



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:17 pm BST

PDB ID : 1NIK  
Title : Wild Type RNA Polymerase II  
Authors : Bushnell, D.A.; Kornberg, R.D.  
Deposited on : 2002-12-24  
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

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

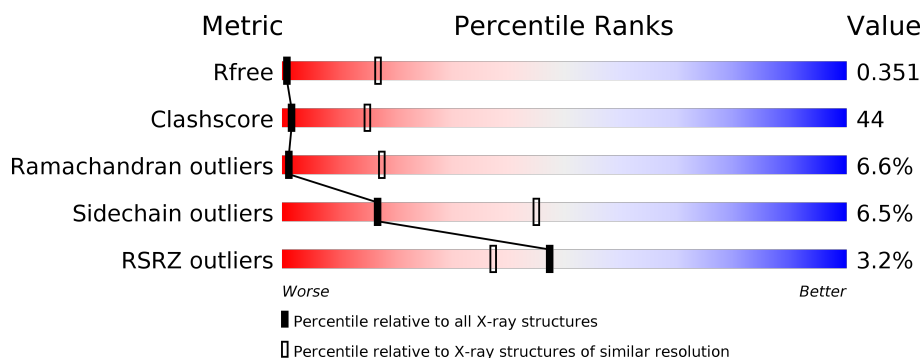
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.10 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))
$R_{free}$	130704	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

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

Mol	Chain	Length	Quality of chain
1	A	1733	<div> <div>2%</div> <div> <div></div> <div>32%</div> <div>40%</div> <div>7%</div> <div>20%</div> </div> </div>
2	B	1224	<div> <div>2%</div> <div> <div></div> <div>32%</div> <div>51%</div> <div>7%</div> <div>10%</div> </div> </div>
3	C	318	<div> <div>2%</div> <div> <div></div> <div>37%</div> <div>40%</div> <div>7%</div> <div>16%</div> </div> </div>
4	D	161	<div> <div></div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>
5	E	215	<div> <div>4%</div> <div> <div></div> <div>42%</div> <div>55%</div> </div> </div>
6	F	155	<div> <div></div> <div> <div></div> <div>18%</div> <div>32%</div> <div>46%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	G	170	<div><div></div><div>95%</div><div>5%</div></div>
8	H	146	<div><div>5%</div><div>30%</div><div>52%</div><div>9%</div><div>9%</div></div>
9	I	122	<div><div>13%</div><div>35%</div><div>51%</div><div>11%</div><div>••</div></div>
10	J	70	<div><div>4%</div><div>31%</div><div>51%</div><div>9%</div><div>•</div><div>7%</div></div>
11	K	120	<div><div>2%</div><div>41%</div><div>50%</div><div>•</div><div>5%</div></div>
12	L	70	<div><div>4%</div><div>17%</div><div>33%</div><div>13%</div><div>•</div><div>34%</div></div>

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 28295 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 RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1388	Total	C	N	O	S	0	0	7
			10864	6858	1899	2046	61			

- Molecule 2 is a protein called ORF YOR151c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1097	Total	C	N	O	S	0	0	0
			8721	5526	1523	1618	54			

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	D	153	Total C 153 153	0	0	153

- Molecule 5 is a protein called DNA-directed RNA polymerase II, chain RPB5.

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
7	G	170	Total	C	0	0	170
			170	170			

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit RPB8.

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

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

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II, chain RPB10.

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

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

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II, chain RPB12.

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

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total	Zn	0	0
			1	1		
13	A	2	Total	Zn	0	0
			2	2		

*Continued on next page...*

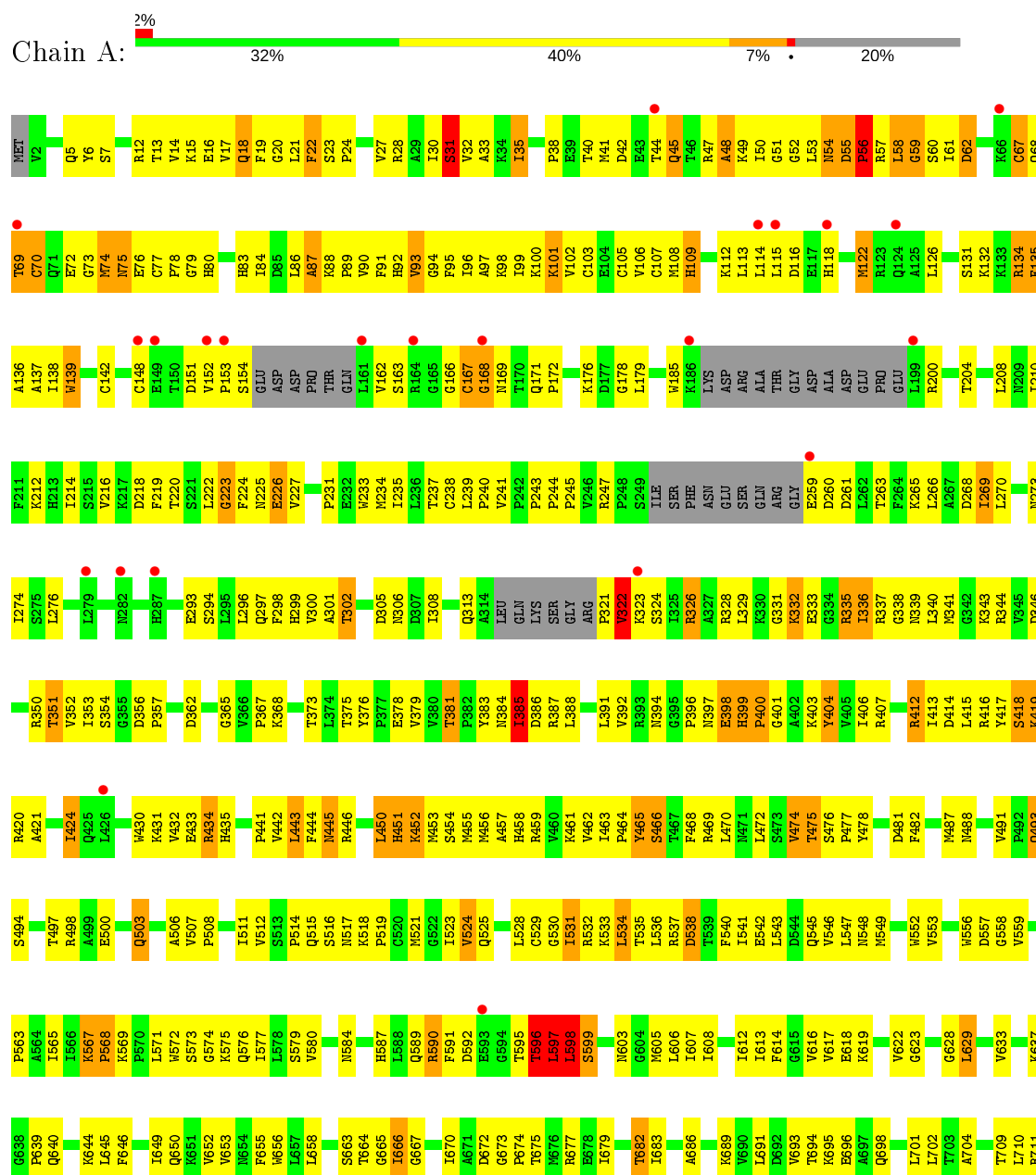
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	1	Total 1	Zn 1	0	0
13	J	1	Total 1	Zn 1	0	0
13	I	2	Total 2	Zn 2	0	0

### 3 Residue-property plots

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

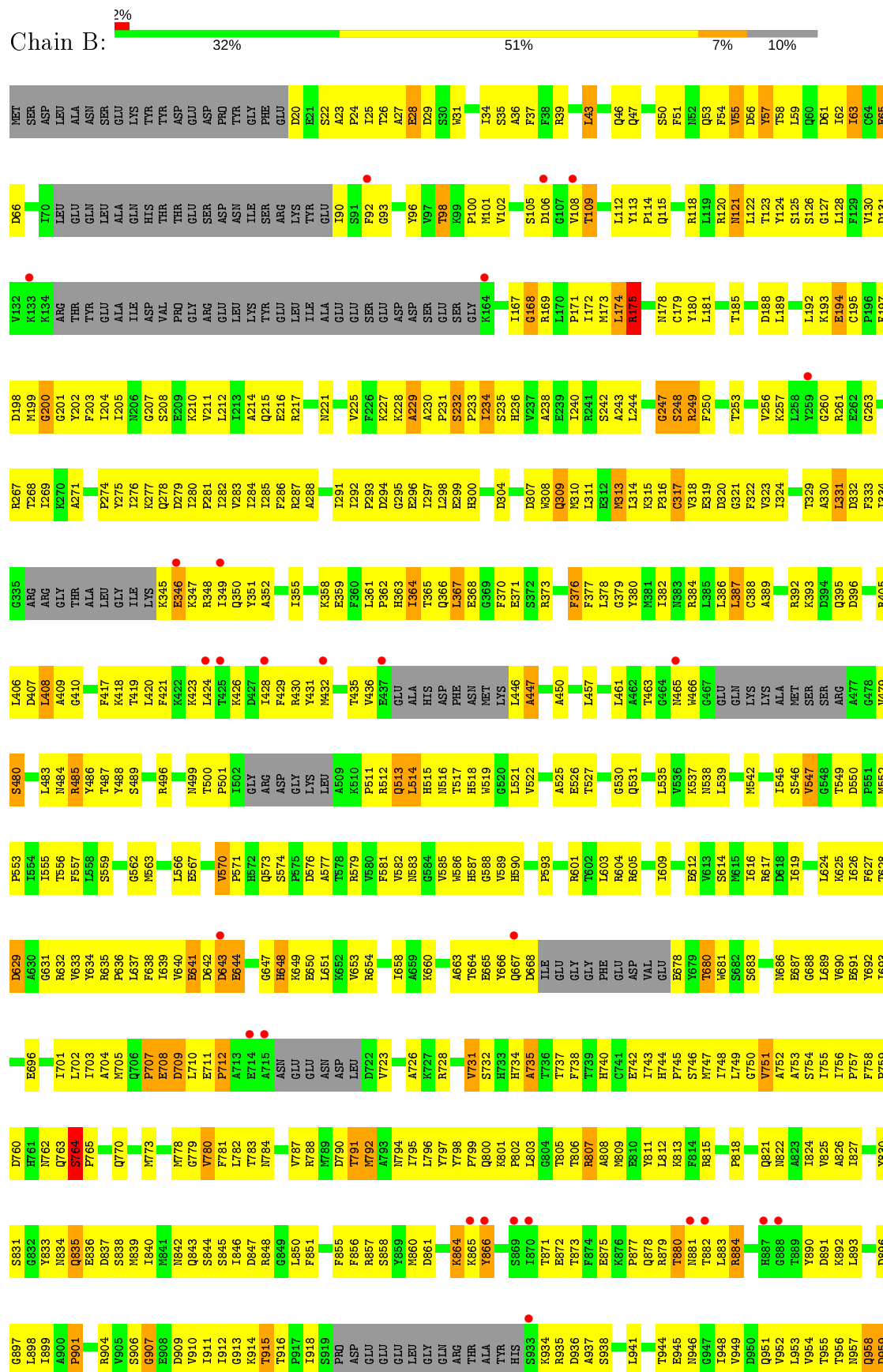
#### • Molecule 1: RPB1

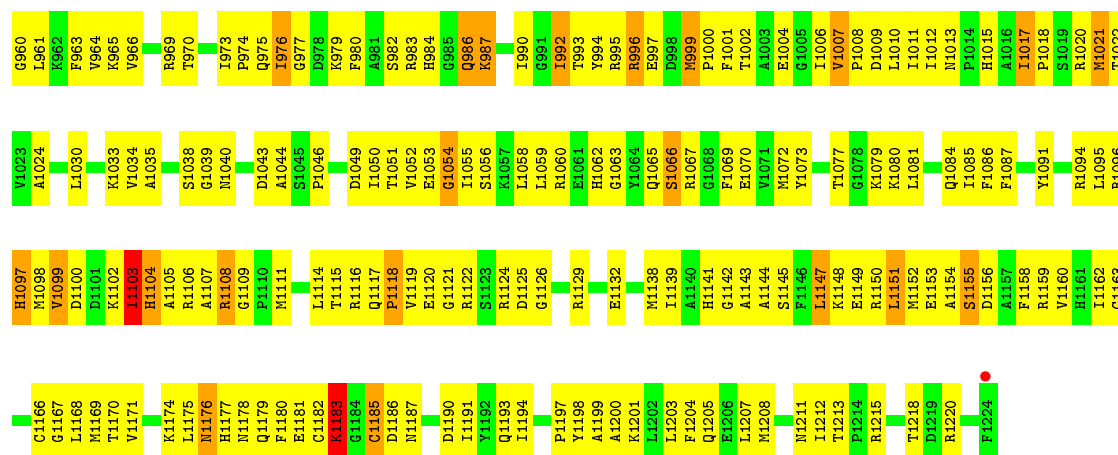




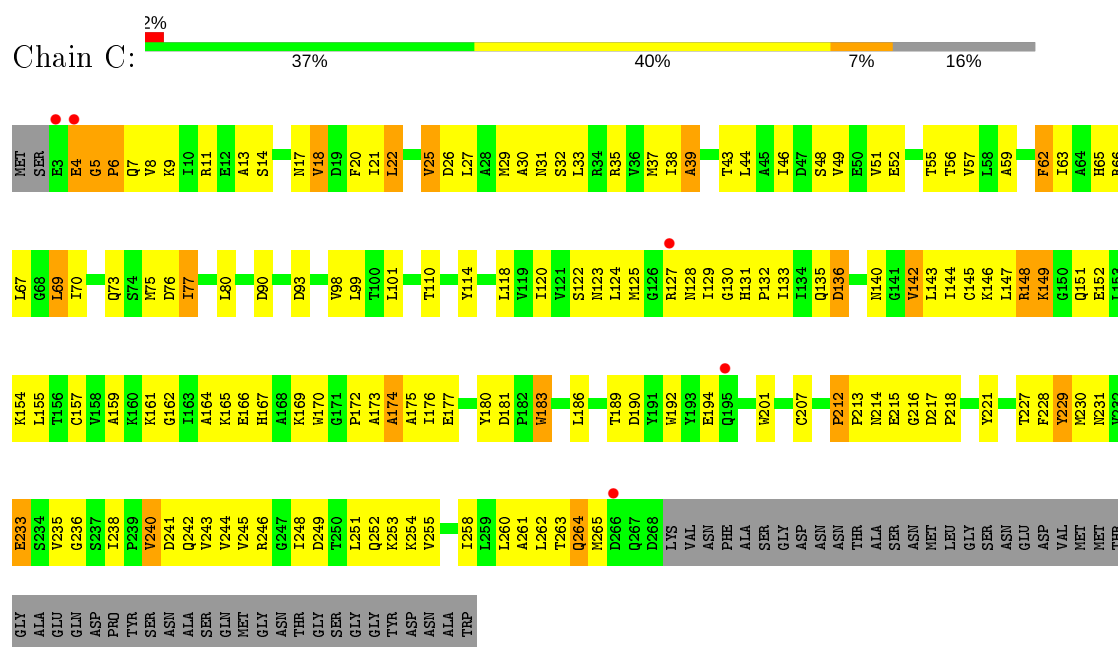


- Molecule 2: ORF YOR151c

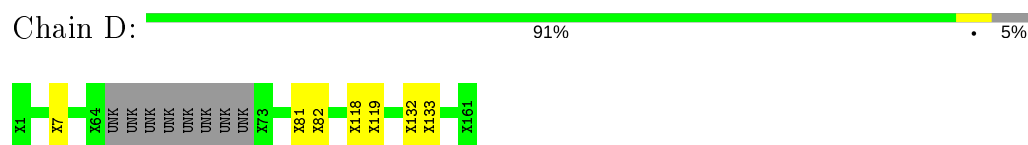




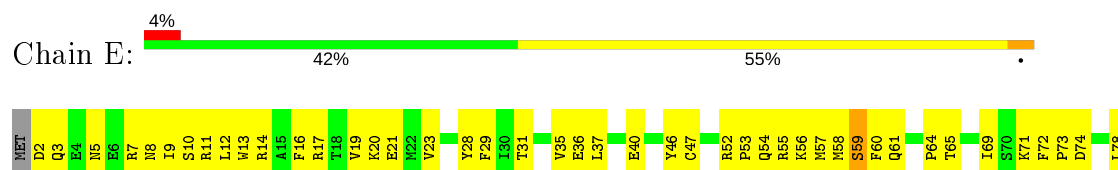
- Molecule 3: DNA-directed RNA polymerase II, chain RPB3

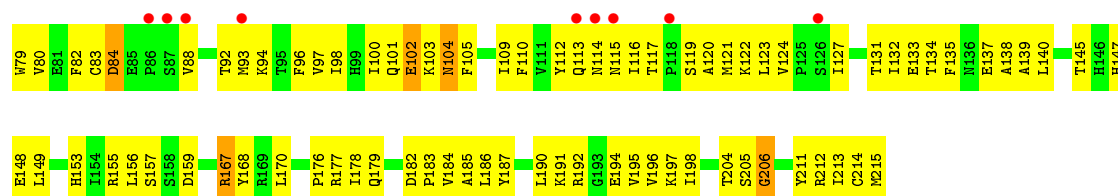


- Molecule 4: DNA-directed RNA polymerase II, chain RPB4

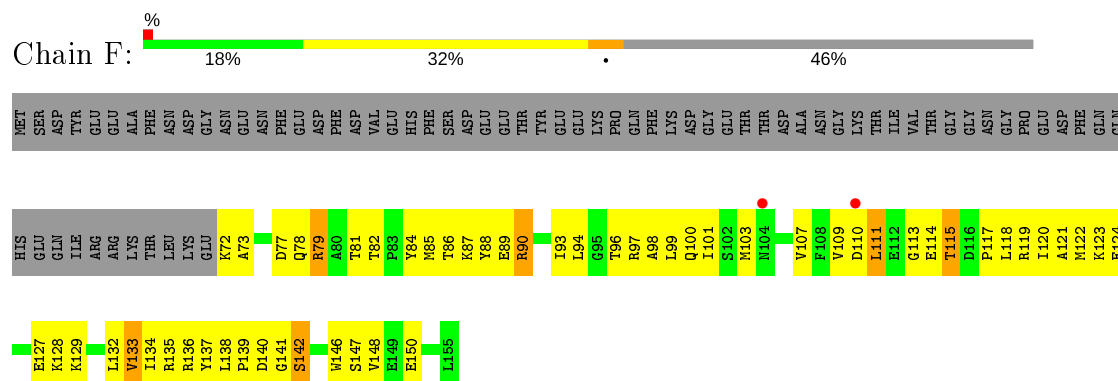


- Molecule 5: DNA-directed RNA polymerase II, chain RPB5

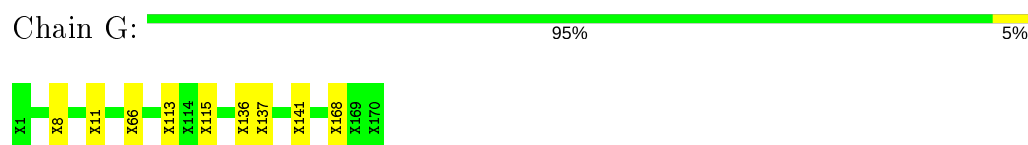




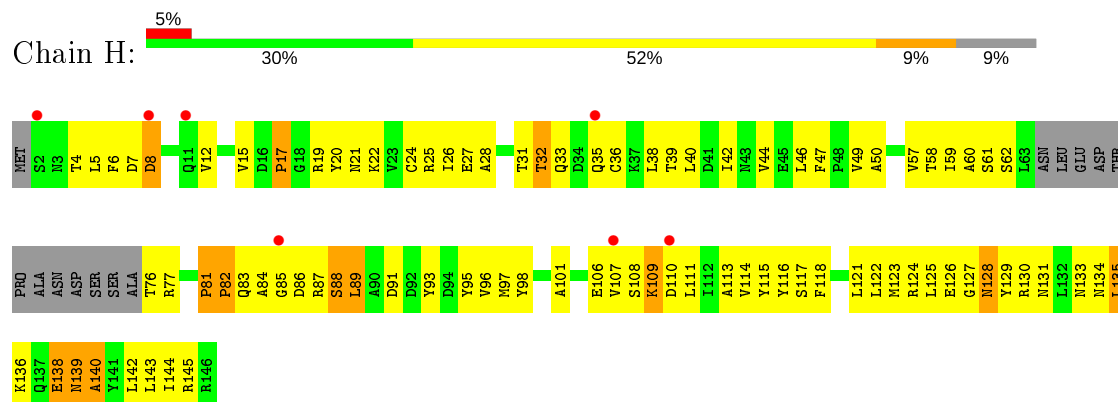
- Molecule 6: DNA-directed RNA polymerase I, II and III 23 kDa polypeptide



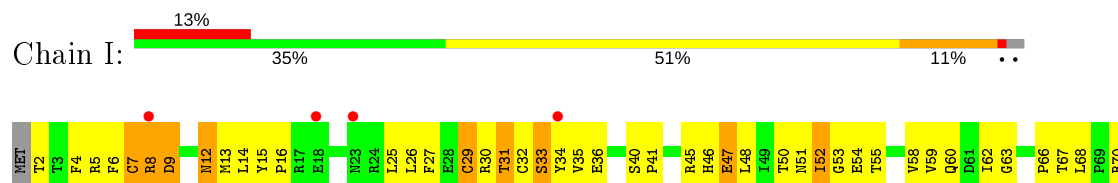
- Molecule 7: DNA-directed RNA polymerase II, chain RPB7



- Molecule 8: DNA-directed RNA polymerase subunit RPB8

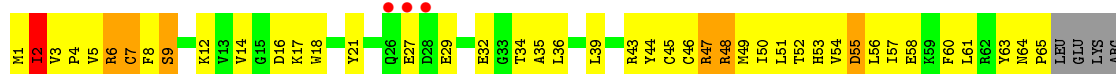


- Molecule 9: DNA-directed RNA polymerase II, chain RPB9



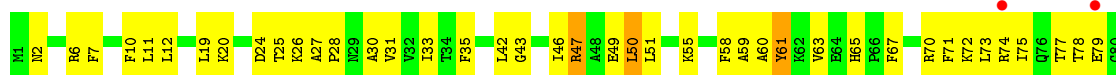


- Molecule 10: DNA-directed RNA polymerase II, chain RPB10

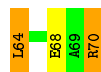


ASP

- Molecule 11: DNA-directed RNA polymerase II, chain RPB11



- Molecule 12: DNA-directed RNA polymerase II, chain RPB12



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	224.10Å 394.46Å 284.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 4.10 39.97 – 4.11	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-4.10) 86.4 (39.97-4.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 4.13Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.334 , 0.360 0.330 , 0.351	Depositor DCC
$R_{free}$ test set	3272 reflections (3.38%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	114.0	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 168.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.044 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.047 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.78	EDS
Total number of atoms	28295	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	194.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.41	0/11048	0.71	6/14936 (0.0%)
2	B	0.46	0/8891	0.71	1/11990 (0.0%)
3	C	0.48	0/2133	0.76	2/2891 (0.1%)
5	E	0.37	0/1788	0.65	0/2406
6	F	0.40	0/691	0.64	0/933
8	H	0.40	0/1086	0.73	0/1470
9	I	0.48	0/989	0.76	1/1331 (0.1%)
10	J	0.53	0/541	0.78	0/727
11	K	0.46	0/937	0.68	0/1265
12	L	0.49	0/366	0.78	0/485
All	All	0.44	0/28470	0.71	10/38434 (0.0%)

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

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1392	SER	N-CA-C	6.34	128.13	111.00
3	C	39	ALA	N-CA-C	6.06	127.35	111.00
1	A	398	GLU	N-CA-C	-5.77	95.43	111.00
3	C	183	TRP	N-CA-C	-5.61	95.86	111.00
2	B	647	GLY	N-CA-C	5.22	126.15	113.10
1	A	1403	GLU	N-CA-C	5.22	125.08	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	750	GLY	N-CA-C	-5.17	100.18	113.10
9	I	75	CYS	N-CA-C	-5.13	97.14	111.00
1	A	452	LYS	N-CA-C	-5.07	97.32	111.00
1	A	466	SER	N-CA-C	5.03	124.59	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	811	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10864	0	10959	1032	1
2	B	8721	0	8746	900	0
3	C	2095	0	2052	162	1
4	D	153	0	0	4	0
5	E	1752	0	1776	129	0
6	F	679	0	701	66	0
7	G	170	0	0	5	0
8	H	1068	0	1040	134	0
9	I	971	0	933	101	0
10	J	532	0	544	77	0
11	K	919	0	929	84	0
12	L	364	0	390	50	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	1	0
13	J	1	0	0	1	0
All	All	28295	0	28070	2499	1

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 44.

