THR
1	D	42	ALA
1	D	81	ALA
1	D	120	THR
1	D	121	ASN
1	D	302	ALA
1	E	43	TYR
1	E	44	GLN
1	E	248	GLY
1	F	43	TYR
1	F	44	GLN
1	G	81	ALA
1	G	121	ASN
1	G	246	PHE
1	G	272	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	273	THR
1	H	152	SER
1	H	248	GLY
1	I	81	ALA
1	I	248	GLY
1	I	307	LEU
1	J	41	LEU
1	J	152	SER
1	J	246	PHE
1	J	272	THR
1	J	301	LEU
1	A	140	GLY
1	A	155	TYR
1	A	306	ASP
1	B	41	LEU
1	B	127	GLY
1	B	152	SER
1	B	249	GLU
1	C	80	THR
1	C	127	GLY
1	C	140	GLY
1	C	188	GLU
1	D	140	GLY
1	D	152	SER
1	E	42	ALA
1	E	80	THR
1	E	140	GLY
1	F	140	GLY
1	F	248	GLY
1	G	44	GLN
1	G	140	GLY
1	G	271	PRO
1	G	307	LEU
1	H	127	GLY
1	H	140	GLY
1	H	238	ILE
1	I	120	THR
1	I	188	GLU
1	I	245	ASP
1	J	114	GLY
1	J	140	GLY
1	J	271	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	J	273	THR
1	A	40	LYS
1	A	243	LEU
1	B	128	THR
1	B	189	GLY
1	D	188	GLU
1	D	299	GLU
1	F	40	LYS
1	F	120	THR
1	F	124	ALA
1	G	188	GLU
1	G	274	GLY
1	H	120	THR
1	I	121	ASN
1	I	149	HIS
1	I	150	TYR
1	J	120	THR
1	J	211	VAL
1	J	250	GLU
1	J	306	ASP
1	B	254	ALA
1	B	288	ASP
1	D	41	LEU
1	E	120	THR
1	E	274	GLY
1	E	289	PHE
1	F	188	GLU
1	G	46	SER
1	G	80	THR
1	I	127	GLY
1	I	268	THR
1	J	274	GLY
1	A	152	SER
1	B	121	ASN
1	C	122	SER
1	C	217	GLY
1	H	137	LYS
1	I	80	THR
1	B	40	LYS
1	E	40	LYS
1	G	51	SER
1	I	140	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	I	254	ALA
1	J	155	TYR
1	A	271	PRO
1	G	175	GLY
1	H	109	PRO
1	D	129	GLY
1	C	238	ILE
1	A	109	PRO
1	E	89	ILE
1	H	122	SER

### 5.3.2 Protein sidechains [i](#)

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	227/246 (92%)	197 (87%)	30 (13%)	5	22
1	B	227/246 (92%)	194 (86%)	33 (14%)	4	18
1	C	223/246 (91%)	187 (84%)	36 (16%)	3	14
1	D	227/246 (92%)	194 (86%)	33 (14%)	4	18
1	E	224/246 (91%)	193 (86%)	31 (14%)	4	20
1	F	227/246 (92%)	202 (89%)	25 (11%)	8	30
1	G	226/246 (92%)	192 (85%)	34 (15%)	3	17
1	H	223/246 (91%)	189 (85%)	34 (15%)	3	16
1	I	227/246 (92%)	198 (87%)	29 (13%)	5	23
1	J	227/246 (92%)	195 (86%)	32 (14%)	4	19
All	All	2258/2460 (92%)	1941 (86%)	317 (14%)	4	19

All (317) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	41	LEU
1	A	60	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	88	LEU
1	A	94	LEU
1	A	101	LEU
1	A	105	VAL
1	A	138	MET
1	A	139	ASN
1	A	144	VAL
1	A	150	TYR
1	A	153	SER
1	A	171	TYR
1	A	176	VAL
1	A	179	VAL
1	A	202	GLU
1	A	207	VAL
1	A	212	ARG
1	A	216	THR
1	A	218	TYR
1	A	221	MET
1	A	236	ASP
1	A	246	PHE
1	A	258	ILE
1	A	268	THR
1	A	272	THR
1	A	273	THR
1	A	275	LYS
1	A	293	LEU
1	A	308	ARG
1	B	39	GLU
1	B	40	LYS
1	B	41	LEU
1	B	49	MET
1	B	74	THR
1	B	88	LEU
1	B	101	LEU
1	B	105	VAL
1	B	118	GLU
1	B	122	SER
1	B	128	THR
1	B	150	TYR
1	B	154	ASP
1	B	157	GLN
1	B	176	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	179	VAL
1	B	182	VAL
1	B	185	ILE
1	B	191	PHE
1	B	210	LYS
1	B	212	ARG
1	B	234	HIS
1	B	236	ASP
