



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:05 am GMT

PDB ID : 3PRX  
Title : Structure of Complement C5 in Complex with CVF and SSL7  
Authors : Laursen, N.S.; Andersen, G.R.; Sottrup-Jensen, L.; Andersen, K.R.; Spillner, E.; Braren, I.  
Deposited on : 2010-11-30  
Resolution : 4.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

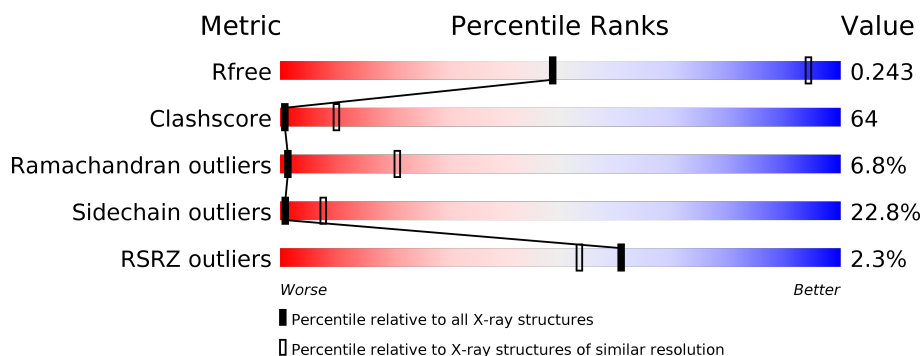
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.30 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))
$R_{free}$	100719	1002 (4.92-3.62)
Clashscore	112137	1001 (4.92-3.68)
Ramachandran outliers	110173	1012 (4.92-3.64)
Sidechain outliers	110143	1021 (4.92-3.62)
RSRZ outliers	101464	1009 (4.92-3.62)

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

Mol	Chain	Length	Quality of chain
1	A	1676	<div> <div>24%</div> <div>50%</div> <div>21%</div> <div>• •</div> </div>
1	C	1676	<div> <div>3%</div> <div>23%</div> <div>51%</div> <div>21%</div> <div>• •</div> </div>
2	B	1642	<div> <div>23%</div> <div>38%</div> <div>13%</div> <div>26%</div> </div>
2	D	1642	<div> <div>22%</div> <div>39%</div> <div>12%</div> <div>26%</div> </div>
3	X	231	<div> <div>11%</div> <div>26%</div> <div>44%</div> <div>11%</div> <div>•</div> <div>17%</div> </div>
3	Y	231	<div> <div>6%</div> <div>24%</div> <div>45%</div> <div>13%</div> <div>•</div> <div>17%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 48236 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 Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1626	Total	C	N	O	S	0	0	0
			12874	8242	2113	2467	52			
1	C	1626	Total	C	N	O	S	0	0	0
			12874	8242	2113	2467	52			

- Molecule 2 is a protein called Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1215	Total	C	N	O	S	0	0	0
			9635	6143	1617	1836	39			
2	D	1215	Total	C	N	O	S	0	0	0
			9635	6143	1617	1836	39			

- Molecule 3 is a protein called Superantigen-like protein 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	191	Total	C	N	O	S	0	0	0
			1539	965	267	306	1			
3	Y	191	Total	C	N	O	S	0	0	0
			1539	965	267	306	1			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

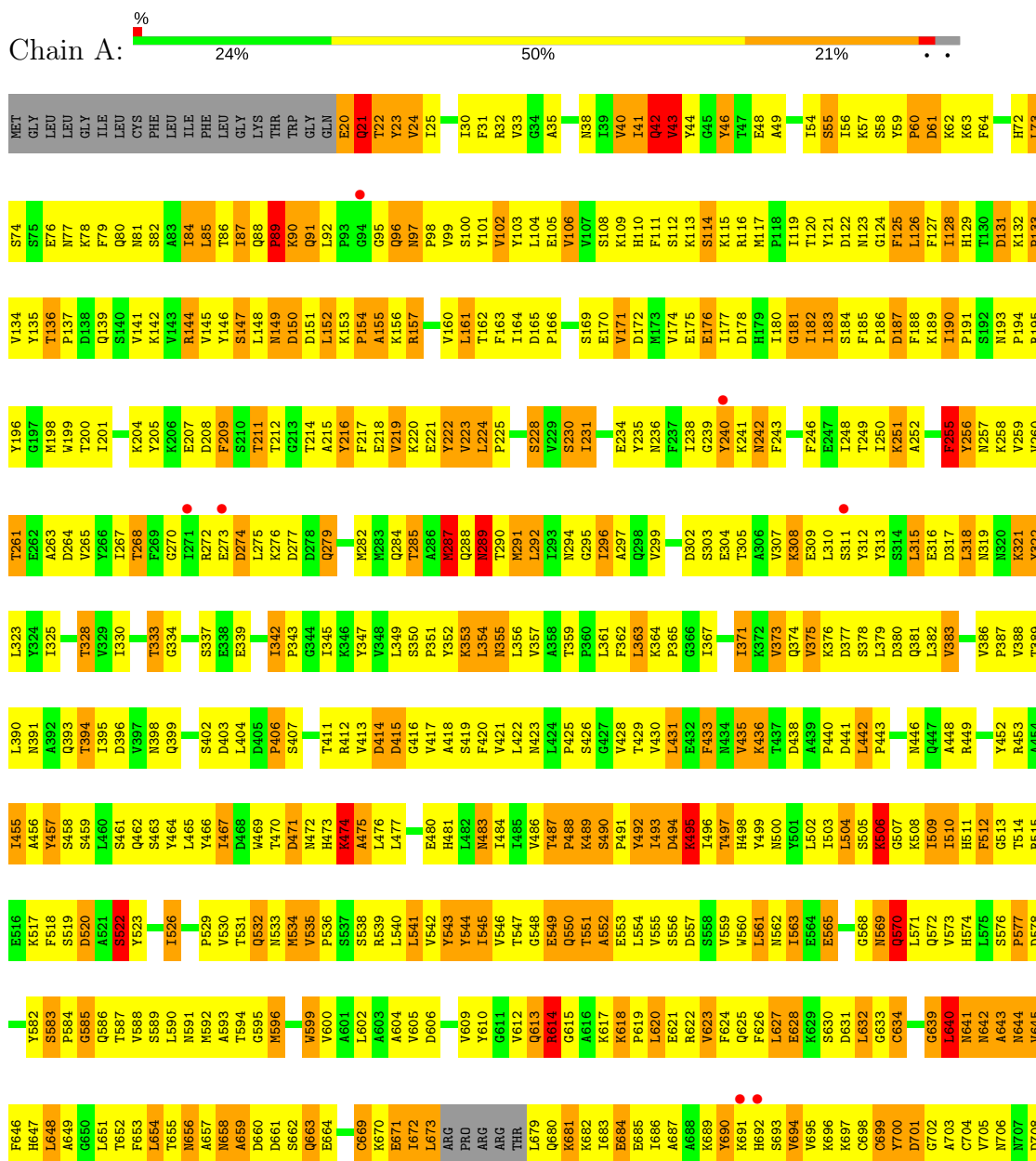
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	D	2	Total	C	N	O	0	0
			28	16	2	10		
5	D	2	Total	C	N	O	0	0
			28	16	2	10		

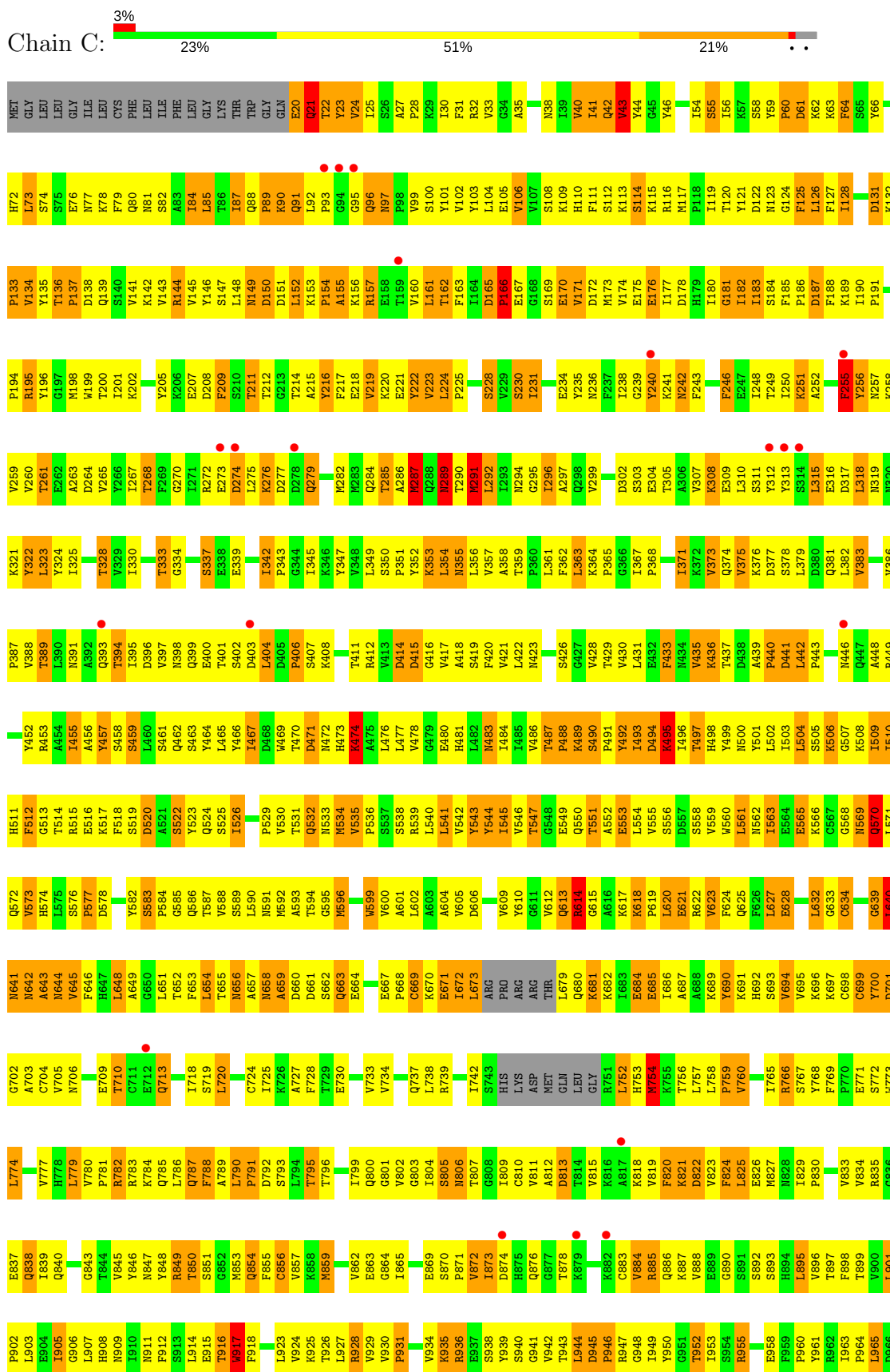
### 3 Residue-property plots

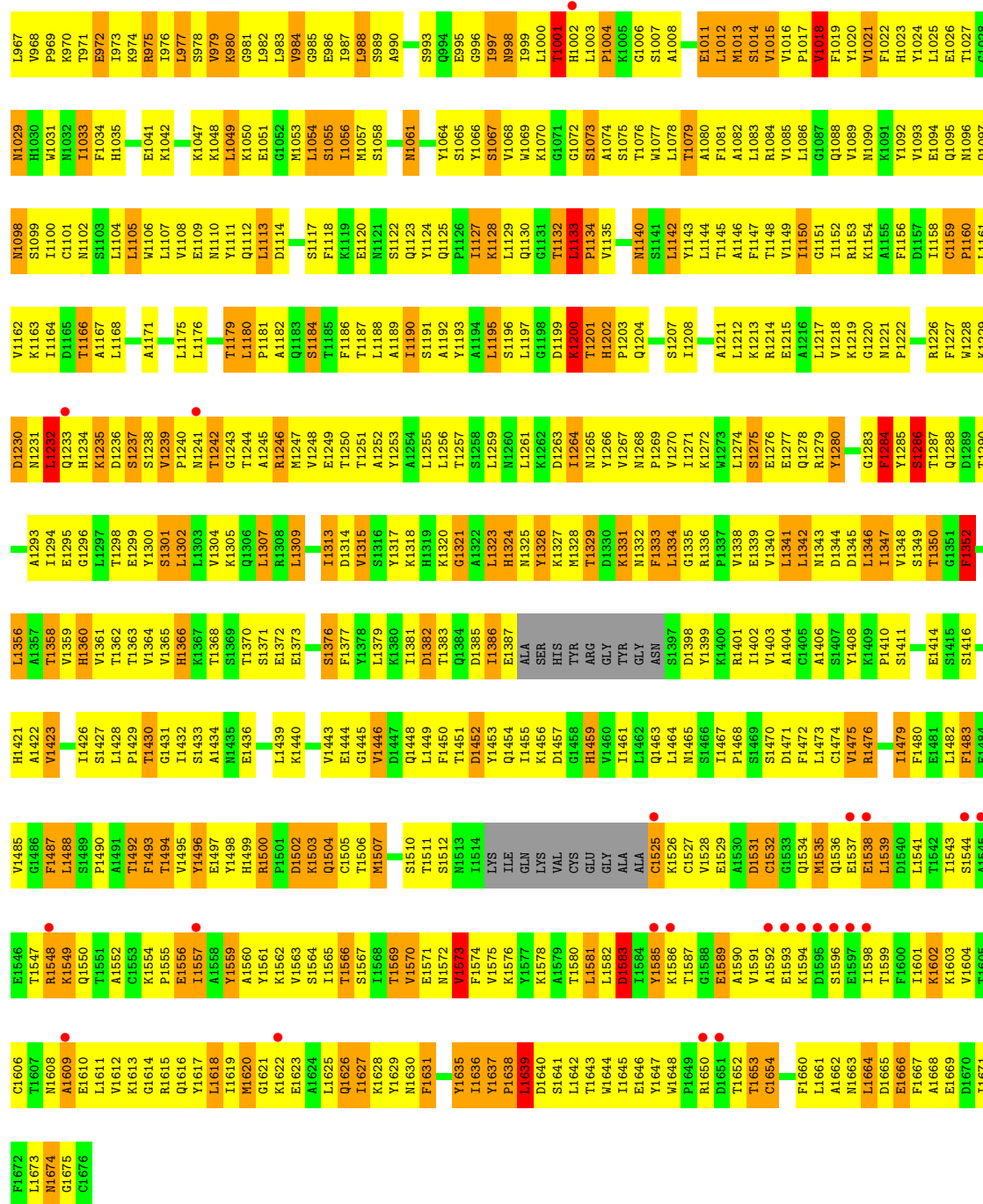
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Complement C5

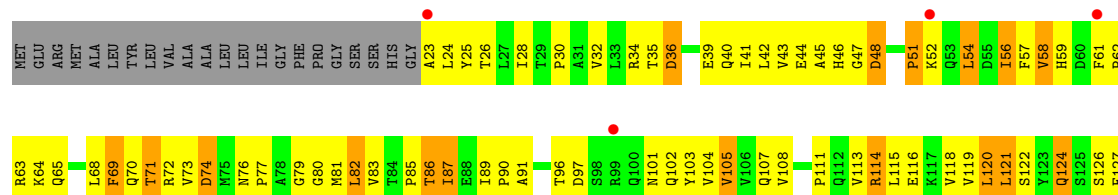
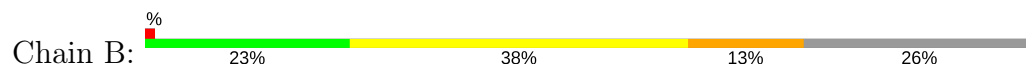