All (2499) 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)
4:D:132:UNK:CA	4:D:133:UNK:CA	2.01	1.36
12:L:60:ARG:HG3	12:L:61:THR:H	1.05	1.17
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.18	1.15
9:I:111:THR:HG22	9:I:113:ASP:H	1.05	1.14
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.65	1.11
1:A:855:THR:HG21	1:A:857:ARG:HE	1.12	1.10
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.33	1.08
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.27	1.08
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.00	1.08
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.33	1.07
1:A:704:ALA:HB2	1:A:710:LEU:HG	1.34	1.07
2:B:512:ARG:HH21	2:B:535:LEU:HD11	1.17	1.06
2:B:708:GLU:HG3	2:B:709:ASP:H	1.17	1.06
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.18	1.05
2:B:345:LYS:HA	2:B:348:ARG:HE	1.11	1.05
2:B:570:VAL:HB	2:B:573:GLN:HB3	1.36	1.05
6:F:81:THR:HG21	6:F:136:ARG:HD3	1.38	1.04
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.40	1.03
1:A:1329:THR:HG22	1:A:1331:SER:H	1.16	1.03
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.40	1.02
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.38	1.02
2:B:1159:ARG:HE	2:B:1193:GLN:NE2	1.56	1.02
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.39	1.02
2:B:1159:ARG:NE	2:B:1193:GLN:HE21	1.57	1.02
1:A:913:LEU:HD12	1:A:914:GLU:H	1.25	1.01
3:C:80:LEU:HD22	3:C:129:ILE:HD11	1.41	1.00
1:A:567:LYS:CB	1:A:568:PRO:HD2	1.91	1.00
2:B:977:GLY:HA3	2:B:1099:VAL:HG21	1.41	0.99
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.44	0.99
1:A:567:LYS:HB3	8:H:96:VAL:H	1.26	0.99
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.22	0.98
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.45	0.98
1:A:244:PRO:HG2	1:A:245:PRO:HD3	1.46	0.98
11:K:113:THR:O	11:K:114:LEU:HB2	1.60	0.97
2:B:842:ASN:ND2	2:B:845:SER:H	1.62	0.97
9:I:7:CYS:HB2	9:I:14:LEU:HD21	1.47	0.97
2:B:1100:ASP:HA	2:B:1103:ILE:HD11	1.46	0.96
3:C:167:HIS:CD2	3:C:169:LYS:H	1.83	0.96
2:B:955:THR:HG22	2:B:956:THR:H	1.31	0.96
2:B:392:ARG:HH21	9:I:52:ILE:HD11	1.30	0.96
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.47	0.95

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:LEU:O	2:B:175:ARG:HB2	1.64	0.95
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.01	0.95
2:B:1051:THR:HG22	2:B:1053:GLU:N	1.81	0.95
3:C:56:THR:HG22	3:C:57:VAL:H	1.28	0.94
2:B:737:THR:HG21	9:I:66:PRO:O	1.68	0.94
1:A:1399:ARG:HB3	1:A:1408:ILE:HD13	1.50	0.94
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.47	0.94
1:A:783:THR:HG22	1:A:784:LEU:HG	1.49	0.93
3:C:73:GLN:HE21	3:C:75:MET:H	1.14	0.93
1:A:1281:ARG:HD2	1:A:1309:ASP:OD2	1.68	0.93
2:B:1002:THR:HG22	2:B:1006:ILE:N	1.84	0.92
2:B:1159:ARG:HE	2:B:1193:GLN:HE21	0.93	0.92
1:A:1116:LEU:HD12	1:A:1329:THR:OG1	1.67	0.92
1:A:1445:ILE:O	1:A:1446:ASP:CA	2.16	0.92
2:B:824:ILE:HG12	10:J:48:ARG:HH12	1.32	0.92
5:E:5:ASN:HD21	5:E:52:ARG:HG2	1.35	0.92
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.33	0.92
12:L:60:ARG:HG3	12:L:61:THR:N	1.85	0.92
2:B:955:THR:HG22	2:B:956:THR:N	1.86	0.91
9:I:75:CYS:HG	13:I:204:ZN:ZN	0.68	0.91
1:A:1435:PRO:HA	1:A:1439:GLY:O	1.69	0.91
2:B:1077:THR:HG22	2:B:1079:LYS:H	1.35	0.90
1:A:590:ARG:NH1	1:A:590:ARG:HG3	1.86	0.90
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	1.87	0.90
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.01	0.90
1:A:15:LYS:HB3	2:B:1220:ARG:HG2	1.51	0.90
2:B:842:ASN:HD22	2:B:845:SER:H	1.17	0.90
7:G:11:UNK:CA	7:G:66:UNK:CA	2.49	0.90
1:A:549:MET:SD	1:A:577:ILE:HD12	2.12	0.90
3:C:167:HIS:HD2	3:C:169:LYS:H	0.90	0.90
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.53	0.89
1:A:381:THR:HG22	1:A:383:TYR:H	1.35	0.89
3:C:22:LEU:HD22	3:C:25:VAL:HG21	1.53	0.89
9:I:111:THR:HG22	9:I:113:ASP:N	1.86	0.89
1:A:567:LYS:NZ	8:H:46:LEU:HB2	1.87	0.89
1:A:962:ARG:HA	1:A:965:GLN:HE21	1.37	0.89
1:A:61:ILE:HG22	1:A:62:ASP:H	1.37	0.89
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.38	0.88
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.55	0.88
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.56	0.88
3:C:57:VAL:HG11	10:J:60:PHE:CB	2.03	0.88

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1410:PHE:CD2	2:B:1212:ILE:HD11	2.08	0.88
2:B:956:THR:HA	2:B:961:LEU:O	1.71	0.88
1:A:337:ARG:NH1	1:A:839:ARG:HH12	1.72	0.88
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.54	0.88
1:A:1105:LEU:HD22	1:A:1384:VAL:HG21	1.53	0.88
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.54	0.88
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.72	0.88
2:B:977:GLY:HA3	2:B:1099:VAL:CG2	2.04	0.87
2:B:955:THR:CG2	2:B:956:THR:H	1.87	0.87
1:A:590:ARG:HH11	1:A:590:ARG:HG3	1.37	0.87
1:A:666:ILE:CD1	2:B:1030:LEU:HD13	2.04	0.87
2:B:228:LYS:HD3	2:B:234:ILE:HD13	1.57	0.86
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.57	0.86
1:A:351:THR:HG23	2:B:1103:ILE:HA	1.53	0.86
1:A:1039:LYS:O	1:A:1043:ASP:HB2	1.75	0.86
2:B:130:VAL:HG21	2:B:167:ILE:HD12	1.56	0.86
2:B:512:ARG:HH21	2:B:535:LEU:CD1	1.88	0.86
1:A:667:GLY:HA2	1:A:670:ILE:HD12	1.56	0.86
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.57	0.86
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.40	0.86
2:B:345:LYS:CA	2:B:348:ARG:HE	1.87	0.86
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.58	0.85
1:A:417:TYR:O	1:A:418:SER:HB2	1.75	0.85
2:B:744:HIS:HD2	2:B:746:SER:H	1.23	0.85
8:H:125:LEU:HG	8:H:130:ARG:NH1	1.92	0.85
1:A:605:MET:HE3	1:A:614:PHE:O	1.75	0.85
11:K:10:PHE:CD1	11:K:11:LEU:HD13	2.11	0.85
2:B:801:LYS:O	10:J:52:THR:HG23	1.76	0.85
5:E:177:ARG:HD3	5:E:215:MET:SD	2.18	0.84
11:K:12:LEU:HD12	11:K:12:LEU:H	1.42	0.84
2:B:108:VAL:HG12	2:B:109:THR:H	1.42	0.84
2:B:345:LYS:HA	2:B:348:ARG:NE	1.91	0.84
2:B:1106:ARG:HH21	2:B:1109:GLY:H	1.24	0.84
2:B:1106:ARG:NH1	2:B:1118:PRO:HB3	1.91	0.83
2:B:912:ILE:O	2:B:938:SER:HB2	1.76	0.83
5:E:2:ASP:O	5:E:3:GLN:HG2	1.78	0.83
1:A:709:THR:HG21	9:I:93:LYS:O	1.77	0.83
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.08	0.83
3:C:11:ARG:NH2	3:C:229:TYR:HD2	1.77	0.83
6:F:147:SER:OG	6:F:150:GLU:HG3	1.78	0.83
1:A:683:ILE:HD11	1:A:764:CYS:HB2	1.61	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:THR:HG21	1:A:617:VAL:H	1.43	0.83
2:B:1002:THR:CG2	2:B:1006:ILE:H	1.91	0.83
1:A:1390:ASN:ND2	1:A:1399:ARG:HA	1.93	0.82
2:B:200:GLY:HA2	2:B:202:TYR:HE2	1.42	0.82
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.61	0.82
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.59	0.82
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.62	0.82
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.60	0.82
2:B:1106:ARG:HH21	2:B:1109:GLY:N	1.78	0.81
8:H:93:TYR:HB3	8:H:144:ILE:O	1.80	0.81
1:A:208:LEU:HD22	1:A:212:LYS:HE3	1.62	0.81
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.29	0.81
2:B:1106:ARG:HE	2:B:1109:GLY:N	1.79	0.81
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.62	0.81
1:A:1017:LEU:HB2	5:E:206:GLY:H	1.44	0.81
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.61	0.81
1:A:885:THR:HG23	1:A:893:PHE:HE1	1.44	0.81
2:B:121:ASN:HD22	2:B:121:ASN:N	1.79	0.81
10:J:48:ARG:HH21	10:J:49:MET:HE1	1.45	0.81
1:A:742:ASN:HA	1:A:745:GLN:HB2	1.63	0.81
3:C:148:ARG:NH1	10:J:64:ASN:HA	1.96	0.81
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.61	0.81
2:B:244:LEU:O	2:B:249:ARG:HG2	1.81	0.81
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.15	0.80
2:B:1106:ARG:NH2	2:B:1109:GLY:H	1.79	0.80
8:H:5:LEU:HD11	8:H:135:LEU:HG	1.63	0.80
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.63	0.80
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.61	0.80
1:A:855:THR:HG21	1:A:857:ARG:NE	1.95	0.80
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.63	0.80
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.11	0.80
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.11	0.80
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.63	0.80
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.17	0.80
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.12	0.80
3:C:167:HIS:HD2	3:C:169:LYS:N	1.76	0.80
9:I:50:THR:CG2	9:I:52:ILE:HG23	2.11	0.80
10:J:46:CYS:HG	13:J:101:ZN:ZN	0.92	0.80
1:A:40:THR:HG22	1:A:41:MET:HG3	1.64	0.80
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.12	0.79
1:A:1299:VAL:HG12	1:A:1300:LYS:H	1.47	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:37:MET:HG2	3:C:243:VAL:HG12	1.62	0.79
8:H:123:MET:HE3	8:H:142:LEU:HD22	1.63	0.79
8:H:81:PRO:HB2	8:H:82:PRO:HD3	1.62	0.79
1:A:523:ILE:HD12	1:A:622:VAL:CG2	2.12	0.79
1:A:32:VAL:HG21	1:A:68:GLN:NE2	1.97	0.79
2:B:1100:ASP:HA	2:B:1103:ILE:CD1	2.12	0.79
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.62	0.79
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.11	0.79
1:A:666:ILE:HD13	2:B:1030:LEU:HD22	1.65	0.79
1:A:298:PHE:O	1:A:302:THR:HB	1.83	0.79
1:A:337:ARG:NH1	1:A:839:ARG:NH1	2.29	0.79
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.63	0.79
1:A:768:GLN:CG	1:A:816:HIS:HA	2.13	0.78
2:B:487:THR:HG22	2:B:489:SER:H	1.48	0.78
2:B:855:PHE:HZ	2:B:857:ARG:NH1	1.81	0.78
1:A:472:LEU:O	1:A:475:THR:HB	1.81	0.78
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.19	0.78
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.63	0.78
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.66	0.78
1:A:313:GLN:HB2	1:A:322:VAL:CG2	2.14	0.78
2:B:842:ASN:ND2	2:B:845:SER:N	2.31	0.78
1:A:313:GLN:HB2	1:A:322:VAL:HG23	1.64	0.78
1:A:399:HIS:O	1:A:401:GLY:N	2.17	0.78
2:B:583:ASN:HD21	2:B:628:THR:HB	1.49	0.78
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.19	0.78
1:A:58:LEU:HD22	1:A:80:HIS:O	1.83	0.78
2:B:1106:ARG:HE	2:B:1109:GLY:H	1.29	0.78
3:C:56:THR:HG22	3:C:57:VAL:N	1.97	0.78
1:A:353:ILE:HD13	1:A:487:MET:CE	2.14	0.77
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.13	0.77
2:B:392:ARG:NH2	9:I:52:ILE:HD11	1.98	0.77
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	1.66	0.77
2:B:1100:ASP:OD1	2:B:1103:ILE:HD11	1.84	0.77
2:B:707:PRO:HG2	2:B:708:GLU:H	1.49	0.77
1:A:1281:ARG:O	1:A:1282:VAL:HG23	1.83	0.77
1:A:913:LEU:HD12	1:A:914:GLU:N	1.98	0.77
3:C:165:LYS:O	11:K:6:ARG:NH1	2.17	0.77
1:A:901:LEU:H	1:A:926:GLN:NE2	1.82	0.77
1:A:31:SER:CB	1:A:83:HIS:HB2	2.15	0.77
2:B:708:GLU:HG3	2:B:709:ASP:N	1.98	0.77
3:C:124:LEU:O	3:C:127:ARG:HG2	1.85	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.49	0.77
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.65	0.77
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.64	0.77
4:D:81:UNK:CA	4:D:82:UNK:CA	2.63	0.77
1:A:70:CYS:O	1:A:72:GLU:HG2	1.84	0.77
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.84	0.77
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	1.84	0.76
3:C:57:VAL:CG1	10:J:60:PHE:HB3	2.15	0.76
11:K:47:ARG:HH11	11:K:47:ARG:HB3	1.49	0.76
1:A:541:ILE:HG21	1:A:549:MET:HE3	1.67	0.76
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.21	0.76
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.51	0.76
8:H:40:LEU:HD23	8:H:42:ILE:HD11	1.65	0.76
2:B:232:SER:OG	2:B:234:ILE:HD12	1.84	0.76
5:E:61:GLN:HE21	5:E:105:PHE:HE2	1.34	0.76
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.68	0.76
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.50	0.76
2:B:496:ARG:NH1	2:B:539:LEU:HB2	1.99	0.76
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.16	0.76
2:B:770:GLN:HG2	2:B:983:ARG:O	1.86	0.76
1:A:24:PRO:HB3	1:A:237:THR:HB	1.67	0.76
2:B:708:GLU:CG	2:B:709:ASP:H	1.97	0.76
2:B:996:ARG:NH2	3:C:174:ALA:O	2.19	0.76
1:A:1323:ASP:OD1	1:A:1325:THR:HB	1.86	0.76
2:B:542:MET:HE3	2:B:747:MET:HG3	1.67	0.76
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.67	0.75
2:B:842:ASN:HD22	2:B:845:SER:N	1.83	0.75
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.66	0.75
1:A:95:PHE:O	1:A:99:ILE:HG13	1.85	0.75
2:B:211:VAL:HG21	2:B:483:LEU:HD13	1.67	0.75
8:H:89:LEU:C	8:H:91:ASP:H	1.90	0.75
12:L:38:LEU:O	12:L:39:SER:HB3	1.85	0.75
1:A:41:MET:HA	1:A:49:LYS:HA	1.68	0.75
2:B:1166:CYS:O	2:B:1168:LEU:N	2.18	0.75
10:J:12:LYS:O	10:J:14:VAL:HG23	1.85	0.75
2:B:118:ARG:HH22	2:B:194:GLU:CD	1.90	0.75
2:B:423:LYS:HA	2:B:426:LYS:HE2	1.68	0.75
2:B:651:LEU:HD11	2:B:707:PRO:HB3	1.69	0.75
1:A:223:GLY:O	1:A:1415:SER:HA	1.86	0.75
1:A:265:LYS:NZ	1:A:323:LYS:H	1.84	0.75
1:A:469:ARG:HH21	2:B:976:ILE:HD13	1.51	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:69:ILE:HG23	5:E:73:PRO:HA	1.67	0.75
1:A:336:ILE:HD12	1:A:1405:THR:HG21	1.68	0.74
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.23	0.74
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.69	0.74
2:B:711:GLU:N	2:B:712:PRO:HD3	2.01	0.74
1:A:1146:VAL:HG11	1:A:1202:MET:SD	2.27	0.74
1:A:1436:ILE:HG22	1:A:1437:GLY:N	2.02	0.74
1:A:535:THR:CG2	1:A:616:VAL:HA	2.18	0.74
1:A:1436:ILE:CG2	2:B:1142:GLY:HA2	2.17	0.74
2:B:62:ILE:HG23	2:B:418:LYS:HG2	1.69	0.74
2:B:542:MET:HE1	2:B:743:ILE:HG21	1.70	0.74
6:F:111:LEU:N	6:F:111:LEU:HD12	2.02	0.74
1:A:1399:ARG:HB2	1:A:1408:ILE:HG21	1.70	0.74
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.51	0.74
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.02	0.74
1:A:443:LEU:HD21	1:A:455:MET:HB3	1.70	0.74
2:B:570:VAL:HB	2:B:573:GLN:CB	2.18	0.74
2:B:46:GLN:HG3	2:B:47:GLN:N	2.03	0.74
2:B:879:ARG:HB3	2:B:883:LEU:HD23	1.70	0.74
2:B:882:THR:HG22	2:B:884:ARG:H	1.50	0.74
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.23	0.74
1:A:575:LYS:HB3	1:A:612:ILE:CG2	2.17	0.74
1:A:534:LEU:O	1:A:574:GLY:HA3	1.88	0.74
1:A:853:ASP:OD1	1:A:855:THR:HB	1.88	0.74
1:A:567:LYS:HB3	8:H:96:VAL:N	2.02	0.73
5:E:61:GLN:NE2	5:E:105:PHE:HE2	1.86	0.73
8:H:89:LEU:HB3	8:H:91:ASP:OD1	1.88	0.73
1:A:925:LEU:O	1:A:929:LEU:HD23	1.88	0.73
1:A:154:SER:HB3	1:A:162:VAL:CG2	2.17	0.73
1:A:710:LEU:H	1:A:710:LEU:HD12	1.52	0.73
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.70	0.73
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.23	0.73
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.70	0.73
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.71	0.73
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.70	0.73
2:B:193:LYS:HD3	2:B:787:VAL:HG11	1.70	0.73
8:H:35:GLN:HB3	8:H:111:LEU:HD21	1.70	0.73
1:A:1258:HIS:ND1	1:A:1262:LYS:HE3	2.04	0.73
2:B:1106:ARG:NE	2:B:1109:GLY:H	1.85	0.73
2:B:363:HIS:O	2:B:364:ILE:HB	1.88	0.73
1:A:500:GLU:OE2	2:B:1145:SER:HB2	1.88	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.23	0.73
1:A:321:PRO:O	1:A:322:VAL:HB	1.87	0.73
1:A:445:ASN:CB	1:A:455:MET:HG2	2.19	0.73
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.23	0.72
1:A:1436:ILE:HG22	1:A:1437:GLY:H	1.52	0.72
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.54	0.72
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.71	0.72
1:A:337:ARG:NE	1:A:839:ARG:HH22	1.88	0.72
2:B:58:THR:O	2:B:62:ILE:HG13	1.89	0.72
2:B:542:MET:HG3	2:B:747:MET:HE3	1.69	0.72
1:A:32:VAL:HB	1:A:57:ARG:HD2	1.71	0.72
2:B:570:VAL:HG21	2:B:573:GLN:NE2	2.04	0.72
2:B:708:GLU:O	2:B:710:LEU:N	2.22	0.72
2:B:745:PRO:O	2:B:748:ILE:HG12	1.89	0.72
1:A:1209:MET:SD	1:A:1236:LEU:HB3	2.30	0.72
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.69	0.72
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.72	0.72
1:A:567:LYS:HZ1	8:H:46:LEU:HB2	1.55	0.72
1:A:857:ARG:HD3	1:A:861:GLY:O	1.88	0.72
11:K:65:HIS:CD2	11:K:67:PHE:H	2.06	0.72
1:A:351:THR:HG21	2:B:1103:ILE:HG23	1.71	0.72
1:A:575:LYS:HB3	1:A:612:ILE:HG23	1.71	0.72
9:I:74:GLU:HB3	9:I:79:HIS:HA	1.70	0.72
1:A:341:MET:HE1	1:A:1401:SER:HB2	1.72	0.72
1:A:567:LYS:HD3	8:H:95:TYR:CD1	2.25	0.72
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.38	0.72
2:B:313:MET:CE	2:B:386:LEU:HD22	2.19	0.72
8:H:5:LEU:HB3	8:H:133:ASN:O	1.88	0.72
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.70	0.72
1:A:900:ASP:OD2	1:A:903:ASN:HB2	1.90	0.72
2:B:955:THR:CG2	2:B:956:THR:N	2.49	0.71
1:A:1397:LEU:O	1:A:1400:CYS:HB2	1.89	0.71
1:A:567:LYS:HE3	8:H:46:LEU:HD12	1.71	0.71
1:A:503:GLN:HE21	6:F:90:ARG:NH2	1.88	0.71
2:B:108:VAL:HG12	2:B:109:THR:N	2.06	0.71
2:B:555:ILE:HD13	2:B:587:HIS:CE1	2.26	0.71
2:B:309:GLN:HG3	9:I:52:ILE:HD13	1.72	0.71
11:K:7:PHE:HB2	11:K:11:LEU:HD22	1.72	0.71
2:B:234:ILE:H	2:B:234:ILE:HD12	1.53	0.71
1:A:598:LEU:HD22	8:H:25:ARG:NH1	2.05	0.71
5:E:168:TYR:HB3	5:E:170:LEU:HD21	1.72	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:TYR:O	1:A:418:SER:CB	2.36	0.71
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.71	0.71
1:A:1152:ILE:HG23	1:A:1260:LEU:HD23	1.71	0.71
1:A:1332:PHE:H	1:A:1332:PHE:HD2	1.38	0.71
1:A:225:ASN:O	1:A:227:VAL:N	2.21	0.71
1:A:340:LEU:HD21	2:B:1200:ALA:HB2	1.72	0.71
1:A:383:TYR:HB3	6:F:115:THR:HG22	1.73	0.71
1:A:44:THR:O	1:A:45:GLN:HB2	1.91	0.71
1:A:672:ASP:HB2	1:A:736:ASN:OD1	1.90	0.71
1:A:75:ASN:O	1:A:76:GLU:HB3	1.88	0.71
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.32	0.70
1:A:451:HIS:NE2	1:A:1074:GLU:HG3	2.07	0.70
1:A:367:PRO:HB3	1:A:466:SER:HA	1.73	0.70
1:A:675:THR:HG21	1:A:736:ASN:ND2	2.06	0.70
2:B:637:LEU:CD1	2:B:693:ILE:HD12	2.20	0.70
11:K:65:HIS:HD2	11:K:67:PHE:H	1.35	0.70
1:A:48:ALA:O	1:A:49:LYS:HG3	1.89	0.70
1:A:691:LEU:HD11	1:A:695:LYS:HE3	1.71	0.70
2:B:636:PRO:O	2:B:637:LEU:HG	1.90	0.70
2:B:737:THR:HG23	9:I:66:PRO:CB	2.20	0.70
2:B:792:MET:HA	2:B:856:PHE:O	1.91	0.70
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.74	0.70
3:C:18:VAL:HG23	3:C:240:VAL:HG11	1.72	0.70
2:B:130:VAL:HG12	2:B:131:ASP:N	2.07	0.70
2:B:463:THR:CG2	2:B:465:ASN:HD22	2.05	0.70
2:B:542:MET:CE	2:B:747:MET:HG3	2.22	0.70
11:K:55:LYS:HD3	11:K:78:THR:CB	2.20	0.70
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.74	0.70
2:B:281:PRO:HG2	2:B:284:ILE:HD12	1.73	0.70
2:B:957:ASN:HD22	2:B:961:LEU:HD12	1.57	0.70
12:L:47:ARG:HG2	12:L:52:GLY:HA2	1.72	0.70
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.57	0.70
2:B:65:GLU:HG3	2:B:66:ASP:H	1.56	0.70
5:E:56:LYS:HG3	5:E:84:ASP:HB2	1.73	0.70
1:A:567:LYS:HE3	8:H:46:LEU:CD1	2.22	0.70
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.57	0.70
11:K:55:LYS:HD3	11:K:78:THR:HB	1.72	0.70
2:B:1066:SER:O	2:B:1067:ARG:HD3	1.90	0.69
8:H:36:CYS:SG	8:H:130:ARG:NH2	2.65	0.69
1:A:72:GLU:OE2	2:B:1175:LEU:HD12	1.92	0.69
1:A:675:THR:CB	1:A:736:ASN:HD21	2.04	0.69