1	B	240	LYS
1	B	245	ASP
1	B	256	ARG
1	B	258	ILE
1	B	266	LEU
1	B	268	THR
1	B	273	THR
1	B	276	THR
1	B	300	MET
1	B	307	LEU
1	C	39	GLU
1	C	44	GLN
1	C	45	GLN
1	C	61	MET
1	C	65	LEU
1	C	88	LEU
1	C	94	LEU
1	C	101	LEU
1	C	121	ASN
1	C	132	VAL
1	C	136	ASN
1	C	138	MET
1	C	139	ASN
1	C	151	ASP
1	C	153	SER
1	C	171	TYR
1	C	174	GLU
1	C	179	VAL
1	C	181	TYR
1	C	183	SER
1	C	190	GLU
1	C	212	ARG
1	C	213	THR
1	C	228	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	236	ASP
1	C	240	LYS
1	C	256	ARG
1	C	258	ILE
1	C	267	GLU
1	C	273	THR
1	C	275	LYS
1	C	276	THR
1	C	277	VAL
1	C	295	VAL
1	C	300	MET
1	C	306	ASP
1	D	39	GLU
1	D	41	LEU
1	D	44	GLN
1	D	51	SER
1	D	52	ASN
1	D	88	LEU
1	D	94	LEU
1	D	101	LEU
1	D	136	ASN
1	D	141	THR
1	D	148	LEU
1	D	150	TYR
1	D	153	SER
1	D	154	ASP
1	D	163	GLU
1	D	176	VAL
1	D	179	VAL
1	D	180	SER
1	D	202	GLU
1	D	210	LYS
1	D	212	ARG
1	D	218	TYR
1	D	221	MET
1	D	222	VAL
1	D	249	GLU
1	D	250	GLU
1	D	251	LEU
1	D	258	ILE
1	D	272	THR
1	D	273	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	275	LYS
1	D	308	ARG
1	D	309	GLU
1	E	39	GLU
1	E	77	SER
1	E	80	THR
1	E	83	ARG
1	E	88	LEU
1	E	94	LEU
1	E	101	LEU
1	E	105	VAL
1	E	120	THR
1	E	122	SER
1	E	132	VAL
1	E	152	SER
1	E	174	GLU
1	E	176	VAL
1	E	179	VAL
1	E	185	ILE
1	E	216	THR
1	E	221	MET
1	E	230	SER
1	E	236	ASP
1	E	240	LYS
1	E	256	ARG
1	E	258	ILE
1	E	266	LEU
1	E	268	THR
1	E	275	LYS
1	E	278	ILE
1	E	286	THR
1	E	293	LEU
1	E	298	GLU
1	E	301	LEU
1	F	41	LEU
1	F	46	SER
1	F	60	ASP
1	F	77	SER
1	F	85	GLU
1	F	88	LEU
1	F	94	LEU
1	F	95	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	101	LEU
1	F	105	VAL
1	F	138	MET
1	F	152	SER
1	F	179	VAL
1	F	212	ARG
1	F	221	MET
1	F	240	LYS
1	F	250	GLU
1	F	258	ILE
1	F	266	LEU
1	F	268	THR
1	F	275	LYS
1	F	286	THR
1	F	293	LEU
1	F	304	VAL
1	F	308	ARG
1	G	39	GLU
1	G	41	LEU
1	G	46	SER
1	G	51	SER
1	G	52	ASN
1	G	88	LEU
1	G	94	LEU
1	G	101	LEU
1	G	120	THR
1	G	122	SER
1	G	130	ARG
1	G	136	ASN
1	G	144	VAL
1	G	153	SER
1	G	154	ASP
1	G	171	TYR
1	G	179	VAL
1	G	180	SER
1	G	185	ILE
1	G	201	LEU
1	G	206	GLU
1	G	210	LYS
1	G	212	ARG
1	G	213	THR
1	G	221	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	222	VAL
1	G	236	ASP
1	G	246	PHE
1	G	251	LEU
1	G	258	ILE
1	G	266	LEU
1	G	273	THR
1	G	275	LYS
1	G	293	LEU
1	H	39	GLU
1	H	44	GLN
1	H	45	GLN
1	H	61	MET
1	H	83	ARG
1	H	88	LEU
1	H	94	LEU
1	H	101	LEU
1	H	109	PRO
1	H	120	THR
1	H	122	SER
1	H	125	HIS
1	H	132	VAL
1	H	139	ASN
1	H	174	GLU
1	H	179	VAL
1	H	182	VAL
1	H	185	ILE
1	H	188	GLU
1	H	208	VAL
1	H	210	LYS
1	H	216	THR
1	H	221	MET
1	H	222	VAL
1	H	225	SER
1	H	240	LYS
1	H	258	ILE
1	H	268	THR
1	H	273	THR
1	H	275	LYS
1	H	276	THR
1	H	277	VAL
1	H	295	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	301	LEU
1	I	39	GLU
1	I	88	LEU
1	I	101	LEU
1	I	105	VAL
1	I	121	ASN
1	I	138	MET
1	I	139	ASN
1	I	141	THR
1	I	150	TYR
1	I	153	SER