- Molecule 1: Complement C5



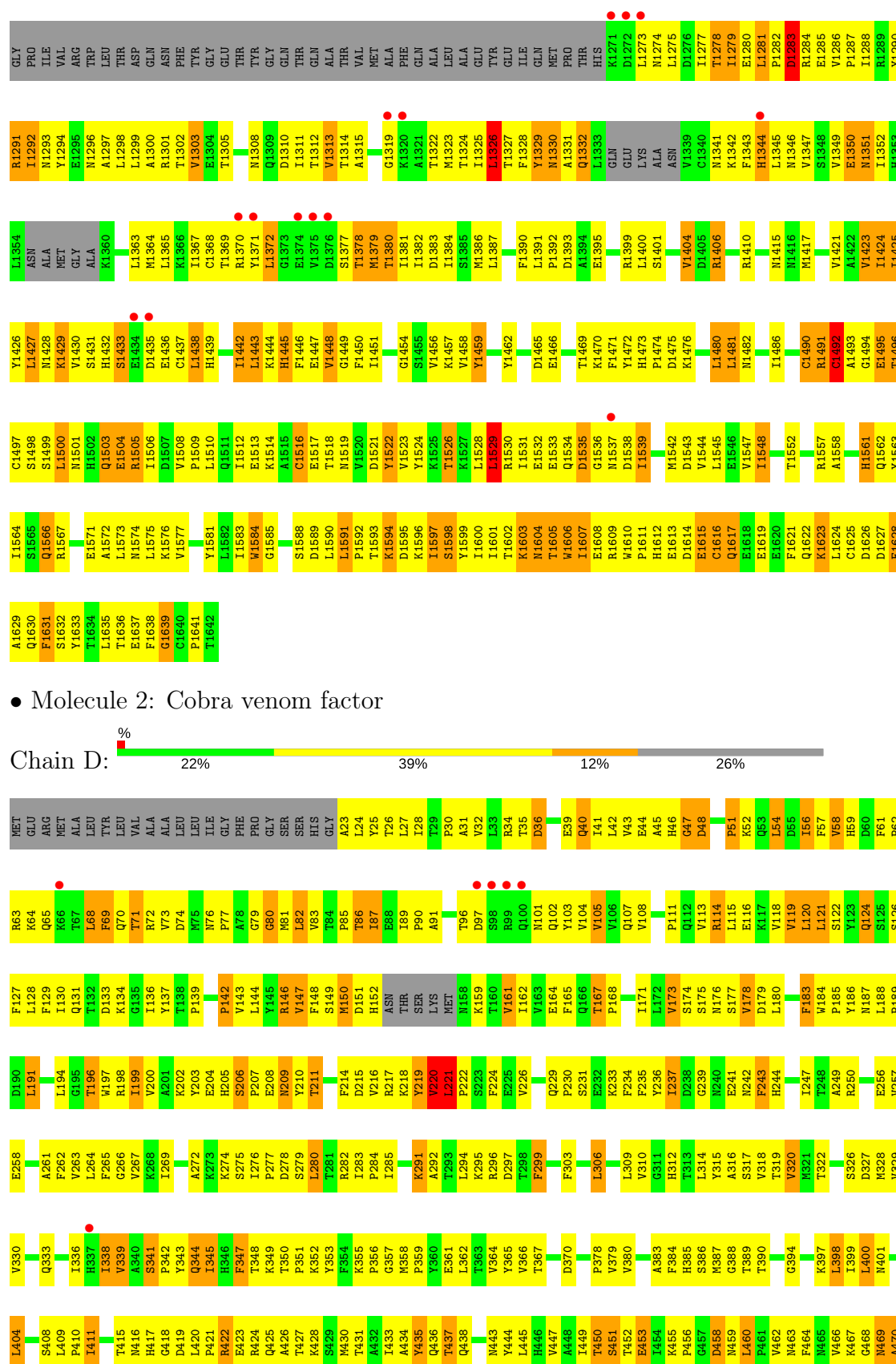


• Molecule 2: Cobra venom factor









K4422	V1349	V1286	LYS	LEU	ALA	ASP	LEU	ILE	I924	T861	I800	G608	V538	K4713
V1423	E1360	P1287	PHE	GLN	PRO	HIS	GLN	ILE	V925	K862	C801	C609	V538	K4713
I1424	E1351	I1288	ASP	ARG	VAL	SER	ARG	ILE	I926	Q863	V802	T610	K541	S472
I1425	I1352	T1289	GLN	PRO	LEU	TYR	THR	THR	I927	Q864	A811	A611	D542	Q475
Y1426	H1353	R1290	THR	THR	SER	ALA	ALA	PRO	V928	R865	R805	R612	T543	L476
L1427	L1354	R1291	GLY	THR	GLY	ALA	GLY	GLY	K929	R866	R806	S613	C544	K477
N1428	ASN	I1292	PRO	THR	THR	PHE	THR	GLY	L930	R867	Y806	G614	M546	Y478
K1429	ALA	M1293	ILE	THR	THR	THR	THR	CYS	D931	Q868	E907	Q615	G546	F479
V1430	MET	Y1294	VAL	LEU	GLN	ASN	GLN	GLY	P932	Q869	I808	N616	T547	T480
S1431	GLY	E1295	ARG	THR	GLY	ARG	GLY	GLY	R933	F870	R809	N617	L548	Y481
H1432	ALA	M1296	TRP	ALA	GLY	ALA	ALA	GLN	Q933	P871	R810	M618	V549	L482
K1433	K1360	A1297	THR	TYR	ILE	SER	ILE	ASN	V937	Q873	M811	G619	V550	L483
E1434	THR	L1298	LEU	ALA	GLN	SER	GLN	MET	G938	K874	K812	T620	K551	L484
L1363	ASP	L1299	ASP	LEU	GLY	SER	GLY	ILE	G939	A874	V813	F621	G552	L488
E1436	GLN	A1300	GLN	ALA	ALA	TRP	ALA	ARG	T940	L875	F814	E622	D553	K489
M1364	ASN	R1301	ASN	ALA	GLU	LEU	LEU	MET	Q941	S876	F815	Q627	N554	L489
K1365	THR	T1302	PHE	ALA	GLU	THR	ALA	ALA	L942	S877	I816	L626	L555	F490
K1366	THR	V1303	THR	GLY	GLU	ALA	ALA	ALA	E943	R878	D817	R627	I566	K491
C1368	GLN	E1304	GLY	VAL	VAL	TYR	TYR	PRO	V944	A879	L818	L628	Q557	Y492
T1369	LEU	T1305	GLY	TYR	TYR	VAL	VAL	VAL	I945	V880	Q819	T629	M558	G493
R1370	ASN	M1308	THR	LEU	VAL	VAL	VAL	ILE	K946	P881	P820	T630	P559	R494
Y1371	ASP	Q1309	ASP	THR	ALA	VAL	VAL	ALA	A947	V882	Y821	Q634	G560	Q497
L1372	GLN	D1310	ARG	PHE	ALA	PHE	ALA	TYR	K949	V884	S823	L634	A561	R497
S1377	THR	I1311	VAL	ILE	ILE	ALA	ALA	TYR	L950	V885	V824	N635	A562	R498
T1378	GLN	T1312	LEU	LEU	LEU	MET	LEU	LEU	D951	P886	V825	K637	K564	Q501
M1379	THR	V1313	VAL	VAL	VAL	ALA	ASP	ASP	D952	L887	K826	Q638	I566	N502
T1380	ALA	T1314	ALA	ALA	ALA	ALA	THR	THR	R953	E888	N827	Q639	K566	L503
V1381	VAL	A1315	THR	ALA	LEU	LYS	THR	THR	V954	Q889	Q828	S640	L567	V504
I1382	MET	I1382	THR	LEU	LEU	MET	GLY	GLY	P955	Q890	V830	A641	E568	T505
D1383	ALA	D1318	ALA	THR	GLY	VAL	GLN	GLN	D956	L891	V831	A642	G569	N506
I1384	PHE	G1319	PHE	SER	SER	ALA	TRP	TRP	P957	E895	E831	K643	D570	N507
S1385	GLN	T1322	GLN	LYS	LYS	GLY	GLU	GLU	E958	E896	I832	C644	D570	L508
S1386	ALA	M1323	ALA	THR	THR	ILE	THR	THR	P959	K896	R833	P645	A573	L509
L1387	ALA	T1324	ALA	THR	THR	SER	LEU	LEU	E960	K897	I835	Q646	R574	L510
F1390	GLY	I1325	ALA	TRP	CYS	HIS	GLY	GLY	T961	A898	L836	PRO	V575	P511
L1391	GLU	L1326	TYR	GLU	ASP	ILE	ASN	ASN	I963	Q901	H837	ALA	V880	P512
P1392	GLY	T1327	GLY	TYR	THR	ILE	ILE	ILE	I964	E902	N838	ASN	D551	D513
F1328	ILE	F1328	ILE	ASN	VAL	CYS	ARG	ARG	I965	A903	Y839	ARG	K552	D514
Y1329	GLN	A1394	ALA	ASN	VAL	GLY	THR	THR	Q966	L904	V840	ARG	A583	L515
N1330	MET	E1395	THR	HIS	SER	GLY	GLY	GLY	G967	Y905	N841	ARG	V584	F518
A1331	PRO	A1331	THR	LEU	LEU	VAL	VAL	ALA	D968	S906	E842	SER	Y585	R519
Q1332	THR	Q1332	THR	ASP	ASP	TRP	VAL	VAL	P969	D907	D843	ILE	Y585	F520
L1333	ASN	L1333	HIS	SER	SER	TRP	ASN	ASN	VAL	G968	I844	VAL	N588	V521
GLN	ILE	GLN	D1271	SER	SER	TRP	GLN	GLN	VAL	V909	Y845	GLY	I593	V522
LYS	GLY	LYS	D1272	ILE	ILE	ILE	ILE	ILE	GLN	R910	V846	VAL	S594	Y523
ALA	ALA	ALA	N1274	LYS	LYS	ASN	VAL	VAL	ILE	K911	R847	ARG	Q595	Y524
ASN	ASN	ASN	L1275	THR	ALA	ARG	GLY	THR	ILE	K912	T786	ASP	Q595	Q525
V1339	V1339	V1339	D1276	THR	THR	GLN	GLY	TYR	VAL	L913	L850	SER	I598	V526
C1340	C1340	C1340	T1277	ALA	ASN	GLN	TYR	TYR	ASN	K914	L851	ASN	I598	G527
M1341	M1341	M1341	T1278	LEU	THR	GLN	ALA	ALA	SER	V915	N852	ALA	M599	N528
K1342	K1342	K1342	T1279	LEU	LEU	PRO	THR	THR	ILE	V916	R853	ARG	D600	N529
E1280	ALA	E1280	E1280	ALA	LEU	ASP	GLN	GLN	ASP	P917	P854	LYS	T601	E530
H1344	H1344	H1344	L1281	LEU	LYS	GLY	GLY	MET	GLY	E918	A855	SER	I602	T531
N1415	N1415	N1415	P1282	LEU	LYS	ALA	VAL	VAL	SER	G919	F856	ALA	I602	T531
N1416	N1416	N1416	D1283	LEU	LYS	PHE	THR	TYR	LYS	V920	C857	GLY	E603	V532
M1417	M1417	M1417	D1284	LYS	TYR	LYS	THR	LYS	LEU	Q921	S858	LEU	E604	A533
V1421	V1421	V1421	E1285	MET	GLU	GLY	GLY	LYS	ASN	K922	A859	PHE	S605	D534
				LYS	LYS	ASN	ASN	ALA	HIS	S923	S860	GLN	D606	S535



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.65Å 181.96Å 392.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 4.30 49.21 – 4.30	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.21-4.30) 96.9 (49.21-4.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.83 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.208 , 0.261 0.191 , 0.243	Depositor DCC
$R_{free}$ test set	1815 reflections (2.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	116.2	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 160.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	48236	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: NAG

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	0.60	1/13151 (0.0%)	0.80	3/17841 (0.0%)
1	C	0.60	0/13151	0.80	5/17841 (0.0%)
2	B	0.53	1/9833 (0.0%)	0.73	2/13345 (0.0%)
2	D	0.54	0/9833	0.74	3/13345 (0.0%)
3	X	0.47	1/1560 (0.1%)	0.67	1/2096 (0.0%)
3	Y	0.49	0/1560	0.69	1/2096 (0.0%)
All	All	0.57	3/49088 (0.0%)	0.77	15/66564 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	210	GLU	C-N	5.35	1.46	1.34
2	B	347	PHE	CB-CG	-5.29	1.42	1.51
1	A	42	GLN	CB-CG	5.16	1.66	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	347	PHE	CB-CA-C	-7.26	95.88	110.40
2	D	347	PHE	CB-CA-C	-6.90	96.60	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	640	LEU	CA-CB-CG	6.49	130.23	115.30
1	C	640	LEU	CA-CB-CG	6.30	129.80	115.30
1	A	871	PRO	CA-N-CD	-6.16	102.87	111.50
2	D	347	PHE	CB-CG-CD2	-6.11	116.52	120.80
1	C	166	PRO	CA-N-CD	-5.83	103.33	111.50
2	D	1326	LEU	CA-CB-CG	5.60	128.18	115.30
1	C	1195	LEU	CA-CB-CG	-5.40	102.89	115.30
1	C	1256	LEU	CA-CB-CG	-5.26	103.20	115.30
2	B	1326	LEU	CA-CB-CG	5.23	127.33	115.30
3	Y	209	PHE	N-CA-C	5.17	124.97	111.00
3	X	209	PHE	N-CA-C	5.16	124.92	111.00
1	C	673	LEU	CA-CB-CG	5.12	127.07	115.30
1	A	673	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1504	GLN	Peptide
1	A	98	PRO	Peptide
1	C	1504	GLN	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12874	0	12814	1855	0
1	C	12874	0	12814	1901	0
2	B	9635	0	9630	1082	0
2	D	9635	0	9630	1079	0
3	X	1539	0	1530	166	0
3	Y	1539	0	1530	194	0
4	A	14	0	13	1	0
4	C	14	0	13	2	0
5	B	56	0	50	6	0
5	D	56	0	50	7	0
All	All	48236	0	48074	6152	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 64.

All (6152) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1525:CYS:O	1:A:1528:VAL:HG22	1.34	1.25
3:X:207:LEU:O	3:X:207:LEU:HD12	1.32	1.24
3:Y:207:LEU:HD12	3:Y:207:LEU:O	1.32	1.23
1:C:386:VAL:H	1:C:411:THR:HG22	1.03	1.17
1:A:500:ASN:HB2	1:A:543:TYR:CE1	1.79	1.17
2:B:518:PHE:HE2	2:B:538:VAL:HB	1.12	1.15
2:D:1607:ILE:H	2:D:1607:ILE:HD12	1.10	1.15
1:C:1562:LYS:HD3	1:C:1664:LEU:HD21	1.19	1.14
1:C:500:ASN:HB2	1:C:543:TYR:CE1	1.80	1.14
1:C:535:VAL:HG23	1:C:536:PRO:HD3	1.27	1.14
2:D:261:ALA:HB2	2:D:320:VAL:HG23	1.30	1.13
1:C:1228:TRP:H	1:C:1251:THR:HG22	1.13	1.13
2:D:518:PHE:CE2	2:D:538:VAL:HB	1.83	1.13
1:A:386:VAL:H	1:A:411:THR:HG22	1.03	1.12
1:A:535:VAL:HG23	1:A:536:PRO:HD3	1.28	1.12
1:C:1525:CYS:O	1:C:1528:VAL:HG22	1.49	1.12
2:B:518:PHE:CE2	2:B:538:VAL:HB	1.84	1.11
1:A:1012:LEU:HD22	1:A:1085:VAL:HG21	1.33	1.10
1:C:979:VAL:HG21	1:C:1326:TYR:CE1	1.86	1.10
1:A:25:ILE:H	1:A:655:THR:CG2	1.64	1.10
2:D:1473:HIS:HD2	2:D:1474:PRO:HD2	1.10	1.10
2:B:1613:GLU:O	2:B:1616:CYS:HB2	1.49	1.09
2:D:829:GLN:HG3	2:D:1480:LEU:HD13	1.12	1.09
1:A:182:ILE:HG12	1:A:804:ILE:HD11	1.10	1.09
1:C:120:THR:HG22	1:C:122:ASP:H	1.17	1.09
2:D:1594:LYS:HE2	2:D:1594:LYS:HA	1.30	1.09
1:A:936:ARG:HG3	1:A:936:ARG:HH11	1.15	1.08
1:C:421:VAL:HG11	2:D:505:THR:HG22	1.35	1.08
1:A:25:ILE:H	1:A:655:THR:HG23	1.18	1.08
1:A:1228:TRP:H	1:A:1251:THR:HG22	1.13	1.08
1:A:944:LEU:HD11	1:A:1313:ILE:HD11	1.35	1.08
1:A:979:VAL:HG21	1:A:1326:TYR:CE1	1.86	1.08
1:A:353:LYS:HE3	1:A:378:SER:HA	1.19	1.07
2:D:518:PHE:HE2	2:D:538:VAL:HB	1.13	1.07
2:B:263:VAL:HG22	2:B:318:VAL:HG23	1.37	1.07
1:C:353:LYS:HE3	1:C:378:SER:HA	1.21	1.07
2:D:380:VAL:HG12	2:D:387:MET:HB3	1.29	1.07

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1068:VAL:HA	1:C:1078:LEU:HD12	1.35	1.06
2:B:261:ALA:HB2	2:B:320:VAL:HG23	1.31	1.05
1:C:591:ASN:HB3	1:C:785:GLN:HE21	1.16	1.05
1:C:936:ARG:HG3	1:C:936:ARG:HH11	1.13	1.05
2:D:954:VAL:HB	2:D:957:THR:HG21	1.38	1.05
1:A:120:THR:HG22	1:A:122:ASP:H	1.11	1.05
1:C:127:PHE:HE2	1:C:623:VAL:HG13	1.21	1.05
1:C:1560:ALA:HB2	1:C:1620:MET:HG3	1.38	1.05
2:B:1594:LYS:HA	2:B:1594:LYS:HE2	1.30	1.04
1:A:955:ARG:HG2	1:A:1350:THR:HG23	1.37	1.04
1:C:128:ILE:HG22	1:C:145:VAL:HG22	1.40	1.04
1:A:222:TYR:CE1	1:A:768:TYR:HB2	1.94	1.03
1:A:830:PRO:HG3	1:A:1483:PHE:CZ	1.94	1.03
1:A:1068:VAL:HA	1:A:1078:LEU:HD12	1.36	1.02
2:D:1473:HIS:CD2	2:D:1474:PRO:HD2	1.92	1.02
2:B:1473:HIS:HD2	2:B:1474:PRO:HD2	1.22	1.02
1:C:1133:LEU:H	1:C:1133:LEU:HD12	1.20	1.02
1:A:1102:ASN:ND2	1:C:1162:VAL:HG22	1.74	1.02
1:C:1623:GLU:HB2	1:C:1638:PRO:HG3	1.38	1.02
1:C:944:LEU:HD11	1:C:1313:ILE:HD11	1.36	1.02
2:B:965:ILE:HG13	2:B:1301:ARG:HB2	1.42	1.02
2:D:563:MET:HG3	2:D:780:LEU:HD23	1.42	1.02
1:C:830:PRO:HG3	1:C:1483:PHE:CZ	1.93	1.01
1:A:470:THR:HG22	2:B:450:THR:HG22	1.42	1.01
1:C:1620:MET:HB2	1:C:1644:TRP:HB3	1.42	1.01
2:B:954:VAL:HB	2:B:957:THR:HG21	1.40	1.01
1:C:869:GLU:O	1:C:871:PRO:HD3	1.58	1.01
2:B:829:GLN:HG3	2:B:1480:LEU:HD13	1.40	1.01
1:A:1133:LEU:H	1:A:1133:LEU:HD12	1.21	1.01
2:B:1505:ARG:HG3	2:B:1505:ARG:HH11	1.24	1.00
2:D:263:VAL:HG22	2:D:318:VAL:HG23	1.42	1.00
1:A:1562:LYS:HD2	1:A:1648:TRP:HZ2	1.26	1.00
1:A:1556:GLU:HB3	1:A:1622:LYS:HE2	1.43	1.00
2:B:469:ASN:HD22	2:B:469:ASN:C	1.65	1.00
1:C:182:ILE:HG12	1:C:804:ILE:HD11	1.40	1.00
1:C:60:PRO:HD2	1:C:61:ASP:H	1.27	1.00
2:B:380:VAL:HG12	2:B:387:MET:HB3	1.40	1.00
1:A:1623:GLU:HB2	1:A:1638:PRO:HG3	1.44	1.00
1:A:591:ASN:HB3	1:A:785:GLN:HE21	1.22	1.00
2:D:829:GLN:CG	2:D:1480:LEU:HD13	1.91	1.00
2:D:840:VAL:HG12	2:D:841:ASN:H	1.27	0.99

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1012:LEU:HD22	1:C:1085:VAL:HG21	1.41	0.99
1:A:656:ASN:OD1	1:A:658:ASN:HB3	1.62	0.99
1:A:373:VAL:HG11	1:A:435:VAL:HG11	1.41	0.99
1:A:869:GLU:O	1:A:871:PRO:HD3	1.62	0.99
1:C:1493:PHE:HD1	1:C:1494:THR:N	1.60	0.99
2:D:482:LEU:HB3	2:D:492:VAL:HG23	1.45	0.99
1:A:222:TYR:HE1	1:A:768:TYR:HB2	1.24	0.99
1:A:838:GLN:HA	1:A:901:LEU:HB2	1.45	0.99
3:X:194:LYS:HZ2	3:X:197:ASN:HB2	1.28	0.98
1:A:371:ILE:HG22	1:A:420:PHE:HB2	1.46	0.98
2:B:851:LEU:HD23	2:B:852:TYR:H	1.28	0.98
1:C:1219:LYS:NZ	1:C:1239:VAL:HG11	1.76	0.98
1:C:1585:TYR:HD1	1:C:1671:ILE:HG21	1.28	0.98
1:A:128:ILE:HG22	1:A:145:VAL:HG22	1.40	0.98
2:D:469:ASN:C	2:D:469:ASN:HD22	1.66	0.98
1:A:292:LEU:HA	1:A:297:ALA:HB2	1.44	0.98
2:D:384:PHE:CD1	2:D:400:LEU:HG	1.97	0.98
1:C:373:VAL:HG11	1:C:435:VAL:HG11	1.42	0.98
2:D:965:ILE:HG13	2:D:1301:ARG:HB2	1.46	0.98
2:B:526:VAL:HG23	2:B:530:GLU:HB3	1.46	0.97
1:A:60:PRO:HD2	1:A:61:ASP:H	1.25	0.97
2:B:384:PHE:CD1	2:B:400:LEU:HG	1.99	0.97
1:A:1525:CYS:O	1:A:1528:VAL:CG2	2.13	0.97
2:D:435:TYR:HD1	2:D:436:GLN:H	1.10	0.97
1:A:1008:ALA:HB3	1:A:1078:LEU:HD11	1.46	0.97
1:A:1526:LYS:O	1:A:1529:GLU:HG3	1.63	0.97
1:C:955:ARG:HG2	1:C:1350:THR:HG23	1.45	0.97
1:A:1365:VAL:HG22	1:A:1366:HIS:H	1.29	0.97
1:A:576:SER:HB3	1:A:577:PRO:HD3	1.45	0.97
1:A:884:VAL:O	1:A:885:ARG:HB2	1.65	0.97
1:C:33:VAL:HG21	1:C:121:TYR:CD1	1.99	0.96
1:C:1612:VAL:HB	1:C:1615:ARG:HB3	1.46	0.96
1:C:576:SER:HB3	1:C:577:PRO:HD3	1.47	0.96
1:A:1560:ALA:HB2	1:A:1620:MET:HG3	1.42	0.96
2:D:526:VAL:HG23	2:D:530:GLU:HB3	1.47	0.96
2:D:244:HIS:HB3	2:D:291:LYS:HD2	1.46	0.96
1:A:234:GLU:HG3	1:A:235:TYR:CD2	2.00	0.96
1:C:234:GLU:HG3	1:C:235:TYR:CD2	2.01	0.96
1:C:656:ASN:OD1	1:C:658:ASN:HB3	1.64	0.96
1:C:702:GLY:HA2	1:C:728:PHE:CE1	2.01	0.96
1:A:1612:VAL:HB	1:A:1615:ARG:HB3	1.46	0.96

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:LEU:HA	1:C:297:ALA:HB2	1.46	0.96
1:C:706:ASN:ND2	1:C:709:GLU:H	1.64	0.96
1:A:1493:PHE:HD1	1:A:1494:THR:N	1.64	0.95
1:A:500:ASN:CB	1:A:543:TYR:HE1	1.79	0.95
1:A:706:ASN:ND2	1:A:709:GLU:H	1.64	0.95
2:B:237:ILE:HD11	2:B:309:LEU:HB2	1.46	0.95
1:C:500:ASN:HB2	1:C:543:TYR:HE1	1.20	0.95
2:B:563:MET:HG3	2:B:780:LEU:HD23	1.47	0.95
1:C:838:GLN:HA	1:C:901:LEU:HB2	1.43	0.95
1:A:868:SER:HA	1:A:1527:CYS:HB2	1.47	0.95
1:C:569:ASN:O	1:C:570:GLN:HB2	1.66	0.95
3:Y:194:LYS:HZ2	3:Y:197:ASN:HB2	1.29	0.94
1:A:33:VAL:HG21	1:A:121:TYR:CD1	2.02	0.94
1:A:500:ASN:HB2	1:A:543:TYR:HE1	1.17	0.94
1:C:706:ASN:HD22	1:C:709:GLU:H	1.02	0.94
2:D:380:VAL:HG12	2:D:387:MET:CB	1.96	0.94
1:C:230:SER:HB3	1:C:251:LYS:HG3	1.49	0.94
1:A:1559:TYR:OH	1:A:1591:VAL:HA	1.67	0.94
1:A:419:SER:HB2	2:B:459:ASN:HD22	1.30	0.94
1:A:702:GLY:HA2	1:A:728:PHE:CE1	2.03	0.94
1:A:706:ASN:HD22	1:A:709:GLU:H	1.01	0.94
2:D:829:GLN:HE22	2:D:883:VAL:HG13	1.33	0.94
2:D:851:LEU:HD23	2:D:852:TYR:H	1.31	0.94
3:X:81:ASN:O	3:X:115:ARG:HB2	1.68	0.94
1:A:430:VAL:HG11	1:A:453:ARG:HH21	1.33	0.94
1:C:1124:TYR:HA	1:C:1465:ASN:OD1	1.66	0.94
1:A:24:VAL:HA	1:A:655:THR:OG1	1.66	0.94
2:B:840:VAL:HG12	2:B:841:ASN:H	1.30	0.94
1:C:1061:ASN:HB2	1:C:1065:SER:O	1.68	0.94
2:B:1528:LEU:HD23	2:B:1576:LYS:O	1.68	0.93
1:A:1219:LYS:NZ	1:A:1239:VAL:HG11	1.83	0.93
1:C:596:MET:H	1:C:782:ARG:HH11	1.03	0.93
3:Y:81:ASN:O	3:Y:115:ARG:HB2	1.68	0.93
1:A:1490:PRO:HB3	1:A:1510:SER:HB2	1.50	0.93
1:A:606:ASP:O	1:A:609:VAL:HG23	1.68	0.93
1:C:830:PRO:HG3	1:C:1483:PHE:HZ	1.33	0.93
1:C:884:VAL:O	1:C:885:ARG:HB2	1.65	0.93
1:A:596:MET:H	1:A:782:ARG:HH11	1.09	0.93
1:C:357:VAL:HA	1:C:672:ILE:HG21	1.50	0.92
1:A:569:ASN:O	1:A:570:GLN:HB2	1.65	0.92
1:A:87:ILE:HD13	1:A:87:ILE:N	1.84	0.92