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:PRO:HG2	2:B:296:GLU:HB3	1.74	0.69
1:A:763:ALA:O	1:A:803:SER:HB3	1.92	0.69
8:H:49:VAL:HG12	8:H:50:ALA:N	2.07	0.69
1:A:584:ASN:O	1:A:637:LYS:HE3	1.92	0.69
1:A:858:ASN:HD22	1:A:858:ASN:C	1.96	0.69
1:A:472:LEU:HD11	2:B:835:GLN:NE2	2.08	0.69
2:B:955:THR:HG23	12:L:54:ARG:O	1.91	0.69
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.75	0.69
5:E:83:CYS:SG	5:E:88:VAL:HG22	2.32	0.69
1:A:343:LYS:HE3	2:B:1151:LEU:O	1.92	0.69
3:C:80:LEU:HD22	3:C:129:ILE:CD1	2.21	0.69
2:B:638:PHE:CE1	2:B:743:ILE:HA	2.26	0.69
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.93	0.69
2:B:280:ILE:CD1	2:B:334:ILE:HG12	2.23	0.69
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.74	0.69
2:B:378:LEU:O	2:B:382:ILE:HG13	1.92	0.69
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.73	0.68
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.74	0.68
1:A:694:THR:O	1:A:698:GLN:HG3	1.94	0.68
8:H:7:ASP:O	8:H:8:ASP:HB2	1.92	0.68
1:A:599:SER:HB2	1:A:603:ASN:H	1.58	0.68
1:A:391:LEU:HD22	1:A:400:PRO:O	1.93	0.68
2:B:54:PHE:HA	2:B:58:THR:HB	1.74	0.68
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.74	0.68
3:C:93:ASP:O	3:C:127:ARG:NH2	2.27	0.68
2:B:22:SER:O	2:B:654:ARG:HD2	1.94	0.68
2:B:884:ARG:O	2:B:936:ASP:HB3	1.93	0.68
2:B:976:ILE:O	2:B:990:ILE:HB	1.94	0.68
6:F:81:THR:HG21	6:F:136:ARG:CD	2.20	0.68
1:A:381:THR:HG22	1:A:383:TYR:N	2.09	0.68
2:B:314:LEU:O	2:B:317:CYS:HB2	1.92	0.68
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.76	0.68
9:I:53:GLY:O	9:I:89:GLN:HB2	1.94	0.68
12:L:46:VAL:HG13	12:L:56:LEU:HD12	1.76	0.68
1:A:1095:THR:HG22	1:A:1100:ARG:HB2	1.74	0.68
1:A:446:ARG:HH11	1:A:446:ARG:HG2	1.59	0.68
2:B:709:ASP:O	2:B:710:LEU:HD23	1.94	0.68
2:B:986:GLN:OE1	2:B:986:GLN:HA	1.92	0.68
3:C:166:GLU:HG3	11:K:10:PHE:CZ	2.29	0.68
3:C:254:LYS:HB3	11:K:42:LEU:HD11	1.75	0.68
2:B:280:ILE:HG22	2:B:285:ILE:HG13	1.76	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:842:ASN:ND2	2:B:844:SER:HB2	2.09	0.68
5:E:93:MET:HE2	5:E:120:ALA:HB1	1.75	0.68
2:B:954:VAL:O	12:L:55:ILE:O	2.11	0.68
1:A:535:THR:HG21	1:A:616:VAL:HA	1.76	0.67
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.29	0.67
2:B:711:GLU:N	2:B:712:PRO:CD	2.57	0.67
1:A:693:VAL:CG2	1:A:721:PHE:HE1	2.07	0.67
2:B:288:ALA:HB1	2:B:331:LEU:HD12	1.75	0.67
1:A:786:HIS:HE1	2:B:742:GLU:OE1	1.76	0.67
2:B:1002:THR:HG23	2:B:1004:GLU:N	2.10	0.67
1:A:351:THR:CG2	2:B:1103:ILE:HG23	2.24	0.67
2:B:882:THR:HG21	2:B:935:ARG:HA	1.75	0.67
1:A:994:GLN:HE21	1:A:1019:CYS:HB3	1.59	0.67
2:B:1106:ARG:CZ	2:B:1109:GLY:H	2.07	0.67
2:B:603:LEU:HB3	2:B:609:ILE:HG13	1.76	0.67
1:A:1390:ASN:HD22	1:A:1399:ARG:HA	1.57	0.67
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.77	0.67
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.28	0.67
5:E:127:ILE:O	5:E:127:ILE:HG13	1.93	0.67
8:H:115:TYR:CE2	8:H:124:ARG:HG3	2.30	0.67
1:A:453:MET:HB3	1:A:477:PRO:HB3	1.76	0.67
3:C:260:LEU:O	3:C:264:GLN:HG3	1.95	0.67
11:K:47:ARG:NH1	11:K:47:ARG:HB3	2.09	0.67
1:A:306:ASN:HD21	1:A:324:SER:H	1.43	0.67
3:C:8:VAL:HG12	3:C:9:LYS:N	2.09	0.67
10:J:58:GLU:HA	10:J:61:LEU:HD12	1.76	0.67
1:A:443:LEU:HD22	1:A:455:MET:HE2	1.74	0.67
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.30	0.67
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.77	0.67
3:C:5:GLY:O	3:C:7:GLN:HG3	1.94	0.67
8:H:26:ILE:HD12	8:H:42:ILE:HD12	1.76	0.67
1:A:816:HIS:CE1	2:B:764:SER:HB2	2.30	0.67
10:J:1:MET:H2	10:J:56:LEU:HB2	1.59	0.67
12:L:45:ALA:O	12:L:46:VAL:HG23	1.95	0.67
1:A:1348:LEU:HD21	1:A:1375:MET:SD	2.35	0.66
1:A:76:GLU:OE2	2:B:1159:ARG:NH1	2.28	0.66
2:B:864:LYS:HB3	2:B:872:GLU:H	1.59	0.66
2:B:311:LEU:HB3	9:I:4:PHE:CZ	2.31	0.66
1:A:814:PHE:O	1:A:817:ALA:HB3	1.95	0.66
1:A:914:GLU:HB2	1:A:979:SER:O	1.95	0.66
2:B:514:LEU:HD12	2:B:515:HIS:N	2.09	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:THR:HG21	3:C:145:CYS:SG	2.35	0.66
3:C:22:LEU:HD22	3:C:25:VAL:CG2	2.25	0.66
1:A:1333:ILE:O	1:A:1336:MET:HB3	1.96	0.66
1:A:1364:ASN:ND2	1:A:1365:TYR:N	2.43	0.66
1:A:381:THR:CG2	1:A:383:TYR:H	2.09	0.66
1:A:563:PRO:HB2	1:A:565:ILE:O	1.94	0.66
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.25	0.66
2:B:1147:LEU:HD22	2:B:1151:LEU:HD22	1.77	0.66
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.77	0.66
1:A:1342:GLU:OE2	5:E:212:ARG:NH1	2.28	0.66
3:C:98:VAL:C	3:C:99:LEU:HD23	2.16	0.66
9:I:32:CYS:SG	9:I:33:SER:N	2.69	0.66
9:I:55:THR:HG23	9:I:58:VAL:HG21	1.76	0.66
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.77	0.66
2:B:363:HIS:O	2:B:364:ILE:CB	2.44	0.66
1:A:590:ARG:HB3	1:A:605:MET:N	2.10	0.66
2:B:128:LEU:HB3	2:B:167:ILE:O	1.95	0.66
2:B:566:LEU:HD13	2:B:588:GLY:HA2	1.78	0.66
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.31	0.66
1:A:741:ASN:HD22	1:A:741:ASN:C	1.99	0.66
2:B:649:LYS:HE2	2:B:738:PHE:O	1.96	0.66
1:A:525:GLN:CB	2:B:835:GLN:HG2	2.25	0.66
6:F:109:VAL:HG12	6:F:110:ASP:N	2.10	0.66
1:A:535:THR:HG21	1:A:617:VAL:N	2.08	0.66
2:B:986:GLN:HE22	2:B:1020:ARG:CZ	2.08	0.66
7:G:113:UNK:CA	7:G:115:UNK:CA	2.74	0.66
2:B:46:GLN:HE22	2:B:496:ARG:HA	1.61	0.66
2:B:957:ASN:O	2:B:959:ASP:N	2.28	0.66
1:A:95:PHE:HE2	1:A:1414:ALA:HB2	1.62	0.65
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.26	0.65
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.77	0.65
1:A:305:ASP:HB3	1:A:308:ILE:HD11	1.77	0.65
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.31	0.65
1:A:751:SER:O	1:A:752:LYS:HG2	1.96	0.65
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.30	0.65
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.79	0.65
1:A:1115:SER:HA	1:A:1308:THR:HG22	1.77	0.65
1:A:523:ILE:HD12	1:A:622:VAL:HG22	1.79	0.65
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.06	0.65
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.79	0.65
2:B:46:GLN:HG3	2:B:47:GLN:H	1.59	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ARG:CG	2:B:955:THR:HG21	2.23	0.65
3:C:11:ARG:HH21	3:C:229:TYR:HD2	1.44	0.65
2:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.77	0.65
2:B:751:VAL:O	2:B:754:SER:HB2	1.95	0.65
5:E:176:PRO:O	5:E:212:ARG:HA	1.95	0.65
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	1.79	0.65
1:A:1111:MET:HE1	1:A:1330:ASN:OD1	1.97	0.65
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.79	0.65
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.26	0.65
5:E:124:VAL:HG22	5:E:132:ILE:HG21	1.78	0.65
12:L:51:CYS:O	12:L:53:HIS:N	2.28	0.65
1:A:512:VAL:HA	1:A:519:PRO:HA	1.79	0.65
8:H:24:CYS:HB2	8:H:44:VAL:CG2	2.27	0.65
1:A:450:LEU:HD13	1:A:1074:GLU:HG2	1.77	0.65
2:B:349:ILE:O	2:B:352:ALA:HB3	1.96	0.65
3:C:8:VAL:HG12	3:C:9:LYS:H	1.60	0.65
8:H:107:VAL:HG21	8:H:126:GLU:HG3	1.79	0.65
9:I:111:THR:HG21	9:I:113:ASP:HB2	1.78	0.65
1:A:1042:PHE:CE2	1:A:1046:LEU:HD11	2.31	0.65
1:A:1111:MET:HE1	1:A:1114:PRO:HA	1.79	0.65
1:A:1224:LEU:HD12	1:A:1241:ARG:O	1.97	0.65
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.79	0.65
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.27	0.64
2:B:805:THR:HG21	2:B:815:ARG:HE	1.62	0.64
1:A:1035:TYR:O	1:A:1037:LEU:N	2.30	0.64
1:A:579:SER:OG	1:A:612:ILE:HG22	1.98	0.64
1:A:329:LEU:HD23	1:A:335:ARG:HG3	1.78	0.64
2:B:1170:THR:O	2:B:1170:THR:HG22	1.97	0.64
1:A:1445:ILE:C	1:A:1446:ASP:CA	2.65	0.64
2:B:25:ILE:HG22	2:B:29:ASP:HB2	1.79	0.64
2:B:879:ARG:HB3	2:B:883:LEU:CD2	2.26	0.64
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.32	0.64
1:A:715:GLU:O	1:A:719:VAL:HG23	1.96	0.64
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.81	0.64
1:A:901:LEU:HA	1:A:907:THR:HG23	1.80	0.64
2:B:604:ARG:HG2	2:B:604:ARG:O	1.98	0.64
6:F:96:THR:O	6:F:100:GLN:HG3	1.97	0.64
6:F:86:THR:OG1	6:F:89:GLU:HG3	1.98	0.64
1:A:1193:LEU:HB2	1:A:1260:LEU:HD11	1.78	0.64
1:A:1394:THR:CG2	1:A:1395:GLY:N	2.60	0.64
1:A:629:LEU:HD13	1:A:645:LEU:HD21	1.79	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.32	0.64
2:B:711:GLU:H	2:B:712:PRO:HD3	1.61	0.64
8:H:106:GLU:C	8:H:108:SER:H	2.02	0.64
1:A:523:ILE:HD12	1:A:622:VAL:HG21	1.80	0.63
2:B:1197:PRO:HG2	2:B:1200:ALA:HB2	1.79	0.63
2:B:824:ILE:CG1	10:J:48:ARG:HH12	2.08	0.63
1:A:225:ASN:O	1:A:226:GLU:HG2	1.99	0.63
1:A:709:THR:HB	1:A:712:GLU:H	1.64	0.63
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.33	0.63
8:H:49:VAL:HG12	8:H:50:ALA:H	1.62	0.63
1:A:994:GLN:HE22	1:A:1023:ARG:NE	1.95	0.63
1:A:84:ILE:HG23	1:A:239:LEU:HB3	1.80	0.63
2:B:1104:HIS:HB2	2:B:1122:ARG:HD2	1.80	0.63
2:B:780:VAL:HG21	10:J:56:LEU:CD1	2.29	0.63
2:B:842:ASN:HD21	2:B:844:SER:HB2	1.63	0.63
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.33	0.63
10:J:9:SER:OG	10:J:48:ARG:NH2	2.30	0.63
2:B:221:ASN:OD1	2:B:242:SER:HA	1.98	0.63
1:A:108:MET:O	1:A:109:HIS:HB2	1.99	0.63
1:A:475:THR:HG22	1:A:476:SER:N	2.12	0.63
1:A:354:SER:HA	1:A:482:PHE:CD2	2.34	0.63
2:B:525:ALA:O	2:B:527:THR:HG22	1.99	0.63
6:F:109:VAL:HG21	6:F:124:GLU:HA	1.80	0.63
8:H:31:THR:O	8:H:32:THR:CB	2.47	0.63
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.12	0.63
1:A:268:ASP:HB3	1:A:299:HIS:ND1	2.14	0.63
2:B:373:ARG:NE	2:B:567:GLU:OE2	2.29	0.63
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.32	0.63
5:E:96:PHE:CZ	5:E:100:ILE:HD11	2.32	0.63
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.29	0.63
6:F:135:ARG:HG2	6:F:137:TYR:CE1	2.34	0.63
1:A:1317:MET:HA	1:A:1322:ILE:HD11	1.81	0.63
1:A:1402:PHE:CD2	1:A:1403:GLU:HG3	2.33	0.63
1:A:418:SER:O	1:A:420:ARG:N	2.32	0.63
1:A:982:THR:HG22	1:A:984:LYS:H	1.64	0.63
2:B:1201:LYS:O	2:B:1205:GLN:HG3	1.97	0.63
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.31	0.63
12:L:40:LEU:HD13	12:L:44:ASP:CG	2.19	0.63
4:D:7:UNK:CA	7:G:8:UNK:CA	2.76	0.62
6:F:111:LEU:H	6:F:111:LEU:HD12	1.61	0.62
1:A:33:ALA:O	1:A:83:HIS:HB3	1.99	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:ARG:HG3	1:A:825:ILE:HD11	1.81	0.62
2:B:1106:ARG:HD2	2:B:1126:GLY:O	1.99	0.62
6:F:97:ARG:O	6:F:101:ILE:HG13	1.99	0.62
8:H:12:VAL:HA	8:H:28:ALA:CB	2.28	0.62
1:A:73:GLY:O	1:A:75:ASN:N	2.32	0.62
2:B:208:SER:OG	2:B:210:LYS:HD3	1.99	0.62
2:B:446:LEU:O	2:B:447:ALA:HB3	1.97	0.62
2:B:616:ILE:N	2:B:616:ILE:HD12	2.14	0.62
2:B:914:LYS:HB3	2:B:937:ALA:O	1.98	0.62
1:A:1054:LEU:O	1:A:1057:VAL:HG23	1.99	0.62
2:B:25:ILE:HG22	2:B:26:THR:H	1.65	0.62
1:A:871:ASP:HB3	5:E:204:THR:HG22	1.82	0.62
3:C:173:ALA:O	3:C:174:ALA:HB3	2.00	0.62
12:L:55:ILE:HG13	12:L:56:LEU:H	1.63	0.62
1:A:1436:ILE:HB	2:B:1144:ALA:HB2	1.80	0.62
1:A:915:SER:O	1:A:919:ILE:HG13	2.00	0.62
5:E:96:PHE:O	5:E:100:ILE:HG13	1.98	0.62
9:I:7:CYS:HB2	9:I:29:CYS:HB2	1.81	0.62
1:A:445:ASN:HB2	1:A:454:SER:O	2.00	0.62
2:B:195:CYS:HB3	2:B:782:LEU:HD22	1.81	0.62
1:A:1212:VAL:O	1:A:1216:ILE:HG13	1.99	0.62
1:A:328:ARG:O	1:A:335:ARG:HG2	1.99	0.62
1:A:672:ASP:OD1	1:A:674:PRO:HD2	2.00	0.62
1:A:689:LYS:O	1:A:693:VAL:HG23	2.00	0.62
1:A:88:LYS:HD2	1:A:293:GLU:CD	2.20	0.62
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.35	0.62
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.28	0.62
8:H:123:MET:HE3	8:H:142:LEU:CD2	2.29	0.62
2:B:1034:VAL:HG23	2:B:1059:LEU:HB2	1.80	0.62
2:B:1051:THR:CG2	2:B:1053:GLU:H	1.93	0.62
2:B:446:LEU:O	2:B:447:ALA:CB	2.48	0.62
2:B:39:ARG:HE	2:B:665:GLU:HG2	1.65	0.62
2:B:787:VAL:O	2:B:787:VAL:HG12	2.00	0.62
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.80	0.62
1:A:871:ASP:HB3	5:E:204:THR:CG2	2.30	0.62
1:A:590:ARG:HB3	1:A:605:MET:H	1.63	0.62
6:F:101:ILE:HD12	6:F:121:ALA:HB2	1.82	0.62
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.34	0.62
1:A:1444:MET:HE1	6:F:135:ARG:NE	2.15	0.61
1:A:148:CYS:O	1:A:168:GLY:HA2	1.99	0.61
1:A:778:GLY:HA3	2:B:516:ASN:HB2	1.80	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:ASP:OD2	5:E:204:THR:HG23	1.99	0.61
2:B:1187:ASN:OD1	2:B:1190:ASP:HB3	1.99	0.61
2:B:496:ARG:HH11	2:B:539:LEU:HB2	1.62	0.61
5:E:178:ILE:HG23	5:E:214:CYS:HA	1.81	0.61
12:L:51:CYS:HB2	12:L:53:HIS:CD2	2.35	0.61
1:A:1021:LEU:O	1:A:1025:ARG:HG2	2.00	0.61
1:A:503:GLN:HE21	6:F:90:ARG:HH21	1.47	0.61
1:A:736:ASN:O	1:A:737:LEU:C	2.38	0.61
2:B:211:VAL:O	2:B:480:SER:HA	2.00	0.61
5:E:93:MET:O	5:E:97:VAL:HG23	2.00	0.61
6:F:111:LEU:H	6:F:111:LEU:CD1	2.12	0.61
2:B:913:GLY:HA2	2:B:938:SER:HB3	1.81	0.61
5:E:156:LEU:HD12	5:E:195:VAL:HG12	1.81	0.61
5:E:78:LEU:C	5:E:78:LEU:HD23	2.20	0.61
6:F:109:VAL:HG23	6:F:124:GLU:HG2	1.82	0.61
1:A:567:LYS:HZ2	8:H:46:LEU:HB2	1.64	0.61
3:C:166:GLU:HA	11:K:6:ARG:HB3	1.82	0.61
1:A:1329:THR:HG22	1:A:1331:SER:N	2.01	0.61
1:A:961:ARG:O	1:A:965:GLN:HG3	2.00	0.61
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.66	0.61
3:C:235:VAL:HG21	10:J:6:ARG:HH21	1.65	0.61
1:A:549:MET:SD	1:A:577:ILE:CD1	2.87	0.61
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.64	0.61
2:B:512:ARG:NH2	2:B:535:LEU:CD1	2.62	0.61
1:A:1364:ASN:HD22	1:A:1364:ASN:C	2.04	0.61
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.82	0.61
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.29	0.61
1:A:1437:GLY:HA3	6:F:88:TYR:CD2	2.36	0.61
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.31	0.61
2:B:185:THR:HG23	2:B:188:ASP:OD2	2.01	0.61
2:B:198:ASP:OD1	2:B:485:ARG:NH2	2.33	0.61
1:A:1132:LYS:O	1:A:1135:ARG:HB3	2.01	0.61
1:A:1192:LEU:HD22	1:A:1239:ARG:NH2	2.16	0.61
1:A:506:ALA:HB1	1:A:508:PRO:HD2	1.83	0.61
1:A:528:LEU:O	1:A:531:ILE:HG22	2.01	0.61
6:F:138:LEU:HB3	6:F:139:PRO:HD2	1.83	0.61
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.66	0.61
1:A:789:LYS:HG3	9:I:67:THR:HB	1.83	0.61
2:B:57:TYR:CD1	2:B:57:TYR:N	2.68	0.61
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.30	0.61
12:L:26:THR:O	12:L:27:LEU:HB3	2.01	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:48:CYS:SG	12:L:49:LYS:N	2.70	0.61
2:B:1169:MET:HE1	2:B:1201:LYS:O	2.00	0.60
3:C:46:ILE:HA	3:C:159:ALA:HA	1.82	0.60
3:C:49:VAL:HG21	3:C:67:LEU:HD12	1.83	0.60
5:E:29:PHE:HB2	5:E:65:THR:HG22	1.83	0.60
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.01	0.60
1:A:244:PRO:CG	1:A:245:PRO:HD3	2.27	0.60
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.32	0.60
5:E:78:LEU:HD23	5:E:79:TRP:N	2.16	0.60
11:K:63:VAL:O	11:K:63:VAL:CG2	2.49	0.60
2:B:114:PRO:HB3	2:B:174:LEU:HD11	1.82	0.60
2:B:463:THR:HG22	2:B:465:ASN:HD22	1.66	0.60
1:A:565:ILE:CG2	1:A:567:LYS:HG2	2.31	0.60
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.30	0.60
2:B:686:ASN:C	2:B:688:GLY:H	2.04	0.60
2:B:839:MET:HE3	2:B:1010:LEU:CD1	2.31	0.60
9:I:5:ARG:HD3	9:I:36:GLU:OE2	2.01	0.60
11:K:90:ALA:O	11:K:94:ILE:HG13	2.01	0.60
1:A:1208:THR:O	1:A:1212:VAL:HG23	2.01	0.60
1:A:663:SER:OG	1:A:664:THR:N	2.34	0.60
1:A:779:PHE:CZ	2:B:517:THR:HA	2.37	0.60
2:B:1051:THR:HG22	2:B:1052:VAL:N	2.17	0.60
2:B:299:GLU:OE1	2:B:571:PRO:HG2	2.01	0.60
2:B:549:THR:HB	2:B:628:THR:CG2	2.30	0.60
2:B:744:HIS:CD2	2:B:746:SER:H	2.14	0.60
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.31	0.60
1:A:322:VAL:O	1:A:323:LYS:HG3	2.01	0.60
1:A:306:ASN:OD1	1:A:324:SER:HB3	2.01	0.60
2:B:975:GLN:HG2	2:B:976:ILE:H	1.67	0.60
8:H:15:VAL:HG22	8:H:26:ILE:HG12	1.83	0.60
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.83	0.60
1:A:709:THR:OG1	1:A:712:GLU:HG3	2.00	0.60
2:B:479:VAL:HG12	2:B:480:SER:N	2.17	0.60
5:E:47:CYS:HA	5:E:53:PRO:HA	1.83	0.60
1:A:1042:PHE:HE2	1:A:1046:LEU:HD11	1.67	0.60
1:A:1223:ASP:HA	1:A:1243:VAL:CG1	2.32	0.60
1:A:338:GLY:HA2	2:B:1129:ARG:NH2	2.10	0.60
1:A:418:SER:O	1:A:419:LYS:C	2.40	0.60
10:J:1:MET:N	10:J:56:LEU:HB2	2.17	0.60
1:A:68:GLN:HE22	1:A:80:HIS:CB	2.15	0.60
1:A:97:ALA:HA	1:A:100:LYS:HE3	1.84	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1115:SER:O	1:A:1329:THR:HG23	2.02	0.60
2:B:1171:VAL:CG1	2:B:1191:ILE:HD13	2.32	0.60
2:B:121:ASN:ND2	2:B:121:ASN:N	2.50	0.60
2:B:995:ARG:NH1	2:B:995:ARG:HB2	2.16	0.60
1:A:1158:PRO:HB3	1:A:1241:ARG:NH1	2.17	0.59
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.37	0.59
1:A:337:ARG:CZ	1:A:839:ARG:NH1	2.64	0.59
1:A:567:LYS:O	1:A:569:LYS:N	2.35	0.59
1:A:886:ILE:CD1	1:A:943:LEU:HB3	2.31	0.59
2:B:211:VAL:CG2	2:B:483:LEU:HD13	2.32	0.59
2:B:666:TYR:C	2:B:668:ASP:H	2.06	0.59
8:H:139:ASN:O	8:H:140:ALA:HB2	2.02	0.59
2:B:1117:GLN:HG3	2:B:1156:ASP:OD1	2.02	0.59
1:A:1394:THR:HG22	1:A:1395:GLY:N	2.17	0.59
1:A:231:PRO:HA	1:A:234:MET:HE2	1.85	0.59
1:A:444:PHE:HB3	1:A:458:HIS:HD2	1.67	0.59
1:A:756:ILE:HG22	1:A:757:ASN:N	2.17	0.59
2:B:1174:LYS:HB2	2:B:1179:GLN:O	2.02	0.59
2:B:1159:ARG:CD	2:B:1193:GLN:HE21	2.15	0.59
2:B:803:LEU:H	2:B:822:ASN:HD21	1.48	0.59
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.84	0.59
9:I:8:ARG:HG3	9:I:9:ASP:N	2.15	0.59
1:A:107:CYS:HB2	1:A:114:LEU:CD2	2.33	0.59
1:A:151:ASP:HA	1:A:162:VAL:O	2.02	0.59
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.84	0.59
1:A:824:LEU:O	1:A:827:THR:HB	2.00	0.59
2:B:405:ARG:NH1	2:B:632:ARG:HG2	2.17	0.59
1:A:1399:ARG:CB	1:A:1408:ILE:HD13	2.28	0.59
9:I:15:TYR:O	9:I:27:PHE:HA	2.02	0.59
1:A:93:VAL:HG11	1:A:308:ILE:CD1	2.33	0.59
2:B:589:VAL:HG12	2:B:590:HIS:N	2.18	0.59
9:I:85:PHE:CD1	9:I:99:LEU:HD22	2.37	0.59
1:A:76:GLU:O	1:A:76:GLU:HG3	2.02	0.59
3:C:166:GLU:CG	11:K:10:PHE:HZ	2.14	0.59
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.33	0.59
1:A:896:ARG:NH2	1:A:1030:ARG:HH21	2.00	0.59
1:A:840:ARG:HB3	1:A:1384:VAL:HG12	1.85	0.59
1:A:511:ILE:HG12	1:A:521:MET:HE3	1.85	0.59
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.35	0.59
2:B:90:ILE:HD12	2:B:432:MET:SD	2.42	0.59
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.18	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.85	0.59
8:H:84:ALA:HA	8:H:87:ARG:CG	2.32	0.59
9:I:111:THR:CG2	9:I:113:ASP:HB2	2.33	0.59
1:A:1385:THR:HG22	1:A:1386:ARG:H	1.68	0.59
1:A:469:ARG:NH2	2:B:976:ILE:HD13	2.18	0.59
2:B:130:VAL:HG12	2:B:131:ASP:H	1.67	0.59
2:B:519:TRP:C	2:B:519:TRP:CD1	2.76	0.59
8:H:89:LEU:C	8:H:91:ASP:N	2.55	0.59
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.33	0.59
1:A:57:ARG:O	1:A:68:GLN:HG3	2.03	0.59
1:A:68:GLN:HE22	1:A:80:HIS:HB3	1.67	0.59
6:F:127:GLU:O	6:F:129:LYS:HG3	2.03	0.59
6:F:81:THR:HG22	6:F:82:THR:N	2.18	0.59
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.03	0.58
1:A:225:ASN:ND2	1:A:227:VAL:HB	2.18	0.58
2:B:642:ASP:O	2:B:644:GLU:N	2.36	0.58
5:E:156:LEU:HD12	5:E:195:VAL:CG1	2.33	0.58
8:H:109:LYS:NZ	8:H:109:LYS:HB2	2.18	0.58
2:B:912:ILE:HD11	2:B:966:VAL:HG23	1.84	0.58
10:J:48:ARG:HE	10:J:49:MET:CE	2.16	0.58
11:K:47:ARG:HD3	11:K:59:ALA:O	2.04	0.58
2:B:1102:LYS:O	2:B:1104:HIS:N	2.32	0.58
2:B:1201:LYS:HE2	2:B:1205:GLN:NE2	2.18	0.58
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.85	0.58
2:B:860:MET:HG2	2:B:861:ASP:N	2.18	0.58
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.86	0.58
1:A:596:THR:O	1:A:598:LEU:N	2.36	0.58
1:A:1325:THR:O	5:E:148:GLU:HB2	2.04	0.58
1:A:90:VAL:HG11	1:A:297:GLN:HA	1.84	0.58
2:B:23:ALA:O	2:B:654:ARG:HB3	2.04	0.58
2:B:46:GLN:O	2:B:408:LEU:HD23	2.03	0.58
1:A:567:LYS:NZ	8:H:95:TYR:CE1	2.71	0.58
1:A:1295:THR:HG23	1:A:1297:GLU:OE1	2.03	0.58
1:A:1364:ASN:ND2	1:A:1364:ASN:C	2.56	0.58
1:A:44:THR:O	1:A:44:THR:HG22	2.02	0.58
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.85	0.58
11:K:46:ILE:HG22	11:K:50:LEU:HD12	1.86	0.58
1:A:219:PHE:O	1:A:222:LEU:N	2.33	0.58
2:B:913:GLY:HA2	2:B:938:SER:CB	2.32	0.58
3:C:244:VAL:O	3:C:248:ILE:HG13	2.03	0.58
3:C:37:MET:HG2	3:C:243:VAL:CG1	2.34	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:157:SER:C	5:E:159:ASP:H	2.07	0.58
5:E:61:GLN:HB2	5:E:79:TRP:CE3	2.38	0.58
9:I:16:PRO:HB3	9:I:27:PHE:CE2	2.38	0.58
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.36	0.58
1:A:1308:THR:HG21	1:A:1310:GLY:O	2.04	0.58
1:A:260:ASP:OD1	1:A:261:ASP:N	2.37	0.58
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.85	0.58
2:B:1077:THR:CG2	2:B:1079:LYS:HB2	2.34	0.58
2:B:287:ARG:NH1	2:B:324:ILE:O	2.37	0.58
8:H:81:PRO:CB	8:H:82:PRO:CD	2.81	0.58
11:K:65:HIS:HD2	11:K:67:PHE:N	2.02	0.58
1:A:1332:PHE:N	1:A:1332:PHE:CD2	2.72	0.58
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.85	0.58
1:A:31:SER:OG	1:A:83:HIS:HB2	2.02	0.58
1:A:86:LEU:HA	1:A:273:ASN:OD1	2.02	0.58
2:B:1106:ARG:HH12	2:B:1118:PRO:HB3	1.67	0.58
2:B:205:ILE:N	2:B:205:ILE:HD12	2.19	0.58
1:A:101:LYS:O	1:A:105:CYS:HB2	2.04	0.58
1:A:1400:CYS:SG	1:A:1409:LEU:HG	2.44	0.58
1:A:225:ASN:HD22	1:A:227:VAL:HB	1.68	0.58
1:A:76:GLU:O	1:A:76:GLU:CG	2.52	0.58
6:F:87:LYS:HE2	6:F:88:TYR:CZ	2.39	0.58
11:K:33:ILE:HD13	11:K:87:LEU:HD22	1.85	0.58
1:A:385:ILE:HG22	1:A:386:ASP:N	2.18	0.57
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.85	0.57
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.39	0.57
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.04	0.57
1:A:41:MET:HB3	1:A:48:ALA:O	2.04	0.57
1:A:452:LYS:HB3	2:B:1141:HIS:CE1	2.40	0.57
1:A:537:ARG:HB2	8:H:20:TYR:CE2	2.39	0.57
2:B:101:MET:HB2	2:B:169:ARG:HH12	1.69	0.57
2:B:25:ILE:HG22	2:B:29:ASP:CB	2.34	0.57
2:B:756:ILE:O	2:B:759:PRO:HD3	2.04	0.57
2:B:806:THR:HB	2:B:809:MET:HG3	1.85	0.57
5:E:61:GLN:HB2	5:E:79:TRP:HE3	1.69	0.57
6:F:111:LEU:N	6:F:111:LEU:CD1	2.67	0.57
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.39	0.57
1:A:1143:LEU:HD23	1:A:1267:MET:HB3	1.86	0.57
1:A:1281:ARG:HB2	1:A:1309:ASP:HB2	1.86	0.57
1:A:1315:GLU:O	1:A:1318:THR:HG23	2.04	0.57
1:A:399:HIS:O	1:A:435:HIS:HD2	1.87	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:LEU:N	1:A:926:GLN:NE2	2.50	0.57
1:A:882:SER:HA	1:A:952:ALA:O	2.05	0.57
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.85	0.57
2:B:803:LEU:N	2:B:822:ASN:HD21	2.02	0.57
5:E:213:ILE:O	5:E:213:ILE:HG23	2.04	0.57
5:E:5:ASN:ND2	5:E:52:ARG:HG2	2.12	0.57
5:E:46:TYR:HA	5:E:57:MET:SD	2.43	0.57
8:H:24:CYS:SG	8:H:44:VAL:HG21	2.44	0.57
9:I:47:GLU:OE1	9:I:50:THR:HG23	2.04	0.57
1:A:166:GLY:O	1:A:167:CYS:HB3	2.03	0.57
1:A:524:VAL:HG12	1:A:525:GLN:H	1.69	0.57
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.85	0.57
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.38	0.57
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.33	0.57
8:H:5:LEU:CD1	8:H:135:LEU:HG	2.34	0.57
8:H:12:VAL:HA	8:H:28:ALA:HB2	1.86	0.57
1:A:1074:GLU:O	1:A:1076:ALA:N	2.37	0.57
1:A:337:ARG:CD	1:A:839:ARG:HH22	2.17	0.57
1:A:1436:ILE:HG22	2:B:1142:GLY:HA2	1.87	0.57
11:K:10:PHE:HD1	11:K:11:LEU:HD13	1.67	0.57
1:A:401:GLY:O	1:A:435:HIS:CD2	2.58	0.57
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.37	0.57
2:B:1077:THR:HG22	2:B:1079:LYS:N	2.13	0.57
2:B:1147:LEU:HD22	2:B:1151:LEU:CD2	2.35	0.57
12:L:49:LYS:O	12:L:50:ASP:HB2	2.03	0.57
1:A:567:LYS:NZ	8:H:46:LEU:CB	2.67	0.57
2:B:429:PHE:HA	2:B:432:MET:CE	2.35	0.57
2:B:855:PHE:HZ	2:B:857:ARG:HH11	1.52	0.57
3:C:55:THR:HB	3:C:152:GLU:H	1.70	0.57
6:F:111:LEU:C	6:F:113:GLY:H	2.07	0.57
1:A:28:ARG:HG2	1:A:83:HIS:CE1	2.39	0.57
3:C:148:ARG:HG3	10:J:61:LEU:O	2.03	0.57
3:C:251:LEU:O	3:C:255:VAL:HG23	2.04	0.57
8:H:106:GLU:C	8:H:108:SER:N	2.57	0.57
2:B:311:LEU:HB3	9:I:4:PHE:CE2	2.40	0.57
2:B:848:ARG:NH1	10:J:8:PHE:O	2.35	0.57
1:A:40:THR:HG21	1:A:259:GLU:OE2	2.04	0.57
1:A:414:ASP:O	1:A:417:TYR:O	2.22	0.57
1:A:901:LEU:H	1:A:926:GLN:HE21	1.50	0.57
2:B:1022:THR:HG23	2:B:1022:THR:O	2.05	0.57
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.87	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1300:LYS:NZ	1:A:1300:LYS:HB3	2.20	0.57
1:A:710:LEU:HD12	1:A:710:LEU:N	2.20	0.57
2:B:1116:ARG:HD2	2:B:1198:TYR:CG	2.40	0.57
5:E:46:TYR:CE2	5:E:58:MET:HA	2.40	0.57
8:H:89:LEU:HD22	8:H:91:ASP:CG	2.25	0.57
2:B:955:THR:OG1	12:L:55:ILE:HA	2.04	0.57
1:A:1017:LEU:HD23	5:E:204:THR:O	2.05	0.56
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.86	0.56
2:B:806:THR:OG1	2:B:809:MET:HE3	2.04	0.56
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	1.87	0.56
3:C:242:GLN:NE2	3:C:246:ARG:HE	2.02	0.56
1:A:742:ASN:CA	1:A:745:GLN:HB2	2.33	0.56
2:B:1180:PHE:O	2:B:1181:GLU:HB2	2.05	0.56
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.70	0.56
8:H:89:LEU:HD22	8:H:91:ASP:OD2	2.05	0.56
11:K:51:LEU:HD13	11:K:59:ALA:HB3	1.86	0.56
2:B:844:SER:OG	2:B:996:ARG:N	2.33	0.56
2:B:864:LYS:HD3	2:B:871:THR:OG1	2.05	0.56
1:A:401:GLY:C	1:A:435:HIS:CD2	2.79	0.56
1:A:511:ILE:HA	1:A:521:MET:HE3	1.87	0.56
1:A:556:TRP:CE3	1:A:558:GLY:HA2	2.41	0.56
1:A:619:LYS:O	1:A:623:GLY:N	2.38	0.56
3:C:229:TYR:N	3:C:229:TYR:CD1	2.74	0.56
8:H:82:PRO:O	8:H:83:GLN:HB2	2.04	0.56