1	I	154	ASP
1	I	167	LEU
1	I	168	THR
1	I	174	GLU
1	I	176	VAL
1	I	185	ILE
1	I	191	PHE
1	I	210	LYS
1	I	236	ASP
1	I	245	ASP
1	I	253	LYS
1	I	258	ILE
1	I	266	LEU
1	I	268	THR
1	I	276	THR
1	I	298	GLU
1	I	306	ASP
1	I	308	ARG
1	I	309	GLU
1	J	39	GLU
1	J	41	LEU
1	J	62	LYS
1	J	79	GLU
1	J	88	LEU
1	J	101	LEU
1	J	120	THR
1	J	136	ASN
1	J	139	ASN
1	J	153	SER
1	J	167	LEU
1	J	171	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	J	179	VAL
1	J	212	ARG
1	J	216	THR
1	J	218	TYR
1	J	221	MET
1	J	222	VAL
1	J	236	ASP
1	J	240	LYS
1	J	246	PHE
1	J	249	GLU
1	J	257	ASP
1	J	258	ILE
1	J	268	THR
1	J	272	THR
1	J	273	THR
1	J	275	LYS
1	J	293	LEU
1	J	300	MET
1	J	301	LEU
1	J	309	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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



There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	271/290 (93%)	0.33	4 (1%) 76 49	57, 74, 97, 127	0
1	B	271/290 (93%)	0.33	5 (1%) 71 43	62, 80, 102, 115	0
1	C	268/290 (92%)	0.31	5 (1%) 70 41	50, 70, 100, 113	0
1	D	271/290 (93%)	0.31	4 (1%) 76 49	20, 71, 97, 113	0
1	E	268/290 (92%)	0.31	4 (1%) 76 49	43, 66, 98, 119	0
1	F	271/290 (93%)	0.29	3 (1%) 82 58	42, 67, 96, 130	0
1	G	270/290 (93%)	0.33	4 (1%) 76 49	48, 71, 94, 107	0
1	H	267/290 (92%)	0.30	6 (2%) 65 35	51, 70, 97, 108	0
1	I	271/290 (93%)	0.33	6 (2%) 65 35	62, 80, 103, 113	0
1	J	271/290 (93%)	0.35	4 (1%) 76 49	58, 74, 97, 123	0
All	All	2699/2900 (93%)	0.32	45 (1%) 73 45	20, 73, 99, 130	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	305	ALA	4.4
1	I	251	LEU	3.6
1	A	293	LEU	3.2
1	I	140	GLY	3.1
1	B	147	LEU	2.8
1	C	240	LYS	2.8
1	E	246	PHE	2.8
1	G	57	PHE	2.7
1	E	52	ASN	2.6
1	D	293	LEU	2.5
1	F	57	PHE	2.5
1	C	40	LYS	2.5
1	J	243	LEU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	173	TYR	2.5
1	G	268	THR	2.4
1	H	41	LEU	2.4
1	H	150	TYR	2.4
1	B	189	GLY	2.3
1	D	121	ASN	2.3
1	I	243	LEU	2.3
1	C	155	TYR	2.3
1	J	213	THR	2.3
1	H	215	ASP	2.3
1	D	217	GLY	2.3
1	I	173	TYR	2.3
1	E	57	PHE	2.2
1	C	304	VAL	2.2
1	H	172	PHE	2.2
1	J	214	PHE	2.2
1	A	258	ILE	2.2
1	F	172	PHE	2.2
1	B	258	ILE	2.2
1	F	48	GLU	2.2
1	H	216	THR	2.2
1	I	106	ALA	2.1
1	E	306	ASP	2.1
1	B	156	TYR	2.1
1	D	57	PHE	2.1
1	G	293	LEU	2.1
1	J	244	TYR	2.1
1	A	44	GLN	2.1
1	G	241	LYS	2.1
1	A	243	LEU	2.1
1	I	258	ILE	2.0
1	C	266	LEU	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	K	B	10	1/1	0.89	0.38	-	130,130,130,130	0
2	K	A	1	1/1	0.94	0.37	-	91,91,91,91	0
2	K	D	5	1/1	0.92	0.34	-	131,131,131,131	0
2	K	G	4	1/1	0.94	0.42	-	122,122,122,122	0
2	K	I	9	1/1	0.90	0.35	-	113,113,113,113	0
2	K	C	3	1/1	0.77	0.41	-	112,112,112,112	0
2	K	F	8	1/1	0.90	0.40	-	107,107,107,107	0
2	K	J	2	1/1	0.91	0.40	-	85,85,85,85	0
2	K	H	7	1/1	0.66	0.42	-	119,119,119,119	0
2	K	E	6	1/1	0.74	0.27	-	104,104,104,104	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.