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:HIS:HB3	2:B:291:LYS:HD2	1.48	0.92
2:B:1473:HIS:CD2	2:B:1474:PRO:HD2	2.03	0.92
2:D:521:VAL:HG13	2:D:535:SER:HB3	1.52	0.92
1:C:135:TYR:HE1	1:C:141:VAL:HA	1.35	0.92
2:B:482:LEU:HB3	2:B:492:VAL:HG23	1.48	0.92
1:A:1012:LEU:CD2	1:A:1085:VAL:HG21	2.00	0.92
1:A:353:LYS:CE	1:A:378:SER:HA	2.01	0.91
1:A:944:LEU:CD1	1:A:1313:ILE:HD11	2.00	0.91
1:C:1556:GLU:HB3	1:C:1622:LYS:HE2	1.51	0.91
2:B:563:MET:HE2	2:B:564:LYS:H	1.35	0.91
1:A:849:ARG:HG2	1:A:849:ARG:HH11	1.36	0.91
1:A:753:HIS:O	1:A:754:MET:HB3	1.68	0.91
3:Y:166:ASP:CG	3:Y:207:LEU:CD2	2.38	0.91
1:A:1562:LYS:HD2	1:A:1648:TRP:CZ2	2.05	0.91
3:X:50:TYR:CE2	3:X:170:ARG:HD2	2.06	0.91
1:C:1008:ALA:HB3	1:C:1078:LEU:HD11	1.52	0.91
1:A:135:TYR:HE1	1:A:141:VAL:HA	1.34	0.91
1:C:553:GLU:HA	1:C:658:ASN:HB2	1.53	0.91
2:D:1528:LEU:HD23	2:D:1576:LYS:O	1.70	0.91
2:D:469:ASN:CG	2:D:472:SER:HB2	1.92	0.91
1:C:1490:PRO:HB3	1:C:1510:SER:HB2	1.53	0.91
2:B:1341:ASN:ND2	2:B:1342:LYS:HG2	1.86	0.90
1:C:849:ARG:HH11	1:C:849:ARG:HG2	1.35	0.90
3:Y:170:ARG:HH22	3:Y:206:LYS:HA	1.37	0.90
1:A:230:SER:HB3	1:A:251:LYS:HG3	1.50	0.90
1:A:33:VAL:HG21	1:A:121:TYR:CE1	2.06	0.90
1:C:1559:TYR:OH	1:C:1591:VAL:HA	1.71	0.90
2:D:1590:LEU:HD23	2:D:1591:LEU:H	1.36	0.90
1:C:430:VAL:HG11	1:C:453:ARG:HH21	1.36	0.90
2:B:221:LEU:HD11	2:B:753:LYS:HG2	1.52	0.90
2:B:435:TYR:HD1	2:B:436:GLN:H	1.11	0.90
1:A:1232:LEU:HD11	1:A:1233:GLN:HE21	1.36	0.90
1:A:315:LEU:HD13	1:A:317:ASP:HB2	1.53	0.90
1:C:25:ILE:H	1:C:655:THR:HG23	1.35	0.90
1:A:481:HIS:CE1	1:A:529:PRO:HB3	2.06	0.90
1:C:315:LEU:HD13	1:C:317:ASP:HB2	1.54	0.90
2:D:221:LEU:HD11	2:D:753:LYS:HG2	1.53	0.90
2:B:120:LEU:HD12	2:B:121:LEU:H	1.37	0.90
1:A:1068:VAL:HG21	1:A:1124:TYR:CD1	2.06	0.89
1:A:502:LEU:HB2	1:A:541:LEU:CD2	2.01	0.89
1:C:1232:LEU:HD11	1:C:1233:GLN:HE21	1.35	0.89

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:584:PRO:HB3	1:C:792:ASP:HA	1.54	0.89
2:D:1273:LEU:HB2	2:D:1319:GLY:HA3	1.52	0.89
3:Y:50:TYR:CE2	3:Y:170:ARG:HD2	2.06	0.89
2:B:1273:LEU:HB2	2:B:1319:GLY:HA3	1.53	0.89
2:B:469:ASN:CG	2:B:472:SER:HB2	1.92	0.89
1:A:1404:ALA:HB1	1:A:1493:PHE:CE2	2.08	0.89
1:C:753:HIS:O	1:C:754:MET:HB3	1.72	0.89
1:C:500:ASN:CB	1:C:543:TYR:HE1	1.83	0.89
1:C:576:SER:HB2	1:C:589:SER:HB2	1.52	0.89
1:C:60:PRO:CD	1:C:61:ASP:H	1.86	0.89
1:A:576:SER:HB2	1:A:589:SER:HB2	1.54	0.89
1:C:481:HIS:CE1	1:C:529:PRO:HB3	2.06	0.89
1:A:60:PRO:CD	1:A:61:ASP:H	1.85	0.89
2:D:237:ILE:HD11	2:D:309:LEU:HB2	1.55	0.89
2:B:416:ASN:HA	2:B:425:GLN:HE22	1.37	0.89
1:C:59:TYR:CG	1:C:60:PRO:HD3	2.07	0.89
1:A:31:PHE:HB2	1:A:119:ILE:HG22	1.53	0.88
1:A:618:LYS:H	1:A:619:PRO:HD3	1.38	0.88
1:A:1576:LYS:HG2	1:A:1601:ILE:HG22	1.53	0.88
1:A:59:TYR:CG	1:A:60:PRO:HD3	2.08	0.88
1:C:23:TYR:CD1	1:C:655:THR:HB	2.09	0.88
1:A:830:PRO:HG3	1:A:1483:PHE:HZ	1.36	0.88
1:A:980:LYS:HD3	1:A:986:GLU:HA	1.55	0.88
2:D:519:ARG:NH1	2:D:608:GLY:HA3	1.89	0.88
3:X:77:PRO:HD2	3:X:80:GLN:O	1.74	0.88
1:C:511:HIS:CE1	3:Y:149:SER:OG	2.26	0.88
2:B:455:LYS:O	2:B:458:ASP:HB2	1.72	0.88
2:B:829:GLN:HE22	2:B:883:VAL:HG13	1.36	0.88
3:Y:77:PRO:HD2	3:Y:80:GLN:O	1.73	0.88
1:C:386:VAL:N	1:C:411:THR:HG22	1.88	0.88
1:C:532:GLN:HE21	1:C:568:GLY:HA2	1.38	0.88
2:D:120:LEU:HD12	2:D:121:LEU:H	1.38	0.87
2:D:750:ASP:OD1	2:D:752:PRO:HD3	1.73	0.87
1:A:1124:TYR:HA	1:A:1465:ASN:OD1	1.74	0.87
1:A:386:VAL:N	1:A:411:THR:HG22	1.88	0.87
1:C:31:PHE:HB2	1:C:119:ILE:HG22	1.54	0.87
1:C:606:ASP:O	1:C:609:VAL:HG23	1.72	0.87
1:A:467:ILE:HG22	1:A:486:VAL:HG22	1.55	0.87
1:C:78:LYS:NZ	3:Y:144:GLU:HA	1.88	0.87
2:B:1590:LEU:HD23	2:B:1591:LEU:H	1.36	0.87
1:A:120:THR:HG22	1:A:122:ASP:N	1.88	0.87

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:PRO:HB3	1:A:792:ASP:HA	1.57	0.87
2:B:494:ARG:HG3	2:B:494:ARG:HH11	1.39	0.87
1:C:944:LEU:CD1	1:C:1313:ILE:HD11	2.05	0.87
2:D:1473:HIS:HB3	2:D:1476:LYS:HB2	1.55	0.87
2:D:1607:ILE:H	2:D:1607:ILE:CD1	1.81	0.87
3:Y:58:SER:HB3	3:Y:102:ASN:ND2	1.90	0.87
1:A:1068:VAL:HG13	1:A:1069:TRP:H	1.39	0.87
3:Y:166:ASP:CG	3:Y:207:LEU:HD21	1.95	0.87
2:B:347:PHE:O	2:B:350:THR:HG22	1.75	0.87
1:C:33:VAL:HG21	1:C:121:TYR:CE1	2.09	0.87
1:C:502:LEU:HB2	1:C:541:LEU:CD2	2.05	0.87
1:A:1365:VAL:HG22	1:A:1366:HIS:N	1.84	0.87
1:C:353:LYS:CE	1:C:378:SER:HA	2.03	0.86
2:D:455:LYS:O	2:D:458:ASP:HB2	1.74	0.86
1:A:1560:ALA:CB	1:A:1620:MET:HG3	2.05	0.86
1:A:182:ILE:HG12	1:A:804:ILE:CD1	2.02	0.86
1:A:855:PHE:HA	2:B:904:LEU:HD11	1.57	0.86
2:B:750:ASP:OD1	2:B:752:PRO:HD3	1.75	0.86
1:C:1068:VAL:HG13	1:C:1069:TRP:H	1.40	0.86
1:C:1585:TYR:CD1	1:C:1671:ILE:HG21	2.10	0.86
1:C:572:GLN:HB2	1:C:593:ALA:HB3	1.56	0.86
1:C:618:LYS:H	1:C:619:PRO:HD3	1.38	0.86
1:C:934:VAL:HG22	1:C:1366:HIS:CD2	2.10	0.86
1:C:599:TRP:O	1:C:803:GLY:HA2	1.74	0.86
2:D:416:ASN:HA	2:D:425:GLN:HE22	1.40	0.86
3:X:166:ASP:CG	3:X:207:LEU:CD2	2.42	0.86
1:A:1546:GLU:O	1:A:1667:PHE:HZ	1.57	0.86
1:A:618:LYS:N	1:A:619:PRO:CD	2.38	0.86
1:A:936:ARG:HG3	1:A:936:ARG:NH1	1.89	0.86
1:C:1562:LYS:HD2	1:C:1648:TRP:CZ2	2.11	0.86
1:C:127:PHE:CE2	1:C:623:VAL:HG13	2.08	0.86
1:C:1560:ALA:CB	1:C:1620:MET:HG3	2.04	0.86
1:C:463:SER:HB3	1:C:491:PRO:HA	1.57	0.86
1:C:618:LYS:N	1:C:619:PRO:CD	2.38	0.86
1:C:120:THR:HG22	1:C:122:ASP:N	1.90	0.86
1:C:1315:VAL:HG12	1:C:1324:HIS:O	1.76	0.86
1:A:23:TYR:CD1	1:A:23:TYR:N	2.40	0.86
1:C:1404:ALA:HB1	1:C:1493:PHE:CE2	2.10	0.86
1:C:504:LEU:CD1	1:C:509:ILE:HG23	2.06	0.86
2:D:1341:ASN:ND2	2:D:1342:LYS:HG2	1.91	0.86
1:A:24:VAL:HG21	1:A:554:LEU:HD11	1.55	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1444:LYS:HE2	2:B:1447:GLU:HA	1.58	0.86
1:C:128:ILE:HD12	1:C:201:ILE:HG22	1.57	0.86
2:B:519:ARG:NH1	2:B:608:GLY:HA3	1.91	0.86
2:B:151:ASP:HB2	2:B:794:PHE:HZ	1.38	0.86
2:B:850:LEU:HB2	2:B:882:PHE:HE1	1.41	0.86
1:C:1068:VAL:HG21	1:C:1124:TYR:CD1	2.10	0.85
1:C:1219:LYS:HZ1	1:C:1239:VAL:HG11	1.40	0.85
1:C:696:LYS:HZ3	1:C:759:PRO:HD2	1.38	0.85
3:X:58:SER:HB3	3:X:102:ASN:ND2	1.91	0.85
1:C:936:ARG:HH11	1:C:936:ARG:CG	1.89	0.85
3:Y:207:LEU:CD1	3:Y:207:LEU:O	2.22	0.85
2:B:1590:LEU:HD23	2:B:1591:LEU:N	1.91	0.85
1:C:1531:ASP:OD2	1:C:1531:ASP:C	2.14	0.85
2:D:151:ASP:HB2	2:D:794:PHE:HZ	1.39	0.85
2:D:850:LEU:HB2	2:D:882:PHE:CE1	2.11	0.85
1:A:1333:PHE:O	1:A:1334:LEU:HB2	1.77	0.85
1:A:641:ASN:ND2	1:A:643:ALA:HB3	1.90	0.85
1:C:1576:LYS:HG2	1:C:1601:ILE:HG22	1.59	0.85
2:D:518:PHE:HE2	2:D:538:VAL:CB	1.88	0.85
3:X:170:ARG:HD3	3:X:203:LEU:HD23	1.59	0.85
1:A:1003:LEU:HD11	1:A:1286:SER:HA	1.59	0.85
2:B:850:LEU:HB2	2:B:882:PHE:CE1	2.12	0.85
1:C:371:ILE:HG22	1:C:420:PHE:HB2	1.56	0.85
1:A:127:PHE:HE2	1:A:623:VAL:HG13	1.40	0.85
1:A:1315:VAL:HG12	1:A:1324:HIS:O	1.76	0.85
1:A:315:LEU:HD12	1:A:318:LEU:HG	1.59	0.85
1:C:467:ILE:HG22	1:C:486:VAL:HG22	1.59	0.85
1:C:222:TYR:CE1	1:C:768:TYR:HB2	2.12	0.85
2:D:161:VAL:HG21	2:D:180:LEU:HD21	1.58	0.85
1:C:1278:GLN:OE1	1:C:1283:GLY:HA2	1.76	0.85
1:C:1365:VAL:HG22	1:C:1366:HIS:H	1.40	0.85
2:D:326:SER:HB2	2:D:819:GLN:HG3	1.59	0.85
1:A:145:VAL:HB	1:A:183:ILE:HG13	1.58	0.84
1:A:391:ASN:HD21	1:A:406:PRO:HG3	1.41	0.84
2:B:1512:ILE:O	2:B:1516:CYS:HB2	1.77	0.84
2:B:380:VAL:HG12	2:B:387:MET:CB	2.06	0.84
2:B:518:PHE:HE2	2:B:538:VAL:CB	1.89	0.84
1:C:315:LEU:HD12	1:C:318:LEU:HG	1.59	0.84
1:A:284:GLN:HG2	1:A:310:LEU:HD21	1.59	0.84
1:C:614:ARG:HD2	1:C:615:GLY:N	1.92	0.84
1:C:641:ASN:ND2	1:C:643:ALA:HB3	1.93	0.84

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:ARG:HD2	1:A:615:GLY:N	1.92	0.84
1:A:696:LYS:HZ3	1:A:759:PRO:HD2	1.42	0.84
2:B:481:TYR:O	2:B:481:TYR:HD2	1.61	0.84
1:A:1123:GLN:HA	1:A:1123:GLN:HE21	1.42	0.84
2:B:175:SER:H	2:B:1300:ALA:HB2	1.42	0.84
1:C:133:PRO:HD2	1:C:609:VAL:HG11	1.60	0.84
2:D:1444:LYS:HE2	2:D:1447:GLU:HA	1.59	0.84
2:D:933:ARG:HG3	2:D:933:ARG:HH11	1.40	0.84
1:A:191:PRO:HD2	1:A:194:PRO:HB3	1.60	0.83
1:C:1575:VAL:HB	1:C:1602:LYS:O	1.76	0.83
1:A:1278:GLN:OE1	1:A:1283:GLY:HA2	1.78	0.83
2:B:925:VAL:HG22	2:B:1326:LEU:HD23	1.60	0.83
1:C:145:VAL:HB	1:C:183:ILE:HG13	1.60	0.83
1:C:1526:LYS:O	1:C:1529:GLU:HB2	1.78	0.83
2:D:1590:LEU:HD23	2:D:1591:LEU:N	1.91	0.83
2:D:925:VAL:HG22	2:D:1326:LEU:HD23	1.59	0.83
3:X:207:LEU:CD1	3:X:207:LEU:O	2.22	0.83
1:A:1061:ASN:HB2	1:A:1065:SER:O	1.77	0.83
1:C:980:LYS:HD3	1:C:986:GLU:HA	1.60	0.83
2:D:563:MET:HE2	2:D:564:LYS:H	1.39	0.83
2:D:824:VAL:HG21	2:D:830:VAL:HG11	1.60	0.83
1:A:1571:GLU:HB2	1:A:1574:PHE:CZ	2.13	0.83
2:B:494:ARG:NH1	2:B:494:ARG:HG3	1.91	0.83
2:D:175:SER:H	2:D:1300:ALA:HB2	1.41	0.83
2:D:347:PHE:O	2:D:350:THR:HG22	1.78	0.83
2:D:847:ARG:HG3	2:D:869:GLN:HG2	1.60	0.83
1:C:284:GLN:HG2	1:C:310:LEU:HD21	1.61	0.83
2:D:494:ARG:HG3	2:D:494:ARG:HH11	1.43	0.83
1:A:1056:ILE:HD11	1:A:1066:TYR:CE2	2.14	0.83
1:C:618:LYS:N	1:C:619:PRO:HD3	1.93	0.83
2:D:481:TYR:HE1	2:D:506:MET:SD	2.02	0.83
1:A:1228:TRP:N	1:A:1251:THR:HG22	1.94	0.83
1:A:572:GLN:HB2	1:A:593:ALA:HB3	1.60	0.83
1:A:895:LEU:HD12	1:A:896:VAL:H	1.42	0.83
1:C:1623:GLU:HB2	1:C:1638:PRO:CG	2.07	0.83
2:D:1500:LEU:HD12	2:D:1501:ASN:H	1.44	0.83
2:D:44:GLU:HG2	2:D:82:LEU:HB2	1.61	0.83
1:A:1066:TYR:H	1:A:1079:THR:HG23	1.44	0.82
2:B:1331:ALA:O	2:B:1332:GLN:HB3	1.79	0.82
1:C:391:ASN:HD21	1:C:406:PRO:HG3	1.42	0.82
2:D:563:MET:HG3	2:D:780:LEU:CD2	2.09	0.82