3:C:248:ILE:CD1	11:K:101:LEU:HD22	2.35	0.56
1:A:69:THR:HB	2:B:1174:LYS:HE2	1.87	0.56
2:B:243:ALA:HA	2:B:250:PHE:O	2.05	0.56
2:B:522:VAL:HG11	2:B:537:LYS:HB3	1.86	0.56
2:B:704:ALA:HB1	2:B:710:LEU:HD12	1.87	0.56
3:C:131:HIS:O	3:C:132:PRO:C	2.43	0.56
3:C:175:ALA:HB3	10:J:43:ARG:NH2	2.20	0.56
3:C:258:ILE:O	3:C:261:ALA:HB3	2.04	0.56
6:F:97:ARG:NE	6:F:124:GLU:OE1	2.31	0.56
6:F:99:LEU:HD12	6:F:99:LEU:O	2.05	0.56
9:I:7:CYS:C	9:I:8:ARG:O	2.43	0.56
1:A:98:LYS:O	1:A:102:VAL:HG23	2.05	0.56
1:A:185:TRP:CZ3	1:A:200:ARG:HG2	2.40	0.56
1:A:577:ILE:O	1:A:580:VAL:HG23	2.04	0.56
2:B:1079:LYS:HA	3:C:27:LEU:HD21	1.87	0.56
1:A:738:LYS:HZ1	3:C:194:GLU:C	2.09	0.56
9:I:111:THR:HG22	9:I:112:SER:N	2.19	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ASN:HA	11:K:60:ALA:HB1	1.87	0.56
5:E:195:VAL:HG22	5:E:213:ILE:HB	1.88	0.56
8:H:97:MET:HE2	8:H:142:LEU:HD23	1.86	0.56
11:K:50:LEU:CD1	11:K:73:LEU:HD21	2.35	0.56
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.69	0.56
1:A:1364:ASN:ND2	1:A:1366:ARG:N	2.53	0.56
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.41	0.56
1:A:974:ASP:HB2	8:H:136:LYS:NZ	2.21	0.56
2:B:839:MET:CE	2:B:980:PHE:HB2	2.35	0.56
8:H:97:MET:CE	8:H:142:LEU:HD23	2.35	0.56
12:L:26:THR:HG22	12:L:27:LEU:N	2.21	0.56
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.36	0.56
2:B:120:ARG:NH1	12:L:54:ARG:NH1	2.54	0.56
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.41	0.56
1:A:1365:TYR:O	1:A:1366:ARG:C	2.43	0.56
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.04	0.56
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.67	0.56
3:C:99:LEU:HD23	3:C:99:LEU:N	2.20	0.56
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.03	0.55
1:A:1328:TYR:CG	1:A:1329:THR:N	2.74	0.55
1:A:1342:GLU:HG2	5:E:212:ARG:NH1	2.20	0.55
2:B:118:ARG:NH2	2:B:194:GLU:CD	2.60	0.55
1:A:825:ILE:HD12	2:B:513:GLN:NE2	2.21	0.55
2:B:864:LYS:N	2:B:872:GLU:OE1	2.39	0.55
8:H:6:PHE:HE1	8:H:130:ARG:HE	1.53	0.55
1:A:1096:SER:O	1:A:1099:PRO:HG2	2.05	0.55
1:A:35:ILE:HG12	1:A:52:GLY:O	2.06	0.55
2:B:1171:VAL:HG11	2:B:1191:ILE:HD13	1.88	0.55
1:A:1261:LYS:HA	1:A:1264:GLU:HB3	1.88	0.55
1:A:92:HIS:HD2	1:A:94:GLY:H	1.53	0.55
2:B:984:HIS:HB3	2:B:1022:THR:OG1	2.05	0.55
2:B:479:VAL:HG12	2:B:480:SER:H	1.72	0.55
2:B:794:ASN:C	2:B:795:ILE:HD12	2.26	0.55
2:B:898:LEU:HD22	2:B:964:VAL:HG11	1.89	0.55
3:C:145:CYS:SG	3:C:146:LYS:N	2.79	0.55
11:K:61:TYR:HA	11:K:72:LYS:O	2.07	0.55
1:A:1389:PHE:O	1:A:1392:SER:HB3	2.06	0.55
1:A:672:ASP:HB3	1:A:675:THR:OG1	2.05	0.55
1:A:838:GLN:O	1:A:842:VAL:HG23	2.06	0.55
1:A:867:ILE:HG22	1:A:872:GLY:N	2.22	0.55
2:B:1159:ARG:CD	2:B:1193:GLN:HG3	2.31	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:ILE:O	2:B:37:PHE:HB3	2.06	0.55
2:B:57:TYR:HD1	2:B:57:TYR:N	2.03	0.55
2:B:780:VAL:HG21	10:J:56:LEU:HD13	1.88	0.55
3:C:56:THR:CG2	3:C:57:VAL:H	2.09	0.55
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.88	0.55
10:J:21:TYR:HA	10:J:39:LEU:HD11	1.89	0.55
1:A:665:GLY:HA3	2:B:1086:PHE:CD1	2.41	0.55
2:B:93:GLY:N	2:B:131:ASP:O	2.37	0.55
2:B:361:LEU:N	2:B:362:PRO:CD	2.69	0.55
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.89	0.55
1:A:1111:MET:CE	1:A:1114:PRO:HA	2.35	0.55
1:A:1222:ASN:O	1:A:1223:ASP:HB3	2.06	0.55
1:A:885:THR:O	1:A:885:THR:HG22	2.05	0.55
1:A:885:THR:O	1:A:940:ARG:HG3	2.07	0.55
2:B:556:THR:HG22	2:B:557:PHE:N	2.20	0.55
2:B:801:LYS:O	10:J:52:THR:CG2	2.52	0.55
1:A:517:ASN:ND2	1:A:1362:TYR:HE2	2.05	0.55
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.41	0.55
2:B:1051:THR:CG2	2:B:1052:VAL:N	2.70	0.55
2:B:566:LEU:HD22	2:B:586:TRP:O	2.06	0.55
6:F:109:VAL:HG13	6:F:127:GLU:OE1	2.07	0.55
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.47	0.55
1:A:216:VAL:O	1:A:219:PHE:HB2	2.06	0.55
1:A:463:ILE:HD11	1:A:469:ARG:HG3	1.89	0.55
1:A:15:LYS:HD2	2:B:1220:ARG:HE	1.72	0.55
2:B:130:VAL:CG2	2:B:167:ILE:HD12	2.34	0.55
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.42	0.55
2:B:515:HIS:H	2:B:518:HIS:CD2	2.24	0.55
2:B:28:GLU:CD	2:B:807:ARG:HH22	2.10	0.55
9:I:111:THR:CG2	9:I:112:SER:N	2.69	0.55
9:I:7:CYS:O	9:I:8:ARG:O	2.24	0.55
12:L:32:ALA:HB3	12:L:55:ILE:CD1	2.26	0.55
1:A:399:HIS:O	1:A:435:HIS:CD2	2.60	0.55
1:A:704:ALA:HB2	1:A:710:LEU:CG	2.23	0.55
1:A:849:MET:HE1	1:A:1061:GLY:HA2	1.87	0.55
2:B:406:LEU:HD12	2:B:545:ILE:HD11	1.89	0.55
2:B:958:GLN:O	2:B:960:GLY:N	2.33	0.55
3:C:248:ILE:HD13	11:K:101:LEU:HD22	1.89	0.55
2:B:308:TRP:CH2	9:I:45:ARG:HG2	2.42	0.55
1:A:1116:LEU:O	1:A:1308:THR:HB	2.07	0.55
1:A:50:ILE:C	1:A:52:GLY:H	2.09	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:843:LYS:HG3	1:A:1402:PHE:HD1	1.72	0.55
2:B:755:ILE:CG2	2:B:755:ILE:O	2.55	0.55
5:E:168:TYR:HB3	5:E:170:LEU:CD2	2.36	0.55
1:A:852:TYR:CE2	6:F:136:ARG:HG2	2.42	0.55
1:A:1308:THR:CG2	1:A:1310:GLY:O	2.55	0.54
1:A:339:ASN:O	1:A:343:LYS:HG2	2.07	0.54
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.47	0.54
2:B:195:CYS:CB	2:B:782:LEU:HD22	2.37	0.54
2:B:429:PHE:HA	2:B:432:MET:HE2	1.89	0.54
2:B:566:LEU:HD13	2:B:588:GLY:CA	2.37	0.54
5:E:197:LYS:HG3	5:E:211:TYR:CE2	2.42	0.54
5:E:176:PRO:HD2	5:E:211:TYR:O	2.07	0.54
8:H:89:LEU:O	8:H:91:ASP:N	2.37	0.54
9:I:2:THR:HG22	9:I:2:THR:O	2.07	0.54
1:A:122:MET:O	1:A:126:LEU:HG	2.07	0.54
1:A:646:PHE:O	1:A:650:GLN:HG3	2.07	0.54
1:A:741:ASN:ND2	1:A:743:VAL:H	2.05	0.54
8:H:59:ILE:HG22	8:H:60:ALA:N	2.21	0.54
1:A:590:ARG:O	1:A:591:PHE:HB2	2.08	0.54
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.88	0.54
2:B:680:THR:HG22	2:B:681:TRP:H	1.72	0.54
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.07	0.54
1:A:350:ARG:HB2	1:A:488:ASN:OD1	2.08	0.54
1:A:556:TRP:CD2	1:A:558:GLY:HA2	2.42	0.54
1:A:821:ARG:O	1:A:822:GLU:C	2.46	0.54
1:A:89:PRO:O	1:A:204:THR:HG21	2.07	0.54
2:B:172:ILE:HD13	2:B:178:ASN:CB	2.37	0.54
5:E:153:HIS:CE1	5:E:184:VAL:HG11	2.43	0.54
1:A:451:HIS:CE1	1:A:1074:GLU:HG3	2.42	0.54
1:A:809:THR:O	1:A:810:PRO:C	2.46	0.54
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.23	0.54
2:B:784:ASN:ND2	2:B:788:ARG:HD2	2.23	0.54
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.37	0.54
3:C:13:ALA:O	11:K:114:LEU:HD13	2.08	0.54
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.42	0.54
5:E:195:VAL:HG22	5:E:213:ILE:CB	2.36	0.54
2:B:783:THR:HA	10:J:60:PHE:HE1	1.72	0.54
12:L:63:ARG:O	12:L:64:LEU:O	2.24	0.54
1:A:1205:LYS:O	1:A:1207:LEU:N	2.41	0.54
1:A:1225:PHE:CE2	1:A:1227:ILE:HD11	2.43	0.54
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.72	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1341:ILE:HD12	1:A:1379:GLY:C	2.28	0.54
1:A:963:ILE:HD12	1:A:1049:ILE:HG12	1.88	0.54
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.88	0.54
5:E:46:TYR:CD2	5:E:58:MET:HG2	2.42	0.54
6:F:107:VAL:HG12	6:F:109:VAL:H	1.72	0.54
6:F:72:LYS:N	6:F:142:SER:HA	2.22	0.54
8:H:84:ALA:HA	8:H:87:ARG:HG3	1.88	0.54
1:A:443:LEU:HD13	1:A:455:MET:HE1	1.89	0.54
1:A:515:GLN:HG3	1:A:516:SER:N	2.22	0.54
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.42	0.54
2:B:292:ILE:H	2:B:293:PRO:HD2	1.73	0.54
2:B:542:MET:HE2	2:B:747:MET:HE2	1.89	0.54
2:B:43:LEU:HD13	2:B:812:LEU:CD2	2.38	0.54
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.42	0.54
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.54	0.54
5:E:61:GLN:NE2	5:E:105:PHE:CE2	2.71	0.54
1:A:1366:ARG:O	1:A:1369:ALA:HB3	2.08	0.54
1:A:367:PRO:HB3	1:A:465:TYR:O	2.08	0.54
1:A:533:LYS:O	1:A:535:THR:N	2.40	0.54
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.89	0.54
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.88	0.54
2:B:640:VAL:O	2:B:641:GLU:C	2.46	0.54
2:B:758:PHE:C	2:B:760:ASP:H	2.10	0.54
2:B:898:LEU:CD2	2:B:964:VAL:HG11	2.38	0.54
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.89	0.54
1:A:710:LEU:H	1:A:710:LEU:CD1	2.19	0.54
2:B:288:ALA:HB1	2:B:331:LEU:CD1	2.38	0.54
2:B:43:LEU:HD13	2:B:812:LEU:HD23	1.90	0.54
2:B:120:ARG:HE	2:B:955:THR:CG2	2.20	0.54
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.91	0.54
1:A:337:ARG:NE	1:A:839:ARG:NH2	2.55	0.54
1:A:845:LEU:N	1:A:845:LEU:HD23	2.22	0.54
2:B:864:LYS:HG3	2:B:865:LYS:N	2.22	0.54
1:A:1341:ILE:HD12	1:A:1379:GLY:O	2.07	0.53
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.89	0.53
1:A:90:VAL:HG13	1:A:297:GLN:HA	1.90	0.53
2:B:287:ARG:CG	2:B:292:ILE:HA	2.26	0.53
2:B:484:ASN:ND2	2:B:486:TYR:CD1	2.76	0.53
6:F:114:GLU:OE1	6:F:119:ARG:HG3	2.08	0.53
6:F:94:LEU:HD21	6:F:122:MET:HA	1.89	0.53
10:J:32:GLU:O	10:J:36:LEU:HG	2.07	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.23	0.53
12:L:60:ARG:CG	12:L:61:THR:H	1.94	0.53
1:A:444:PHE:HB3	1:A:458:HIS:CD2	2.43	0.53
1:A:61:ILE:HG22	1:A:62:ASP:N	2.16	0.53
2:B:1169:MET:HE3	2:B:1205:GLN:HG2	1.90	0.53
2:B:549:THR:HB	2:B:628:THR:HG23	1.89	0.53
2:B:837:ASP:OD1	2:B:1020:ARG:NH2	2.41	0.53
1:A:1375:MET:HG2	1:A:1382:THR:O	2.08	0.53
1:A:233:TRP:C	1:A:235:ILE:N	2.60	0.53
1:A:898:ARG:HD2	1:A:899:VAL:H	1.73	0.53
1:A:92:HIS:CD2	1:A:94:GLY:H	2.26	0.53
2:B:956:THR:CG2	2:B:960:GLY:HA2	2.38	0.53
12:L:27:LEU:HD13	12:L:37:LYS:HB3	1.90	0.53
1:A:696:GLU:OE2	1:A:702:LEU:HD23	2.08	0.53
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.38	0.53
2:B:644:GLU:HG3	2:B:654:ARG:HH22	1.74	0.53
2:B:756:ILE:HG21	2:B:759:PRO:HB3	1.90	0.53
2:B:899:ILE:HD11	2:B:910:VAL:O	2.09	0.53
3:C:189:THR:HG22	3:C:190:ASP:N	2.24	0.53
9:I:29:CYS:O	9:I:29:CYS:SG	2.66	0.53
1:A:1029:ARG:HG3	1:A:1029:ARG:HH11	1.74	0.53
1:A:1111:MET:CE	1:A:1330:ASN:OD1	2.57	0.53
1:A:32:VAL:HG21	1:A:68:GLN:HE22	1.74	0.53
1:A:38:PRO:N	1:A:270:LEU:HD23	2.22	0.53
1:A:557:ASP:OD2	1:A:559:VAL:HB	2.08	0.53
1:A:567:LYS:HZ2	8:H:46:LEU:CB	2.21	0.53
1:A:693:VAL:HG21	1:A:721:PHE:CE1	2.39	0.53
2:B:235:SER:OG	2:B:236:HIS:HD2	1.91	0.53
2:B:405:ARG:HA	2:B:631:GLY:O	2.09	0.53
9:I:62:ILE:HG23	9:I:63:GLY:N	2.22	0.53
12:L:70:ARG:HG2	12:L:70:ARG:NH1	2.22	0.53
1:A:1195:LEU:HD11	1:A:1267:MET:HE3	1.91	0.53
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.38	0.53
1:A:683:ILE:HD11	1:A:764:CYS:CB	2.35	0.53
1:A:529:CYS:HB2	2:B:1015:HIS:CE1	2.44	0.53
2:B:287:ARG:HA	2:B:291:ILE:O	2.09	0.53
5:E:23:VAL:HG12	5:E:28:TYR:HB2	1.89	0.53
6:F:118:LEU:O	6:F:122:MET:HG3	2.08	0.53
1:A:13:THR:HG23	1:A:1432:GLN:NE2	2.24	0.53
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.91	0.53
1:A:552:TRP:NE1	1:A:655:PHE:CD1	2.77	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:ILE:HD11	2:B:461:LEU:HD23	1.90	0.53
8:H:38:LEU:CD1	8:H:125:LEU:HD13	2.38	0.53
1:A:1220:PHE:O	1:A:1222:ASN:N	2.42	0.53
1:A:114:LEU:HD22	1:A:171:GLN:NE2	2.23	0.53
1:A:185:TRP:HZ3	1:A:200:ARG:HG2	1.74	0.53
1:A:384:ASN:OD1	1:A:385:ILE:N	2.42	0.53
1:A:741:ASN:ND2	1:A:741:ASN:C	2.62	0.53
1:A:852:TYR:CZ	6:F:136:ARG:HG2	2.44	0.53
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.08	0.53
2:B:90:ILE:CD1	2:B:432:MET:SD	2.97	0.53
2:B:542:MET:HE1	2:B:743:ILE:CG2	2.39	0.53
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.91	0.53
2:B:806:THR:C	2:B:808:ALA:H	2.13	0.53
2:B:857:ARG:HD2	2:B:945:GLU:OE1	2.08	0.53
6:F:132:LEU:O	6:F:148:VAL:HG23	2.09	0.53
9:I:46:HIS:CD2	9:I:48:LEU:HD21	2.44	0.53
1:A:1161:THR:HG22	1:A:1162:VAL:N	2.24	0.53
1:A:1193:LEU:HD21	1:A:1267:MET:HE2	1.91	0.53
1:A:1436:ILE:CG2	1:A:1437:GLY:H	2.22	0.53
1:A:442:VAL:O	1:A:457:ALA:HA	2.09	0.53
1:A:902:LEU:HD21	1:A:923:LEU:HD23	1.90	0.53
2:B:59:LEU:HD11	2:B:417:PHE:CZ	2.44	0.53
1:A:91:PHE:HB2	1:A:297:GLN:OE1	2.09	0.53
2:B:240:ILE:HG23	2:B:240:ILE:O	2.09	0.53
2:B:547:VAL:H	2:B:612:GLU:CD	2.13	0.53
3:C:46:ILE:HD13	3:C:157:CYS:CB	2.39	0.53
3:C:57:VAL:HG11	10:J:60:PHE:HB2	1.88	0.53
5:E:28:TYR:CE1	5:E:78:LEU:HD12	2.44	0.53
8:H:6:PHE:O	8:H:58:THR:HA	2.08	0.53
9:I:73:ARG:O	9:I:81:ARG:HA	2.09	0.53
2:B:120:ARG:NH2	12:L:54:ARG:HD2	2.24	0.53
1:A:134:ARG:HH12	1:A:220:THR:HG22	1.74	0.52
1:A:928:LEU:O	1:A:931:GLU:N	2.43	0.52
2:B:234:ILE:H	2:B:234:ILE:CD1	2.16	0.52
2:B:234:ILE:HG21	2:B:257:LYS:HB3	1.91	0.52
2:B:484:ASN:ND2	2:B:486:TYR:CE1	2.77	0.52
3:C:241:ASP:O	3:C:245:VAL:HG23	2.08	0.52
5:E:12:LEU:HD22	5:E:55:ARG:CZ	2.39	0.52
5:E:17:ARG:O	5:E:21:GLU:HG3	2.09	0.52
5:E:78:LEU:HD21	5:E:109:ILE:HD12	1.90	0.52
8:H:32:THR:HG22	8:H:33:GLN:HG3	1.90	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:PRO:HA	9:I:12:ASN:HD21	1.74	0.52
12:L:38:LEU:HG	12:L:39:SER:N	2.24	0.52
1:A:1116:LEU:N	1:A:1308:THR:HG22	2.24	0.52
1:A:1365:TYR:O	1:A:1367:HIS:N	2.42	0.52
1:A:225:ASN:O	1:A:227:VAL:HG23	2.08	0.52
1:A:226:GLU:HG2	1:A:227:VAL:HG23	1.90	0.52
1:A:666:ILE:HD11	2:B:1030:LEU:CD1	2.20	0.52
2:B:284:ILE:HD13	2:B:324:ILE:HD12	1.91	0.52
2:B:875:GLU:O	2:B:877:PRO:HD3	2.09	0.52
2:B:911:ILE:HD11	2:B:941:LEU:HD12	1.91	0.52
5:E:155:ARG:HD2	5:E:194:GLU:OE2	2.09	0.52
6:F:77:ASP:O	6:F:78:GLN:HB2	2.09	0.52
1:A:1299:VAL:CG1	1:A:1300:LYS:N	2.72	0.52
1:A:670:ILE:HD13	2:B:1067:ARG:CZ	2.39	0.52
2:B:46:GLN:NE2	2:B:496:ARG:HA	2.24	0.52
2:B:916:THR:HG22	2:B:918:ILE:HG13	1.90	0.52
3:C:93:ASP:OD1	3:C:122:SER:HB2	2.09	0.52
9:I:75:CYS:C	9:I:77:LYS:N	2.59	0.52
11:K:46:ILE:O	11:K:50:LEU:HB2	2.09	0.52
1:A:1147:THR:HA	1:A:1197:LEU:HD23	1.90	0.52
1:A:1392:SER:O	1:A:1393:ASN:CB	2.58	0.52
1:A:233:TRP:C	1:A:235:ILE:H	2.13	0.52
1:A:387:ARG:O	1:A:391:LEU:HG	2.09	0.52
2:B:25:ILE:HG22	2:B:26:THR:N	2.24	0.52
10:J:9:SER:CB	10:J:45:CYS:HB2	2.40	0.52
12:L:38:LEU:O	12:L:39:SER:CB	2.56	0.52
1:A:1319:VAL:CG1	1:A:1320:PRO:HD2	2.39	0.52
1:A:507:VAL:N	1:A:508:PRO:CD	2.72	0.52
1:A:754:SER:O	1:A:755:PHE:C	2.48	0.52
2:B:271:ALA:HB3	2:B:285:ILE:CD1	2.40	0.52
2:B:98:THR:OG1	2:B:127:GLY:HA3	2.09	0.52
7:G:141:UNK:CA	7:G:168:UNK:CA	2.87	0.52
9:I:50:THR:HG22	9:I:52:ILE:H	1.75	0.52
10:J:52:THR:O	10:J:52:THR:HG22	2.08	0.52
11:K:65:HIS:HD2	11:K:67:PHE:HB2	1.74	0.52
1:A:1336:MET:HE1	1:A:1381:LEU:HG	1.90	0.52
1:A:261:ASP:OD2	1:A:323:LYS:HD2	2.10	0.52
1:A:340:LEU:HD21	2:B:1200:ALA:CB	2.40	0.52
1:A:399:HIS:C	1:A:401:GLY:H	2.10	0.52
2:B:552:MET:N	2:B:553:PRO:HD2	2.24	0.52
2:B:842:ASN:HD22	2:B:845:SER:CB	2.21	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:35:VAL:C	5:E:37:LEU:H	2.12	0.52
9:I:29:CYS:C	9:I:31:THR:H	2.13	0.52
1:A:167:CYS:HB2	1:A:169:ASN:ND2	2.24	0.52
1:A:219:PHE:O	1:A:222:LEU:O	2.28	0.52
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.45	0.52
2:B:108:VAL:CG1	2:B:109:THR:H	2.18	0.52
2:B:614:SER:OG	2:B:627:PHE:HB2	2.09	0.52
3:C:164:ALA:HA	3:C:167:HIS:O	2.10	0.52
6:F:109:VAL:CG1	6:F:110:ASP:N	2.73	0.52
1:A:1300:LYS:HZ2	1:A:1300:LYS:HB3	1.74	0.52
1:A:326:ARG:HG2	1:A:1406:VAL:CG2	2.39	0.52
1:A:365:GLY:HA3	1:A:469:ARG:HB2	1.91	0.52
1:A:817:ALA:HA	2:B:764:SER:OG	2.10	0.52
11:K:49:GLU:OE2	11:K:97:LYS:HE3	2.10	0.52
1:A:443:LEU:HD11	2:B:1138:MET:SD	2.50	0.52
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.43	0.52
2:B:1065:GLN:NE2	2:B:1067:ARG:HG2	2.24	0.52
2:B:1197:PRO:HG2	2:B:1200:ALA:CB	2.40	0.52
1:A:96:ILE:O	1:A:100:LYS:HG3	2.10	0.52
1:A:384:ASN:OD1	1:A:388:LEU:HD12	2.10	0.52
1:A:41:MET:HG2	1:A:49:LYS:HG2	1.92	0.52
1:A:737:LEU:HD11	1:A:758:ILE:HG21	1.92	0.52
1:A:907:THR:HG22	1:A:908:LEU:N	2.25	0.52
2:B:248:SER:O	2:B:249:ARG:HB2	2.09	0.52
2:B:25:ILE:CG2	2:B:29:ASP:HB3	2.40	0.52
2:B:515:HIS:H	2:B:518:HIS:HD2	1.55	0.52
2:B:755:ILE:HG22	2:B:755:ILE:O	2.09	0.52
1:A:738:LYS:HZ2	3:C:194:GLU:HA	1.75	0.51
2:B:1163:CYS:SG	2:B:1182:CYS:SG	3.09	0.51
2:B:287:ARG:HG2	2:B:292:ILE:CA	2.27	0.51
2:B:864:LYS:HD3	2:B:871:THR:HA	1.91	0.51
11:K:63:VAL:HG23	11:K:63:VAL:O	2.08	0.51
1:A:134:ARG:NH1	1:A:220:THR:O	2.42	0.51
1:A:384:ASN:O	1:A:385:ILE:C	2.48	0.51
1:A:50:ILE:HG22	1:A:51:GLY:N	2.24	0.51
2:B:563:MET:HG3	2:B:563:MET:O	2.10	0.51
2:B:737:THR:CG2	9:I:66:PRO:HB2	2.40	0.51
2:B:751:VAL:HG12	2:B:752:ALA:N	2.26	0.51
2:B:846:ILE:HD13	2:B:974:PRO:HG2	1.91	0.51
3:C:73:GLN:HE21	3:C:75:MET:N	1.97	0.51
12:L:27:LEU:HD13	12:L:37:LYS:CG	2.41	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1326:ARG:O	1:A:1327:ILE:C	2.49	0.51
5:E:5:ASN:O	5:E:9:ILE:HG13	2.11	0.51
12:L:47:ARG:HG2	12:L:52:GLY:CA	2.39	0.51
1:A:1299:VAL:CG1	1:A:1300:LYS:H	2.20	0.51
1:A:1359:ASP:C	1:A:1361:SER:H	2.13	0.51
1:A:470:LEU:HD21	1:A:487:MET:HE3	1.92	0.51
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.45	0.51
1:A:675:THR:CG2	1:A:736:ASN:HD21	2.22	0.51
1:A:821:ARG:HG3	1:A:825:ILE:CD1	2.40	0.51
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.45	0.51
2:B:1035:ALA:HB1	2:B:1040:ASN:O	2.10	0.51
2:B:130:VAL:CG1	2:B:131:ASP:N	2.74	0.51
3:C:80:LEU:CD2	3:C:129:ILE:HD11	2.28	0.51
5:E:124:VAL:HG22	5:E:132:ILE:CG2	2.39	0.51
8:H:84:ALA:C	8:H:86:ASP:N	2.64	0.51
9:I:75:CYS:HG	9:I:106:CYS:HG	1.59	0.51
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.92	0.51
1:A:753:GLY:HA2	1:A:757:ASN:HD22	1.74	0.51
1:A:898:ARG:HD2	1:A:899:VAL:N	2.26	0.51
1:A:929:LEU:H	1:A:929:LEU:CD2	2.23	0.51
2:B:31:TRP:CD1	2:B:807:ARG:NH1	2.78	0.51
1:A:357:PRO:HG2	2:B:833:TYR:CE1	2.45	0.51
3:C:177:GLU:HG3	3:C:231:ASN:HB3	1.93	0.51
5:E:23:VAL:HG13	5:E:28:TYR:CD1	2.45	0.51
6:F:109:VAL:CG2	6:F:124:GLU:HG2	2.40	0.51
1:A:1150:SER:HB2	1:A:1195:LEU:HD23	1.93	0.51
1:A:1362:TYR:OH	1:A:1364:ASN:HA	2.11	0.51
1:A:27:VAL:HG13	1:A:240:PRO:HB3	1.91	0.51
1:A:306:ASN:HD21	1:A:324:SER:N	2.09	0.51
1:A:444:PHE:CB	1:A:458:HIS:HD2	2.24	0.51
1:A:847:ASP:OD2	1:A:858:ASN:HB2	2.10	0.51
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.10	0.51
2:B:120:ARG:HB2	2:B:122:LEU:HG	1.91	0.51
2:B:463:THR:HG21	2:B:465:ASN:HD22	1.74	0.51
2:B:514:LEU:HD12	2:B:515:HIS:H	1.74	0.51
2:B:825:VAL:HG12	2:B:826:ALA:N	2.24	0.51
5:E:121:MET:C	5:E:123:LEU:H	2.13	0.51
11:K:24:ASP:HB3	11:K:30:ALA:HB3	1.93	0.51
1:A:1152:ILE:CG2	1:A:1260:LEU:HD23	2.38	0.51
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	2.09	0.51
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.93	0.51
6:F:101:ILE:HD13	6:F:120:ILE:HG22	1.91	0.51
10:J:7:CYS:SG	10:J:9:SER:HB2	2.50	0.51
12:L:62:LYS:O	12:L:64:LEU:HG	2.11	0.51
12:L:62:LYS:C	12:L:64:LEU:H	2.13	0.51
1:A:1214:GLU:O	1:A:1218:GLN:HG2	2.10	0.51
1:A:332:LYS:H	1:A:337:ARG:HD2	1.76	0.51
1:A:596:THR:O	1:A:597:LEU:C	2.48	0.51
1:A:649:ILE:O	1:A:653:VAL:HG23	2.11	0.51
2:B:185:THR:O	2:B:189:LEU:HG	2.11	0.51
2:B:271:ALA:O	2:B:279:ASP:HA	2.11	0.51
2:B:283:VAL:HG13	2:B:297:ILE:CD1	2.41	0.51
2:B:428:ILE:O	2:B:431:TYR:HB3	2.10	0.51
2:B:707:PRO:CG	2:B:708:GLU:H	2.21	0.51
1:A:817:ALA:HA	2:B:764:SER:HG	1.76	0.51
11:K:101:LEU:HD23	11:K:101:LEU:O	2.11	0.51
1:A:115:LEU:HB2	1:A:122:MET:CE	2.41	0.51
1:A:1269:GLU:OE2	2:B:263:GLY:HA3	2.10	0.51
1:A:1351:GLU:O	1:A:1352:VAL:C	2.49	0.51
1:A:722:LEU:HD11	1:A:794:PRO:HB3	1.92	0.51
1:A:15:LYS:CB	2:B:1220:ARG:HG2	2.33	0.51
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.76	0.51
5:E:168:TYR:HB3	5:E:170:LEU:CG	2.41	0.51
5:E:54:GLN:O	5:E:57:MET:HB3	2.11	0.51
8:H:83:GLN:C	8:H:85:GLY:H	2.14	0.51
1:A:107:CYS:HB2	1:A:114:LEU:HD23	1.93	0.51
1:A:376:TYR:OH	1:A:498:ARG:HD2	2.10	0.51
1:A:901:LEU:HD23	1:A:907:THR:HG23	1.92	0.51
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.92	0.51
1:A:500:GLU:OE1	2:B:1143:ALA:HB1	2.11	0.51
2:B:365:THR:HG23	2:B:367:LEU:HG	1.93	0.51
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.11	0.50
1:A:49:LYS:HB3	1:A:55:ASP:HB2	1.92	0.50
1:A:709:THR:CB	1:A:712:GLU:HG3	2.41	0.50
1:A:786:HIS:CE1	2:B:705:MET:HE1	2.46	0.50
2:B:1177:HIS:HB3	2:B:1179:GLN:HE21	1.74	0.50
2:B:101:MET:HE2	2:B:169:ARG:HH12	1.76	0.50
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.45	0.50
2:B:827:ILE:HG12	2:B:1012:ILE:HD11	1.93	0.50
2:B:1084:GLN:CD	2:B:1084:GLN:H	2.14	0.50
2:B:1106:ARG:HH12	2:B:1118:PRO:CB	2.24	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:47:ARG:CB	11:K:47:ARG:HH11	2.23	0.50
1:A:1376:THR:HG23	1:A:1376:THR:O	2.12	0.50
1:A:857:ARG:HG2	1:A:863:VAL:HA	1.94	0.50
2:B:1177:HIS:CB	2:B:1179:GLN:HE21	2.24	0.50
5:E:157:SER:C	5:E:159:ASP:N	2.64	0.50
1:A:1376:THR:HG23	5:E:212:ARG:NH2	2.26	0.50
8:H:128:ASN:O	8:H:131:ASN:ND2	2.45	0.50
8:H:84:ALA:C	8:H:86:ASP:H	2.13	0.50
8:H:95:TYR:HE2	8:H:97:MET:HG3	1.74	0.50
1:A:587:HIS:HA	1:A:607:ILE:O	2.11	0.50
2:B:1119:VAL:O	2:B:1126:GLY:HA3	2.11	0.50
2:B:485:ARG:NH2	2:B:782:LEU:HD11	2.27	0.50
2:B:581:PHE:HB2	2:B:625:LYS:HG2	1.93	0.50
2:B:737:THR:HG23	9:I:66:PRO:HB2	1.93	0.50
9:I:68:LEU:HB3	9:I:84:VAL:HG22	1.94	0.50
10:J:36:LEU:HD13	10:J:47:ARG:HG2	1.92	0.50
11:K:91:CYS:O	11:K:95:ILE:HG13	2.11	0.50
1:A:1384:VAL:O	1:A:1384:VAL:HG12	2.11	0.50
1:A:573:SER:O	1:A:576:GLN:HB2	2.11	0.50
1:A:810:PRO:O	1:A:813:PHE:HB3	2.11	0.50
1:A:829:VAL:C	1:A:831:THR:H	2.15	0.50
2:B:271:ALA:HB3	2:B:285:ILE:HD11	1.93	0.50
2:B:559:SER:HA	2:B:563:MET:HB3	1.91	0.50
2:B:542:MET:CG	2:B:747:MET:HE3	2.38	0.50
10:J:54:VAL:O	10:J:56:LEU:N	2.43	0.50
1:A:418:SER:C	1:A:420:ARG:N	2.63	0.50
2:B:292:ILE:N	2:B:293:PRO:HD2	2.25	0.50
2:B:800:GLN:OE1	2:B:822:ASN:HB2	2.12	0.50
9:I:101:PHE:O	9:I:109:ILE:HA	2.12	0.50
9:I:15:TYR:N	9:I:15:TYR:CD1	2.79	0.50
9:I:25:LEU:HD12	9:I:26:LEU:H	1.76	0.50
9:I:75:CYS:O	9:I:77:LYS:N	2.44	0.50
3:C:66:ARG:NH2	10:J:2:ILE:CG2	2.74	0.50
12:L:51:CYS:C	12:L:53:HIS:H	2.11	0.50
1:A:100:LYS:NZ	1:A:176:LYS:HD2	2.27	0.50
1:A:341:MET:CE	1:A:1401:SER:HB2	2.40	0.50
1:A:751:SER:O	1:A:752:LYS:CG	2.59	0.50
2:B:1053:GLU:O	2:B:1054:GLY:C	2.50	0.50
2:B:35:SER:O	2:B:36:ALA:C	2.50	0.50
5:E:177:ARG:O	5:E:212:ARG:HD3	2.11	0.50
1:A:1153:TYR:HA	9:I:41:PRO:O	2.12	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:THR:HG23	1:A:575:LYS:HE2	1.93	0.50
1:A:893:PHE:CE1	1:A:940:ARG:HD2	2.46	0.50
1:A:888:GLY:O	1:A:940:ARG:NH2	2.44	0.50
2:B:977:GLY:CA	2:B:1099:VAL:CG2	2.86	0.50
2:B:519:TRP:HZ2	2:B:705:MET:CE	2.24	0.50
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.41	0.50
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.42	0.50
2:B:858:SER:HA	2:B:966:VAL:O	2.12	0.50
2:B:975:GLN:O	2:B:990:ILE:HD12	2.12	0.50
3:C:142:VAL:H	10:J:16:ASP:HB3	1.77	0.50
5:E:80:VAL:HG22	5:E:109:ILE:HD12	1.94	0.50
12:L:40:LEU:HD13	12:L:44:ASP:OD1	2.11	0.50
1:A:1094:VAL:HG13	1:A:1113:THR:CG2	2.37	0.50
1:A:1194:ARG:HH22	1:A:1237:ILE:HD13	1.73	0.50
1:A:346:ASP:CG	2:B:1108:ARG:HA	2.31	0.50
1:A:511:ILE:HG12	1:A:521:MET:CE	2.42	0.50
1:A:612:ILE:O	1:A:612:ILE:HG23	2.12	0.50
1:A:329:LEU:HD22	2:B:1203:LEU:CD1	2.41	0.50
2:B:648:HIS:NE2	2:B:650:GLU:OE1	2.43	0.50
3:C:254:LYS:HE2	11:K:42:LEU:HD13	1.94	0.50
5:E:98:ILE:O	5:E:102:GLU:HG3	2.12	0.50
5:E:46:TYR:HE2	5:E:58:MET:HA	1.76	0.50
6:F:82:THR:HG22	6:F:84:TYR:N	2.27	0.50
9:I:99:LEU:HB2	9:I:112:SER:HB3	1.94	0.50
9:I:29:CYS:SG	9:I:31:THR:HG22	2.52	0.50
1:A:105:CYS:SG	1:A:138:ILE:HG22	2.52	0.49
1:A:332:LYS:HG3	1:A:333:GLU:HG2	1.94	0.49
1:A:819:GLY:O	1:A:820:GLY:C	2.49	0.49
1:A:929:LEU:HD21	1:A:983:ILE:HG21	1.94	0.49
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.51	0.49
2:B:240:ILE:O	2:B:253:THR:HG23	2.11	0.49
3:C:33:LEU:HG	3:C:37:MET:CE	2.41	0.49
8:H:76:THR:HG22	8:H:76:THR:O	2.11	0.49
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.94	0.49
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.93	0.49
1:A:466:SER:HB3	11:K:2:ASN:ND2	2.27	0.49
1:A:1142:THR:O	1:A:1273:LEU:HD22	2.12	0.49
1:A:741:ASN:ND2	1:A:743:VAL:N	2.60	0.49
1:A:808:LEU:O	2:B:728:ARG:NH1	2.43	0.49
2:B:1043:ASP:O	2:B:1050:ILE:HD12	2.12	0.49
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.27	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:708:GLU:C	2:B:710:LEU:H	2.16	0.49
2:B:873:THR:O	2:B:914:LYS:HA	2.12	0.49
3:C:75:MET:HG3	3:C:246:ARG:NH2	2.28	0.49
5:E:56:LYS:HG3	5:E:84:ASP:CB	2.42	0.49
1:A:135:PHE:HD1	1:A:222:LEU:HD22	1.76	0.49
1:A:394:ASN:OD1	1:A:398:GLU:OE1	2.30	0.49
1:A:675:THR:HG21	1:A:736:ASN:HD21	1.77	0.49
1:A:821:ARG:CG	1:A:825:ILE:HD11	2.41	0.49
2:B:260:GLY:O	2:B:267:ARG:HD3	2.12	0.49
2:B:542:MET:HG3	2:B:747:MET:CE	2.38	0.49
2:B:570:VAL:HG11	2:B:573:GLN:OE1	2.13	0.49
2:B:734:HIS:O	2:B:735:ALA:HB2	2.12	0.49
3:C:77:ILE:HG23	3:C:161:LYS:HE3	1.94	0.49
6:F:133:VAL:HG22	6:F:147:SER:HA	1.94	0.49
8:H:6:PHE:HE1	8:H:130:ARG:NE	2.10	0.49
8:H:93:TYR:HA	8:H:145:ARG:CB	2.41	0.49
1:A:1349:TYR:CD2	1:A:1349:TYR:C	2.84	0.49
2:B:1118:PRO:HD3	2:B:1155:SER:HA	1.95	0.49
2:B:65:GLU:HG3	2:B:66:ASP:N	2.27	0.49
2:B:660:LYS:O	2:B:663:ALA:HB3	2.13	0.49
8:H:31:THR:O	8:H:32:THR:HB	2.11	0.49
8:H:47:PHE:HB2	8:H:95:TYR:HD1	1.76	0.49
1:A:1099:PRO:O	1:A:1102:LYS:HB3	2.13	0.49
1:A:1134:ILE:O	1:A:1138:ILE:HG13	2.12	0.49