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:86:LEU:HG	3:Y:91:LYS:HB2	1.61	0.82
1:A:1153:ARG:HD2	1:A:1197:LEU:HB3	1.58	0.82
1:C:1573:VAL:HB	1:C:1603:LYS:HD3	1.60	0.82
1:C:493:ILE:HG23	1:C:495:LYS:H	1.43	0.82
1:A:936:ARG:HH11	1:A:936:ARG:CG	1.92	0.82
1:C:250:ILE:HD11	1:C:265:VAL:HG11	1.61	0.82
1:C:824:PHE:HD2	1:C:824:PHE:H	1.27	0.82
3:X:70:SER:HB3	3:X:91:LYS:HE3	1.61	0.82
1:A:1219:LYS:HZ1	1:A:1239:VAL:HG11	1.44	0.82
1:A:1546:GLU:HG2	1:A:1663:ASN:ND2	1.95	0.82
2:B:521:VAL:HG13	2:B:535:SER:HB3	1.60	0.82
1:C:1123:GLN:HE21	1:C:1123:GLN:HA	1.45	0.82
2:B:326:SER:HB2	2:B:819:GLN:HG3	1.60	0.82
2:D:481:TYR:O	2:D:481:TYR:HD2	1.62	0.82
3:X:86:LEU:HG	3:X:91:LYS:HB2	1.59	0.82
1:C:500:ASN:HB2	1:C:543:TYR:CD1	2.14	0.82
2:D:168:PRO:HG3	2:D:196:THR:C	2.00	0.82
1:A:1570:VAL:HA	1:A:1574:PHE:O	1.80	0.82
1:A:1585:TYR:CE2	1:A:1586:LYS:HB3	2.15	0.82
1:A:1590:ALA:HB1	1:A:1635:TYR:CE1	2.14	0.82
1:A:546:VAL:O	1:A:553:GLU:HB3	1.78	0.82
2:D:850:LEU:HB2	2:D:882:PHE:HE1	1.41	0.82
1:A:171:VAL:HG12	1:A:172:ASP:N	1.93	0.81
2:D:250:ARG:HG2	2:D:256:GLU:HA	1.61	0.81
1:A:1488:LEU:O	1:A:1488:LEU:HD12	1.80	0.81
2:B:200:VAL:HG12	2:B:211:THR:OG1	1.80	0.81
1:A:1575:VAL:HB	1:A:1602:LYS:O	1.79	0.81
1:C:1228:TRP:N	1:C:1251:THR:HG22	1.94	0.81
1:C:1582:LEU:HD21	1:C:1616:GLN:HG2	1.62	0.81
1:A:1582:LEU:HD21	1:A:1616:GLN:HG2	1.62	0.81
1:A:25:ILE:N	1:A:655:THR:CG2	2.44	0.81
2:B:435:TYR:HD1	2:B:436:GLN:N	1.78	0.81
2:B:933:ARG:HH11	2:B:933:ARG:HG3	1.44	0.81
1:C:696:LYS:HZ3	1:C:759:PRO:CD	1.93	0.81
2:B:168:PRO:HG3	2:B:196:THR:C	2.01	0.81
1:C:1020:TYR:HE1	1:C:1295:GLU:HG3	1.45	0.81
1:C:1049:LEU:HD11	1:C:1089:VAL:HG13	1.63	0.81
1:C:1218:VAL:HG12	1:C:1219:LYS:H	1.46	0.81
1:A:1576:LYS:HG2	1:A:1601:ILE:CG2	2.10	0.81
1:A:500:ASN:HB2	1:A:543:TYR:CD1	2.16	0.81
2:B:795:THR:HG22	2:B:796:PRO:HD2	1.61	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1607:ILE:N	2:D:1607:ILE:HD12	1.94	0.81
2:D:435:TYR:HD1	2:D:436:GLN:N	1.78	0.81
1:A:123:ASN:HB3	1:A:209:PHE:CD1	2.16	0.81
1:A:618:LYS:N	1:A:619:PRO:HD3	1.94	0.81
2:B:322:THR:HG22	2:B:327:ASP:O	1.80	0.81
2:D:961:THR:HG22	2:D:1327:THR:HG23	1.63	0.81
1:A:23:TYR:CD1	1:A:655:THR:HB	2.16	0.81
1:C:1531:ASP:O	1:C:1531:ASP:OD2	1.97	0.81
1:A:267:ILE:CD1	1:A:299:VAL:HG11	2.11	0.81
1:C:1067:SER:HA	1:C:1074:ALA:HA	1.63	0.81
1:C:87:ILE:N	1:C:87:ILE:HD13	1.96	0.81
2:D:954:VAL:HG12	2:D:955:PRO:HD2	1.63	0.81
1:C:1199:ASP:OD1	1:C:1201:THR:HG23	1.81	0.81
2:D:795:THR:HG22	2:D:796:PRO:HD2	1.63	0.81
2:B:469:ASN:HD22	2:B:470:ALA:N	1.79	0.80
1:C:149:ASN:HD22	1:C:149:ASN:H	1.26	0.80
1:C:1620:MET:HB2	1:C:1644:TRP:CB	2.10	0.80
1:C:1623:GLU:CB	1:C:1638:PRO:HG3	2.11	0.80
1:C:523:TYR:CE1	2:D:359:PRO:HG2	2.16	0.80
1:A:22:THR:HG21	1:A:657:ALA:HB2	1.62	0.80
1:A:504:LEU:CD1	1:A:509:ILE:HG23	2.11	0.80
1:C:617:LYS:HD2	1:C:622:ARG:HH21	1.46	0.80
3:Y:70:SER:HB3	3:Y:91:LYS:HE3	1.61	0.80
1:A:1190:ILE:HG12	1:A:1253:TYR:CD1	2.17	0.80
1:A:584:PRO:HD3	1:A:820:PHE:HB2	1.63	0.80
1:C:584:PRO:HD3	1:C:820:PHE:HB2	1.63	0.80
3:X:166:ASP:CG	3:X:207:LEU:HD21	2.01	0.80
1:A:1573:VAL:HB	1:A:1603:LYS:HD3	1.63	0.80
2:B:824:VAL:HG21	2:B:830:VAL:HG11	1.62	0.80
2:D:69:PHE:CE2	2:D:71:THR:HB	2.16	0.80
1:A:1213:LYS:HG2	1:A:1266:TYR:HE2	1.45	0.80
1:A:1232:LEU:HG	1:A:1233:GLN:HG3	1.63	0.80
2:B:161:VAL:HG21	2:B:180:LEU:HD21	1.62	0.80
1:C:1152:ILE:CG2	1:C:1168:LEU:HD21	2.10	0.80
1:C:1333:PHE:O	1:C:1334:LEU:HB2	1.79	0.80
2:D:344:GLN:HA	2:D:344:GLN:HE21	1.46	0.80
2:B:1341:ASN:HD22	2:B:1342:LYS:HG2	1.44	0.80
1:C:1571:GLU:HB2	1:C:1574:PHE:CZ	2.16	0.80
1:C:371:ILE:HD11	1:C:433:PHE:CE2	2.16	0.80
2:B:69:PHE:CE2	2:B:71:THR:HB	2.17	0.80
1:C:1067:SER:HB3	1:C:1072:GLY:O	1.81	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:TYR:CD2	1:C:493:ILE:N	2.50	0.80
1:A:243:PHE:CE1	1:A:316:GLU:HB3	2.17	0.80
1:A:599:TRP:O	1:A:803:GLY:HA2	1.81	0.80
1:A:796:THR:HG23	1:A:818:LYS:HB3	1.64	0.80
2:B:1562:GLN:HE22	2:B:1596:LYS:NZ	1.78	0.80
2:B:44:GLU:HG2	2:B:82:LEU:HB2	1.63	0.80
1:C:243:PHE:CE1	1:C:316:GLU:HB3	2.16	0.80
1:A:706:ASN:HD22	1:A:709:GLU:N	1.79	0.80
3:Y:165:LEU:O	3:Y:169:ILE:HG12	1.82	0.80
3:Y:188:LYS:HD3	3:Y:202:ASP:HA	1.64	0.80
1:C:1066:TYR:H	1:C:1079:THR:HG23	1.46	0.79
1:C:1570:VAL:HA	1:C:1574:PHE:O	1.82	0.79
2:D:1383:ASP:HB3	2:D:1457:LYS:HB2	1.63	0.79
2:D:344:GLN:HA	2:D:344:GLN:NE2	1.96	0.79
2:D:818:LEU:HB3	2:D:911:LYS:HD2	1.63	0.79
1:A:1546:GLU:O	1:A:1667:PHE:CZ	2.35	0.79
1:A:442:LEU:HD23	1:A:443:PRO:HD2	1.64	0.79
2:B:151:ASP:HB2	2:B:794:PHE:CZ	2.18	0.79
3:X:125:LYS:HA	3:X:127:ASN:N	1.98	0.79
2:B:1284:ARG:HD2	2:B:1285:GLU:H	1.45	0.79
1:C:1341:LEU:HB2	1:C:1342:LEU:HD23	1.63	0.79
2:B:137:TYR:CZ	2:B:143:VAL:HG22	2.17	0.79
1:C:1232:LEU:HG	1:C:1233:GLN:HG3	1.62	0.79
1:C:799:ILE:HG22	1:C:815:VAL:O	1.82	0.79
2:D:1341:ASN:HD22	2:D:1342:LYS:HG2	1.48	0.79
2:D:557:GLN:HA	2:D:557:GLN:OE1	1.82	0.79
1:A:696:LYS:NZ	1:A:759:PRO:HD2	1.98	0.79
2:B:218:LYS:HB3	2:B:822:TYR:CD2	2.17	0.79
1:C:1562:LYS:HD3	1:C:1664:LEU:CD2	2.10	0.79
2:B:481:TYR:HE1	2:B:506:MET:SD	2.05	0.79
1:C:135:TYR:CE1	1:C:141:VAL:HA	2.17	0.79
1:C:1153:ARG:HD2	1:C:1197:LEU:HB3	1.64	0.79
1:A:78:LYS:NZ	3:X:144:GLU:HA	1.98	0.79
3:X:170:ARG:HH22	3:X:206:LYS:HA	1.47	0.79
1:C:1012:LEU:CD2	1:C:1085:VAL:HG21	2.12	0.79
1:C:191:PRO:HD2	1:C:194:PRO:HB3	1.64	0.79
1:C:706:ASN:HD22	1:C:709:GLU:N	1.79	0.79
2:D:165:PHE:CZ	2:D:199:ILE:HD11	2.18	0.79
1:A:934:VAL:HG22	1:A:1366:HIS:CD2	2.17	0.79
1:A:830:PRO:CG	1:A:1483:PHE:HZ	1.95	0.79
1:A:532:GLN:HA	1:A:532:GLN:OE1	1.83	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:THR:HB	2:D:450:THR:O	1.81	0.79
2:D:1284:ARG:HD2	2:D:1285:GLU:H	1.46	0.79
2:D:872:ILE:HG22	2:D:878:ARG:HG3	1.65	0.79
2:B:961:THR:HG22	2:B:1327:THR:HG23	1.64	0.79
2:B:872:ILE:HG22	2:B:878:ARG:HG3	1.65	0.79
1:C:765:ILE:O	1:C:765:ILE:HD12	1.82	0.79
1:A:1497:GLU:OE1	1:A:1500:ARG:HD3	1.83	0.78
1:A:371:ILE:HD11	1:A:433:PHE:CE2	2.18	0.78
1:A:824:PHE:HD2	1:A:824:PHE:H	1.30	0.78
1:C:1031:TRP:CZ2	1:C:1042:LYS:HG3	2.17	0.78
2:D:1505:ARG:CZ	2:D:1623:LYS:HZ1	1.95	0.78
1:A:1133:LEU:CD1	1:A:1133:LEU:H	1.96	0.78
1:A:1573:VAL:CG1	1:A:1603:LYS:HD3	2.13	0.78
2:B:847:ARG:HG3	2:B:869:GLN:HG2	1.64	0.78
1:C:20:GLU:C	1:C:21:GLN:HG3	2.03	0.78
1:C:696:LYS:NZ	1:C:759:PRO:HD2	1.97	0.78
2:D:1349:VAL:HA	2:D:1364:MET:O	1.83	0.78
1:A:1573:VAL:O	1:A:1603:LYS:HG2	1.84	0.78
1:A:471:ASP:OD2	1:A:474:LYS:HB3	1.83	0.78
1:A:492:TYR:CD2	1:A:493:ILE:N	2.50	0.78
1:A:830:PRO:HG3	1:A:1483:PHE:CE2	2.18	0.78
2:B:265:PHE:CD2	2:B:294:LEU:HB2	2.18	0.78
1:C:111:PHE:CE2	1:C:113:LYS:HB2	2.18	0.78
1:C:1622:LYS:NZ	1:C:1642:LEU:HD23	1.98	0.78
2:D:494:ARG:HG3	2:D:494:ARG:NH1	1.97	0.78
1:A:1623:GLU:HB2	1:A:1638:PRO:CG	2.12	0.78
1:A:617:LYS:HD2	1:A:622:ARG:HH21	1.49	0.78
1:C:1108:VAL:HG21	1:C:1167:ALA:HB2	1.65	0.78
1:A:1049:LEU:HD11	1:A:1089:VAL:HG13	1.65	0.78
1:A:1190:ILE:HG12	1:A:1253:TYR:CE1	2.18	0.78
1:A:804:ILE:HG22	1:A:809:ILE:HG13	1.65	0.78
2:B:563:MET:HG3	2:B:780:LEU:CD2	2.13	0.78
1:C:23:TYR:HD1	1:C:23:TYR:N	1.81	0.78
1:A:391:ASN:ND2	1:A:406:PRO:HG3	1.99	0.78
3:Y:132:THR:HG23	3:Y:155:ILE:HB	1.65	0.78
2:D:385:HIS:CE1	3:Y:142:ASN:HD21	2.01	0.78
3:Y:166:ASP:OD1	3:Y:207:LEU:HD23	1.82	0.78
1:A:284:GLN:HG2	1:A:310:LEU:CD2	2.13	0.78
2:B:598:ILE:CD1	2:B:800:ILE:HG21	2.14	0.78
1:C:442:LEU:HD23	1:C:443:PRO:HD2	1.66	0.78
2:D:69:PHE:HE2	2:D:71:THR:HB	1.47	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:PRO:HG2	1:C:1098:ASN:OD1	1.83	0.78
1:A:1199:ASP:OD1	1:A:1201:THR:HG23	1.84	0.78
1:A:250:ILE:HD11	1:A:265:VAL:HG11	1.64	0.78
1:C:23:TYR:N	1:C:23:TYR:CD1	2.42	0.78
2:B:1383:ASP:HB3	2:B:1457:LYS:HB2	1.66	0.78
2:D:1331:ALA:O	2:D:1332:GLN:HB3	1.82	0.78
2:D:261:ALA:HB2	2:D:320:VAL:CG2	2.13	0.78
2:D:151:ASP:HB2	2:D:794:PHE:CZ	2.18	0.78
1:A:1056:ILE:HD11	1:A:1066:TYR:CD2	2.18	0.78
1:A:1535:MET:H	1:A:1608:ASN:HB3	1.49	0.78
1:C:1593:GLU:HB2	1:C:1596:SER:OG	1.83	0.78
1:A:42:GLN:HA	1:A:80:GLN:HG3	1.65	0.77
2:B:69:PHE:HE2	2:B:71:THR:HB	1.47	0.77
1:C:391:ASN:ND2	1:C:406:PRO:HG3	1.98	0.77
2:D:137:TYR:CZ	2:D:143:VAL:HG22	2.19	0.77
2:D:285:ILE:N	2:D:285:ILE:HD12	1.97	0.77
2:D:422:ARG:HH12	3:Y:44:ARG:HA	1.49	0.77
2:D:218:LYS:HB3	2:D:822:TYR:CD2	2.18	0.77
1:A:22:THR:CG2	1:A:657:ALA:HB2	2.15	0.77
2:B:557:GLN:HA	2:B:557:GLN:OE1	1.82	0.77
1:C:1190:ILE:HG12	1:C:1253:TYR:CD1	2.19	0.77
1:C:1213:LYS:HG2	1:C:1266:TYR:HE2	1.48	0.77
1:C:463:SER:CB	1:C:491:PRO:HA	2.13	0.77
1:C:532:GLN:NE2	1:C:568:GLY:HA2	1.98	0.77
1:A:20:GLU:C	1:A:21:GLN:HG3	2.04	0.77
1:A:1162:VAL:H	1:C:1102:ASN:ND2	1.82	0.77
1:C:535:VAL:CG2	1:C:536:PRO:HD3	2.13	0.77
1:C:830:PRO:CG	1:C:1483:PHE:HZ	1.96	0.77
1:C:968:VAL:HG23	1:C:971:THR:HG21	1.67	0.77
1:A:1179:THR:CG2	1:A:1208:ILE:HD13	2.15	0.77
1:A:576:SER:CB	1:A:577:PRO:HD3	2.15	0.77
1:C:1573:VAL:HG12	1:C:1603:LYS:HB3	1.66	0.77
1:C:1585:TYR:HD1	1:C:1671:ILE:CG2	1.97	0.77
1:C:55:SER:O	1:C:56:ILE:HD13	1.85	0.77
2:D:1446:PHE:HD2	2:D:1448:VAL:HG22	1.49	0.77
1:A:1213:LYS:HG2	1:A:1266:TYR:CE2	2.20	0.77
1:C:471:ASP:OD2	1:C:474:LYS:HB3	1.84	0.77
1:A:765:ILE:O	1:A:765:ILE:HD12	1.84	0.77
1:A:979:VAL:HG21	1:A:1326:TYR:HE1	1.50	0.77
2:B:285:ILE:HD12	2:B:285:ILE:N	2.00	0.77
1:C:284:GLN:HG2	1:C:310:LEU:CD2	2.15	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:GLN:HB2	1:C:80:GLN:NE2	1.99	0.77
1:A:23:TYR:HD1	1:A:23:TYR:N	1.79	0.77
1:A:906:GLY:H	1:A:929:VAL:HB	1.50	0.77
1:C:576:SER:CB	1:C:577:PRO:HD3	2.15	0.77
1:C:613:GLN:O	1:C:613:GLN:HG3	1.85	0.77
2:D:598:ILE:CD1	2:D:800:ILE:HG21	2.13	0.77
1:A:1161:LEU:HD12	1:C:1105:LEU:HD13	1.67	0.77
1:A:135:TYR:CE1	1:A:141:VAL:HA	2.17	0.77
2:B:224:PHE:CZ	2:B:329:VAL:HG22	2.20	0.77
1:C:532:GLN:OE1	1:C:532:GLN:HA	1.83	0.77
2:D:1613:GLU:O	2:D:1616:CYS:HB2	1.85	0.77
2:B:954:VAL:HG12	2:B:955:PRO:HD2	1.67	0.76
3:Y:87:LEU:HA	3:Y:91:LYS:HD3	1.67	0.76
1:A:1218:VAL:HG12	1:A:1219:LYS:H	1.50	0.76
1:A:1161:LEU:HA	1:C:1102:ASN:HD21	1.49	0.76
1:C:1576:LYS:HG2	1:C:1601:ILE:CG2	2.16	0.76
1:C:128:ILE:HG13	1:C:215:ALA:HB2	1.66	0.76
1:C:25:ILE:H	1:C:655:THR:CG2	1.98	0.76
1:A:23:TYR:H	1:A:23:TYR:HD1	1.29	0.76
2:B:469:ASN:ND2	2:B:469:ASN:C	2.37	0.76
1:C:1003:LEU:HD11	1:C:1286:SER:HA	1.65	0.76
1:C:1560:ALA:HB3	1:C:1585:TYR:HE2	1.50	0.76
1:C:1573:VAL:CG1	1:C:1603:LYS:HD3	2.15	0.76
1:C:267:ILE:CD1	1:C:299:VAL:HG11	2.15	0.76
2:D:478:TYR:HD1	2:D:478:TYR:O	1.68	0.76
3:Y:170:ARG:HD3	3:Y:203:LEU:HD23	1.65	0.76
2:D:1496:THR:HG23	2:D:1603:LYS:HD2	1.66	0.76
1:C:78:LYS:HZ2	3:Y:144:GLU:HA	1.50	0.76
2:B:478:TYR:O	2:B:478:TYR:HD1	1.67	0.76
1:A:696:LYS:HZ3	1:A:759:PRO:CD	1.98	0.76
1:C:1320:LYS:CD	1:C:1321:GLY:H	1.99	0.76
1:C:1562:LYS:HD2	1:C:1648:TRP:HZ2	1.49	0.76
1:C:171:VAL:HG12	1:C:172:ASP:N	1.97	0.76
1:C:43:VAL:HG13	1:C:79:PHE:HB3	1.68	0.76
2:D:1280:GLU:HG2	2:D:1287:PRO:HB3	1.66	0.76
3:X:150:ILE:HD12	3:X:150:ILE:O	1.86	0.76
2:B:250:ARG:HG2	2:B:256:GLU:HA	1.68	0.76
2:B:422:ARG:HD3	2:B:422:ARG:H	1.49	0.76
1:C:1494:THR:HB	1:C:1506:THR:HG23	1.68	0.76
1:C:315:LEU:CD1	1:C:318:LEU:HG	2.15	0.76
1:C:849:ARG:HG2	1:C:849:ARG:NH1	1.95	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:125:LYS:HA	3:Y:127:ASN:N	2.00	0.76
1:A:1213:LYS:HE2	1:A:1266:TYR:CD2	2.21	0.76
1:A:641:ASN:HD21	1:A:643:ALA:HB3	1.50	0.76
1:A:25:ILE:N	1:A:655:THR:HG23	1.99	0.76
1:C:1304:VAL:HG12	1:C:1305:LYS:N	2.01	0.76
1:C:351:PRO:HG2	1:C:352:TYR:CD2	2.20	0.76
1:C:830:PRO:HG3	1:C:1483:PHE:CE2	2.21	0.76
3:Y:136:LEU:O	3:Y:136:LEU:HG	1.84	0.76
1:A:386:VAL:H	1:A:411:THR:CG2	1.92	0.76
1:C:1497:GLU:OE1	1:C:1500:ARG:HD3	1.86	0.76
2:D:415:THR:OG1	2:D:425:GLN:HB2	1.85	0.76
1:C:144:ARG:HD2	1:C:146:TYR:CE1	2.20	0.76
1:C:804:ILE:HG22	1:C:809:ILE:HG13	1.67	0.76
2:D:322:THR:HG22	2:D:327:ASP:O	1.84	0.76
1:A:111:PHE:CE2	1:A:113:LYS:HB2	2.21	0.75
1:C:1179:THR:CG2	1:C:1208:ILE:HD13	2.16	0.75
2:D:954:VAL:HB	2:D:957:THR:CG2	2.15	0.75
1:A:315:LEU:CD1	1:A:318:LEU:HG	2.15	0.75
2:B:261:ALA:HB2	2:B:320:VAL:CG2	2.13	0.75
1:C:1488:LEU:HD12	1:C:1488:LEU:O	1.85	0.75
1:A:463:SER:HB3	1:A:491:PRO:HA	1.68	0.75
1:C:796:THR:HG23	1:C:818:LYS:HB3	1.67	0.75
2:D:200:VAL:HG12	2:D:211:THR:OG1	1.87	0.75
1:A:1067:SER:HB3	1:A:1072:GLY:O	1.85	0.75
1:A:1379:LEU:HD11	1:A:1505:CYS:O	1.86	0.75
2:B:1583:ILE:HG12	2:B:1607:ILE:HG23	1.66	0.75
2:B:344:GLN:HA	2:B:344:GLN:NE2	2.02	0.75
2:B:825:VAL:O	2:B:828:GLU:HG3	1.87	0.75
1:C:1585:TYR:CE2	1:C:1586:LYS:HB3	2.22	0.75
1:C:596:MET:N	1:C:782:ARG:HD3	2.01	0.75
1:A:1108:VAL:HG21	1:A:1167:ALA:HB2	1.69	0.75
1:A:1560:ALA:HB3	1:A:1585:TYR:HE2	1.52	0.75
2:B:42:LEU:HD11	2:B:82:LEU:HD12	1.67	0.75
1:A:1162:VAL:H	1:C:1102:ASN:HD21	1.34	0.75
2:D:148:PHE:CE2	2:D:792:VAL:HG11	2.21	0.75
1:C:1068:VAL:HA	1:C:1078:LEU:CD1	2.15	0.75
1:C:180:ILE:HB	1:C:599:TRP:CZ3	2.22	0.75
1:C:539:ARG:NH2	1:C:634:CYS:H	1.84	0.75
2:D:1424:ILE:HG12	2:D:1426:TYR:CE2	2.22	0.75
2:D:422:ARG:HD3	2:D:422:ARG:H	1.50	0.75
1:A:1244:THR:HG23	1:A:1502:ASP:OD2	1.85	0.75

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:PHE:CE1	1:A:452:TYR:HB2	2.21	0.75
1:A:539:ARG:NH2	1:A:634:CYS:H	1.85	0.75
2:B:1284:ARG:CD	2:B:1285:GLU:H	2.00	0.75
2:B:948:ARG:HH21	2:B:948:ARG:HB2	1.51	0.75
1:C:1104:LEU:O	1:C:1108:VAL:HG12	1.87	0.75
2:D:469:ASN:C	2:D:469:ASN:ND2	2.39	0.75
1:A:1638:PRO:O	1:A:1639:LEU:HB2	1.87	0.75
1:A:128:ILE:HD12	1:A:201:ILE:HG22	1.67	0.75
1:A:535:VAL:CG2	1:A:536:PRO:HD3	2.13	0.75
2:B:818:LEU:HB3	2:B:911:LYS:HD2	1.69	0.75
1:C:1504:GLN:HG3	1:C:1505:CYS:HA	1.69	0.75
1:C:260:VAL:HG12	1:C:261:THR:H	1.50	0.75
1:C:38:ASN:HA	1:C:84:ILE:HG22	1.68	0.75
2:D:1347:VAL:HG22	2:D:1367:ILE:HG23	1.69	0.75
2:D:265:PHE:CD2	2:D:294:LEU:HB2	2.21	0.75
1:A:255:PHE:HE1	1:A:258:LYS:CB	1.98	0.75
2:B:829:GLN:CG	2:B:1480:LEU:HD13	2.17	0.75
1:C:1320:LYS:HD2	1:C:1321:GLY:H	1.51	0.75
1:C:44:TYR:HB2	1:C:545:ILE:HD12	1.69	0.75
1:C:549:GLU:CD	1:C:550:GLN:H	1.89	0.75
1:A:111:PHE:HE2	1:A:113:LYS:HB2	1.52	0.74
1:A:1402:ILE:HG13	1:A:1479:ILE:HD11	1.69	0.74
2:B:508:LEU:HD12	2:B:509:HIS:H	1.52	0.74
1:C:1218:VAL:HG12	1:C:1219:LYS:N	2.02	0.74
1:C:1314:ASP:HA	1:C:1325:ASN:HB2	1.68	0.74
1:A:849:ARG:HG2	1:A:849:ARG:NH1	1.94	0.74
1:C:1244:THR:HG23	1:C:1502:ASP:OD2	1.87	0.74
1:C:415:ASP:HB2	1:C:417:VAL:HB	1.69	0.74
2:D:261:ALA:CB	2:D:320:VAL:HG23	2.15	0.74
2:D:42:LEU:HD11	2:D:82:LEU:HD12	1.68	0.74
1:C:224:LEU:HD23	1:C:225:PRO:HD2	1.70	0.74
1:A:613:GLN:HG3	1:A:613:GLN:O	1.85	0.74
2:B:1473:HIS:HB3	2:B:1476:LYS:HB2	1.68	0.74
1:C:33:VAL:HG21	1:C:121:TYR:HD1	1.51	0.74
2:D:615:GLN:HB2	2:D:616:ASN:ND2	2.03	0.74
3:X:87:LEU:HA	3:X:91:LYS:HD3	1.69	0.74
1:C:961:TYR:HE2	1:C:1343:ASN:HA	1.53	0.74
1:A:1067:SER:HA	1:A:1074:ALA:HA	1.68	0.74
1:A:1314:ASP:HA	1:A:1325:ASN:HB2	1.70	0.74
1:A:1562:LYS:HD3	1:A:1664:LEU:HD21	1.70	0.74
1:C:285:THR:HG22	1:C:285:THR:O	1.86	0.74

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:640:LEU:H	1:C:644:ASN:HB3	1.53	0.74
1:C:895:LEU:HD12	1:C:896:VAL:H	1.52	0.74
1:A:1047:LYS:HE2	1:A:1051:GLU:OE2	1.86	0.74
1:A:1402:ILE:HG13	1:A:1479:ILE:CD1	2.17	0.74
1:A:258:LYS:HD3	1:A:893:SER:OG	1.85	0.74
1:C:1056:ILE:HD11	1:C:1066:TYR:CE2	2.23	0.74
2:D:34:ARG:HD3	2:D:124:GLN:HG2	1.69	0.74
2:D:469:ASN:HD22	2:D:470:ALA:N	1.86	0.74
1:A:620:LEU:O	1:A:623:VAL:HG23	1.88	0.74
1:C:1024:TYR:HA	1:C:1302:LEU:HD21	1.69	0.74
1:C:123:ASN:HB3	1:C:209:PHE:CD1	2.23	0.74
1:C:538:SER:O	1:C:561:LEU:HB2	1.88	0.74
1:C:695:VAL:HG13	1:C:724:CYS:HA	1.70	0.74
2:D:758:LEU:HD13	2:D:760:LYS:HE2	1.69	0.74
1:A:1031:TRP:CZ2	1:A:1042:LYS:HG3	2.22	0.74
1:A:1152:ILE:CG2	1:A:1168:LEU:HD21	2.17	0.74
1:A:128:ILE:HG13	1:A:215:ALA:HB2	1.69	0.74
1:A:42:GLN:HB2	1:A:80:GLN:NE2	2.02	0.74
1:C:993:SER:C	1:C:995:GLU:H	1.91	0.74
2:D:1525:LYS:HD2	2:D:1610:TRP:CZ2	2.22	0.74
2:D:620:VAL:HG12	2:D:621:PHE:HD2	1.53	0.74
1:A:144:ARG:HD2	1:A:146:TYR:CE1	2.22	0.73
1:A:538:SER:O	1:A:561:LEU:HB2	1.86	0.73
2:B:344:GLN:HA	2:B:344:GLN:HE21	1.52	0.73
1:C:1013:MET:SD	1:C:1016:VAL:HG21	2.28	0.73
1:C:1186:PHE:HA	1:C:1250:THR:HG22	1.70	0.73
1:C:1622:LYS:HZ3	1:C:1642:LEU:HD23	1.52	0.73
3:X:132:THR:HG23	3:X:155:ILE:HB	1.70	0.73
1:A:1020:TYR:HE1	1:A:1295:GLU:HG3	1.52	0.73
1:A:503:ILE:HB	1:A:511:HIS:HB2	1.69	0.73
2:B:1435:ASP:OD1	5:B:2003:NAG:H81	1.88	0.73
1:C:1627:ILE:HD12	1:C:1629:TYR:HB3	1.69	0.73
1:C:133:PRO:HD2	1:C:609:VAL:CG1	2.17	0.73
1:C:127:PHE:CD2	1:C:623:VAL:HG22	2.23	0.73
1:A:1341:LEU:HB2	1:A:1342:LEU:HD23	1.69	0.73
1:A:1370:THR:HG23	1:A:1373:GLU:OE1	1.88	0.73
1:A:1593:GLU:HB2	1:A:1596:SER:OG	1.88	0.73
1:C:1133:LEU:H	1:C:1133:LEU:CD1	1.95	0.73
1:C:222:TYR:HE1	1:C:768:TYR:HB2	1.51	0.73
2:D:948:ARG:HB2	2:D:948:ARG:HH21	1.53	0.73
3:X:111:ASP:OD1	3:X:112:PRO:HD2	1.89	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1349:VAL:HA	2:B:1364:MET:O	1.88	0.73
1:C:1190:ILE:HG12	1:C:1253:TYR:CE1	2.23	0.73
1:C:1365:VAL:HG22	1:C:1366:HIS:N	2.01	0.73
1:C:433:PHE:CE1	1:C:452:TYR:HB2	2.23	0.73
1:A:1068:VAL:HA	1:A:1078:LEU:CD1	2.17	0.73
1:A:160:VAL:HG22	1:A:175:GLU:HB3	1.71	0.73
2:B:484:LEU:HB2	2:B:519:ARG:HG3	1.70	0.73
1:C:1056:ILE:HD11	1:C:1066:TYR:CD2	2.23	0.73
1:C:42:GLN:NE2	1:C:44:TYR:N	2.37	0.73
1:C:936:ARG:NH1	1:C:936:ARG:HG3	1.87	0.73
2:B:1607:ILE:H	2:B:1607:ILE:HD12	1.53	0.73
1:C:1493:PHE:CD1	1:C:1494:THR:N	2.52	0.73
2:B:620:VAL:HG12	2:B:621:PHE:HD2	1.52	0.73
1:C:906:GLY:H	1:C:929:VAL:HB	1.53	0.73
2:D:1508:VAL:HB	2:D:1509:PRO:HD3	1.70	0.73
3:X:165:LEU:O	3:X:169:ILE:HG12	1.89	0.73
1:A:182:ILE:CG1	1:A:804:ILE:HD11	2.06	0.73
1:A:968:VAL:HG23	1:A:971:THR:OG1	1.88	0.73
2:B:415:THR:OG1	2:B:425:GLN:HB2	1.89	0.73
1:C:111:PHE:HE2	1:C:113:LYS:HB2	1.50	0.73
1:C:489:LYS:CG	1:C:490:SER:N	2.50	0.73
1:A:470:THR:HB	2:B:450:THR:O	1.89	0.73
1:C:1573:VAL:O	1:C:1603:LYS:HG2	1.89	0.73
1:C:1626:GLN:HB2	1:C:1635:TYR:HD1	1.53	0.73
1:C:255:PHE:HE1	1:C:258:LYS:CB	2.02	0.73
1:A:700:TYR:C	1:A:700:TYR:HD2	1.92	0.73
2:B:548:LEU:HD22	2:B:793:SER:HB3	1.70	0.73
1:C:1527:CYS:C	1:C:1529:GLU:N	2.34	0.73
1:C:160:VAL:HG22	1:C:175:GLU:HB3	1.71	0.73
1:C:220:LYS:HD3	1:C:765:ILE:HG23	1.69	0.73
2:D:825:VAL:O	2:D:828:GLU:HG3	1.88	0.73
1:A:415:ASP:HB2	1:A:417:VAL:HB	1.69	0.72
1:A:993:SER:C	1:A:995:GLU:H	1.93	0.72
2:B:844:ILE:HG13	2:B:872:ILE:HG12	1.71	0.72
1:C:494:ASP:O	1:C:496:ILE:N	2.22	0.72
2:D:1482:ASN:HB2	2:D:1495:GLU:HG2	1.69	0.72
1:A:514:THR:O	1:A:515:ARG:HD3	1.89	0.72
1:A:517:LYS:HG2	1:A:518:PHE:N	2.04	0.72
2:B:148:PHE:CE2	2:B:792:VAL:HG11	2.24	0.72
1:C:1152:ILE:HG21	1:C:1168:LEU:HD21	1.70	0.72
1:C:1213:LYS:HG2	1:C:1266:TYR:CE2	2.24	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:963:ILE:HG23	1:C:967:LEU:HD23	1.72	0.72
1:A:149:ASN:H	1:A:149:ASN:HD22	1.36	0.72
1:A:1573:VAL:HG12	1:A:1603:LYS:HB3	1.70	0.72
1:A:493:ILE:HG23	1:A:495:LYS:H	1.55	0.72
1:A:695:VAL:HG13	1:A:724:CYS:HA	1.70	0.72
2:B:1347:VAL:HG22	2:B:1367:ILE:HG23	1.70	0.72
1:C:1358:THR:HB	1:C:1360:HIS:CE1	2.24	0.72
1:C:365:PRO:HD2	1:C:464:TYR:CD2	2.25	0.72
1:C:700:TYR:C	1:C:700:TYR:HD2	1.92	0.72
2:D:834:ALA:O	2:D:835:ILE:HD13	1.89	0.72
2:D:850:LEU:HD12	2:D:851:LEU:H	1.53	0.72
1:A:483:ASN:ND2	2:B:399:ILE:HB	2.04	0.72
1:A:799:ILE:HG22	1:A:815:VAL:O	1.90	0.72
2:B:1279:ILE:HG22	2:B:1288:ILE:HB	1.71	0.72
2:B:34:ARG:HD3	2:B:124:GLN:HG2	1.71	0.72
1:C:238:ILE:HD12	1:C:347:TYR:HE1	1.53	0.72
1:C:330:ILE:HG22	1:C:337:SER:CB	2.20	0.72
2:D:844:ILE:HG13	2:D:872:ILE:HG12	1.72	0.72
1:A:148:LEU:HD23	1:A:152:LEU:CD1	2.19	0.72
1:C:1255:LEU:O	1:C:1255:LEU:HD12	1.90	0.72
1:C:374:GLN:HA	1:C:416:GLY:O	1.88	0.72
3:X:68:ASN:CG	3:X:69:GLY:H	1.92	0.72
1:A:1228:TRP:H	1:A:1251:THR:CG2	1.98	0.72
1:A:830:PRO:CG	1:A:1483:PHE:CZ	2.72	0.72
1:A:1623:GLU:CB	1:A:1638:PRO:HG3	2.18	0.72
1:C:1278:GLN:OE1	1:C:1283:GLY:CA	2.37	0.72
1:C:1573:VAL:CB	1:C:1603:LYS:HD3	2.19	0.72
1:C:24:VAL:N	1:C:655:THR:HG21	2.04	0.72
1:C:495:LYS:CE	1:C:495:LYS:HA	2.19	0.72
1:A:260:VAL:HG12	1:A:261:THR:H	1.54	0.72
1:A:38:ASN:HA	1:A:84:ILE:HG22	1.71	0.72
1:A:43:VAL:HG13	1:A:79:PHE:HB3	1.69	0.72
2:B:261:ALA:CB	2:B:320:VAL:HG23	2.16	0.72
1:C:234:GLU:HG3	1:C:235:TYR:HD2	1.51	0.72
1:C:365:PRO:HD2	1:C:464:TYR:CE2	2.24	0.72
1:A:1560:ALA:HB3	1:A:1585:TYR:CE2	2.25	0.72
1:C:1108:VAL:HG11	1:C:1164:ILE:HG22	1.70	0.72
1:C:1329:THR:OG1	1:C:1331:LYS:HG2	1.90	0.72
2:D:1506:ILE:HD11	2:D:1628:PHE:HE1	1.53	0.72
1:A:1347:ILE:O	1:A:1347:ILE:HG22	1.89	0.72
1:A:373:VAL:HG23	1:A:418:ALA:HB3	1.70	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1313:VAL:HG11	2:B:1323:MET:SD	2.29	0.72
1:C:1560:ALA:HB3	1:C:1585:TYR:CE2	2.24	0.72
3:X:64:VAL:HG11	3:X:95:LYS:O	1.90	0.72
1:A:1076:THR:CG2	1:A:1120:GLU:HA	2.18	0.72
1:A:1304:VAL:HG12	1:A:1305:LYS:N	2.03	0.72
1:A:1493:PHE:CD1	1:A:1494:THR:N	2.55	0.72
1:A:225:PRO:HG3	1:A:766:ARG:HB2	1.71	0.72
2:B:162:ILE:CG2	2:B:202:LYS:HG2	2.20	0.72
1:C:596:MET:HA	1:C:782:ARG:HG2	1.70	0.72
1:C:1163:LYS:O	1:C:1166:THR:HG22	1.90	0.71
1:C:489:LYS:HG3	1:C:490:SER:H	1.55	0.71
1:C:491:PRO:HB2	1:C:493:ILE:O	1.89	0.71
1:C:620:LEU:O	1:C:623:VAL:HG23	1.88	0.71
2:D:481:TYR:HB2	2:D:520:PHE:CE1	2.25	0.71
2:B:563:MET:HB3	2:B:778:PHE:CE2	2.25	0.71
1:C:1068:VAL:HG13	1:C:1069:TRP:N	2.06	0.71
1:C:1567:SER:HB3	1:C:1578:LYS:HB2	1.70	0.71
1:C:386:VAL:H	1:C:411:THR:CG2	1.92	0.71
1:A:1104:LEU:O	1:A:1108:VAL:HG12	1.91	0.71
1:A:351:PRO:HG2	1:A:352:TYR:CD2	2.25	0.71
2:B:618:LEU:HD11	2:B:635:ASN:O	1.90	0.71
1:C:1423:VAL:HG13	1:C:1496:TYR:CD2	2.24	0.71
2:D:23:ALA:HB3	2:D:528:ASN:HD22	1.55	0.71
3:Y:166:ASP:OD2	3:Y:207:LEU:HG	1.89	0.71
3:Y:68:ASN:CG	3:Y:69:GLY:H	1.93	0.71
1:A:1069:TRP:CZ3	1:A:1451:THR:HG21	2.25	0.71
1:C:61:ASP:O	1:C:62:LYS:HB2	1.90	0.71
1:C:979:VAL:HG21	1:C:1326:TYR:HE1	1.52	0.71
2:D:1523:VAL:HG22	2:D:1584:TRP:HB2	1.72	0.71
1:A:42:GLN:NE2	1:A:44:TYR:N	2.38	0.71
1:A:491:PRO:O	1:A:492:TYR:C	2.28	0.71
1:A:552:ALA:HB2	1:A:657:ALA:HB3	1.73	0.71
1:A:981:GLY:CA	1:A:1333:PHE:HB2	2.21	0.71
2:B:435:TYR:CD1	2:B:436:GLN:N	2.59	0.71
1:C:1381:ILE:HG12	1:C:1382:ASP:N	2.05	0.71
1:C:1450:PHE:CZ	1:C:1475:VAL:HB	2.24	0.71
1:C:222:TYR:HD2	1:C:223:VAL:N	1.88	0.71
1:C:42:GLN:HA	1:C:80:GLN:HG3	1.72	0.71
2:D:1371:TYR:CG	2:D:1377:SER:HB3	2.25	0.71
1:A:224:LEU:HD23	1:A:225:PRO:HD2	1.71	0.71
1:C:530:VAL:HG23	1:C:534:MET:HE2	1.71	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1284:ARG:CD	2:D:1285:GLU:H	2.02	0.71
2:D:1562:GLN:HE22	2:D:1596:LYS:NZ	1.88	0.71
1:A:374:GLN:HA	1:A:416:GLY:O	1.91	0.71
1:A:44:TYR:HB2	1:A:545:ILE:HD12	1.71	0.71
1:A:489:LYS:CG	1:A:490:SER:N	2.53	0.71
1:A:491:PRO:HB2	1:A:493:ILE:O	1.89	0.71
1:A:961:TYR:HE2	1:A:1343:ASN:HA	1.55	0.71
2:B:1280:GLU:HG2	2:B:1287:PRO:HB3	1.73	0.71
1:C:906:GLY:O	1:C:908:HIS:CE1	2.44	0.71
1:A:774:LEU:HD12	1:A:799:ILE:HD11	1.71	0.71
1:C:1219:LYS:HZ3	1:C:1239:VAL:HG11	1.55	0.71
1:C:961:TYR:CE2	1:C:1343:ASN:HA	2.25	0.71
1:A:1268:ASN:HD22	1:A:1268:ASN:H	1.38	0.71
1:A:1024:TYR:HA	1:A:1302:LEU:HD21	1.73	0.71
1:A:423:ASN:OD1	2:B:504:VAL:HG22	1.91	0.71
2:B:1446:PHE:HD2	2:B:1448:VAL:HG22	1.54	0.71
1:C:967:LEU:HD12	1:C:968:VAL:N	2.04	0.71
3:X:64:VAL:HG23	3:X:71:ASN:OD1	1.91	0.71
1:A:1179:THR:HG21	1:A:1208:ILE:HD13	1.72	0.71
1:A:1573:VAL:CB	1:A:1603:LYS:HD3	2.21	0.71
1:A:40:VAL:HG21	1:A:512:PHE:HD1	1.55	0.71
1:A:640:LEU:H	1:A:644:ASN:HB3	1.56	0.71
1:A:99:VAL:O	1:A:119:ILE:HD11	1.90	0.71
2:B:1593:THR:HG22	2:B:1594:LYS:N	2.06	0.71
2:B:165:PHE:CZ	2:B:199:ILE:HD11	2.26	0.71
2:B:481:TYR:HB2	2:B:520:PHE:CE1	2.25	0.71
1:C:1638:PRO:O	1:C:1639:LEU:HB2	1.89	0.71
1:A:1076:THR:HG22	1:A:1120:GLU:OE2	1.91	0.70
1:A:234:GLU:HG3	1:A:235:TYR:HD2	1.50	0.70
1:A:255:PHE:CE1	1:A:258:LYS:HB3	2.25	0.70
1:A:365:PRO:HD2	1:A:464:TYR:CD2	2.25	0.70
1:A:398:ASN:O	1:A:399:GLN:HB2	1.90	0.70
1:A:906:GLY:O	1:A:908:HIS:CE1	2.43	0.70
2:B:850:LEU:HD12	2:B:851:LEU:H	1.55	0.70
2:D:162:ILE:CG2	2:D:202:LYS:HG2	2.20	0.70
2:D:508:LEU:HD12	2:D:509:HIS:H	1.55	0.70
2:B:758:LEU:HD13	2:B:760:LYS:HE2	1.72	0.70
1:C:1543:ILE:O	1:C:1547:THR:HG23	1.90	0.70
1:A:1186:PHE:HA	1:A:1250:THR:HG22	1.73	0.70
1:A:765:ILE:HD13	1:A:767:SER:O	1.91	0.70
1:A:963:ILE:HG23	1:A:967:LEU:HD23	1.72	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:LYS:HD3	1:C:110:HIS:CE1	2.26	0.70
1:A:1013:MET:SD	1:A:1016:VAL:HG21	2.31	0.70
1:A:1127:ILE:HD11	1:A:1143:TYR:CD2	2.27	0.70
1:A:1525:CYS:C	1:A:1528:VAL:HG22	2.12	0.70
1:A:238:ILE:HD12	1:A:347:TYR:HE1	1.55	0.70
2:B:1482:ASN:HB2	2:B:1495:GLU:HG2	1.72	0.70
3:X:166:ASP:OD1	3:X:207:LEU:HD23	1.91	0.70
1:A:131:ASP:HB3	1:A:142:LYS:HB2	1.74	0.70
1:A:504:LEU:HD21	1:A:651:LEU:HG	1.74	0.70
2:B:615:GLN:HB2	2:B:616:ASN:ND2	2.06	0.70
1:C:1127:ILE:H	1:C:1127:ILE:HD12	1.56	0.70
1:C:131:ASP:O	1:C:132:LYS:HG2	1.91	0.70
1:C:968:VAL:HG12	1:C:1368:THR:HG22	1.73	0.70
1:C:152:LEU:HD11	1:C:627:LEU:HD11	1.73	0.70
1:C:491:PRO:O	1:C:492:TYR:C	2.26	0.70
1:C:503:ILE:HB	1:C:511:HIS:HB2	1.72	0.70
2:D:1381:ILE:HG21	2:D:1459:TYR:HE1	1.56	0.70
3:Y:80:GLN:HG3	3:Y:114:GLY:C	2.12	0.70
1:A:1076:THR:HG21	1:A:1120:GLU:HA	1.72	0.70
1:A:961:TYR:CE2	1:A:1343:ASN:HA	2.27	0.70
1:A:685:GLU:HA	1:A:685:GLU:OE1	1.92	0.70
2:B:950:LEU:HD22	2:B:1329:TYR:CZ	2.26	0.70
2:B:1615:GLU:HB3	2:B:1621:PHE:CD1	2.26	0.70
2:B:28:ILE:HD12	2:B:42:LEU:HD23	1.73	0.70
1:C:1112:GLN:HE21	1:C:1171:ALA:HB2	1.54	0.70
1:C:869:GLU:C	1:C:871:PRO:HD3	2.11	0.70
2:D:1445:HIS:CG	2:D:1446:PHE:N	2.59	0.70
2:D:618:LEU:HD11	2:D:635:ASN:O	1.92	0.70
3:Y:146:LEU:HD22	3:Y:147:ASP:N	2.06	0.70
1:C:255:PHE:CE1	1:C:258:LYS:HB3	2.27	0.70
3:Y:47:HIS:HE1	3:Y:181:LYS:HE2	1.56	0.70
1:A:1504:GLN:HG3	1:A:1505:CYS:HA	1.72	0.70
2:B:1424:ILE:H	2:B:1424:ILE:HD13	1.56	0.70
1:C:975:ARG:NH2	1:C:1346:LEU:HD22	2.06	0.70
1:C:517:LYS:HG2	1:C:518:PHE:N	2.05	0.70
1:C:690:TYR:O	1:C:690:TYR:CG	2.43	0.70
2:D:262:PHE:HE1	2:D:282:ARG:HG3	1.56	0.70
1:A:285:THR:HG22	1:A:285:THR:O	1.91	0.70
2:B:954:VAL:HB	2:B:957:THR:CG2	2.19	0.70
1:C:1047:LYS:HE2	1:C:1051:GLU:OE2	1.92	0.70
1:C:419:SER:HB2	2:D:459:ASN:HD22	1.56	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:968:VAL:CG2	1:C:971:THR:HG21	2.22	0.70
1:A:1616:GLN:OE1	1:A:1650:ARG:HD3	1.92	0.70
1:A:330:ILE:HG22	1:A:337:SER:CB	2.21	0.70
1:C:99:VAL:O	1:C:119:ILE:HD11	1.91	0.70
1:C:1625:LEU:O	1:C:1627:ILE:HG23	1.91	0.70
1:C:639:GLY:HA2	1:C:648:LEU:HD13	1.74	0.70
1:C:938:SER:O	1:C:940:SER:N	2.25	0.70
2:D:237:ILE:O	2:D:306:LEU:HD11	1.92	0.70
3:X:136:LEU:HG	3:X:136:LEU:O	1.91	0.70
3:Y:111:ASP:OD1	3:Y:112:PRO:HD2	1.91	0.70
1:C:476:LEU:HB3	1:C:563:ILE:HA	1.73	0.69
2:D:1480:LEU:HD12	2:D:1481:LEU:N	2.06	0.69
1:A:1278:GLN:OE1	1:A:1283:GLY:CA	2.40	0.69
1:A:148:LEU:HD23	1:A:152:LEU:HD12	1.74	0.69
1:A:1567:SER:HB3	1:A:1578:LYS:HB2	1.74	0.69
1:A:587:THR:HG22	1:A:789:ALA:HB2	1.72	0.69
1:C:1219:LYS:CE	1:C:1239:VAL:HG21	2.22	0.69
1:C:1370:THR:HG23	1:C:1373:GLU:OE1	1.91	0.69
2:D:484:LEU:HB2	2:D:519:ARG:HG3	1.73	0.69
3:X:73:VAL:HG23	3:X:74:ARG:N	2.07	0.69
3:Y:170:ARG:NH2	3:Y:206:LYS:HA	2.06	0.69
1:A:1543:ILE:O	1:A:1547:THR:HG23	1.91	0.69
1:A:1646:GLU:OE2	1:A:1660:PHE:HZ	1.75	0.69
1:A:495:LYS:HA	1:A:495:LYS:CE	2.17	0.69
1:A:596:MET:HA	1:A:782:ARG:HG2	1.74	0.69
1:A:849:ARG:NH2	2:B:555:LEU:HB2	2.07	0.69
2:B:834:ALA:O	2:B:835:ILE:HD13	1.92	0.69
1:C:1429:PRO:HB2	1:C:1432:ILE:CG1	2.22	0.69
1:C:1646:GLU:OE2	1:C:1660:PHE:HZ	1.75	0.69
2:D:148:PHE:HB3	2:D:800:ILE:HD11	1.75	0.69
2:D:825:VAL:N	2:D:828:GLU:OE1	2.25	0.69
1:A:33:VAL:HG21	1:A:121:TYR:HD1	1.57	0.69
1:C:1019:PHE:C	1:C:1019:PHE:CD2	2.65	0.69
1:C:1404:ALA:HB1	1:C:1493:PHE:HE2	1.57	0.69
1:C:1585:TYR:CE1	1:C:1671:ILE:HG12	2.28	0.69
2:D:435:TYR:CD1	2:D:436:GLN:N	2.58	0.69
3:Y:73:VAL:HG23	3:Y:74:ARG:N	2.07	0.69
1:A:1329:THR:OG1	1:A:1331:LYS:HG2	1.92	0.69
1:A:1494:THR:HB	1:A:1506:THR:HG23	1.74	0.69
1:A:463:SER:CB	1:A:491:PRO:HA	2.23	0.69
2:B:1445:HIS:CG	2:B:1446:PHE:N	2.59	0.69