2:B:896:ASP:OD2	12:L:58:LYS:HE3	2.13	0.49
1:A:738:LYS:NZ	3:C:194:GLU:HA	2.26	0.49
3:C:43:THR:CG2	3:C:44:LEU:N	2.75	0.49
6:F:81:THR:HG22	6:F:82:THR:H	1.78	0.49
8:H:44:VAL:O	8:H:44:VAL:HG12	2.12	0.49
11:K:97:LYS:O	11:K:100:ALA:HB3	2.12	0.49
12:L:52:GLY:O	12:L:54:ARG:HG3	2.12	0.49
1:A:474:VAL:HG13	1:A:478:TYR:CE1	2.48	0.49
1:A:538:ASP:OD1	8:H:22:LYS:HB2	2.12	0.49
2:B:171:PRO:HD2	2:B:457:LEU:CD1	2.43	0.49
3:C:75:MET:HG3	3:C:246:ARG:HH22	1.77	0.49
5:E:191:LYS:O	5:E:192:ARG:C	2.51	0.49
10:J:7:CYS:O	10:J:8:PHE:C	2.50	0.49
1:A:226:GLU:CG	1:A:227:VAL:N	2.75	0.49
1:A:391:LEU:O	1:A:394:ASN:N	2.46	0.49
1:A:545:GLN:O	1:A:548:ASN:N	2.44	0.49
1:A:74:MET:O	1:A:75:ASN:HB2	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:726:ALA:HB1	2:B:1051:THR:CG2	2.43	0.49
2:B:1208:MET:HA	2:B:1212:ILE:O	2.12	0.49
1:A:974:ASP:HB2	8:H:136:LYS:HZ1	1.77	0.49
8:H:88:SER:O	8:H:89:LEU:HG	2.12	0.49
9:I:85:PHE:O	9:I:86:PHE:HB3	2.12	0.49
1:A:225:ASN:C	1:A:227:VAL:H	2.10	0.49
1:A:418:SER:HB3	1:A:421:ALA:HB2	1.94	0.49
2:B:25:ILE:CG2	2:B:29:ASP:CB	2.91	0.49
1:A:795:GLU:HG2	2:B:731:VAL:HG21	1.93	0.49
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.45	0.49
3:C:4:GLU:O	3:C:5:GLY:O	2.31	0.49
11:K:55:LYS:CD	11:K:78:THR:HB	2.42	0.49
1:A:1100:ARG:NH2	1:A:1330:ASN:HB2	2.28	0.49
2:B:225:VAL:HG11	2:B:388:CYS:HB3	1.95	0.49
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.48	0.49
2:B:380:TYR:CE1	2:B:384:ARG:HD3	2.48	0.49
2:B:488:TYR:CE2	2:B:813:LYS:HB2	2.48	0.49
2:B:756:ILE:CG2	2:B:759:PRO:HB3	2.42	0.49
2:B:890:TYR:O	2:B:892:LYS:N	2.46	0.49
2:B:906:SER:O	2:B:907:GLY:C	2.50	0.49
2:B:839:MET:HE2	2:B:980:PHE:CD1	2.48	0.49
2:B:737:THR:CG2	9:I:66:PRO:CB	2.89	0.49
10:J:16:ASP:OD1	10:J:17:LYS:HE3	2.12	0.49
1:A:1392:SER:O	1:A:1393:ASN:CG	2.52	0.49
1:A:378:GLU:HG2	1:A:388:LEU:HD11	1.94	0.49
1:A:337:ARG:CZ	1:A:839:ARG:HH12	2.22	0.49
2:B:1106:ARG:HH21	2:B:1109:GLY:C	2.16	0.49
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.46	0.49
2:B:781:PHE:O	2:B:782:LEU:HG	2.12	0.49
4:D:118:UNK:CA	4:D:119:UNK:CA	2.91	0.49
8:H:59:ILE:O	8:H:60:ALA:HB3	2.12	0.49
11:K:83:PRO:HA	11:K:86:ALA:HB3	1.95	0.49
1:A:1001:ARG:HG2	1:A:1001:ARG:HH11	1.77	0.48
1:A:89:PRO:C	1:A:204:THR:HG21	2.33	0.48
2:B:1053:GLU:O	2:B:1055:ILE:N	2.46	0.48
2:B:1106:ARG:NH2	2:B:1109:GLY:C	2.67	0.48
2:B:821:GLN:OE1	2:B:850:LEU:HD12	2.13	0.48
1:A:332:LYS:N	1:A:337:ARG:HD2	2.28	0.48
1:A:491:VAL:O	1:A:493:GLN:NE2	2.46	0.48
1:A:589:GLN:OE1	1:A:591:PHE:HE1	1.96	0.48
1:A:69:THR:HG22	1:A:69:THR:O	2.12	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:LYS:HB3	8:H:19:ARG:HH22	1.79	0.48
1:A:61:ILE:HA	1:A:74:MET:SD	2.53	0.48
1:A:918:GLU:O	1:A:918:GLU:HG3	2.12	0.48
2:B:1060:ARG:O	2:B:1063:GLY:N	2.45	0.48
2:B:1065:GLN:HE22	2:B:1067:ARG:HG2	1.79	0.48
2:B:1160:VAL:HG11	2:B:1169:MET:SD	2.53	0.48
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.95	0.48
5:E:100:ILE:CG2	5:E:105:PHE:HB2	2.42	0.48
8:H:39:THR:O	8:H:123:MET:HA	2.14	0.48
8:H:49:VAL:CG1	8:H:50:ALA:N	2.75	0.48
1:A:1189:SER:OG	1:A:1190:PRO:HD2	2.12	0.48
1:A:68:GLN:NE2	1:A:80:HIS:CB	2.76	0.48
2:B:283:VAL:O	2:B:286:PHE:HB2	2.11	0.48
2:B:351:TYR:O	2:B:355:ILE:HG13	2.12	0.48
2:B:227:LYS:HB2	2:B:395:GLN:OE1	2.13	0.48
1:A:1406:VAL:CG1	1:A:1410:PHE:HE1	2.26	0.48
1:A:1436:ILE:CG2	1:A:1437:GLY:N	2.72	0.48
1:A:606:LEU:HB2	1:A:614:PHE:CE2	2.47	0.48
1:A:783:THR:HG21	1:A:815:PHE:CE2	2.48	0.48
2:B:1162:ILE:HD11	2:B:1194:ILE:CD1	2.41	0.48
2:B:653:VAL:HG12	2:B:654:ARG:N	2.28	0.48
2:B:911:ILE:HD11	2:B:941:LEU:HB2	1.94	0.48
3:C:11:ARG:NH2	3:C:229:TYR:CD2	2.68	0.48
3:C:142:VAL:H	10:J:16:ASP:CB	2.26	0.48
3:C:254:LYS:O	3:C:258:ILE:HD13	2.13	0.48
5:E:102:GLU:O	5:E:104:ASN:N	2.46	0.48
6:F:87:LYS:HE2	6:F:88:TYR:CE1	2.48	0.48
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.54	0.48
1:A:1412:ALA:HA	1:A:1417:GLU:OE2	2.14	0.48
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.92	0.48
1:A:381:THR:O	1:A:384:ASN:N	2.41	0.48
1:A:475:THR:CG2	1:A:476:SER:N	2.76	0.48
1:A:874:ASP:HA	1:A:1058:VAL:HG22	1.95	0.48
1:A:913:LEU:HD11	1:A:981:LEU:O	2.14	0.48
6:F:82:THR:HG22	6:F:84:TYR:H	1.77	0.48
7:G:136:UNK:CA	7:G:137:UNK:CA	2.91	0.48
11:K:43:GLY:HA2	11:K:71:PHE:CZ	2.49	0.48
1:A:31:SER:HB2	1:A:83:HIS:HB2	1.91	0.48
1:A:365:GLY:O	1:A:468:PHE:HA	2.14	0.48
1:A:674:PRO:O	1:A:677:ARG:HB3	2.13	0.48
1:A:89:PRO:HG3	1:A:208:LEU:CD1	2.44	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:LEU:N	2:B:298:LEU:HD23	2.29	0.48
2:B:363:HIS:CD2	2:B:585:VAL:HG22	2.49	0.48
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.95	0.48
9:I:62:ILE:CG2	9:I:63:GLY:N	2.77	0.48
11:K:27:ALA:HB1	11:K:28:PRO:HD2	1.96	0.48
1:A:742:ASN:O	1:A:745:GLN:HB2	2.13	0.48
2:B:1077:THR:HG22	2:B:1079:LYS:HB2	1.94	0.48
2:B:994:TYR:HD1	2:B:999:MET:HE3	1.78	0.48
8:H:33:GLN:OE1	8:H:129:TYR:CE2	2.67	0.48
8:H:36:CYS:HA	8:H:126:GLU:O	2.13	0.48
1:A:112:LYS:HG2	1:A:113:LEU:H	1.79	0.48
1:A:178:GLY:O	1:A:179:LEU:HD23	2.13	0.48
1:A:376:TYR:CD2	1:A:376:TYR:C	2.87	0.48
1:A:531:ILE:CD1	1:A:617:VAL:HG11	2.44	0.48
2:B:284:ILE:CD1	2:B:324:ILE:HD12	2.43	0.48
2:B:821:GLN:HB2	2:B:851:PHE:CE2	2.49	0.48
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.14	0.48
1:A:167:CYS:O	1:A:169:ASN:N	2.45	0.48
1:A:1410:PHE:CE2	2:B:1212:ILE:HD11	2.45	0.48
2:B:566:LEU:CD1	2:B:588:GLY:HA2	2.44	0.48
2:B:825:VAL:CG1	2:B:826:ALA:N	2.76	0.48
1:A:1066:VAL:O	1:A:1068:ALA:N	2.46	0.48
1:A:1074:GLU:C	1:A:1076:ALA:N	2.67	0.48
1:A:18:GLN:O	2:B:1215:ARG:CG	2.62	0.48
1:A:226:GLU:HG2	1:A:227:VAL:N	2.29	0.48
1:A:54:ASN:HA	1:A:58:LEU:HD12	1.95	0.48
1:A:834:THR:HG21	1:A:1077:THR:CA	2.43	0.48
1:A:954:TRP:O	1:A:956:LEU:HG	2.14	0.48
2:B:315:LYS:O	2:B:318:VAL:N	2.46	0.48
3:C:43:THR:HG22	3:C:44:LEU:N	2.29	0.48
6:F:79:ARG:HG2	6:F:146:TRP:CZ2	2.49	0.48
6:F:98:ALA:O	6:F:117:PRO:HB2	2.14	0.48
11:K:10:PHE:CE1	11:K:11:LEU:HD13	2.49	0.48
12:L:62:LYS:O	12:L:64:LEU:N	2.37	0.48
1:A:1192:LEU:HD11	1:A:1239:ARG:CB	2.37	0.47
1:A:1284:MET:HG2	1:A:1306:LEU:CD2	2.43	0.47
2:B:55:VAL:HG12	2:B:56:ASP:N	2.27	0.47
3:C:258:ILE:HG23	11:K:19:LEU:HD11	1.96	0.47
5:E:102:GLU:C	5:E:104:ASN:N	2.67	0.47
8:H:118:PHE:HB2	8:H:121:LEU:HB2	1.95	0.47
9:I:50:THR:HG22	9:I:51:ASN:N	2.28	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:LEU:CD2	1:A:455:MET:HB3	2.42	0.47
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.96	0.47
2:B:1156:ASP:HB3	2:B:1197:PRO:HA	1.95	0.47
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.29	0.47
2:B:324:ILE:HG23	2:B:329:THR:HB	1.96	0.47
2:B:864:LYS:HB3	2:B:871:THR:HA	1.96	0.47
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.95	0.47
3:C:35:ARG:O	3:C:38:ILE:N	2.47	0.47
8:H:138:GLU:O	8:H:139:ASN:C	2.53	0.47
10:J:48:ARG:HE	10:J:49:MET:HE2	1.79	0.47
1:A:1386:ARG:HE	1:A:1387:HIS:CE1	2.32	0.47
2:B:1158:PHE:HE2	2:B:1201:LYS:HE3	1.80	0.47
2:B:284:ILE:HD13	2:B:333:PHE:CD2	2.49	0.47
2:B:269:ILE:CD1	2:B:386:LEU:HD21	2.39	0.47
2:B:871:THR:HG22	2:B:872:GLU:O	2.14	0.47
3:C:62:PHE:O	3:C:66:ARG:HG3	2.13	0.47
9:I:54:GLU:O	9:I:89:GLN:HG2	2.14	0.47
3:C:66:ARG:CZ	10:J:2:ILE:HG21	2.44	0.47
10:J:57:ILE:HG12	10:J:61:LEU:HD11	1.94	0.47
11:K:59:ALA:HA	11:K:74:ARG:O	2.15	0.47
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.29	0.47
1:A:1225:PHE:O	1:A:1240:CYS:HA	2.14	0.47
1:A:1134:ILE:HD11	1:A:1321:GLY:HA3	1.96	0.47
2:B:1182:CYS:O	2:B:1183:LYS:O	2.31	0.47
2:B:51:PHE:CD2	2:B:173:MET:HB3	2.49	0.47
2:B:46:GLN:HE21	2:B:496:ARG:HG2	1.78	0.47
2:B:726:ALA:CB	2:B:1051:THR:HG21	2.45	0.47
5:E:78:LEU:HD21	5:E:80:VAL:HG22	1.95	0.47
8:H:40:LEU:CD2	8:H:42:ILE:HD11	2.39	0.47
12:L:30:ILE:CD1	12:L:59:ALA:HA	2.45	0.47
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.60	0.47
1:A:20:GLY:HA2	1:A:1413:GLY:O	2.14	0.47
1:A:563:PRO:HG3	1:A:572:TRP:CH2	2.48	0.47
1:A:994:GLN:NE2	1:A:1019:CYS:HB3	2.27	0.47
2:B:1054:GLY:O	2:B:1058:LEU:HG	2.13	0.47
2:B:1169:MET:SD	2:B:1201:LYS:HG2	2.54	0.47
2:B:780:VAL:HG21	10:J:56:LEU:HD11	1.97	0.47
2:B:842:ASN:HD22	2:B:845:SER:HB3	1.80	0.47
8:H:47:PHE:CD1	8:H:95:TYR:HB2	2.50	0.47
9:I:75:CYS:O	9:I:76:PRO:C	2.52	0.47
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.61	0.47
2:B:1051:THR:HG21	2:B:1053:GLU:HB2	1.97	0.47
2:B:1124:ARG:O	2:B:1125:ASP:HB3	2.14	0.47
2:B:123:THR:O	2:B:125:SER:N	2.47	0.47
2:B:230:ALA:C	2:B:232:SER:H	2.17	0.47
2:B:845:SER:HB2	10:J:8:PHE:HB3	1.96	0.47
1:A:12:ARG:HD3	2:B:1218:THR:HB	1.97	0.47
1:A:848:ILE:CD1	1:A:1374:VAL:HG21	2.45	0.47
1:A:167:CYS:C	1:A:169:ASN:H	2.18	0.47
1:A:381:THR:CG2	1:A:383:TYR:CD1	2.98	0.47
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.78	0.47
2:B:1013:ASN:OD1	2:B:1015:HIS:HB2	2.15	0.47
1:A:22:PHE:HB2	2:B:1211:ASN:CG	2.35	0.47
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.49	0.47
2:B:750:GLY:O	2:B:751:VAL:C	2.53	0.47
3:C:262:LEU:O	3:C:265:MET:HB3	2.15	0.47
1:A:517:ASN:ND2	1:A:1362:TYR:CE2	2.83	0.47
1:A:83:HIS:CE1	1:A:238:CYS:SG	3.08	0.47
2:B:1116:ARG:NH1	2:B:1198:TYR:CD1	2.83	0.47
2:B:332:ASP:C	2:B:334:ILE:N	2.68	0.47
2:B:62:ILE:HG21	2:B:417:PHE:HD2	1.80	0.47
2:B:860:MET:HB2	2:B:965:LYS:HG2	1.97	0.47
5:E:7:ARG:C	5:E:9:ILE:H	2.17	0.47
6:F:109:VAL:HG11	6:F:123:LYS:HG2	1.96	0.47
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.30	0.47
1:A:294:SER:HA	1:A:297:GLN:HB3	1.96	0.47
1:A:515:GLN:HA	1:A:1367:HIS:NE2	2.29	0.47
1:A:666:ILE:O	1:A:667:GLY:C	2.53	0.47
1:A:90:VAL:HG21	1:A:296:LEU:HG	1.95	0.47
2:B:1198:TYR:HE1	2:B:1201:LYS:HZ2	1.61	0.47
2:B:512:ARG:NH2	2:B:535:LEU:HD11	2.02	0.47
5:E:58:MET:O	5:E:59:SER:C	2.53	0.47
8:H:125:LEU:HG	8:H:130:ARG:CZ	2.43	0.47
9:I:100:PHE:HZ	9:I:118:ARG:HH12	1.62	0.47
1:A:1364:ASN:HD22	1:A:1365:TYR:N	2.13	0.47
1:A:783:THR:CG2	1:A:815:PHE:CE2	2.97	0.47
1:A:829:VAL:O	1:A:831:THR:N	2.48	0.47
2:B:773:MET:SD	2:B:987:LYS:HD2	2.54	0.47
6:F:101:ILE:HD11	6:F:124:GLU:OE1	2.15	0.47
9:I:74:GLU:OE1	9:I:79:HIS:ND1	2.47	0.47
2:B:798:TYR:CD2	10:J:4:PRO:HG3	2.49	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:83:PRO:O	11:K:87:LEU:N	2.46	0.47
1:A:116:ASP:HB2	1:A:118:HIS:CD2	2.49	0.47
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.78	0.47
1:A:1392:SER:O	1:A:1393:ASN:ND2	2.48	0.47
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.45	0.47
1:A:530:GLY:O	1:A:531:ILE:C	2.54	0.47
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.45	0.47
2:B:210:LYS:HE2	2:B:461:LEU:O	2.14	0.47
5:E:96:PHE:CE1	5:E:100:ILE:HD11	2.50	0.47
8:H:49:VAL:CG1	8:H:50:ALA:H	2.27	0.47
1:A:975:HIS:ND1	1:A:1036:ARG:HG3	2.30	0.46
1:A:1364:ASN:HD21	1:A:1366:ARG:HG2	1.67	0.46
1:A:352:VAL:HG12	1:A:353:ILE:N	2.29	0.46
1:A:540:PHE:C	1:A:541:ILE:HD12	2.35	0.46
1:A:645:LEU:O	1:A:649:ILE:HG13	2.16	0.46
1:A:67:CYS:SG	1:A:77:CYS:SG	3.11	0.46
1:A:964:ILE:HD13	1:A:1035:TYR:CZ	2.50	0.46
2:B:314:LEU:O	2:B:315:LYS:C	2.53	0.46
2:B:640:VAL:HG12	2:B:640:VAL:O	2.15	0.46
2:B:96:TYR:CD1	2:B:96:TYR:N	2.83	0.46
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.79	0.46
6:F:101:ILE:HD13	6:F:120:ILE:CG2	2.45	0.46
8:H:113:ALA:HA	8:H:125:LEU:O	2.15	0.46
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.51	0.46
1:A:573:SER:OG	1:A:576:GLN:HG3	2.15	0.46
2:B:487:THR:HG22	2:B:489:SER:N	2.24	0.46
2:B:519:TRP:HE1	2:B:635:ARG:HH22	1.64	0.46
2:B:806:THR:HG22	2:B:808:ALA:H	1.79	0.46
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.79	0.46
2:B:906:SER:CB	2:B:946:ASN:HB2	2.45	0.46
3:C:258:ILE:N	3:C:258:ILE:HD12	2.30	0.46
8:H:26:ILE:HD13	8:H:49:VAL:HG11	1.97	0.46
1:A:849:MET:HB2	1:A:1063:MET:SD	2.55	0.46
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.50	0.46
1:A:804:TYR:HE1	2:B:1021:MET:CE	2.28	0.46
2:B:100:PRO:O	2:B:180:TYR:OH	2.31	0.46
2:B:377:PHE:C	2:B:379:GLY:N	2.68	0.46
2:B:864:LYS:H	2:B:872:GLU:CG	2.28	0.46
10:J:1:MET:O	10:J:2:ILE:O	2.33	0.46
1:A:1209:MET:CG	1:A:1236:LEU:HD22	2.45	0.46
1:A:222:LEU:O	1:A:224:PHE:N	2.46	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:GLY:O	5:E:204:THR:HG21	2.14	0.46
1:A:923:LEU:O	1:A:927:VAL:HG23	2.14	0.46
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.50	0.46
2:B:321:GLY:C	2:B:323:VAL:H	2.17	0.46
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.50	0.46
2:B:851:PHE:O	2:B:974:PRO:HD3	2.15	0.46
1:A:1017:LEU:O	1:A:1018:PHE:C	2.53	0.46
1:A:329:LEU:HA	1:A:335:ARG:HB2	1.98	0.46
1:A:477:PRO:HG2	1:A:521:MET:HG2	1.98	0.46
1:A:549:MET:HE1	1:A:656:TRP:CD1	2.39	0.46
2:B:167:ILE:HG22	2:B:167:ILE:O	2.14	0.46
2:B:708:GLU:CG	2:B:709:ASP:N	2.69	0.46
11:K:91:CYS:O	11:K:94:ILE:HB	2.16	0.46
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.16	0.46
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.98	0.46
1:A:1410:PHE:C	1:A:1412:ALA:N	2.67	0.46
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.78	0.46
2:B:230:ALA:N	2:B:231:PRO:HD2	2.31	0.46
2:B:653:VAL:C	2:B:654:ARG:HG2	2.36	0.46
2:B:800:GLN:HB3	10:J:52:THR:HG22	1.97	0.46
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.97	0.46
6:F:117:PRO:O	6:F:120:ILE:HB	2.16	0.46
9:I:7:CYS:CB	9:I:14:LEU:HD21	2.33	0.46
1:A:1074:GLU:C	1:A:1076:ALA:H	2.18	0.46
1:A:1390:ASN:HD21	1:A:1399:ARG:HA	1.78	0.46
1:A:658:LEU:HD13	2:B:831:SER:HA	1.98	0.46
1:A:666:ILE:CD1	2:B:1030:LEU:HD22	2.41	0.46
2:B:1100:ASP:HA	2:B:1103:ILE:CG1	2.46	0.46
2:B:201:GLY:H	2:B:202:TYR:HD2	1.63	0.46
2:B:282:ILE:HG13	2:B:283:VAL:N	2.31	0.46
2:B:316:PRO:HA	2:B:319:GLU:HG2	1.98	0.46
2:B:680:THR:O	2:B:683:SER:OG	2.34	0.46
3:C:180:TYR:O	3:C:181:ASP:HB3	2.15	0.46
5:E:179:GLN:OE1	5:E:179:GLN:HA	2.16	0.46
1:A:852:TYR:OH	6:F:89:GLU:OE2	2.28	0.46
8:H:114:VAL:O	8:H:124:ARG:HA	2.16	0.46
2:B:294:ASP:H	9:I:12:ASN:ND2	2.13	0.46
9:I:2:THR:OG1	9:I:45:ARG:HB3	2.15	0.46
1:A:420:ARG:O	1:A:424:ILE:HG13	2.16	0.46
1:A:55:ASP:HB3	1:A:56:PRO:HD3	1.98	0.46
1:A:679:ILE:HG23	1:A:729:ALA:CB	2.39	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.98	0.46
2:B:1072:MET:O	2:B:1081:LEU:HB2	2.15	0.46
2:B:332:ASP:C	2:B:334:ILE:H	2.17	0.46
2:B:300:HIS:ND1	2:B:376:PHE:CE2	2.83	0.46
3:C:252:GLN:CG	11:K:95:ILE:HG23	2.46	0.46
5:E:190:LEU:HD11	5:E:196:VAL:HG11	1.98	0.46
1:A:112:LYS:HG2	1:A:113:LEU:N	2.30	0.46
1:A:1327:ILE:O	5:E:147:HIS:HE1	1.98	0.46
1:A:383:TYR:HB3	6:F:115:THR:CG2	2.44	0.46
1:A:881:GLN:OE1	1:A:959:ASN:HA	2.15	0.46
1:A:890:ASP:N	1:A:1296:GLY:HA3	2.30	0.46
2:B:1085:ILE:HG22	2:B:1086:PHE:N	2.31	0.46
2:B:322:PHE:CG	2:B:322:PHE:O	2.69	0.46
3:C:62:PHE:CD2	3:C:62:PHE:C	2.89	0.46
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.46	0.46
1:A:701:LEU:HA	9:I:115:LYS:HE3	1.98	0.46
9:I:34:TYR:O	9:I:35:VAL:HG23	2.16	0.46
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.56	0.46
1:A:53:LEU:HD13	1:A:263:THR:HG23	1.97	0.46
1:A:446:ARG:HG2	1:A:446:ARG:NH1	2.28	0.46
1:A:50:ILE:HG22	1:A:51:GLY:H	1.81	0.46
1:A:517:ASN:OD1	1:A:517:ASN:O	2.34	0.46
1:A:535:THR:HG22	1:A:616:VAL:HA	1.98	0.46
1:A:87:ALA:HB3	1:A:276:LEU:CD2	2.45	0.46
1:A:958:VAL:HG22	1:A:1052:GLN:HB3	1.98	0.46
2:B:1085:ILE:CG2	2:B:1086:PHE:N	2.78	0.46
2:B:1104:HIS:HB2	2:B:1122:ARG:CD	2.44	0.46
2:B:1106:ARG:CD	2:B:1126:GLY:O	2.62	0.46
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.95	0.46
2:B:589:VAL:HG12	2:B:590:HIS:H	1.81	0.46
1:A:786:HIS:CE1	2:B:742:GLU:OE1	2.64	0.46
2:B:893:LEU:HD22	2:B:897:GLY:O	2.16	0.46
1:A:738:LYS:NZ	3:C:194:GLU:CA	2.79	0.46
5:E:112:TYR:CE2	5:E:134:THR:HB	2.51	0.46
9:I:7:CYS:HB2	9:I:14:LEU:CD2	2.34	0.46
10:J:32:GLU:CD	10:J:32:GLU:H	2.19	0.46
1:A:1041:ALA:O	1:A:1044:TRP:HB3	2.15	0.45
1:A:1410:PHE:C	1:A:1412:ALA:H	2.19	0.45
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.51	0.45
1:A:893:PHE:CD1	1:A:940:ARG:HD2	2.51	0.45
2:B:1106:ARG:HG2	2:B:1107:ALA:N	2.31	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1120:GLU:HG2	2:B:1121:GLY:N	2.31	0.45
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.99	0.45
2:B:50:SER:O	2:B:53:GLN:HB3	2.16	0.45
2:B:686:ASN:C	2:B:688:GLY:N	2.70	0.45
5:E:96:PHE:CE2	5:E:110:PHE:HB2	2.50	0.45
9:I:91:ARG:HD3	9:I:91:ARG:HA	1.75	0.45
12:L:45:ALA:O	12:L:46:VAL:CG2	2.64	0.45
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.81	0.45
1:A:592:ASP:N	1:A:595:THR:OG1	2.48	0.45
2:B:1072:MET:HE3	2:B:1085:ILE:HD12	1.98	0.45
2:B:1098:MET:O	2:B:1099:VAL:C	2.53	0.45
2:B:345:LYS:O	2:B:347:LYS:N	2.49	0.45
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.66	0.45
2:B:25:ILE:HD11	2:B:653:VAL:CB	2.46	0.45
2:B:664:THR:HG1	2:B:678:GLU:N	2.14	0.45
2:B:704:ALA:HB2	2:B:738:PHE:CE1	2.51	0.45
2:B:758:PHE:C	2:B:760:ASP:N	2.68	0.45
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.50	0.45
2:B:890:TYR:C	2:B:892:LYS:H	2.19	0.45
2:B:914:LYS:H	2:B:938:SER:HB3	1.81	0.45
2:B:956:THR:HG21	2:B:960:GLY:HA2	1.96	0.45
3:C:18:VAL:O	3:C:18:VAL:HG12	2.15	0.45
3:C:263:THR:C	3:C:265:MET:H	2.18	0.45
1:A:1037:LEU:HD13	1:A:1042:PHE:HA	1.98	0.45
1:A:223:GLY:HA3	1:A:1415:SER:HB3	1.98	0.45
1:A:542:GLU:C	1:A:546:VAL:HG23	2.36	0.45
1:A:567:LYS:CB	1:A:568:PRO:CD	2.67	0.45
1:A:848:ILE:HD13	1:A:864:ILE:HD13	1.98	0.45
2:B:1177:HIS:C	2:B:1179:GLN:N	2.68	0.45
2:B:1200:ALA:O	2:B:1201:LYS:C	2.54	0.45
2:B:168:GLY:H	2:B:450:ALA:HB1	1.82	0.45
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.98	0.45
2:B:574:SER:HB3	2:B:577:ALA:HB2	1.98	0.45
2:B:963:PHE:HE2	2:B:965:LYS:HE3	1.81	0.45
5:E:10:SER:O	5:E:14:ARG:HG3	2.16	0.45
1:A:1155:ASP:CG	1:A:1162:VAL:HG23	2.37	0.45
1:A:1336:MET:SD	1:A:1381:LEU:HG	2.56	0.45
2:B:1171:VAL:HG13	2:B:1191:ILE:HD13	1.99	0.45
2:B:295:GLY:O	2:B:299:GLU:HG3	2.16	0.45
2:B:371:GLU:N	2:B:371:GLU:OE1	2.49	0.45
2:B:515:HIS:O	2:B:516:ASN:C	2.54	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:549:THR:H	2:B:628:THR:HG22	1.81	0.45
5:E:94:LYS:O	5:E:98:ILE:HG13	2.16	0.45
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.99	0.45
11:K:61:TYR:CD1	11:K:61:TYR:C	2.89	0.45
1:A:1209:MET:CE	1:A:1236:LEU:HB3	2.47	0.45
1:A:456:MET:HB2	1:A:478:TYR:OH	2.17	0.45
2:B:1060:ARG:C	2:B:1062:HIS:N	2.69	0.45
2:B:1182:CYS:O	2:B:1183:LYS:HD2	2.15	0.45
2:B:205:ILE:HG12	2:B:461:LEU:HB3	1.99	0.45
2:B:955:THR:HG1	12:L:55:ILE:HA	1.81	0.45
3:C:249:ASP:O	3:C:252:GLN:HB3	2.16	0.45
5:E:185:ALA:CB	5:E:190:LEU:HD12	2.47	0.45
5:E:205:SER:O	5:E:206:GLY:C	2.54	0.45
8:H:111:LEU:HA	8:H:127:GLY:O	2.17	0.45
9:I:92:ARG:CG	9:I:93:LYS:H	2.30	0.45
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.17	0.45
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.98	0.45
2:B:824:ILE:CG2	2:B:1087:PHE:CE2	3.00	0.45
2:B:977:GLY:C	2:B:1099:VAL:HG23	2.37	0.45
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.70	0.45
2:B:121:ASN:HA	2:B:207:GLY:CA	2.46	0.45
2:B:100:PRO:HA	2:B:125:SER:O	2.16	0.45
2:B:215:GLN:HB2	2:B:407:ASP:HB2	1.98	0.45
2:B:260:GLY:HA3	2:B:267:ARG:HG2	1.98	0.45
2:B:276:ILE:HD13	2:B:334:ILE:CG2	2.46	0.45
2:B:995:ARG:HH11	2:B:995:ARG:HB2	1.81	0.45
3:C:242:GLN:OE1	3:C:242:GLN:HA	2.16	0.45
3:C:5:GLY:O	3:C:6:PRO:C	2.54	0.45
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.98	0.45
9:I:29:CYS:O	9:I:31:THR:N	2.49	0.45
1:A:1405:THR:O	1:A:1406:VAL:C	2.54	0.45
1:A:335:ARG:HA	1:A:335:ARG:HD3	1.87	0.45
1:A:418:SER:O	1:A:421:ALA:N	2.49	0.45
1:A:535:THR:HG21	1:A:616:VAL:CA	2.43	0.45
1:A:573:SER:H	1:A:576:GLN:HG3	1.81	0.45
1:A:845:LEU:O	1:A:848:ILE:HG13	2.17	0.45
1:A:994:GLN:HE21	1:A:1019:CYS:CB	2.26	0.45
2:B:1117:GLN:NE2	2:B:1156:ASP:OD2	2.48	0.45
2:B:1185:CYS:O	2:B:1186:ASP:HB2	2.17	0.45
2:B:408:LEU:HA	2:B:408:LEU:HD12	1.71	0.45
2:B:763:GLN:CG	2:B:765:PRO:HD2	2.40	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.99	0.45
3:C:62:PHE:C	3:C:62:PHE:HD2	2.20	0.45
8:H:101:ALA:HB2	8:H:116:TYR:CD2	2.51	0.45
8:H:38:LEU:HD13	8:H:125:LEU:CD1	2.46	0.45
10:J:5:VAL:O	10:J:6:ARG:HB2	2.15	0.45
1:A:960:ILE:HD12	1:A:1021:LEU:HD21	1.99	0.45
1:A:1208:THR:HG22	1:A:1210:GLY:N	2.31	0.45
1:A:1317:MET:CA	1:A:1322:ILE:HD11	2.46	0.45
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.99	0.45
1:A:340:LEU:HD21	2:B:1200:ALA:CA	2.47	0.45
2:B:361:LEU:O	2:B:363:HIS:O	2.35	0.45
3:C:69:LEU:HA	3:C:69:LEU:HD12	1.76	0.45
9:I:34:TYR:O	9:I:35:VAL:CG2	2.65	0.45
1:A:1114:PRO:O	1:A:1330:ASN:OD1	2.35	0.45
1:A:778:GLY:HA3	2:B:516:ASN:CB	2.46	0.45
1:A:829:VAL:C	1:A:831:THR:N	2.70	0.45
2:B:1013:ASN:OD1	2:B:1015:HIS:N	2.44	0.45
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.59	0.45
1:A:351:THR:CG2	2:B:1103:ILE:HA	2.36	0.45
2:B:1158:PHE:CD2	2:B:1198:TYR:HD1	2.35	0.45
2:B:973:ILE:CG2	2:B:974:PRO:HD2	2.47	0.45
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.49	0.45
3:C:17:ASN:OD1	3:C:233:GLU:HG2	2.16	0.45
3:C:8:VAL:CG1	3:C:9:LYS:N	2.80	0.45
8:H:116:TYR:HE2	8:H:140:ALA:CB	2.30	0.45
9:I:8:ARG:HG3	9:I:9:ASP:CG	2.37	0.45
12:L:38:LEU:HG	12:L:39:SER:H	1.82	0.45
1:A:210:ILE:O	1:A:214:ILE:HG13	2.17	0.45
1:A:47:ARG:O	1:A:48:ALA:HB2	2.16	0.45
1:A:78:PRO:O	1:A:79:GLY:C	2.56	0.45
1:A:80:HIS:O	1:A:243:PRO:HB3	2.17	0.45
1:A:815:PHE:O	1:A:818:MET:N	2.50	0.45
2:B:1159:ARG:NE	2:B:1193:GLN:NE2	2.33	0.45
2:B:361:LEU:N	2:B:362:PRO:HD2	2.31	0.45
2:B:365:THR:CG2	2:B:367:LEU:H	2.30	0.45
2:B:370:PHE:N	2:B:371:GLU:OE1	2.50	0.45
2:B:426:LYS:O	2:B:430:ARG:HG3	2.17	0.45
2:B:605:ARG:CZ	2:B:639:ILE:HD13	2.46	0.45
2:B:640:VAL:HG23	2:B:740:HIS:HA	1.97	0.45
2:B:805:THR:HA	2:B:809:MET:HE1	1.98	0.45
3:C:76:ASP:OD2	3:C:128:ASN:N	2.47	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:98:TYR:O	8:H:118:PHE:HD2	1.99	0.45
9:I:75:CYS:C	9:I:77:LYS:H	2.20	0.45
10:J:48:ARG:HH21	10:J:49:MET:CE	2.24	0.45
11:K:73:LEU:CD2	11:K:75:ILE:HD11	2.46	0.45
1:A:1208:THR:N	1:A:1211:GLN:OE1	2.49	0.44
1:A:1428:VAL:HG13	2:B:1151:LEU:HD23	2.00	0.44
1:A:388:LEU:O	1:A:392:VAL:HG23	2.17	0.44
2:B:1154:ALA:O	2:B:1155:SER:CB	2.64	0.44
2:B:707:PRO:O	2:B:708:GLU:O	2.35	0.44
3:C:31:ASN:O	3:C:35:ARG:HG3	2.17	0.44
3:C:73:GLN:NE2	3:C:75:MET:H	1.97	0.44
5:E:147:HIS:CD2	5:E:149:LEU:H	2.35	0.44
8:H:57:VAL:HG12	8:H:58:THR:N	2.32	0.44
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.97	0.44
1:A:1152:ILE:HG23	1:A:1260:LEU:CD2	2.43	0.44
1:A:1436:ILE:O	1:A:1437:GLY:C	2.56	0.44
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.99	0.44
1:A:709:THR:C	1:A:711:ARG:N	2.67	0.44
2:B:332:ASP:O	2:B:334:ILE:N	2.50	0.44
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.52	0.44
2:B:847:ASP:O	3:C:65:HIS:HE1	2.01	0.44
5:E:102:GLU:C	5:E:104:ASN:H	2.20	0.44
11:K:24:ASP:HB3	11:K:30:ALA:CB	2.47	0.44
11:K:78:THR:O	11:K:79:GLU:C	2.56	0.44
1:A:1207:LEU:HA	1:A:1211:GLN:OE1	2.17	0.44
1:A:219:PHE:CE2	1:A:231:PRO:HD2	2.52	0.44
1:A:265:LYS:HZ1	1:A:323:LYS:H	1.62	0.44
1:A:50:ILE:C	1:A:52:GLY:N	2.69	0.44
1:A:84:ILE:HG23	1:A:84:ILE:O	2.17	0.44
1:A:885:THR:HG23	1:A:893:PHE:CE1	2.36	0.44
2:B:986:GLN:OE1	2:B:986:GLN:CA	2.64	0.44
3:C:120:ILE:HD11	3:C:130:GLY:O	2.17	0.44
3:C:148:ARG:HD3	3:C:149:LYS:H	1.83	0.44
3:C:236:GLY:C	3:C:238:ILE:N	2.69	0.44
5:E:138:ALA:C	5:E:140:LEU:H	2.21	0.44
6:F:111:LEU:C	6:F:113:GLY:N	2.71	0.44
9:I:106:CYS:O	9:I:107:SER:HB2	2.18	0.44
1:A:1441:PHE:HB2	6:F:134:ILE:HG23	2.00	0.44
1:A:571:LEU:HD22	8:H:46:LEU:HD11	1.99	0.44
2:B:247:GLY:O	2:B:248:SER:HB3	2.17	0.44
3:C:77:ILE:CG2	3:C:161:LYS:HE3	2.48	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:7:ARG:C	5:E:9:ILE:N	2.71	0.44
8:H:5:LEU:O	8:H:133:ASN:HB3	2.17	0.44
8:H:40:LEU:HG	8:H:42:ILE:HG13	1.98	0.44
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.45	0.44
1:A:1348:LEU:CD2	1:A:1372:VAL:HG13	2.39	0.44
1:A:233:TRP:O	1:A:235:ILE:N	2.50	0.44
2:B:281:PRO:HG2	2:B:284:ILE:CD1	2.45	0.44
2:B:642:ASP:O	2:B:643:ASP:C	2.56	0.44
2:B:744:HIS:CD2	2:B:746:SER:OG	2.70	0.44
2:B:904:ARG:CZ	2:B:948:ILE:HD11	2.48	0.44
2:B:915:THR:HG21	2:B:934:LYS:HG2	2.00	0.44
9:I:99:LEU:HB2	9:I:112:SER:CB	2.46	0.44
9:I:84:VAL:CG1	9:I:84:VAL:O	2.65	0.44
1:A:1384:VAL:O	1:A:1389:PHE:HE2	2.01	0.44
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	2.00	0.44
1:A:42:ASP:OD1	1:A:45:GLN:O	2.36	0.44
2:B:1002:THR:HG21	2:B:1006:ILE:HB	2.00	0.44
2:B:200:GLY:HA2	2:B:202:TYR:CD2	2.50	0.44
2:B:288:ALA:HA	2:B:331:LEU:HD13	1.99	0.44
2:B:745:PRO:C	2:B:747:MET:N	2.70	0.44
1:A:974:ASP:CB	8:H:136:LYS:NZ	2.80	0.44
1:A:968:GLN:NE2	1:A:1035:TYR:HB2	2.32	0.44
1:A:1046:LEU:O	1:A:1047:SER:C	2.55	0.44
1:A:1121:GLU:O	1:A:1122:PRO:C	2.56	0.44
1:A:326:ARG:HE	1:A:1406:VAL:HG11	1.82	0.44
1:A:367:PRO:CB	1:A:466:SER:HA	2.47	0.44
2:B:1002:THR:CG2	2:B:1004:GLU:HB2	2.47	0.44