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:TYR:CZ	2:B:424:ARG:HD2	2.27	0.69
1:C:131:ASP:HB3	1:C:142:LYS:HB2	1.72	0.69
1:C:238:ILE:HB	1:C:347:TYR:CD1	2.28	0.69
1:C:658:ASN:O	1:C:659:ALA:HB3	1.91	0.69
2:D:422:ARG:NH1	3:Y:44:ARG:HA	2.07	0.69
2:D:859:ALA:HB1	2:D:866:TYR:CD1	2.27	0.69
1:A:1108:VAL:HG11	1:A:1164:ILE:HG22	1.73	0.69
1:A:1404:ALA:HB1	1:A:1493:PHE:HE2	1.57	0.69
1:A:234:GLU:HG3	1:A:235:TYR:CE2	2.28	0.69
1:C:1228:TRP:H	1:C:1251:THR:CG2	1.98	0.69
1:C:1366:HIS:N	1:C:1366:HIS:ND1	2.40	0.69
1:C:1627:ILE:O	1:C:1627:ILE:HD12	1.92	0.69
3:Y:50:TYR:HE2	3:Y:170:ARG:NH1	1.90	0.69
1:A:1423:VAL:HG13	1:A:1496:TYR:CD2	2.27	0.69
2:B:1371:TYR:CG	2:B:1377:SER:HB3	2.27	0.69
2:B:230:PRO:HG3	2:B:333:GLN:HG2	1.73	0.69
1:C:144:ARG:HD2	1:C:146:TYR:HE1	1.58	0.69
1:C:257:ASN:HD21	1:C:892:SER:HA	1.58	0.69
1:C:24:VAL:HA	1:C:655:THR:OG1	1.93	0.69
2:D:127:PHE:HE2	2:D:602:ILE:HG23	1.57	0.69
2:D:224:PHE:CZ	2:D:329:VAL:HG22	2.27	0.69
2:D:262:PHE:CE1	2:D:282:ARG:HG3	2.27	0.69
2:D:824:VAL:HG22	2:D:825:VAL:H	1.58	0.69
1:A:1429:PRO:HB2	1:A:1432:ILE:CG1	2.23	0.69
1:A:700:TYR:CD2	1:A:700:TYR:C	2.64	0.69
2:B:859:ALA:HB1	2:B:866:TYR:CD1	2.28	0.69
1:C:1347:ILE:O	1:C:1347:ILE:HG22	1.93	0.69
1:C:1423:VAL:HG13	1:C:1496:TYR:CE2	2.27	0.69
1:C:837:GLU:HG2	1:C:1488:LEU:HA	1.75	0.69
1:C:1525:CYS:O	1:C:1529:GLU:HG3	1.93	0.69
1:C:1549:LYS:NZ	1:C:1667:PHE:HB3	2.07	0.69
1:C:77:ASN:HD21	1:C:81:ASN:HB2	1.57	0.69
2:D:950:LEU:HD22	2:D:1329:TYR:CZ	2.28	0.69
1:A:127:PHE:CE2	1:A:623:VAL:HG13	2.27	0.69
1:C:148:LEU:HD23	1:C:152:LEU:CD1	2.22	0.69
1:C:307:VAL:CG1	1:C:313:TYR:HB2	2.23	0.69
1:C:115:LYS:HB2	1:C:654:LEU:HD21	1.74	0.69
1:C:587:THR:HG22	1:C:789:ALA:HB2	1.74	0.69
2:D:1382:ILE:HB	2:D:1425:ILE:HB	1.74	0.69
2:D:840:VAL:HG12	2:D:841:ASN:N	2.06	0.69
3:X:188:LYS:HD3	3:X:202:ASP:HA	1.75	0.69

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1086:LEU:HD12	1:A:1095:GLN:HG3	1.75	0.69
1:A:549:GLU:CD	1:A:549:GLU:H	1.96	0.69
1:C:1069:TRP:CZ3	1:C:1451:THR:HG21	2.28	0.69
2:D:148:PHE:CB	2:D:800:ILE:HD11	2.22	0.69
2:D:1593:THR:HG22	2:D:1594:LYS:N	2.07	0.69
1:A:1218:VAL:HG12	1:A:1219:LYS:N	2.07	0.69
1:A:123:ASN:HB3	1:A:209:PHE:HD1	1.56	0.69
1:A:92:LEU:HD12	1:C:1029:ASN:ND2	2.07	0.69
2:B:1381:ILE:HG21	2:B:1459:TYR:HE1	1.57	0.69
2:B:136:ILE:HA	2:B:215:ASP:O	1.92	0.69
1:C:166:PRO:HD3	1:C:199:TRP:HA	1.75	0.69
1:C:596:MET:N	1:C:782:ARG:HH11	1.85	0.69
2:D:114:ARG:O	2:D:115:LEU:HD23	1.93	0.69
2:D:1610:TRP:CD2	2:D:1628:PHE:CD2	2.81	0.69
2:D:1435:ASP:OD1	5:D:2003:NAG:H81	1.92	0.69
2:D:813:VAL:HG12	2:D:840:VAL:HG22	1.75	0.69
1:A:1180:LEU:O	1:A:1182:ALA:N	2.26	0.68
1:A:1320:LYS:CD	1:A:1321:GLY:H	2.06	0.68
1:A:222:TYR:HD2	1:A:223:VAL:N	1.90	0.68
1:A:467:ILE:CG2	1:A:486:VAL:HG22	2.23	0.68
2:B:950:LEU:HD22	2:B:1329:TYR:CE1	2.27	0.68
2:D:1446:PHE:CD2	2:D:1448:VAL:HG22	2.27	0.68
3:X:98:LEU:HD22	3:X:101:GLN:OE1	1.93	0.68
1:A:1525:CYS:N	1:A:1528:VAL:HG13	2.07	0.68
1:A:494:ASP:O	1:A:496:ILE:N	2.27	0.68
2:D:1279:ILE:HG22	2:D:1288:ILE:HB	1.74	0.68
2:D:548:LEU:HD22	2:D:793:SER:HB3	1.75	0.68
1:A:255:PHE:HE1	1:A:258:LYS:HB2	1.56	0.68
1:A:25:ILE:H	1:A:655:THR:HG21	1.56	0.68
1:A:61:ASP:O	1:A:62:LYS:HB2	1.92	0.68
1:A:639:GLY:HA2	1:A:648:LEU:HD13	1.74	0.68
2:B:1424:ILE:HG12	2:B:1426:TYR:CE2	2.28	0.68
1:C:1268:ASN:H	1:C:1268:ASN:HD22	1.42	0.68
1:C:1504:GLN:HG3	1:C:1505:CYS:N	2.09	0.68
1:C:705:VAL:N	1:C:739:ARG:HH22	1.92	0.68
1:C:91:GLN:O	1:C:92:LEU:HG	1.92	0.68
2:D:1424:ILE:HD13	2:D:1424:ILE:H	1.59	0.68
2:D:197:TRP:HB2	2:D:214:PHE:CE1	2.28	0.68
2:D:913:LEU:HD23	2:D:914:LYS:N	2.09	0.68
1:A:1366:HIS:ND1	1:A:1366:HIS:N	2.41	0.68
1:A:228:SER:O	1:A:252:ALA:HA	1.93	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:TYR:O	1:A:543:TYR:HD1	1.77	0.68
1:A:690:TYR:CG	1:A:690:TYR:O	2.46	0.68
2:B:114:ARG:O	2:B:115:LEU:HD23	1.93	0.68
1:C:1671:ILE:HA	1:C:1675:GLY:H	1.57	0.68
3:Y:64:VAL:HG11	3:Y:95:LYS:O	1.93	0.68
1:A:1608:ASN:O	1:A:1610:GLU:N	2.27	0.68
1:A:938:SER:O	1:A:940:SER:N	2.27	0.68
2:B:1345:LEU:HA	2:B:1368:CYS:O	1.93	0.68
1:C:1226:ARG:CZ	1:C:1266:TYR:HE1	2.07	0.68
1:C:307:VAL:HG13	1:C:313:TYR:HB2	1.76	0.68
1:A:1386:ILE:HG13	1:A:1387:GLU:H	1.59	0.68
1:A:1673:LEU:O	1:A:1674:ASN:HB2	1.94	0.68
1:A:174:VAL:HG22	1:A:175:GLU:N	2.09	0.68
2:B:464:PHE:HB2	2:B:504:VAL:O	1.94	0.68
1:C:104:LEU:HD12	1:C:105:GLU:H	1.59	0.68
1:C:774:LEU:HD12	1:C:799:ILE:HD11	1.76	0.68
2:D:1313:VAL:HG11	2:D:1323:MET:SD	2.34	0.68
1:A:1068:VAL:HG13	1:A:1069:TRP:N	2.08	0.68
1:A:1127:ILE:H	1:A:1127:ILE:HD12	1.59	0.68
1:A:255:PHE:CE1	1:A:258:LYS:CB	2.77	0.68
1:C:1323:LEU:HD12	1:C:1324:HIS:H	1.59	0.68
1:C:148:LEU:HD23	1:C:152:LEU:HD12	1.76	0.68
1:C:1673:LEU:O	1:C:1674:ASN:HB2	1.94	0.68
1:C:25:ILE:HD13	1:C:41:ILE:HB	1.76	0.68
1:C:641:ASN:HD21	1:C:643:ALA:HB3	1.58	0.68
1:C:742:ILE:HG13	1:C:752:LEU:O	1.94	0.68
1:A:1585:TYR:CD2	1:A:1586:LYS:N	2.61	0.68
1:A:698:CYS:C	1:A:700:TYR:H	1.97	0.68
1:A:77:ASN:HD21	1:A:81:ASN:HB2	1.59	0.68
1:A:829:ILE:HG12	1:A:925:LYS:HG2	1.74	0.68
1:C:1034:PHE:CE2	1:C:1041:GLU:HG2	2.29	0.68
1:C:1179:THR:HG21	1:C:1208:ILE:HD13	1.76	0.68
1:A:101:TYR:CE2	1:C:1305:LYS:HE3	2.28	0.68
3:X:134:THR:HG22	3:X:153:PHE:O	1.94	0.68
3:X:228:ILE:O	3:X:228:ILE:HG22	1.94	0.68
3:Y:86:LEU:HG	3:Y:91:LYS:CB	2.24	0.68
1:A:1123:GLN:NE2	1:A:1123:GLN:HA	2.08	0.68
1:C:1631:PHE:CD2	1:C:1631:PHE:N	2.60	0.68
1:C:382:LEU:HD13	1:C:415:ASP:C	2.14	0.68
1:C:700:TYR:C	1:C:700:TYR:CD2	2.63	0.68
1:C:784:LYS:HG2	1:C:785:GLN:N	2.07	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:28:ILE:HD12	2:D:42:LEU:HD23	1.74	0.68
3:X:166:ASP:OD2	3:X:207:LEU:HG	1.94	0.68
1:A:161:LEU:HD11	1:A:185:PHE:CD1	2.29	0.68
1:A:706:ASN:ND2	1:A:709:GLU:N	2.38	0.68
2:B:218:LYS:HB3	2:B:822:TYR:HD2	1.59	0.68
2:B:133:ASP:HA	2:B:757:TRP:HZ3	1.59	0.68
1:C:1266:TYR:O	1:C:1266:TYR:CD1	2.45	0.68
1:C:222:TYR:C	1:C:222:TYR:HD2	1.97	0.68
1:C:330:ILE:HG22	1:C:337:SER:HB2	1.76	0.68
1:C:373:VAL:HG23	1:C:418:ALA:HB3	1.74	0.68
1:C:938:SER:C	1:C:940:SER:H	1.96	0.68
1:A:1320:LYS:HD2	1:A:1321:GLY:H	1.58	0.67
1:A:1309:LEU:HD13	1:A:1328:MET:HG3	1.75	0.67
1:A:1450:PHE:CZ	1:A:1475:VAL:HB	2.28	0.67
1:A:365:PRO:HD2	1:A:464:TYR:CE2	2.28	0.67
1:A:40:VAL:CG2	1:A:512:PHE:HD1	2.06	0.67
2:B:243:PHE:HD1	2:B:314:LEU:HD23	1.58	0.67
1:C:1341:LEU:HB2	1:C:1342:LEU:CD2	2.24	0.67
1:C:517:LYS:HG2	1:C:518:PHE:H	1.59	0.67
3:Y:150:ILE:HD12	3:Y:150:ILE:O	1.93	0.67
1:A:1358:THR:HB	1:A:1360:HIS:CE1	2.29	0.67
1:A:517:LYS:HG2	1:A:518:PHE:H	1.58	0.67
1:A:612:VAL:HG21	1:A:769:PHE:CZ	2.29	0.67
1:C:1159:CYS:O	1:C:1161:LEU:N	2.27	0.67
1:C:1202:HIS:CD2	1:C:1203:PRO:HD2	2.28	0.67
1:C:471:ASP:OD2	1:C:474:LYS:HD2	1.94	0.67
2:D:28:ILE:HG12	2:D:628:LEU:HD13	1.75	0.67
3:X:179:LEU:HD12	3:X:180:TYR:N	2.10	0.67
1:A:267:ILE:HD11	1:A:299:VAL:HG11	1.74	0.67
1:A:357:VAL:HA	1:A:672:ILE:HG21	1.76	0.67
1:A:470:THR:HG22	2:B:450:THR:CG2	2.22	0.67
2:B:261:ALA:CB	2:B:285:ILE:HD11	2.24	0.67
1:C:576:SER:HB2	1:C:589:SER:CB	2.24	0.67
1:A:1112:GLN:HE21	1:A:1171:ALA:HB2	1.59	0.67
1:A:1423:VAL:HG13	1:A:1496:TYR:CE2	2.30	0.67
1:A:704:CYS:C	1:A:739:ARG:HH22	1.98	0.67
1:A:88:GLN:O	1:A:90:LYS:HD3	1.94	0.67
1:C:1142:LEU:HD11	1:C:1179:THR:HA	1.77	0.67
3:X:80:GLN:HG3	3:X:114:GLY:C	2.15	0.67
3:Y:166:ASP:CG	3:Y:207:LEU:HD23	2.14	0.67
1:A:1034:PHE:CE2	1:A:1041:GLU:HG2	2.29	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1244:THR:HG22	1:A:1246:ARG:N	2.08	0.67
1:A:1266:TYR:CD1	1:A:1266:TYR:O	2.48	0.67
1:A:207:GLU:O	1:A:209:PHE:N	2.28	0.67
1:A:640:LEU:O	1:A:640:LEU:HD12	1.93	0.67
2:B:149:SER:O	2:B:794:PHE:HE1	1.78	0.67
1:C:596:MET:H	1:C:782:ARG:NH1	1.87	0.67
2:D:1539:ILE:HD12	2:D:1539:ILE:H	1.59	0.67
2:D:556:ILE:H	2:D:556:ILE:HD12	1.58	0.67
1:A:1019:PHE:CD2	1:A:1019:PHE:C	2.67	0.67
1:A:104:LEU:HD12	1:A:105:GLU:H	1.59	0.67
1:A:1163:LYS:O	1:A:1166:THR:HG22	1.94	0.67
1:A:1341:LEU:H	1:A:1341:LEU:HD22	1.60	0.67
1:A:222:TYR:C	1:A:222:TYR:HD2	1.98	0.67
1:A:586:GLN:O	1:A:586:GLN:HG3	1.95	0.67
2:B:1480:LEU:HD12	2:B:1481:LEU:N	2.10	0.67
2:B:1602:THR:C	2:B:1604:ASN:H	1.97	0.67
2:B:262:PHE:HE1	2:B:282:ARG:HG3	1.60	0.67
2:B:299:PHE:HE1	2:B:303:PHE:HD2	1.43	0.67
1:C:1049:LEU:HD11	1:C:1089:VAL:CG1	2.24	0.67
1:C:1493:PHE:CD1	1:C:1493:PHE:C	2.67	0.67
1:C:765:ILE:HD13	1:C:767:SER:O	1.94	0.67
2:D:531:ILE:HD11	2:D:634:LEU:HD23	1.76	0.67
1:A:109:LYS:HD3	1:A:110:HIS:CE1	2.30	0.67
1:A:1142:LEU:HD11	1:A:1179:THR:HA	1.77	0.67
1:A:190:ILE:HG22	1:A:191:PRO:N	2.09	0.67
1:A:742:ILE:HG13	1:A:752:LEU:O	1.94	0.67
1:A:596:MET:N	1:A:782:ARG:HD3	2.10	0.67
1:A:865:ILE:O	1:A:866:CYS:O	2.11	0.67
1:C:180:ILE:HB	1:C:599:TRP:CE3	2.30	0.67
1:C:690:TYR:C	1:C:692:HIS:H	1.98	0.67
2:D:1444:LYS:CE	2:D:1447:GLU:HA	2.25	0.67
3:Y:47:HIS:CE1	3:Y:181:LYS:HE2	2.30	0.67
2:B:1505:ARG:NH1	2:B:1505:ARG:HG3	1.93	0.67
2:B:1562:GLN:HE22	2:B:1596:LYS:HZ2	1.42	0.67
1:C:1077:TRP:NE1	1:C:1147:PHE:CE1	2.62	0.67
1:C:1535:MET:H	1:C:1608:ASN:HB3	1.60	0.67
1:C:474:LYS:H	1:C:474:LYS:HD3	1.60	0.67
3:Y:41:HIS:O	3:Y:42:ASP:HB2	1.95	0.67
2:B:30:PRO:HG3	2:B:489:ILE:HG13	1.77	0.67
2:B:783:SER:HB2	2:B:787:TRP:HZ2	1.60	0.67
2:B:824:VAL:HG22	2:B:825:VAL:H	1.60	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1341:LEU:H	1:C:1341:LEU:HD22	1.60	0.67
1:C:1504:GLN:HG3	1:C:1505:CYS:CA	2.24	0.67
1:C:473:HIS:O	1:C:473:HIS:CD2	2.47	0.67
1:C:493:ILE:HG23	1:C:495:LYS:N	2.10	0.67
2:D:1594:LYS:HA	2:D:1594:LYS:CE	2.15	0.67
2:D:603:GLU:O	2:D:605:SER:N	2.27	0.67
1:A:459:SER:OG	1:A:461:SER:HB3	1.94	0.67
1:A:796:THR:HG23	1:A:818:LYS:CB	2.25	0.67
1:C:944:LEU:HD23	1:C:944:LEU:N	2.10	0.67
2:D:144:LEU:H	2:D:144:LEU:HD23	1.59	0.67
2:D:243:PHE:HD1	2:D:314:LEU:HD23	1.58	0.67
2:D:829:GLN:HG3	2:D:1480:LEU:CD1	2.07	0.67
3:X:86:LEU:HG	3:X:91:LYS:CB	2.23	0.67
1:A:1219:LYS:CE	1:A:1239:VAL:HG21	2.25	0.66
1:A:530:VAL:HG23	1:A:534:MET:HE2	1.75	0.66
1:A:947:ARG:O	1:A:949:ILE:HG12	1.95	0.66
2:B:1382:ILE:HB	2:B:1425:ILE:HB	1.77	0.66
2:B:196:THR:HG23	2:B:215:ASP:OD1	1.95	0.66
2:B:422:ARG:H	2:B:422:ARG:CD	2.08	0.66
1:C:1323:LEU:HD12	1:C:1324:HIS:N	2.10	0.66
1:C:222:TYR:C	1:C:222:TYR:CD2	2.68	0.66
1:C:583:SER:O	1:C:586:GLN:HG2	1.94	0.66
1:C:698:CYS:C	1:C:700:TYR:H	1.97	0.66
2:D:481:TYR:HB2	2:D:520:PHE:HE1	1.58	0.66
3:Y:128:LYS:HB2	3:Y:158:GLU:HB2	1.77	0.66
1:A:1643:THR:HG22	1:A:1644:TRP:N	2.09	0.66
1:A:474:LYS:H	1:A:474:LYS:HD3	1.59	0.66
2:B:1444:LYS:CE	2:B:1447:GLU:HA	2.25	0.66
2:B:1450:PHE:CD1	2:B:1451:ILE:N	2.64	0.66
2:B:599:TRP:HA	2:B:599:TRP:CE3	2.29	0.66
1:C:1226:ARG:HB3	1:C:1269:PRO:HB2	1.75	0.66
3:X:166:ASP:CG	3:X:207:LEU:HD23	2.14	0.66
1:A:473:HIS:CD2	1:A:473:HIS:O	2.49	0.66
1:A:115:LYS:CB	1:A:654:LEU:HD21	2.25	0.66
1:C:1113:LEU:CD2	1:C:1114:ASP:H	2.07	0.66
1:C:1643:THR:HG22	1:C:1644:TRP:N	2.11	0.66
1:C:480:GLU:O	1:C:530:VAL:HG12	1.95	0.66
2:D:131:GLN:OE1	2:D:146:ARG:NH1	2.28	0.66
1:C:525:SER:H	2:D:401:ASN:HD21	1.40	0.66
1:A:25:ILE:HD13	1:A:41:ILE:HB	1.77	0.66
2:B:1606:TRP:C	2:B:1606:TRP:CD1	2.69	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1076:THR:CG2	1:C:1120:GLU:HA	2.24	0.66
1:C:1309:LEU:HD13	1:C:1328:MET:HG3	1.77	0.66
1:C:640:LEU:HD12	1:C:640:LEU:O	1.95	0.66
2:D:1602:THR:C	2:D:1604:ASN:H	1.99	0.66
3:Y:205:ASP:O	3:Y:206:LYS:C	2.33	0.66
1:C:1219:LYS:HD3	1:C:1239:VAL:HG21	1.77	0.66
1:C:467:ILE:CG2	1:C:486:VAL:HG22	2.25	0.66
1:C:706:ASN:ND2	1:C:709:GLU:N	2.38	0.66
2:D:241:GLU:O	2:D:296:ARG:HD3	1.95	0.66
1:A:1226:ARG:HB3	1:A:1269:PRO:HB2	1.78	0.66
1:A:307:VAL:HG13	1:A:313:TYR:HB2	1.78	0.66
1:A:471:ASP:OD2	1:A:474:LYS:HD2	1.96	0.66
1:C:685:GLU:OE1	1:C:685:GLU:HA	1.94	0.66
2:D:1450:PHE:CD1	2:D:1451:ILE:N	2.64	0.66
3:Y:228:ILE:HG22	3:Y:228:ILE:O	1.93	0.66
1:A:238:ILE:HB	1:A:347:TYR:CD1	2.31	0.66
1:A:484:ILE:CD1	1:A:540:LEU:HD21	2.26	0.66
1:A:632:LEU:N	1:A:632:LEU:HD23	2.11	0.66
1:A:690:TYR:CD2	1:A:690:TYR:O	2.49	0.66
1:A:702:GLY:CA	1:A:728:PHE:CE1	2.78	0.66
2:B:961:THR:CG2	2:B:1327:THR:HG23	2.25	0.66
2:B:147:VAL:HG12	2:B:183:PHE:HE1	1.60	0.66
2:B:476:ILE:HD11	2:B:524:TYR:CG	2.30	0.66
1:C:127:PHE:HD2	1:C:623:VAL:HG22	1.60	0.66
1:C:1024:TYR:HA	1:C:1302:LEU:CD2	2.26	0.66
1:C:1352:PHE:CD2	1:C:1352:PHE:N	2.62	0.66
1:C:1562:LYS:CD	1:C:1664:LEU:HD21	2.12	0.66
1:C:190:ILE:HG22	1:C:191:PRO:N	2.11	0.66
1:C:234:GLU:HG3	1:C:235:TYR:CE2	2.29	0.66
1:C:931:PRO:HB2	1:C:1366:HIS:CD2	2.30	0.66
2:D:1445:HIS:CG	2:D:1446:PHE:H	2.14	0.66
2:D:964:ILE:HG13	2:D:1302:THR:HG23	1.77	0.66
1:A:869:GLU:C	1:A:871:PRO:HD3	2.15	0.66
2:B:1417:MET:HG2	2:B:1443:LEU:HD23	1.76	0.66
1:C:228:SER:O	1:C:252:ALA:HA	1.96	0.66
1:C:255:PHE:HE1	1:C:258:LYS:HB2	1.61	0.66
1:C:639:GLY:H	1:C:645:VAL:HA	1.60	0.66
1:C:670:LYS:HD2	1:C:671:GLU:HG2	1.78	0.66
1:C:935:LYS:HD3	1:C:1373:GLU:OE2	1.94	0.66
2:D:961:THR:CG2	2:D:1327:THR:HG23	2.25	0.66
3:Y:98:LEU:HD22	3:Y:101:GLN:OE1	1.96	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1566:THR:O	1:A:1613:LYS:HE3	1.95	0.66
1:A:1618:LEU:HD22	1:A:1619:ILE:H	1.60	0.66
1:A:371:ILE:CG2	1:A:420:PHE:HB2	2.23	0.66
1:A:968:VAL:HG12	1:A:1368:THR:HG22	1.78	0.66
2:B:131:GLN:OE1	2:B:146:ARG:NH1	2.29	0.66
2:B:523:TYR:CD1	2:B:523:TYR:C	2.68	0.66
1:C:1127:ILE:HD11	1:C:1143:TYR:CD2	2.31	0.66
1:C:1213:LYS:HE2	1:C:1266:TYR:CD2	2.31	0.66
1:C:436:LYS:HB2	1:C:449:ARG:HG2	1.77	0.66
2:D:1345:LEU:HA	2:D:1368:CYS:O	1.96	0.66
2:D:236:TYR:CZ	2:D:424:ARG:HD2	2.31	0.66
2:D:69:PHE:CG	2:D:87:ILE:HG22	2.31	0.66
1:A:1202:HIS:CD2	1:A:1203:PRO:HD2	2.31	0.66
1:C:1034:PHE:CD2	1:C:1041:GLU:HG2	2.30	0.66
1:C:981:GLY:CA	1:C:1333:PHE:HB2	2.25	0.66
1:C:1379:LEU:HD11	1:C:1505:CYS:O	1.95	0.66
1:C:671:GLU:O	1:C:672:ILE:HB	1.96	0.66
2:D:230:PRO:HG3	2:D:333:GLN:HG2	1.77	0.66
2:D:57:PHE:HD1	2:D:59:HIS:HE2	1.44	0.66
1:A:62:LYS:HE2	1:A:103:TYR:CE2	2.31	0.65
1:A:955:ARG:NH1	1:A:1352:PHE:HA	2.11	0.65
2:B:194:LEU:HD12	2:B:217:ARG:HA	1.78	0.65
1:A:1163:LYS:HZ1	1:C:1109:GLU:CD	1.99	0.65
1:C:495:LYS:HE2	1:C:495:LYS:HA	1.76	0.65
1:C:705:VAL:HA	1:C:739:ARG:NH1	2.11	0.65
2:D:563:MET:HB3	2:D:778:PHE:CE2	2.31	0.65
1:A:436:LYS:HB2	1:A:449:ARG:HG2	1.78	0.65
1:A:489:LYS:HG3	1:A:490:SER:H	1.60	0.65
1:A:633:GLY:O	1:A:634:CYS:HB2	1.96	0.65
1:A:641:ASN:O	1:A:643:ALA:N	2.29	0.65
1:A:25:ILE:HB	1:A:654:LEU:HB2	1.78	0.65
1:A:87:ILE:HD13	1:A:87:ILE:H	1.61	0.65
1:A:895:LEU:HD12	1:A:896:VAL:N	2.11	0.65
1:C:704:CYS:C	1:C:739:ARG:HH22	2.00	0.65
1:C:511:HIS:CE1	3:Y:149:SER:HG	2.14	0.65
1:A:935:LYS:HD3	1:A:1373:GLU:OE2	1.95	0.65
1:A:884:VAL:CG1	1:A:886:GLN:HG2	2.26	0.65
1:C:123:ASN:HB3	1:C:209:PHE:HD1	1.61	0.65
1:C:505:SER:OG	1:C:506:LYS:HD3	1.97	0.65
1:C:934:VAL:CG2	1:C:1366:HIS:CD2	2.79	0.65
1:A:1585:TYR:CG	1:A:1586:LYS:N	2.64	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1491:ARG:HG3	2:B:1492:CYS:H	1.62	0.65
1:C:1145:THR:O	1:C:1149:VAL:HG23	1.97	0.65
1:C:443:PRO:HD2	1:C:446:ASN:HB2	1.78	0.65
1:C:884:VAL:O	1:C:885:ARG:CB	2.42	0.65
2:D:128:LEU:O	2:D:129:PHE:CD1	2.49	0.65
2:D:481:TYR:CE2	2:D:493:GLY:CA	2.79	0.65
3:X:47:HIS:HE1	3:X:181:LYS:HE2	1.62	0.65
2:B:69:PHE:CG	2:B:87:ILE:HG22	2.32	0.65
1:A:875:HIS:HB3	2:B:901:GLN:NE2	2.11	0.65
1:C:1667:PHE:O	1:C:1671:ILE:HG22	1.97	0.65
1:C:535:VAL:HG23	1:C:536:PRO:CD	2.15	0.65
2:D:133:ASP:HA	2:D:757:TRP:HZ3	1.60	0.65
3:X:41:HIS:O	3:X:42:ASP:HB2	1.96	0.65
3:Y:207:LEU:HD12	3:Y:207:LEU:C	2.14	0.65
1:A:1034:PHE:CD2	1:A:1041:GLU:HG2	2.32	0.65
1:A:505:SER:OG	1:A:506:LYS:HD3	1.97	0.65
1:A:884:VAL:O	1:A:885:ARG:CB	2.41	0.65
1:C:1123:GLN:NE2	1:C:1123:GLN:HA	2.11	0.65
1:C:1180:LEU:O	1:C:1182:ALA:N	2.29	0.65
1:C:1564:SER:HB2	1:C:1616:GLN:HG3	1.78	0.65
1:C:504:LEU:HD12	1:C:509:ILE:HG23	1.77	0.65
1:C:40:VAL:HG21	1:C:512:PHE:HD1	1.62	0.65
1:C:514:THR:O	1:C:515:ARG:HD3	1.95	0.65