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.53	0.44
2:B:800:GLN:CB	10:J:52:THR:HG22	2.47	0.44
5:E:28:TYR:CE2	5:E:64:PRO:HG3	2.53	0.44
8:H:47:PHE:CB	8:H:95:TYR:HD1	2.31	0.44
10:J:16:ASP:OD1	10:J:17:LYS:HG3	2.17	0.44
11:K:24:ASP:OD1	11:K:26:LYS:N	2.51	0.44
1:A:13:THR:HG23	1:A:1432:GLN:CD	2.38	0.44
1:A:591:PHE:HD2	1:A:595:THR:HB	1.83	0.44
1:A:21:LEU:HD21	1:A:95:PHE:CZ	2.53	0.44
2:B:185:THR:H	2:B:188:ASP:HB2	1.81	0.44
2:B:315:LYS:N	2:B:316:PRO:HD2	2.32	0.44
2:B:56:ASP:HB3	2:B:57:TYR:CD1	2.52	0.44
2:B:650:GLU:HG2	2:B:654:ARG:NH1	2.33	0.44
2:B:702:LEU:HD21	2:B:735:ALA:HB1	1.98	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:864:LYS:HD3	2:B:871:THR:CB	2.47	0.44
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.99	0.44
3:C:186:LEU:HA	3:C:186:LEU:HD12	1.86	0.44
3:C:22:LEU:CD2	3:C:25:VAL:HG21	2.37	0.44
5:E:133:GLU:HB3	5:E:135:PHE:HE1	1.83	0.44
1:A:1441:PHE:HB2	6:F:134:ILE:CG2	2.47	0.44
1:A:1094:VAL:HG12	1:A:1095:THR:N	2.32	0.44
1:A:1415:SER:O	1:A:1416:ALA:C	2.56	0.44
1:A:825:ILE:C	1:A:827:THR:N	2.70	0.44
2:B:216:GLU:OE1	2:B:537:LYS:CE	2.66	0.44
2:B:274:PRO:O	2:B:276:ILE:N	2.51	0.44
2:B:640:VAL:HG23	2:B:740:HIS:CA	2.48	0.44
3:C:39:ALA:HA	3:C:164:ALA:CB	2.46	0.44
1:A:1166:ASP:CG	1:A:1194:ARG:HH21	2.19	0.43
1:A:115:LEU:HB2	1:A:122:MET:HE1	1.99	0.43
1:A:148:CYS:HB3	1:A:167:CYS:O	2.18	0.43
1:A:401:GLY:H	1:A:435:HIS:HD2	1.66	0.43
1:A:466:SER:HB3	11:K:2:ASN:HD22	1.82	0.43
1:A:533:LYS:C	1:A:535:THR:N	2.72	0.43
1:A:54:ASN:O	1:A:55:ASP:HB2	2.18	0.43
1:A:595:THR:HG22	1:A:596:THR:N	2.33	0.43
1:A:69:THR:O	2:B:1174:LYS:HG2	2.17	0.43
1:A:741:ASN:HD22	1:A:743:VAL:N	2.16	0.43
1:A:742:ASN:C	1:A:745:GLN:HB2	2.38	0.43
2:B:102:VAL:HG21	2:B:112:LEU:HD13	1.99	0.43
2:B:130:VAL:CG1	2:B:131:ASP:H	2.29	0.43
2:B:101:MET:HE2	2:B:169:ARG:NH1	2.33	0.43
2:B:203:PHE:HE1	2:B:212:LEU:CD1	2.31	0.43
2:B:212:LEU:HD13	2:B:409:ALA:HA	2.00	0.43
2:B:855:PHE:HZ	2:B:857:ARG:HH12	1.64	0.43
2:B:957:ASN:O	2:B:958:GLN:C	2.55	0.43
3:C:135:GLN:C	3:C:136:ASP:O	2.56	0.43
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.99	0.43
11:K:55:LYS:HD3	11:K:78:THR:OG1	2.18	0.43
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.39	0.43
1:A:1148:ILE:HD12	1:A:1196:GLU:HG2	2.01	0.43
1:A:131:SER:OG	1:A:132:LYS:N	2.51	0.43
1:A:1342:GLU:HG2	5:E:212:ARG:HH11	1.83	0.43
1:A:1364:ASN:HD22	1:A:1366:ARG:N	2.16	0.43
1:A:306:ASN:OD1	1:A:313:GLN:NE2	2.51	0.43
1:A:673:GLY:N	1:A:674:PRO:HD2	2.33	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:SER:OG	2:B:1193:GLN:NE2	2.51	0.43
1:A:858:ASN:ND2	1:A:858:ASN:C	2.68	0.43
2:B:1116:ARG:CZ	2:B:1198:TYR:CE1	3.01	0.43
2:B:577:ALA:HB1	2:B:589:VAL:HG12	2.00	0.43
2:B:806:THR:C	2:B:808:ALA:N	2.71	0.43
2:B:864:LYS:HD3	2:B:871:THR:CA	2.47	0.43
3:C:59:ALA:O	3:C:63:ILE:HG13	2.18	0.43
5:E:138:ALA:O	5:E:140:LEU:N	2.50	0.43
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.53	0.43
8:H:81:PRO:HD2	8:H:82:PRO:HD2	1.98	0.43
9:I:46:HIS:O	9:I:47:GLU:HB2	2.18	0.43
9:I:55:THR:HG21	9:I:109:ILE:CD1	2.48	0.43
9:I:98:VAL:CG1	9:I:99:LEU:N	2.81	0.43
12:L:27:LEU:HD13	12:L:37:LYS:CB	2.48	0.43
1:A:103:CYS:O	1:A:106:VAL:O	2.35	0.43
1:A:362:ASP:OD1	1:A:459:ARG:HD3	2.18	0.43
1:A:518:LYS:HB2	1:A:519:PRO:HD2	2.00	0.43
1:A:852:TYR:CE2	6:F:136:ARG:NE	2.86	0.43
1:A:901:LEU:HD13	1:A:919:ILE:CG2	2.48	0.43
2:B:1038:SER:HB3	2:B:1062:HIS:NE2	2.32	0.43
2:B:1175:LEU:O	2:B:1176:ASN:CG	2.56	0.43
2:B:295:GLY:H	2:B:298:LEU:HG	1.84	0.43
2:B:358:LYS:O	2:B:359:GLU:OE1	2.36	0.43
2:B:56:ASP:HB3	2:B:57:TYR:CE1	2.53	0.43
2:B:705:MET:H	2:B:710:LEU:CD1	2.32	0.43
3:C:8:VAL:HA	3:C:21:ILE:O	2.19	0.43
11:K:92:ASN:O	11:K:93:SER:C	2.56	0.43
12:L:43:THR:HG22	12:L:43:THR:O	2.18	0.43
1:A:850:VAL:O	1:A:1060:PRO:HA	2.18	0.43
1:A:84:ILE:CG2	1:A:239:LEU:HB3	2.48	0.43
1:A:494:SER:HB2	1:A:497:THR:OG1	2.18	0.43
1:A:751:SER:OG	2:B:1015:HIS:CE1	2.71	0.43
2:B:1106:ARG:NH1	2:B:1118:PRO:CB	2.72	0.43
1:A:343:LYS:NZ	2:B:1156:ASP:OD2	2.49	0.43
2:B:526:GLU:CD	2:B:752:ALA:HB3	2.38	0.43
5:E:69:ILE:O	5:E:73:PRO:HG3	2.19	0.43
1:A:834:THR:HG21	1:A:1077:THR:HA	2.00	0.43
1:A:86:LEU:HB3	1:A:296:LEU:HD21	1.99	0.43
1:A:344:ARG:O	2:B:1118:PRO:HG2	2.19	0.43
2:B:194:GLU:HA	2:B:194:GLU:OE1	2.18	0.43
2:B:276:ILE:HD13	2:B:334:ILE:HG23	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:709:ASP:C	2:B:710:LEU:HD23	2.38	0.43
2:B:781:PHE:CE2	2:B:795:ILE:HD11	2.53	0.43
3:C:135:GLN:O	3:C:136:ASP:O	2.37	0.43
3:C:249:ASP:OD1	3:C:253:LYS:HE3	2.19	0.43
3:C:9:LYS:HB2	3:C:21:ILE:HB	1.98	0.43
8:H:12:VAL:HG13	8:H:26:ILE:HG23	2.01	0.43
1:A:1118:VAL:O	1:A:1305:VAL:HG13	2.18	0.43
1:A:1347:ALA:O	1:A:1348:LEU:C	2.55	0.43
1:A:102:VAL:HG21	1:A:234:MET:HE1	1.99	0.43
1:A:68:GLN:O	1:A:70:CYS:N	2.52	0.43
1:A:774:ARG:O	1:A:775:ILE:C	2.57	0.43
2:B:562:GLY:O	2:B:563:MET:C	2.56	0.43
2:B:690:VAL:HG12	2:B:691:GLU:N	2.33	0.43
2:B:969:ARG:HG2	2:B:970:THR:N	2.33	0.43
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.31	0.43
1:A:1116:LEU:HD12	1:A:1329:THR:HG1	1.77	0.43
1:A:1158:PRO:HB3	1:A:1241:ARG:HH12	1.83	0.43
1:A:404:TYR:HA	1:A:413:ILE:O	2.18	0.43
1:A:565:ILE:HD13	1:A:567:LYS:HE2	2.01	0.43
1:A:760:GLN:HB2	2:B:1021:MET:HE1	2.00	0.43
2:B:1152:MET:SD	2:B:1197:PRO:HD3	2.59	0.43
2:B:781:PHE:HE2	2:B:795:ILE:HD11	1.83	0.43
3:C:5:GLY:O	3:C:6:PRO:O	2.37	0.43
5:E:59:SER:HA	5:E:80:VAL:O	2.19	0.43
5:E:9:ILE:C	5:E:11:ARG:N	2.71	0.43
6:F:89:GLU:HB3	6:F:134:ILE:HD13	2.00	0.43
9:I:50:THR:HG22	9:I:52:ILE:N	2.33	0.43
10:J:48:ARG:NH2	10:J:49:MET:HE1	2.25	0.43
1:A:1068:ALA:O	1:A:1069:ALA:C	2.55	0.43
1:A:644:LYS:O	1:A:645:LEU:C	2.55	0.43
1:A:853:ASP:OD1	1:A:855:THR:CB	2.64	0.43
1:A:907:THR:HG22	1:A:908:LEU:H	1.82	0.43
2:B:1108:ARG:O	2:B:1108:ARG:CG	2.67	0.43
2:B:126:SER:OG	2:B:172:ILE:HD11	2.18	0.43
2:B:214:ALA:HB2	2:B:408:LEU:CD1	2.48	0.43
2:B:329:THR:O	2:B:332:ASP:HB3	2.19	0.43
2:B:446:LEU:HD23	2:B:446:LEU:N	2.33	0.43
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.84	0.43
2:B:834:ASN:HB2	2:B:838:SER:O	2.19	0.43
3:C:46:ILE:HG23	3:C:157:CYS:HB3	2.00	0.43
5:E:114:ASN:O	5:E:115:ASN:HB3	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:82:PHE:N	5:E:82:PHE:CD1	2.85	0.43
6:F:140:ASP:OD1	6:F:141:GLY:N	2.52	0.43
1:A:709:THR:HG23	9:I:94:ASP:HA	2.00	0.43
10:J:21:TYR:CA	10:J:39:LEU:HD11	2.49	0.43
10:J:9:SER:HB2	10:J:45:CYS:HB2	2.01	0.43
11:K:95:ILE:O	11:K:98:LEU:HB2	2.19	0.43
1:A:113:LEU:HG	1:A:218:ASP:OD1	2.19	0.43
1:A:114:LEU:HD12	1:A:142:CYS:O	2.18	0.43
1:A:266:LEU:HD23	1:A:266:LEU:HA	1.81	0.43
1:A:396:PRO:HG3	1:A:416:ARG:HB3	2.00	0.43
1:A:458:HIS:ND1	1:A:507:VAL:HG21	2.33	0.43
1:A:457:ALA:O	1:A:507:VAL:HG23	2.19	0.43
1:A:709:THR:O	1:A:712:GLU:N	2.52	0.43
1:A:711:ARG:HA	9:I:97:MET:HE1	2.01	0.43
2:B:1103:ILE:O	2:B:1104:HIS:C	2.56	0.43
2:B:702:LEU:HD22	2:B:737:THR:CG2	2.49	0.43
9:I:84:VAL:HG13	9:I:84:VAL:O	2.19	0.43
1:A:1150:SER:HB2	1:A:1195:LEU:CD2	2.49	0.43
1:A:1336:MET:HE1	1:A:1381:LEU:N	2.34	0.43
1:A:1409:LEU:HD23	1:A:1409:LEU:HA	1.83	0.43
1:A:633:VAL:HG11	1:A:645:LEU:HD22	2.00	0.43
1:A:672:ASP:O	1:A:675:THR:HB	2.19	0.43
1:A:679:ILE:O	1:A:682:THR:HB	2.18	0.43
1:A:89:PRO:HG3	1:A:208:LEU:HD12	2.00	0.43
2:B:202:TYR:CD2	2:B:202:TYR:N	2.87	0.43
2:B:484:ASN:CG	2:B:486:TYR:HE1	2.23	0.43
2:B:55:VAL:O	2:B:59:LEU:HB3	2.19	0.43
2:B:519:TRP:CZ2	2:B:705:MET:CE	2.99	0.43
2:B:850:LEU:CD2	2:B:1009:ASP:HB3	2.48	0.43
6:F:94:LEU:HD23	6:F:94:LEU:HA	1.83	0.43
8:H:123:MET:HE1	8:H:142:LEU:CD1	2.49	0.43
8:H:5:LEU:O	8:H:6:PHE:HB2	2.19	0.43
8:H:84:ALA:CA	8:H:87:ARG:HB2	2.48	0.43
9:I:50:THR:HG22	9:I:52:ILE:HG23	1.98	0.43
1:A:30:ILE:O	1:A:31:SER:O	2.37	0.42
1:A:337:ARG:CZ	1:A:839:ARG:CZ	2.97	0.42
1:A:541:ILE:HG12	1:A:549:MET:HE3	2.01	0.42
1:A:815:PHE:C	1:A:817:ALA:N	2.72	0.42
2:B:115:GLN:HG2	2:B:193:LYS:HB2	2.01	0.42
2:B:366:GLN:O	2:B:367:LEU:O	2.36	0.42
2:B:877:PRO:O	2:B:878:GLN:HG2	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:228:PHE:HB2	3:C:230:MET:HE2	2.01	0.42
5:E:168:TYR:O	5:E:170:LEU:HD23	2.19	0.42
8:H:111:LEU:HD23	8:H:127:GLY:O	2.18	0.42
8:H:83:GLN:C	8:H:85:GLY:N	2.73	0.42
12:L:61:THR:HG22	12:L:62:LYS:N	2.33	0.42
1:A:1390:ASN:HD22	1:A:1399:ARG:CA	2.30	0.42
1:A:412:ARG:CZ	2:B:1108:ARG:NH2	2.81	0.42
1:A:545:GLN:O	1:A:546:VAL:C	2.55	0.42
1:A:614:PHE:C	1:A:614:PHE:CD1	2.92	0.42
1:A:645:LEU:HD11	1:A:649:ILE:HD11	2.01	0.42
1:A:534:LEU:HD13	1:A:656:TRP:CD1	2.54	0.42
1:A:373:THR:HG21	2:B:1105:ALA:O	2.18	0.42
2:B:310:MET:O	2:B:313:MET:HB2	2.18	0.42
2:B:705:MET:N	2:B:710:LEU:HD12	2.34	0.42
3:C:148:ARG:H	3:C:151:GLN:HG3	1.84	0.42
5:E:117:THR:C	5:E:119:SER:N	2.73	0.42
8:H:143:LEU:N	8:H:143:LEU:HD12	2.34	0.42
8:H:93:TYR:CA	8:H:145:ARG:HB3	2.45	0.42
1:A:782:ARG:NH2	9:I:67:THR:HG22	2.34	0.42
1:A:1049:ILE:O	1:A:1050:GLU:C	2.56	0.42
1:A:1155:ASP:O	1:A:1190:PRO:O	2.37	0.42
1:A:134:ARG:O	1:A:137:ALA:N	2.52	0.42
1:A:49:LYS:NZ	1:A:60:SER:HA	2.34	0.42
1:A:845:LEU:O	1:A:846:GLU:C	2.57	0.42
2:B:1073:TYR:N	2:B:1073:TYR:CD1	2.87	0.42
2:B:880:THR:O	2:B:881:ASN:HB2	2.20	0.42
5:E:79:TRP:HD1	5:E:96:PHE:HE1	1.67	0.42
6:F:85:MET:HE1	6:F:148:VAL:HG13	2.00	0.42
2:B:784:ASN:HB3	10:J:63:TYR:OH	2.18	0.42
1:A:1004:ASN:O	1:A:1008:GLN:HB2	2.19	0.42
1:A:1066:VAL:O	1:A:1067:LEU:C	2.55	0.42
1:A:1161:THR:OG1	1:A:1170:ILE:HD11	2.20	0.42
1:A:1242:VAL:CG1	1:A:1243:VAL:H	2.22	0.42
1:A:151:ASP:OD1	1:A:163:SER:HA	2.19	0.42
1:A:541:ILE:HD12	1:A:541:ILE:N	2.34	0.42
1:A:753:GLY:HA2	1:A:757:ASN:ND2	2.34	0.42
1:A:80:HIS:N	1:A:243:PRO:HB3	2.34	0.42
2:B:1033:LYS:NZ	2:B:1070:GLU:OE1	2.46	0.42
2:B:1197:PRO:O	2:B:1200:ALA:HB3	2.19	0.42
2:B:1204:PHE:O	2:B:1207:LEU:HB2	2.19	0.42
2:B:203:PHE:HE1	2:B:212:LEU:HD12	1.85	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:546:SER:OG	2:B:631:GLY:N	2.52	0.42
2:B:794:ASN:O	2:B:795:ILE:HD12	2.19	0.42
2:B:806:THR:O	2:B:808:ALA:N	2.53	0.42
2:B:980:PHE:HE1	2:B:990:ILE:CD1	2.30	0.42
2:B:831:SER:CB	2:B:994:TYR:OH	2.67	0.42
3:C:251:LEU:HG	11:K:98:LEU:HD11	2.01	0.42
5:E:168:TYR:CB	5:E:170:LEU:HG	2.49	0.42
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.34	0.42
1:A:88:LYS:HD2	1:A:293:GLU:OE1	2.20	0.42
1:A:337:ARG:HH11	1:A:839:ARG:HH12	1.62	0.42
2:B:269:ILE:HB	2:B:317:CYS:SG	2.60	0.42
2:B:34:ILE:HG12	2:B:542:MET:CE	2.49	0.42
2:B:34:ILE:HG12	2:B:542:MET:HE1	2.00	0.42
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.53	0.42
9:I:101:PHE:HD1	9:I:110:PHE:O	2.02	0.42
10:J:53:HIS:CD2	10:J:54:VAL:N	2.88	0.42
1:A:1027:ALA:O	1:A:1030:ARG:HB2	2.20	0.42
1:A:1242:VAL:CG1	1:A:1243:VAL:N	2.83	0.42
1:A:451:HIS:HB2	1:A:454:SER:OG	2.19	0.42
1:A:35:ILE:HD13	1:A:53:LEU:HD23	2.01	0.42
1:A:568:PRO:CB	3:C:221:TYR:CZ	3.03	0.42
1:A:84:ILE:HG21	1:A:239:LEU:HD23	2.01	0.42
1:A:99:ILE:O	1:A:102:VAL:HB	2.18	0.42
2:B:1177:HIS:O	2:B:1179:GLN:N	2.52	0.42
2:B:300:HIS:ND1	2:B:376:PHE:CD2	2.81	0.42
2:B:666:TYR:C	2:B:668:ASP:N	2.72	0.42
2:B:749:LEU:HD22	2:B:753:ALA:CB	2.49	0.42
2:B:955:THR:HA	12:L:54:ARG:O	2.19	0.42
3:C:31:ASN:O	3:C:32:SER:C	2.56	0.42
5:E:113:GLN:HG2	5:E:137:GLU:OE1	2.19	0.42
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.54	0.42
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.49	0.42
1:A:873:MET:C	1:A:1058:VAL:HG23	2.40	0.42
1:A:383:TYR:O	6:F:115:THR:HG22	2.20	0.42
1:A:751:SER:O	1:A:752:LYS:CB	2.67	0.42
1:A:756:ILE:CG2	1:A:757:ASN:N	2.80	0.42
1:A:760:GLN:CB	2:B:1021:MET:HE1	2.49	0.42
2:B:1106:ARG:HH12	2:B:1118:PRO:CA	2.33	0.42
2:B:315:LYS:O	2:B:317:CYS:N	2.53	0.42
5:E:28:TYR:CE1	5:E:78:LEU:CD1	3.03	0.42
1:A:567:LYS:CD	8:H:95:TYR:CD1	3.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:52:THR:CG2	10:J:52:THR:O	2.68	0.42
10:J:53:HIS:CE1	10:J:55:ASP:HA	2.54	0.42
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.51	0.42
1:A:1015:VAL:O	1:A:1015:VAL:HG12	2.18	0.42
1:A:108:MET:O	1:A:109:HIS:CB	2.66	0.42
1:A:1329:THR:HG22	1:A:1330:ASN:N	2.35	0.42
1:A:166:GLY:O	1:A:167:CYS:CB	2.67	0.42
1:A:458:HIS:CE1	1:A:507:VAL:CG2	3.00	0.42
1:A:530:GLY:O	1:A:532:ARG:N	2.53	0.42
1:A:533:LYS:C	1:A:535:THR:H	2.23	0.42
1:A:514:PRO:HB2	1:A:875:ALA:HB3	2.01	0.42
1:A:908:LEU:O	1:A:909:ASP:C	2.58	0.42
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.34	0.42
2:B:487:THR:O	2:B:488:TYR:C	2.56	0.42
2:B:634:TYR:CD1	2:B:692:TYR:HB3	2.55	0.42
5:E:137:GLU:O	5:E:138:ALA:C	2.57	0.42
8:H:24:CYS:CB	8:H:44:VAL:HG21	2.47	0.42
12:L:60:ARG:CG	12:L:61:THR:N	2.62	0.42
1:A:1173:HIS:NE2	1:A:1227:ILE:HG23	2.35	0.42
1:A:1349:TYR:O	1:A:1350:LYS:C	2.56	0.42
1:A:14:VAL:O	1:A:15:LYS:HD3	2.20	0.42
1:A:474:VAL:O	1:A:474:VAL:HG13	2.20	0.42
1:A:683:ILE:O	1:A:686:ALA:N	2.53	0.42
2:B:1115:THR:CG2	2:B:1199:ALA:HB2	2.50	0.42
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.85	0.42
2:B:435:THR:O	2:B:435:THR:HG22	2.20	0.42
2:B:995:ARG:CB	2:B:995:ARG:HH11	2.33	0.42
3:C:214:ASN:CB	3:C:217:ASP:OD2	2.68	0.42
6:F:138:LEU:HD23	6:F:138:LEU:HA	1.83	0.42
1:A:1126:ALA:O	1:A:1128:GLN:N	2.53	0.42
1:A:1366:ARG:HH11	1:A:1366:ARG:HG2	1.84	0.42
1:A:14:VAL:HB	1:A:1430:LEU:HD13	2.02	0.42
1:A:76:GLU:O	1:A:78:PRO:CD	2.68	0.42
2:B:1148:LYS:O	2:B:1152:MET:HB2	2.19	0.42
2:B:1149:GLU:HG3	2:B:1153:GLU:OE1	2.20	0.42
2:B:1177:HIS:C	2:B:1179:GLN:H	2.22	0.42
2:B:280:ILE:CG2	2:B:285:ILE:HG13	2.47	0.42
2:B:368:GLU:O	2:B:371:GLU:OE1	2.37	0.42
2:B:499:ASN:OD1	2:B:500:THR:N	2.53	0.42
2:B:640:VAL:HG22	2:B:651:LEU:CD2	2.50	0.42
2:B:737:THR:HG23	9:I:66:PRO:HB3	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:911:ILE:HG21	2:B:966:VAL:HG11	2.01	0.42
3:C:146:LYS:O	3:C:147:LEU:HD23	2.20	0.42
3:C:166:GLU:CG	11:K:10:PHE:CZ	2.96	0.42
3:C:242:GLN:O	3:C:246:ARG:N	2.52	0.42
5:E:100:ILE:O	5:E:101:GLN:C	2.58	0.42
8:H:109:LYS:HZ2	8:H:109:LYS:HB2	1.84	0.42
8:H:138:GLU:HG2	8:H:139:ASN:N	2.35	0.42
9:I:63:GLY:O	9:I:70:ARG:NH2	2.53	0.42
1:A:101:LYS:HG2	1:A:139:TRP:CZ2	2.55	0.41
1:A:1168:GLU:O	1:A:1172:LEU:HG	2.19	0.41
1:A:1254:ALA:O	1:A:1255:GLU:HB2	2.19	0.41
1:A:1394:THR:HG22	1:A:1395:GLY:O	2.19	0.41
1:A:481:ASP:C	1:A:481:ASP:OD1	2.58	0.41
1:A:598:LEU:HD22	8:H:25:ARG:CZ	2.50	0.41
1:A:760:GLN:OE1	2:B:1021:MET:HE2	2.20	0.41
2:B:1177:HIS:O	2:B:1179:GLN:HG3	2.19	0.41
2:B:167:ILE:O	2:B:168:GLY:O	2.38	0.41
2:B:230:ALA:O	2:B:232:SER:N	2.47	0.41
2:B:640:VAL:HG22	2:B:651:LEU:HD23	2.01	0.41
2:B:707:PRO:HG2	2:B:708:GLU:N	2.27	0.41
3:C:27:LEU:HD12	3:C:27:LEU:O	2.20	0.41
9:I:25:LEU:HD12	9:I:26:LEU:N	2.35	0.41
3:C:14:SER:HA	11:K:114:LEU:HD22	2.02	0.41
11:K:82:ASP:O	11:K:85:ASP:HB2	2.20	0.41
1:A:1343:ALA:O	1:A:1346:ALA:HB3	2.20	0.41
1:A:474:VAL:HG13	1:A:478:TYR:HE1	1.85	0.41
1:A:639:PRO:HG2	1:A:640:GLN:H	1.84	0.41
1:A:982:THR:HB	1:A:985:ASP:CG	2.40	0.41
2:B:1106:ARG:HH12	2:B:1118:PRO:HA	1.85	0.41
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.60	0.41
2:B:92:PHE:HD2	2:B:130:VAL:HG11	1.85	0.41
2:B:405:ARG:CZ	2:B:632:ARG:HG2	2.49	0.41
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.54	0.41
2:B:901:PRO:O	2:B:949:VAL:O	2.38	0.41
6:F:109:VAL:HG12	6:F:110:ASP:H	1.82	0.41
9:I:16:PRO:HA	9:I:26:LEU:O	2.20	0.41
1:A:547:LEU:HD22	11:K:58:PHE:HD1	1.84	0.41
11:K:65:HIS:HD2	11:K:67:PHE:CB	2.33	0.41
1:A:399:HIS:C	1:A:401:GLY:N	2.71	0.41
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.60	0.41
1:A:629:LEU:CD1	1:A:645:LEU:HD21	2.48	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:LEU:HD12	1:A:808:LEU:N	2.35	0.41
2:B:1177:HIS:HB2	2:B:1179:GLN:HG3	2.03	0.41
2:B:350:GLN:O	2:B:351:TYR:C	2.59	0.41
5:E:19:VAL:O	5:E:19:VAL:HG12	2.20	0.41
8:H:84:ALA:HA	8:H:87:ARG:CB	2.50	0.41
12:L:28:LYS:O	12:L:29:TYR:CG	2.74	0.41
1:A:1406:VAL:CG1	1:A:1410:PHE:CE1	3.03	0.41
1:A:388:LEU:HA	1:A:388:LEU:HD23	1.88	0.41
1:A:894:GLU:C	1:A:896:ARG:N	2.74	0.41
1:A:913:LEU:CD1	1:A:981:LEU:O	2.69	0.41
2:B:1033:LYS:NZ	2:B:1087:PHE:O	2.51	0.41
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.55	0.41
2:B:879:ARG:O	2:B:880:THR:HB	2.20	0.41
3:C:252:GLN:HG3	11:K:95:ILE:HG23	2.03	0.41
3:C:252:GLN:NE2	11:K:99:GLY:N	2.68	0.41
1:A:871:ASP:CB	5:E:204:THR:CG2	2.99	0.41
11:K:106:GLU:O	11:K:110:ASN:ND2	2.54	0.41
1:A:1026:LEU:HA	1:A:1026:LEU:HD23	1.90	0.41
1:A:113:LEU:C	1:A:115:LEU:H	2.23	0.41
1:A:441:PRO:HG2	1:A:441:PRO:O	2.20	0.41
1:A:679:ILE:CG2	1:A:729:ALA:HB1	2.43	0.41
1:A:771:GLU:N	1:A:822:GLU:OE1	2.53	0.41
1:A:984:LYS:O	1:A:988:LEU:HB2	2.19	0.41
2:B:1020:ARG:O	2:B:1021:MET:C	2.58	0.41
2:B:1120:GLU:CG	2:B:1121:GLY:N	2.84	0.41
2:B:175:ARG:HH11	2:B:175:ARG:CG	2.34	0.41
2:B:276:ILE:HD11	2:B:355:ILE:CD1	2.50	0.41
2:B:835:GLN:HE21	2:B:835:GLN:HB2	1.74	0.41
2:B:865:LYS:HB3	2:B:866:TYR:H	1.72	0.41
2:B:911:ILE:HD11	2:B:941:LEU:CB	2.51	0.41
5:E:71:LYS:C	5:E:73:PRO:HD3	2.40	0.41
1:A:567:LYS:NZ	8:H:95:TYR:CD1	2.80	0.41
1:A:960:ILE:HD12	1:A:1021:LEU:CD2	2.50	0.41
1:A:1193:LEU:HD21	1:A:1267:MET:CE	2.51	0.41
1:A:1139:GLU:HG3	1:A:1280:GLU:O	2.20	0.41
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.85	0.41
1:A:38:PRO:CA	1:A:270:LEU:HD23	2.49	0.41
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.56	0.41
1:A:531:ILE:CG2	1:A:532:ARG:N	2.84	0.41
1:A:960:ILE:O	1:A:961:ARG:C	2.57	0.41
1:A:338:GLY:CA	2:B:1129:ARG:HH22	2.17	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:ILE:HD12	2:B:234:ILE:N	2.29	0.41
2:B:307:ASP:O	2:B:308:TRP:C	2.59	0.41
2:B:329:THR:O	2:B:333:PHE:N	2.48	0.41
2:B:418:LYS:O	2:B:420:LEU:N	2.54	0.41
2:B:53:GLN:HG2	2:B:547:VAL:HG13	2.02	0.41
2:B:601:ARG:O	2:B:605:ARG:HG3	2.19	0.41
5:E:13:TRP:O	5:E:16:PHE:HB3	2.21	0.41
8:H:4:THR:O	8:H:5:LEU:HD23	2.20	0.41
9:I:40:SER:HB2	9:I:41:PRO:HD2	2.03	0.41
9:I:59:VAL:HG12	9:I:60:GLN:N	2.34	0.41
9:I:98:VAL:HG12	9:I:99:LEU:N	2.36	0.41
10:J:3:VAL:CG2	10:J:18:TRP:CG	3.02	0.41
11:K:71:PHE:CD1	11:K:71:PHE:C	2.93	0.41
11:K:93:SER:O	11:K:97:LYS:HG3	2.20	0.41
1:A:542:GLU:OE1	1:A:569:LYS:HE2	2.20	0.41
2:B:185:THR:N	2:B:188:ASP:HB2	2.36	0.41
2:B:240:ILE:C	2:B:253:THR:HG23	2.41	0.41
2:B:702:LEU:HD12	2:B:702:LEU:HA	1.76	0.41
5:E:72:PHE:CD2	5:E:155:ARG:NH2	2.83	0.41
11:K:35:PHE:O	11:K:70:ARG:HB2	2.21	0.41
2:B:955:THR:CG2	12:L:54:ARG:O	2.65	0.41
1:A:1187:GLN:HA	1:A:1243:VAL:HG23	2.02	0.41
1:A:225:ASN:C	1:A:227:VAL:N	2.71	0.41
1:A:407:ARG:HG2	1:A:430:TRP:CE2	2.54	0.41
1:A:515:GLN:CG	1:A:516:SER:N	2.84	0.41
1:A:866:PHE:C	1:A:867:ILE:HG13	2.40	0.41
2:B:105:SER:O	2:B:106:ASP:HB2	2.20	0.41
2:B:1104:HIS:HB2	2:B:1122:ARG:CB	2.51	0.41
2:B:1152:MET:O	2:B:1156:ASP:O	2.39	0.41
2:B:346:GLU:O	2:B:347:LYS:C	2.58	0.41
1:A:525:GLN:HB2	2:B:835:GLN:HG2	2.00	0.41
5:E:7:ARG:HG3	5:E:8:ASN:N	2.36	0.41
8:H:126:GLU:N	8:H:130:ARG:HH12	2.19	0.41
9:I:92:ARG:CG	9:I:93:LYS:N	2.84	0.41
10:J:27:GLU:C	10:J:29:GLU:H	2.23	0.41
2:B:800:GLN:CB	10:J:52:THR:CG2	2.89	0.41
12:L:41:SER:O	12:L:44:ASP:HB2	2.21	0.41
1:A:1116:LEU:CD2	1:A:1316:VAL:HG21	2.51	0.41
1:A:134:ARG:O	1:A:136:ALA:N	2.53	0.41
1:A:598:LEU:O	1:A:599:SER:C	2.59	0.41
2:B:199:MET:N	2:B:199:MET:SD	2.87	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:387:LEU:HD23	2:B:393:LYS:HD2	2.03	0.41
2:B:616:ILE:HG12	2:B:696:GLU:HG3	2.03	0.41
2:B:784:ASN:HD21	2:B:788:ARG:HD2	1.84	0.41
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.47	0.41
3:C:5:GLY:HA3	3:C:6:PRO:HD2	1.78	0.41
5:E:117:THR:O	5:E:120:ALA:N	2.54	0.41
8:H:57:VAL:CG1	8:H:58:THR:N	2.83	0.41
9:I:6:PHE:HD2	9:I:13:MET:HA	1.86	0.41
1:A:18:GLN:O	2:B:1215:ARG:HG3	2.21	0.41
1:A:530:GLY:O	1:A:533:LYS:N	2.53	0.41
1:A:909:ASP:OD1	1:A:910:PRO:HD2	2.21	0.41
2:B:1197:PRO:O	2:B:1200:ALA:N	2.51	0.41
2:B:51:PHE:O	2:B:54:PHE:N	2.54	0.41
2:B:843:GLN:HB2	2:B:993:THR:OG1	2.20	0.41
2:B:872:GLU:HA	2:B:915:THR:O	2.21	0.41
3:C:46:ILE:CG2	3:C:157:CYS:HB3	2.51	0.41
3:C:66:ARG:NH2	10:J:3:VAL:O	2.54	0.41
5:E:116:ILE:CG2	5:E:117:THR:N	2.84	0.41
9:I:34:TYR:C	9:I:35:VAL:HG23	2.41	0.41
9:I:99:LEU:HB2	9:I:112:SER:OG	2.21	0.41
11:K:103:THR:O	11:K:106:GLU:N	2.53	0.41
11:K:98:LEU:O	11:K:99:GLY:C	2.58	0.41
2:B:120:ARG:HH12	12:L:54:ARG:NH1	2.18	0.41
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.45	0.41
1:A:401:GLY:N	1:A:435:HIS:HD2	2.18	0.41
1:A:354:SER:CA	1:A:482:PHE:CD2	3.03	0.41
1:A:725:ALA:HA	1:A:728:LYS:HE2	2.02	0.41
2:B:850:LEU:HD22	2:B:1009:ASP:HB3	2.01	0.41
2:B:818:PRO:HG3	10:J:54:VAL:HG21	2.03	0.41
2:B:941:LEU:HD21	2:B:946:ASN:HA	2.02	0.41
2:B:1084:GLN:NE2	3:C:192:TRP:HB2	2.37	0.41
5:E:72:PHE:CD1	5:E:72:PHE:N	2.89	0.41
10:J:34:THR:O	10:J:35:ALA:C	2.58	0.41
1:A:15:LYS:HD2	2:B:1220:ARG:NE	2.35	0.40
1:A:379:VAL:HG22	1:A:431:LYS:HG2	2.03	0.40
1:A:399:HIS:NE2	1:A:462:VAL:HG21	2.36	0.40
1:A:738:LYS:CB	8:H:19:ARG:HH22	2.34	0.40
1:A:878:ILE:HG22	1:A:879:GLU:N	2.37	0.40
1:A:962:ARG:O	1:A:963:ILE:C	2.57	0.40
1:A:751:SER:OG	2:B:1015:HIS:HE1	2.03	0.40
2:B:1103:ILE:HG13	2:B:1103:ILE:H	1.52	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ILE:HG12	2:B:324:ILE:HD12	2.03	0.40
2:B:321:GLY:C	2:B:323:VAL:N	2.74	0.40
2:B:627:PHE:O	2:B:632:ARG:NH1	2.54	0.40
2:B:758:PHE:HB2	2:B:1024:ALA:HB1	2.04	0.40
2:B:992:ILE:CD1	2:B:994:TYR:CE2	3.04	0.40
3:C:29:MET:O	3:C:30:ALA:C	2.59	0.40
5:E:127:ILE:O	5:E:127:ILE:CG1	2.63	0.40
1:A:1322:ILE:HD12	1:A:1327:ILE:HD12	2.03	0.40
1:A:1345:ARG:CG	1:A:1372:VAL:HG12	2.51	0.40
1:A:172:PRO:HB3	1:A:185:TRP:CZ2	2.56	0.40
1:A:19:PHE:HB3	1:A:1413:GLY:HA2	2.03	0.40
1:A:270:LEU:O	1:A:274:ILE:HG13	2.21	0.40
1:A:384:ASN:O	1:A:386:ASP:N	2.54	0.40
1:A:508:PRO:O	1:A:511:ILE:HG13	2.22	0.40
1:A:598:LEU:HD22	8:H:25:ARG:HH12	1.83	0.40
1:A:804:TYR:HE1	2:B:1021:MET:HE3	1.85	0.40
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.57	0.40
2:B:446:LEU:HG	2:B:446:LEU:O	2.21	0.40
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.36	0.40
2:B:707:PRO:O	2:B:708:GLU:C	2.59	0.40
5:E:157:SER:OG	5:E:159:ASP:HB2	2.22	0.40
5:E:3:GLN:HG3	5:E:5:ASN:H	1.85	0.40
8:H:40:LEU:HD13	8:H:123:MET:HE2	2.02	0.40
2:B:801:LYS:HE2	10:J:51:LEU:O	2.22	0.40
1:A:1029:ARG:O	1:A:1032:LEU:N	2.55	0.40
1:A:1039:LYS:NZ	1:A:1043:ASP:OD1	2.47	0.40
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	2.03	0.40
1:A:1316:VAL:O	1:A:1322:ILE:HD13	2.21	0.40
1:A:1364:ASN:HD21	1:A:1366:ARG:NH1	2.19	0.40
1:A:332:LYS:H	1:A:337:ARG:CB	2.33	0.40
1:A:403:LYS:O	1:A:404:TYR:O	2.39	0.40
1:A:556:TRP:CE2	1:A:558:GLY:HA2	2.56	0.40
1:A:19:PHE:HA	2:B:1213:THR:O	2.22	0.40
2:B:113:TYR:CE2	2:B:192:LEU:HD22	2.57	0.40
2:B:188:ASP:O	2:B:192:LEU:HG	2.21	0.40
2:B:233:PRO:HG2	2:B:234:ILE:HG13	2.03	0.40
2:B:244:LEU:HB2	2:B:249:ARG:HA	2.03	0.40
2:B:288:ALA:HB2	2:B:330:ALA:HB1	2.04	0.40
2:B:348:ARG:H	2:B:348:ARG:HG2	1.67	0.40
2:B:345:LYS:N	2:B:348:ARG:HE	2.15	0.40
2:B:549:THR:HG22	2:B:550:ASP:N	2.36	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:ASP:CB	2:B:57:TYR:HD1	2.33	0.40
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.03	0.40
2:B:864:LYS:H	2:B:872:GLU:HB2	1.87	0.40
2:B:952:VAL:HG13	2:B:966:VAL:HG22	2.03	0.40
3:C:175:ALA:HB3	10:J:43:ARG:CZ	2.51	0.40
5:E:131:THR:HG21	5:E:191:LYS:HE2	2.02	0.40
8:H:33:GLN:OE1	8:H:129:TYR:HE2	2.05	0.40
1:A:1220:PHE:O	1:A:1221:LYS:C	2.60	0.40
1:A:1283:VAL:O	1:A:1306:LEU:HA	2.21	0.40
1:A:336:ILE:CD1	1:A:1405:THR:HG21	2.45	0.40
1:A:331:GLY:O	1:A:332:LYS:O	2.39	0.40
1:A:432:VAL:O	1:A:434:ARG:N	2.54	0.40
1:A:535:THR:O	1:A:536:LEU:C	2.59	0.40
1:A:553:VAL:HG22	1:A:652:VAL:CG2	2.51	0.40
2:B:283:VAL:HG13	2:B:297:ILE:HD12	2.03	0.40
2:B:348:ARG:O	2:B:349:ILE:C	2.60	0.40
2:B:365:THR:HG22	2:B:367:LEU:H	1.87	0.40
2:B:380:TYR:O	2:B:384:ARG:HG2	2.21	0.40
2:B:424:LEU:HD12	2:B:424:LEU:HA	1.91	0.40
2:B:994:TYR:CD1	2:B:999:MET:HE3	2.56	0.40
3:C:114:TYR:CG	3:C:140:ASN:HB3	2.56	0.40
8:H:117:SER:HA	8:H:122:LEU:HD23	2.02	0.40
9:I:101:PHE:HB2	9:I:110:PHE:CE2	2.57	0.40
1:A:709:THR:CG2	9:I:94:ASP:HA	2.52	0.40
11:K:46:ILE:CG2	11:K:50:LEU:HD12	2.51	0.40
1:A:1116:LEU:H	1:A:1308:THR:CG2	2.35	0.40
1:A:1378:GLN:O	1:A:1380:GLY:N	2.55	0.40
1:A:396:PRO:HB3	1:A:403:LYS:HG2	2.03	0.40
1:A:783:THR:CG2	1:A:815:PHE:CZ	2.98	0.40
1:A:768:GLN:HG2	1:A:816:HIS:N	2.37	0.40
1:A:929:LEU:N	1:A:929:LEU:CD2	2.85	0.40
2:B:1114:LEU:O	2:B:1198:TYR:HE2	2.04	0.40
1:A:17:VAL:HA	2:B:1215:ARG:O	2.22	0.40
2:B:56:ASP:CB	2:B:57:TYR:CD1	3.04	0.40
2:B:57:TYR:O	2:B:58:THR:C	2.60	0.40
2:B:637:LEU:O	2:B:690:VAL:HG13	2.22	0.40
2:B:121:ASN:HD21	2:B:965:LYS:HE3	1.86	0.40
3:C:214:ASN:HB2	3:C:217:ASP:OD2	2.22	0.40
5:E:182:ASP:O	5:E:186:LEU:HG	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:LYS:NZ	3:C:90:ASP:N[4_555]	1.74	0.46

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1365/1733 (79%)	1022 (75%)	251 (18%)	92 (7%)	1	17
2	B	1077/1224 (88%)	839 (78%)	169 (16%)	69 (6%)	1	18
3	C	264/318 (83%)	208 (79%)	40 (15%)	16 (6%)	1	19
5	E	212/215 (99%)	170 (80%)	33 (16%)	9 (4%)	3	24
6	F	82/155 (53%)	64 (78%)	15 (18%)	3 (4%)	3	27
8	H	129/146 (88%)	93 (72%)	21 (16%)	15 (12%)	0	6
9	I	117/122 (96%)	93 (80%)	15 (13%)	9 (8%)	1	15
10	J	63/70 (90%)	47 (75%)	12 (19%)	4 (6%)	1	19
11	K	112/120 (93%)	96 (86%)	15 (13%)	1 (1%)	17	54
12	L	44/70 (63%)	22 (50%)	13 (30%)	9 (20%)	0	2
All	All	3465/4173 (83%)	2654 (77%)	584 (17%)	227 (7%)	1	18

All (227) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	48	ALA
1	A	55	ASP
1	A	56	PRO
1	A	74	MET
1	A	75	ASN
1	A	167	CYS
1	A	322	VAL
1	A	404	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	418	SER
1	A	543	LEU
1	A	567	LYS
1	A	597	LEU
1	A	598	LEU
1	A	628	GLY
1	A	752	LYS
1	A	846	GLU
1	A	998	LEU
1	A	1036	ARG
1	A	1127	ASP
1	A	1206	ASP
1	A	1221	LYS
1	A	1223	ASP
1	A	1392	SER
1	A	1393	ASN
1	A	1403	GLU
1	A	1406	VAL
1	A	1416	ALA
2	B	65	GLU
2	B	124	TYR
2	B	174	LEU
2	B	175	ARG
2	B	200	GLY
2	B	229	ALA
2	B	364	ILE
2	B	367	LEU
2	B	531	GLN
2	B	708	GLU
2	B	709	ASP
2	B	731	VAL
2	B	751	VAL
2	B	958	GLN
2	B	959	ASP
2	B	1046	PRO
2	B	1103	ILE
2	B	1167	GLY
2	B	1176	ASN
2	B	1183	LYS
3	C	4	GLU
3	C	5	GLY
3	C	6	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	C	110	THR
3	C	142	VAL
3	C	215	GLU
6	F	73	ALA
8	H	32	THR
8	H	81	PRO
8	H	140	ALA
9	I	8	ARG
10	J	2	ILE
10	J	55	ASP
12	L	27	LEU
12	L	38	LEU
12	L	64	LEU
1	A	35	ILE
1	A	54	ASN
1	A	62	ASP
1	A	87	ALA
1	A	109	HIS
1	A	135	PHE
1	A	168	GLY
1	A	332	LYS
1	A	385	ILE
1	A	419	LYS
1	A	534	LEU
1	A	568	PRO
1	A	790	ASP
1	A	986	ILE
1	A	1114	PRO
1	A	1365	TYR
1	A	1366	ARG
1	A	1379	GLY
2	B	55	VAL
2	B	168	GLY
2	B	275	TYR
2	B	346	GLU
2	B	410	GLY
2	B	480	SER
2	B	641	GLU
2	B	643	ASP
2	B	792	MET
2	B	864	LYS
2	B	866	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	884	ARG
2	B	891	ASP
2	B	992	ILE
2	B	1066	SER
2	B	1155	SER
3	C	136	ASP
6	F	142	SER
8	H	61	SER
8	H	77	ARG
8	H	88	SER
8	H	128	ASN
9	I	30	ARG
9	I	79	HIS
12	L	39	SER
12	L	52	GLY
1	A	6	TYR
1	A	45	GLN
1	A	59	GLY
1	A	67	CYS
1	A	69	THR
1	A	335	ARG
1	A	433	GLU
1	A	596	THR
1	A	737	LEU
1	A	775	ILE
1	A	830	LYS
1	A	920	LEU
2	B	28	GLU
2	B	249	ARG
2	B	277	LYS
2	B	447	ALA
2	B	629	ASP
2	B	735	ALA
2	B	880	THR
2	B	1017	ILE
2	B	1099	VAL
2	B	1104	HIS
2	B	1178	ASN
3	C	48	SER
3	C	212	PRO
3	C	227	THR
5	E	31	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
5	E	102	GLU
5	E	103	LYS
5	E	122	LYS
5	E	139	ALA
5	E	206	GLY
6	F	128	LYS
8	H	8	ASP
8	H	17	PRO
8	H	82	PRO
8	H	135	LEU
8	H	139	ASN
9	I	9	ASP
9	I	33	SER
9	I	86	PHE
10	J	9	SER
12	L	63	ARG
1	A	101	LYS
1	A	134	ARG
1	A	139	TRP
1	A	424	ILE
1	A	599	SER
1	A	1067	LEU
1	A	1097	GLY
1	A	1115	SER
1	A	1122	PRO
1	A	1405	THR
2	B	248	SER
2	B	304	ASP
2	B	436	VAL
2	B	501	PRO
2	B	667	GLN
2	B	791	THR
2	B	807	ARG
2	B	1054	GLY
2	B	1097	HIS
3	C	18	VAL
3	C	149	LYS
3	C	174	ALA
5	E	59	SER
10	J	6	ARG
12	L	50	ASP
12	L	56	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	58	LEU
1	A	223	GLY
1	A	399	HIS
1	A	400	PRO
1	A	958	VAL
1	A	972	HIS
1	A	1098	VAL
1	A	1130	GLN
1	A	1282	VAL
1	A	1351	GLU
1	A	1378	GLN
2	B	419	THR
2	B	619	ILE
2	B	648	HIS
2	B	687	GLU
2	B	707	PRO
2	B	712	PRO
2	B	764	SER
2	B	907	GLY
2	B	982	SER
2	B	1108	ARG
5	E	36	GLU
8	H	62	SER
8	H	89	LEU
9	I	47	GLU
9	I	88	SER
1	A	226	GLU
1	A	368	LYS
1	A	465	TYR
1	A	531	ILE
1	A	903	ASN
1	A	1014	ALA
1	A	1314	SER
1	A	1352	VAL
2	B	27	ALA
5	E	167	ARG
8	H	138	GLU
9	I	98	VAL
11	K	107	THR
2	B	247	GLY
1	A	336	ILE
1	A	1104	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	L	55	ILE
1	A	810	PRO
1	A	1075	PRO
1	A	1242	VAL
3	C	172	PRO
3	C	216	GLY
2	B	511	PRO
3	C	218	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1206/1520 (79%)	1128 (94%)	78 (6%)	17	45
2	B	952/1061 (90%)	886 (93%)	66 (7%)	15	43
3	C	234/274 (85%)	222 (95%)	12 (5%)	24	52
5	E	196/197 (100%)	189 (96%)	7 (4%)	35	60
6	F	74/137 (54%)	68 (92%)	6 (8%)	11	38
8	H	117/128 (91%)	112 (96%)	5 (4%)	29	56
9	I	113/116 (97%)	104 (92%)	9 (8%)	12	39
10	J	60/65 (92%)	56 (93%)	4 (7%)	16	44
11	K	99/102 (97%)	90 (91%)	9 (9%)	9	33
12	L	40/57 (70%)	35 (88%)	5 (12%)	4	22
All	All	3091/3657 (84%)	2890 (94%)	201 (6%)	17	45

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	22	PHE
1	A	31	SER
1	A	56	PRO
1	A	70	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	93	VAL
1	A	122	MET
1	A	247	ARG
1	A	269	ILE
1	A	302	THR
1	A	322	VAL
1	A	326	ARG
1	A	351	THR
1	A	375	THR
1	A	381	THR
1	A	385	ILE
1	A	397	ASN
1	A	412	ARG
1	A	434	ARG
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	461	LYS
1	A	474	VAL
1	A	475	THR
1	A	493	GLN
1	A	503	GLN
1	A	524	VAL
1	A	538	ASP
1	A	590	ARG
1	A	596	THR
1	A	597	LEU
1	A	598	LEU
1	A	618	GLU
1	A	629	LEU
1	A	666	ILE
1	A	682	THR
1	A	740	LEU
1	A	741	ASN
1	A	745	GLN
1	A	756	ILE
1	A	768	GLN
1	A	774	ARG
1	A	821	ARG
1	A	845	LEU
1	A	849	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	855	THR
1	A	858	ASN
1	A	920	LEU
1	A	929	LEU
1	A	948	VAL
1	A	949	ASP
1	A	979	SER
1	A	1029	ARG
1	A	1035	TYR
1	A	1043	ASP
1	A	1055	ARG
1	A	1057	VAL
1	A	1077	THR
1	A	1128	GLN
1	A	1222	ASN
1	A	1232	ASN
1	A	1258	HIS
1	A	1264	GLU
1	A	1295	THR
1	A	1308	THR
1	A	1318	THR
1	A	1332	PHE
1	A	1335	ILE
1	A	1351	GLU
1	A	1359	ASP
1	A	1364	ASN
1	A	1366	ARG
1	A	1375	MET
1	A	1376	THR
1	A	1425	SER
1	A	1442	ASP
2	B	20	ASP
2	B	43	LEU
2	B	57	TYR
2	B	61	ASP
2	B	63	ILE
2	B	98	THR
2	B	109	THR
2	B	121	ASN
2	B	175	ARG
2	B	194	GLU
2	B	232	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	234	ILE
2	B	261	ARG
2	B	268	THR
2	B	278	GLN
2	B	309	GLN
2	B	313	MET
2	B	317	CYS
2	B	320	ASP
2	B	331	LEU
2	B	376	PHE
2	B	387	LEU
2	B	396	ASP
2	B	408	LEU
2	B	466	TRP
2	B	485	ARG
2	B	513	GLN
2	B	514	LEU
2	B	538	ASN
2	B	547	VAL
2	B	570	VAL
2	B	576	ASP
2	B	624	LEU
2	B	629	ASP
2	B	644	GLU
2	B	680	THR
2	B	723	VAL
2	B	732	SER
2	B	762	ASN
2	B	764	SER
2	B	780	VAL
2	B	791	THR
2	B	835	GLN
2	B	901	PRO
2	B	909	ASP
2	B	915	THR
2	B	944	THR
2	B	951	GLN
2	B	953	LEU
2	B	976	ILE
2	B	986	GLN
2	B	987	LYS
2	B	996	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	999	MET
2	B	1007	VAL
2	B	1021	MET
2	B	1049	ASP
2	B	1103	ILE
2	B	1111	MET
2	B	1118	PRO
2	B	1132	GLU
2	B	1147	LEU
2	B	1150	ARG
2	B	1151	LEU
2	B	1183	LYS
2	B	1185	CYS
3	C	22	LEU
3	C	25	VAL
3	C	26	ASP
3	C	62	PHE
3	C	69	LEU
3	C	77	ILE
3	C	133	ILE
3	C	148	ARG
3	C	229	TYR
3	C	233	GLU
3	C	240	VAL
3	C	264	GLN
5	E	40	GLU
5	E	60	PHE
5	E	74	ASP
5	E	84	ASP
5	E	92	THR
5	E	104	ASN
5	E	183	PRO
6	F	79	ARG
6	F	90	ARG
6	F	103	MET
6	F	111	LEU
6	F	115	THR
6	F	133	VAL
8	H	21	ASN
8	H	27	GLU
8	H	109	LYS
8	H	110	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	H	134	ASN
9	I	7	CYS
9	I	12	ASN
9	I	29	CYS
9	I	31	THR
9	I	52	ILE
9	I	75	CYS
9	I	76	PRO
9	I	87	GLN
9	I	103	CYS
10	J	2	ILE
10	J	7	CYS
10	J	47	ARG
10	J	48	ARG
11	K	20	LYS
11	K	25	THR
11	K	31	VAL
11	K	47	ARG
11	K	50	LEU
11	K	61	TYR
11	K	77	THR
11	K	81	TYR
11	K	114	LEU
12	L	50	ASP
12	L	54	ARG
12	L	55	ILE
12	L	68	GLU
12	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	92	HIS
1	A	118	HIS
1	A	169	ASN
1	A	225	ASN
1	A	339	ASN
1	A	358	ASN
1	A	435	HIS
1	A	445	ASN
1	A	493	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	503	GLN
1	A	517	ASN
1	A	631	HIS
1	A	723	ASN
1	A	736	ASN
1	A	741	ASN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	926	GLN
1	A	965	GLN
1	A	968	GLN
1	A	994	GLN
1	A	1364	ASN
1	A	1387	HIS
1	A	1390	ASN
1	A	1432	GLN
2	B	46	GLN
2	B	53	GLN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	325	GLN
2	B	363	HIS
2	B	465	ASN
2	B	484	ASN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	657	HIS
2	B	744	HIS
2	B	822	ASN
2	B	842	ASN
2	B	862	GLN
2	B	957	ASN
2	B	975	GLN
2	B	1015	HIS
2	B	1065	GLN
2	B	1117	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	1179	GLN
2	B	1193	GLN
3	C	65	HIS
3	C	73	GLN
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	242	GLN
3	C	252	GLN
5	E	5	ASN
5	E	32	GLN
5	E	101	GLN
5	E	104	ASN
5	E	114	ASN
5	E	147	HIS
8	H	33	GLN
9	I	12	ASN
10	J	53	HIS
11	K	52	ASN
11	K	65	HIS
11	K	76	GLN
11	K	110	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1388/1733 (80%)	-0.07	38 (2%) 54 44	20, 181, 283, 321	0
2	B	1097/1224 (89%)	-0.02	28 (2%) 56 45	74, 189, 297, 321	0
3	C	266/318 (83%)	0.00	5 (1%) 66 58	87, 180, 262, 321	0
4	D	0/161	-	-	-	-
5	E	214/215 (99%)	0.20	9 (4%) 36 29	88, 223, 305, 321	0
6	F	84/155 (54%)	0.05	2 (2%) 59 49	90, 163, 254, 321	0
7	G	0/170	-	-	-	-
8	H	133/146 (91%)	0.40	7 (5%) 26 23	139, 242, 318, 321	0
9	I	119/122 (97%)	0.71	16 (13%) 3 4	139, 241, 318, 321	0
10	J	65/70 (92%)	-0.11	3 (4%) 32 27	68, 173, 284, 313	0
11	K	114/120 (95%)	-0.03	2 (1%) 68 59	98, 170, 245, 304	0
12	L	46/70 (65%)	0.19	3 (6%) 18 15	134, 233, 304, 321	0
All	All	3526/4504 (78%)	0.02	113 (3%) 47 37	20, 189, 294, 321	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	199	LEU	5.2
1	A	114	LEU	5.1
2	B	869	SER	4.7
2	B	715	ALA	4.6
5	E	88	VAL	4.6
1	A	149	GLU	4.4
3	C	4	GLU	4.2
9	I	73	ARG	4.1
2	B	882	THR	4.1
1	A	1236	LEU	4.0
1	A	153	PRO	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
8	H	8	ASP	3.9
9	I	74	GLU	3.9
9	I	83	ASN	3.8
2	B	887	HIS	3.8
9	I	119	THR	3.6
9	I	76	PRO	3.6
5	E	113	GLN	3.6
8	H	35	GLN	3.6
2	B	428	ILE	3.4
5	E	114	ASN	3.4
12	L	46	VAL	3.3
1	A	593	GLU	3.3
1	A	69	THR	3.2
8	H	107	VAL	3.2
9	I	72	ASP	3.2
2	B	933	SER	3.1
1	A	1221	LYS	3.1
1	A	1256	GLU	3.1
8	H	2	SER	3.1
2	B	865	LYS	3.0
10	J	26	GLN	3.0
9	I	34	TYR	3.0
9	I	18	GLU	3.0
1	A	161	LEU	3.0
1	A	1159	ARG	3.0
3	C	266	ASP	3.0
1	A	282	ASN	2.9
1	A	152	VAL	2.9
5	E	93	MET	2.8
2	B	133	LYS	2.8
2	B	346	GLU	2.7
2	B	714	GLU	2.7
10	J	28	ASP	2.7
1	A	426	LEU	2.7
1	A	44	THR	2.7
5	E	126	SER	2.7
1	A	186	LYS	2.7
2	B	106	ASP	2.6
2	B	881	ASN	2.6
3	C	3	GLU	2.6
5	E	115	ASN	2.6
2	B	164	LYS	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	866	TYR	2.6
1	A	1188	GLN	2.6
1	A	168	GLY	2.5
9	I	8	ARG	2.5
2	B	437	GLU	2.5
10	J	27	GLU	2.5
1	A	1161	THR	2.5
6	F	110	ASP	2.5
1	A	115	LEU	2.5
8	H	85	GLY	2.5
1	A	124	GLN	2.5
2	B	870	ILE	2.4
12	L	49	LYS	2.4
11	K	74	ARG	2.4
2	B	108	VAL	2.4
1	A	1127	ASP	2.4
3	C	195	GLN	2.4
1	A	1175	SER	2.4
1	A	164	ARG	2.4
1	A	287	HIS	2.4
2	B	643	ASP	2.4
1	A	66	LYS	2.3
9	I	71	SER	2.3
8	H	110	ASP	2.3
8	H	11	GLN	2.3
1	A	323	LYS	2.3
1	A	1079	MET	2.3
1	A	1095	THR	2.3
3	C	127	ARG	2.3
5	E	86	PRO	2.3
2	B	465	ASN	2.3
1	A	1126	ALA	2.2
2	B	667	GLN	2.2
5	E	118	PRO	2.2
2	B	888	GLY	2.2
2	B	1224	PHE	2.2
1	A	259	GLU	2.2
2	B	92	PHE	2.2
2	B	432	MET	2.2
9	I	84	VAL	2.2
1	A	118	HIS	2.2
1	A	279	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
6	F	104	ASN	2.1
9	I	104	LEU	2.1
9	I	102	VAL	2.1
1	A	1108	ALA	2.1
1	A	1003	LYS	2.1
2	B	259	TYR	2.1
5	E	87	SER	2.1
1	A	1300	LYS	2.1
9	I	23	ASN	2.1
1	A	1206	ASP	2.1
9	I	118	ARG	2.0
12	L	47	ARG	2.0
9	I	114	GLN	2.0
11	K	79	GLU	2.0
1	A	148	CYS	2.0
2	B	425	THR	2.0
2	B	424	LEU	2.0
2	B	349	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
13	ZN	I	203	1/1	0.90	0.19	172,172,172,172	0
13	ZN	A	1735	1/1	0.90	0.11	172,172,172,172	0
13	ZN	I	204	1/1	0.92	0.25	172,172,172,172	0
13	ZN	A	1734	1/1	0.93	0.17	172,172,172,172	0
13	ZN	C	319	1/1	0.94	0.06	172,172,172,172	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
13	ZN	J	101	1/1	0.94	0.13	172,172,172,172	0
13	ZN	B	1307	1/1	0.99	0.06	172,172,172,172	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.