2:D:282:ARG:C	2:D:283:ILE:HD12	2.17	0.65
2:D:239:GLY:H	2:D:296:ARG:NH2	1.95	0.65
2:D:421:PRO:HB2	2:D:423:GLU:OE2	1.96	0.65
2:D:422:ARG:CD	2:D:422:ARG:H	2.08	0.65
2:D:127:PHE:CE2	2:D:602:ILE:HG23	2.32	0.65
3:Y:179:LEU:HD12	3:Y:180:TYR:N	2.11	0.65
3:Y:43:ILE:HG23	3:Y:44:ARG:H	1.60	0.65
1:A:1381:ILE:HG12	1:A:1382:ASP:N	2.12	0.65
1:A:222:TYR:C	1:A:222:TYR:CD2	2.70	0.65
1:A:60:PRO:CD	1:A:61:ASP:N	2.56	0.65
1:A:705:VAL:N	1:A:739:ARG:HH22	1.94	0.65
2:B:783:SER:HB2	2:B:787:TRP:CZ2	2.32	0.65
1:C:1076:THR:HG21	1:C:1120:GLU:HA	1.79	0.65
1:C:1075:SER:HB2	1:C:1120:GLU:OE1	1.96	0.65
1:C:24:VAL:HG11	1:C:543:TYR:CE2	2.31	0.65
1:C:936:ARG:NH2	1:C:1284:PHE:CE1	2.64	0.65
1:A:131:ASP:O	1:A:132:LYS:HG2	1.97	0.65
1:A:865:ILE:O	1:A:866:CYS:C	2.35	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:LEU:H	2:B:144:LEU:HD23	1.62	0.65
2:B:237:ILE:HD11	2:B:309:LEU:CB	2.24	0.65
2:B:460:LEU:O	2:B:460:LEU:HD23	1.97	0.65
2:B:23:ALA:HB3	2:B:528:ASN:HD22	1.61	0.65
1:C:1231:ASN:HB2	1:C:1235:LYS:HG3	1.77	0.65
1:C:863:GLU:H	1:C:863:GLU:CD	2.00	0.65
2:D:557:GLN:HE21	2:D:563:MET:CE	2.10	0.65
3:Y:53:GLU:HB3	3:Y:55:PHE:CE2	2.32	0.65
2:B:1371:TYR:O	2:B:1432:HIS:HA	1.97	0.65
2:B:1445:HIS:CG	2:B:1446:PHE:H	2.15	0.65
2:B:887:LEU:CD2	2:B:1490:CYS:HB3	2.27	0.65
2:B:262:PHE:CE1	2:B:282:ARG:HG3	2.30	0.65
2:B:825:VAL:N	2:B:828:GLU:OE1	2.29	0.65
1:C:1429:PRO:HB2	1:C:1432:ILE:HG13	1.78	0.65
1:C:492:TYR:HD2	1:C:493:ILE:H	1.44	0.65
1:C:690:TYR:CD2	1:C:690:TYR:O	2.49	0.65
2:D:1515:ALA:HB1	2:D:1523:VAL:HG21	1.79	0.65
2:D:167:THR:HG23	2:D:171:ILE:H	1.61	0.65
1:A:1259:LEU:HD11	1:A:1300:TYR:HB2	1.78	0.65
1:A:931:PRO:HB2	1:A:1366:HIS:CD2	2.32	0.65
1:A:690:TYR:C	1:A:692:HIS:H	2.00	0.65
2:B:481:TYR:HB2	2:B:520:PHE:HE1	1.59	0.65
2:B:603:GLU:O	2:B:605:SER:N	2.28	0.65
1:C:1304:VAL:CG1	1:C:1305:LYS:N	2.60	0.65
1:C:24:VAL:CG1	1:C:24:VAL:O	2.45	0.65
1:C:884:VAL:CG1	1:C:886:GLN:HG2	2.27	0.65
2:D:1387:LEU:HB2	2:D:1390:PHE:CD2	2.32	0.65
3:X:50:TYR:HE2	3:X:170:ARG:NH1	1.94	0.65
1:A:1244:THR:H	1:A:1247:MET:HE3	1.62	0.64
1:A:307:VAL:CG1	1:A:313:TYR:HB2	2.27	0.64
1:A:492:TYR:HD2	1:A:493:ILE:H	1.45	0.64
1:A:705:VAL:HA	1:A:739:ARG:NH1	2.12	0.64
2:B:364:VAL:HG21	2:B:379:VAL:HG21	1.79	0.64
2:D:299:PHE:HE1	2:D:303:PHE:HD2	1.45	0.64
2:D:433:ILE:HG22	2:D:434:ALA:O	1.96	0.64
1:A:1352:PHE:N	1:A:1352:PHE:CD2	2.62	0.64
1:A:554:LEU:H	1:A:658:ASN:HD22	1.43	0.64
1:A:423:ASN:HB3	2:B:501:GLN:NE2	2.13	0.64
2:B:838:ASN:OD1	2:B:840:VAL:HG23	1.97	0.64
2:B:814:PHE:HZ	2:B:846:VAL:HG21	1.62	0.64
2:B:913:LEU:HD23	2:B:914:LYS:N	2.12	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1244:THR:HG22	1:C:1246:ARG:N	2.13	0.64
3:X:70:SER:CB	3:X:91:LYS:HE3	2.27	0.64
1:A:1627:ILE:HG13	1:A:1627:ILE:O	1.98	0.64
1:A:494:ASP:OD1	1:A:495:LYS:HE2	1.97	0.64
2:B:524:TYR:O	2:B:524:TYR:HD1	1.79	0.64
1:C:1427:SER:HB3	1:C:1492:THR:HG23	1.79	0.64
1:C:207:GLU:O	1:C:209:PHE:N	2.29	0.64
2:D:1506:ILE:CD1	2:D:1628:PHE:HE1	2.09	0.64
3:X:170:ARG:O	3:X:174:VAL:HG23	1.97	0.64
3:X:179:LEU:HD12	3:X:180:TYR:H	1.62	0.64
1:A:656:ASN:HB3	1:A:659:ALA:H	1.63	0.64
1:A:837:GLU:HG2	1:A:1488:LEU:HA	1.78	0.64
1:A:947:ARG:O	1:A:949:ILE:N	2.30	0.64
1:A:917:TRP:HB3	2:B:558:MET:SD	2.38	0.64
1:C:1086:LEU:HD12	1:C:1095:GLN:HG3	1.79	0.64
1:C:119:ILE:O	1:C:119:ILE:HD12	1.97	0.64
1:C:1423:VAL:CG1	1:C:1496:TYR:CE2	2.80	0.64
1:C:1566:THR:O	1:C:1613:LYS:HE3	1.98	0.64
1:C:24:VAL:HG11	1:C:543:TYR:OH	1.97	0.64
1:C:829:ILE:HG12	1:C:925:LYS:HG2	1.80	0.64
2:D:26:THR:OG1	2:D:44:GLU:HB2	1.98	0.64
1:C:429:THR:HA	1:C:456:ALA:HB2	1.80	0.64
3:X:205:ASP:O	3:X:206:LYS:C	2.33	0.64
1:A:1077:TRP:NE1	1:A:1147:PHE:CE1	2.66	0.64
1:A:1504:GLN:HG3	1:A:1505:CYS:N	2.11	0.64
1:A:820:PHE:O	1:A:821:LYS:HG3	1.98	0.64
2:B:1623:LYS:HA	2:B:1623:LYS:HZ3	1.63	0.64
1:C:1548:ARG:HD3	1:C:1548:ARG:H	1.63	0.64
1:C:255:PHE:CE1	1:C:258:LYS:CB	2.80	0.64
2:D:1446:PHE:HB3	2:D:1448:VAL:HG22	1.79	0.64
2:D:1547:VAL:HG23	2:D:1557:ARG:NH1	2.12	0.64
2:D:523:TYR:C	2:D:523:TYR:CD1	2.70	0.64
3:X:170:ARG:HD3	3:X:203:LEU:CD2	2.27	0.64
3:Y:64:VAL:HG23	3:Y:71:ASN:OD1	1.97	0.64
1:A:583:SER:O	1:A:586:GLN:HG2	1.96	0.64
2:B:421:PRO:HB2	2:B:423:GLU:OE2	1.98	0.64
1:C:161:LEU:H	1:C:161:LEU:HD12	1.62	0.64
1:C:60:PRO:HD2	1:C:61:ASP:N	2.09	0.64
1:C:362:PHE:CE1	1:C:640:LEU:HB2	2.33	0.64
2:D:149:SER:O	2:D:794:PHE:HE1	1.80	0.64
1:A:1024:TYR:HA	1:A:1302:LEU:CD2	2.28	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1365:VAL:CG2	1:A:1366:HIS:H	2.08	0.64
1:A:24:VAL:CG1	1:A:24:VAL:O	2.45	0.64
1:A:535:VAL:HG23	1:A:536:PRO:CD	2.16	0.64
2:B:1615:GLU:HB3	2:B:1621:PHE:HD1	1.63	0.64
1:C:260:VAL:HG12	1:C:261:THR:N	2.12	0.64
2:D:136:ILE:HA	2:D:215:ASP:O	1.97	0.64
2:D:1505:ARG:CZ	2:D:1623:LYS:NZ	2.61	0.64
2:D:130:ILE:HD13	2:D:199:ILE:HG22	1.80	0.64
2:D:464:PHE:HB2	2:D:504:VAL:O	1.98	0.64
2:D:599:TRP:HA	2:D:599:TRP:CE3	2.31	0.64
1:A:1232:LEU:CD1	1:A:1233:GLN:HE21	2.11	0.64
1:A:1323:LEU:HD12	1:A:1324:HIS:H	1.63	0.64
1:A:480:GLU:O	1:A:530:VAL:HG12	1.98	0.64
1:A:24:VAL:CG2	1:A:554:LEU:HD11	2.27	0.64
1:C:1525:CYS:N	1:C:1528:VAL:HG13	2.13	0.64
1:C:436:LYS:HA	1:C:448:ALA:O	1.97	0.64
1:C:883:CYS:O	1:C:884:VAL:O	2.16	0.64
1:A:1304:VAL:CG1	1:A:1305:LYS:N	2.61	0.64
1:A:144:ARG:HD2	1:A:146:TYR:HE1	1.62	0.64
1:C:1402:ILE:HG13	1:C:1479:ILE:CD1	2.28	0.64
1:C:632:LEU:HD23	1:C:632:LEU:N	2.13	0.64
1:C:612:VAL:HG21	1:C:769:PHE:CZ	2.32	0.64
2:D:218:LYS:HB3	2:D:822:TYR:HD2	1.59	0.64
2:D:964:ILE:CG2	2:D:964:ILE:O	2.46	0.64
3:X:128:LYS:HB2	3:X:158:GLU:HB2	1.78	0.64
3:X:194:LYS:NZ	3:X:197:ASN:HB2	2.10	0.64
3:X:73:VAL:HG22	3:X:84:LEU:HB3	1.80	0.64
3:Y:70:SER:CB	3:Y:91:LYS:HE3	2.28	0.64
2:B:1446:PHE:CD2	2:B:1448:VAL:HG22	2.33	0.63
2:B:534:ASP:HA	2:B:620:VAL:HG21	1.80	0.63
1:C:693:SER:C	1:C:695:VAL:H	2.01	0.63
2:D:1417:MET:HG2	2:D:1443:LEU:HD23	1.80	0.63
2:D:1591:LEU:HD23	2:D:1591:LEU:C	2.19	0.63
2:D:543:THR:OG1	2:D:544:CYS:N	2.30	0.63
1:A:1101:CYS:HB3	1:C:1161:LEU:HD11	1.81	0.63
1:A:653:PHE:CD1	1:A:660:ASP:HB3	2.33	0.63
2:D:355:LYS:O	2:D:358:MET:HB3	1.97	0.63
1:C:483:ASN:ND2	2:D:399:ILE:HB	2.14	0.63
1:A:671:GLU:O	1:A:672:ILE:HB	1.97	0.63
2:B:221:LEU:CD1	2:B:753:LYS:HG2	2.25	0.63
1:C:1286:SER:HB2	1:C:1499:HIS:HA	1.80	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:GLN:HG2	1:C:403:ASP:OD1	1.99	0.63
1:C:459:SER:OG	1:C:461:SER:HB3	1.97	0.63
1:C:633:GLY:O	1:C:634:CYS:HB2	1.98	0.63
1:C:982:LEU:C	1:C:984:VAL:H	2.01	0.63
2:D:1371:TYR:O	2:D:1432:HIS:HA	1.97	0.63
2:D:58:VAL:HG12	2:D:104:VAL:HG22	1.80	0.63
3:X:50:TYR:CE2	3:X:170:ARG:CD	2.80	0.63
3:Y:134:THR:HG22	3:Y:153:PHE:O	1.97	0.63
3:Y:179:LEU:HD12	3:Y:180:TYR:H	1.62	0.63
1:A:1219:LYS:HD3	1:A:1239:VAL:HG21	1.80	0.63
1:A:1459:HIS:CD2	1:A:1459:HIS:N	2.66	0.63
1:A:91:GLN:O	1:A:92:LEU:HG	1.96	0.63
2:B:58:VAL:HG12	2:B:104:VAL:HG22	1.80	0.63
2:B:829:GLN:HG2	2:B:885:VAL:CG1	2.28	0.63
2:D:194:LEU:HD12	2:D:217:ARG:HA	1.80	0.63
1:C:423:ASN:CG	2:D:504:VAL:HG22	2.18	0.63
3:X:207:LEU:HD12	3:X:207:LEU:C	2.14	0.63
3:X:43:ILE:HG23	3:X:44:ARG:H	1.62	0.63
1:A:1286:SER:HB2	1:A:1499:HIS:HA	1.80	0.63
1:A:153:LYS:HB3	1:A:154:PRO:HD2	1.80	0.63
1:A:1618:LEU:HD22	1:A:1619:ILE:N	2.12	0.63
1:A:330:ILE:HG22	1:A:337:SER:HB2	1.79	0.63
1:A:443:PRO:HD2	1:A:446:ASN:HB2	1.80	0.63
1:A:531:THR:O	1:A:534:MET:HG3	1.98	0.63
1:A:476:LEU:HB3	1:A:563:ILE:HA	1.80	0.63
1:A:60:PRO:HD2	1:A:61:ASP:N	2.08	0.63
2:B:1539:ILE:H	2:B:1539:ILE:HD12	1.62	0.63
2:B:127:PHE:HE2	2:B:602:ILE:HG23	1.62	0.63
1:C:238:ILE:HB	1:C:347:TYR:HD1	1.62	0.63
1:C:473:HIS:ND1	2:D:455:LYS:HE3	2.13	0.63
1:C:512:PHE:CD2	1:C:512:PHE:O	2.51	0.63
1:C:947:ARG:O	1:C:949:ILE:N	2.31	0.63
1:A:199:TRP:HB2	1:A:217:PHE:CE1	2.34	0.63
1:A:977:LEU:HD22	1:A:978:SER:H	1.63	0.63
2:B:965:ILE:CG1	2:B:1301:ARG:HB2	2.25	0.63
1:C:104:LEU:HD12	1:C:105:GLU:N	2.13	0.63
1:C:830:PRO:CG	1:C:1483:PHE:CZ	2.74	0.63
1:C:238:ILE:HD12	1:C:347:TYR:CE1	2.33	0.63
1:C:512:PHE:HE2	3:Y:148:ALA:HB3	1.63	0.63
1:A:1236:ASP:O	1:A:1238:SER:N	2.29	0.63
1:A:1013:MET:CE	1:A:1287:THR:HB	2.28	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:ALA:HB3	2:B:285:ILE:HD11	1.80	0.63
1:C:1459:HIS:CD2	1:C:1459:HIS:N	2.66	0.63
1:C:1629:TYR:CE1	1:C:1631:PHE:CD1	2.86	0.63
1:C:614:ARG:HD2	1:C:615:GLY:H	1.63	0.63
1:C:702:GLY:CA	1:C:728:PHE:CE1	2.77	0.63
1:C:949:ILE:HG22	1:C:950:TYR:CE1	2.33	0.63
2:D:965:ILE:CG1	2:D:1301:ARG:HB2	2.26	0.63
2:D:1447:GLU:HG3	2:D:1447:GLU:O	1.98	0.63
2:D:963:ILE:HD11	2:D:1311:ILE:HG21	1.81	0.63
2:B:1591:LEU:C	2:B:1591:LEU:HD23	2.19	0.63
1:C:653:PHE:CD1	1:C:660:ASP:HB3	2.33	0.63
1:C:24:VAL:CA	1:C:655:THR:HG21	2.28	0.63
2:D:142:PRO:HB3	2:D:187:ASN:ND2	2.14	0.63
2:D:1431:SER:HB3	2:D:1433:SER:H	1.64	0.63
2:D:296:ARG:HG3	2:D:296:ARG:HH11	1.63	0.63
1:A:938:SER:C	1:A:940:SER:H	2.01	0.63
2:B:1500:LEU:HD11	2:B:1608:GLU:HA	1.80	0.63
2:B:1500:LEU:HD13	2:B:1607:ILE:O	1.99	0.63
2:B:620:VAL:HG12	2:B:621:PHE:CD2	2.32	0.63
1:C:1229:LYS:NZ	1:C:1240:PRO:HD2	2.14	0.63
1:C:195:ARG:HD3	1:C:1058:SER:HA	1.80	0.63
1:C:491:PRO:C	1:C:493:ILE:N	2.49	0.63
1:C:543:TYR:HD1	1:C:543:TYR:O	1.82	0.63
1:C:824:PHE:CE2	1:C:846:TYR:HB2	2.34	0.63
1:C:88:GLN:O	1:C:90:LYS:HD3	1.99	0.63
1:A:1152:ILE:HG21	1:A:1168:LEU:HD21	1.81	0.62
1:A:152:LEU:HD11	1:A:627:LEU:HD11	1.81	0.62
1:A:1626:GLN:HG2	1:A:1626:GLN:O	1.98	0.62
1:A:502:LEU:HB2	1:A:541:LEU:HD23	1.79	0.62
1:C:1641:SER:C	1:C:1643:THR:H	2.03	0.62
1:C:656:ASN:HB3	1:C:659:ALA:H	1.64	0.62
1:C:752:LEU:HG	1:C:752:LEU:O	1.99	0.62
2:D:364:VAL:HG21	2:D:379:VAL:HG21	1.81	0.62
3:Y:170:ARG:O	3:Y:174:VAL:HG23	1.98	0.62
1:A:614:ARG:HD2	1:A:615:GLY:H	1.63	0.62
1:A:967:LEU:HD12	1:A:968:VAL:N	2.14	0.62
2:B:1607:ILE:N	2:B:1607:ILE:HD12	2.14	0.62
1:C:101:TYR:CE1	1:C:116:ARG:NH2	2.67	0.62
1:A:92:LEU:HD12	1:C:1029:ASN:HD21	1.64	0.62
1:C:1493:PHE:HD1	1:C:1493:PHE:C	2.00	0.62
2:D:1505:ARG:NE	2:D:1623:LYS:NZ	2.47	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:950:LEU:HD22	2:D:1329:TYR:CE1	2.33	0.62
1:A:123:ASN:O	1:A:211:THR:HG21	1.98	0.62
1:A:1556:GLU:CB	1:A:1622:LYS:HE2	2.24	0.62
2:B:57:PHE:HD1	2:B:59:HIS:HE2	1.47	0.62
2:B:964:ILE:HG13	2:B:1302:THR:HG23	1.82	0.62
1:C:1527:CYS:O	1:C:1528:VAL:C	2.36	0.62
1:C:1622:LYS:HD2	1:C:1642:LEU:HB3	1.81	0.62
1:C:59:TYR:CD1	1:C:60:PRO:HD3	2.34	0.62
2:D:30:PRO:HG3	2:D:489:ILE:HG13	1.81	0.62
1:A:506:LYS:HE2	1:A:533:ASN:O	1.98	0.62
1:A:543:TYR:CD1	1:A:543:TYR:O	2.51	0.62
1:A:551:THR:O	1:A:552:ALA:CB	2.47	0.62
2:B:1387:LEU:HB2	2:B:1390:PHE:CD2	2.34	0.62
2:B:1623:LYS:HD2	2:B:1623:LYS:N	2.11	0.62
2:B:265:PHE:CE2	2:B:294:LEU:HB2	2.34	0.62
2:B:355:LYS:N	2:B:355:LYS:HD2	2.15	0.62
2:B:76:ASN:HB2	2:B:77:PRO:HD2	1.82	0.62
1:C:1219:LYS:HE2	1:C:1239:VAL:HG21	1.81	0.62
1:C:1627:ILE:O	1:C:1627:ILE:CG1	2.46	0.62
1:C:267:ILE:HD11	1:C:299:VAL:HG11	1.81	0.62
1:C:270:GLY:HA3	1:C:282:MET:HG2	1.80	0.62
1:C:506:LYS:HE2	1:C:533:ASN:O	1.99	0.62
1:C:834:VAL:O	1:C:837:GLU:HB2	2.00	0.62
2:D:294:LEU:HD12	2:D:295:LYS:N	2.14	0.62
2:D:384:PHE:O	2:D:385:HIS:C	2.38	0.62
2:D:524:TYR:HD1	2:D:524:TYR:O	1.83	0.62
2:D:850:LEU:HD12	2:D:851:LEU:N	2.14	0.62
1:A:938:SER:OG	1:A:1284:PHE:CZ	2.53	0.62
1:A:1423:VAL:CG1	1:A:1496:TYR:CE2	2.81	0.62
1:A:20:GLU:O	1:A:20:GLU:CD	2.37	0.62
1:A:682:LYS:HZ3	1:A:686:ILE:HD11	1.64	0.62
1:A:837:GLU:O	1:A:901:LEU:HD12	2.00	0.62
2:B:1547:VAL:HG23	2:B:1557:ARG:NH1	2.14	0.62
1:C:1386:ILE:HG13	1:C:1387:GLU:H	1.63	0.62
1:C:199:TRP:HB2	1:C:217:PHE:CE1	2.34	0.62
1:C:222:TYR:CD2	1:C:223:VAL:N	2.66	0.62
1:C:623:VAL:O	1:C:624:PHE:C	2.38	0.62
1:C:824:PHE:N	1:C:824:PHE:HD2	1.97	0.62
2:D:61:PHE:CG	2:D:62:PRO:HA	2.35	0.62
3:X:146:LEU:HD22	3:X:147:ASP:N	2.14	0.62
1:A:511:HIS:CE1	3:X:149:SER:OG	2.52	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1616:GLN:OE1	1:C:1650:ARG:HB3	1.98	0.62
2:D:147:VAL:HG12	2:D:183:PHE:HE1	1.64	0.62
1:A:1056:ILE:CD1	1:A:1066:TYR:CE2	2.82	0.62
1:A:1429:PRO:HB2	1:A:1432:ILE:HG13	1.80	0.62
1:A:884:VAL:HG12	1:A:885:ARG:N	2.15	0.62
1:C:1271:ILE:O	1:C:1275:SER:HB3	2.00	0.62
1:C:412:ARG:HD2	2:D:458:ASP:OD1	2.00	0.62
1:C:968:VAL:HG23	1:C:971:THR:CG2	2.30	0.62
2:D:510:ILE:HG23	2:D:514:LEU:HD12	1.81	0.62
2:D:563:MET:CG	2:D:780:LEU:HD23	2.25	0.62
1:A:238:ILE:HD12	1:A:347:TYR:CE1	2.33	0.62
1:A:495:LYS:HA	1:A:495:LYS:HE2	1.80	0.62
2:B:1446:PHE:HB3	2:B:1448:VAL:HG22	1.81	0.62
1:C:1142:LEU:HD13	1:C:1187:THR:HG21	1.82	0.62
1:C:1585:TYR:CD2	1:C:1586:LYS:N	2.67	0.62
2:D:1532:GLU:O	2:D:1539:ILE:HD12	1.99	0.62
2:D:162:ILE:HG21	2:D:202:LYS:HG2	1.82	0.62
2:D:355:LYS:N	2:D:355:LYS:HD2	2.14	0.62
2:D:69:PHE:CD2	2:D:70:GLN:N	2.68	0.62
2:D:221:LEU:CD1	2:D:753:LYS:HG2	2.29	0.62
2:D:923:SER:O	2:D:924:ILE:HD12	2.00	0.62
1:C:512:PHE:CE2	3:Y:148:ALA:HB3	2.35	0.62
3:Y:179:LEU:HG	3:Y:180:TYR:CD2	2.35	0.62
1:A:104:LEU:HD12	1:A:105:GLU:N	2.15	0.62
1:A:1226:ARG:CZ	1:A:1266:TYR:HE1	2.13	0.62
1:A:161:LEU:HD11	1:A:185:PHE:CE1	2.35	0.62
2:B:922:LYS:HE3	2:B:1329:TYR:CZ	2.34	0.62
2:B:1562:GLN:NE2	2:B:1596:LYS:NZ	2.48	0.62
2:B:148:PHE:CB	2:B:800:ILE:HD11	2.30	0.62
1:C:936:ARG:NH2	1:C:1284:PHE:HE1	1.98	0.62
1:C:1333:PHE:CD1	1:C:1334:LEU:HD13	2.34	0.62
1:C:442:LEU:HD23	1:C:443:PRO:CD	2.29	0.62
1:C:125:PHE:CE1	1:C:627:LEU:HD21	2.34	0.62
1:C:976:ILE:HB	1:C:1362:THR:HG22	1.82	0.62
2:D:534:ASP:HA	2:D:620:VAL:HG21	1.82	0.62
1:A:1493:PHE:CD1	1:A:1493:PHE:C	2.73	0.62
1:A:1646:GLU:OE2	1:A:1660:PHE:CZ	2.53	0.62
1:A:317:ASP:C	1:A:319:ASN:H	2.03	0.62
1:A:382:LEU:HD13	1:A:415:ASP:C	2.19	0.62
1:A:488:PRO:HG3	1:A:499:TYR:OH	2.00	0.62
2:B:1431:SER:HB3	2:B:1433:SER:H	1.64	0.62

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1523:VAL:HG22	2:B:1584:TRP:HB2	1.81	0.62
2:B:344:GLN:HB2	2:B:367:THR:O	2.00	0.62
2:B:829:GLN:HA	2:B:885:VAL:HG12	1.81	0.62
1:C:690:TYR:CE1	1:C:692:HIS:HA	2.34	0.62
2:D:873:LYS:HD2	2:D:873:LYS:N	2.15	0.62
2:D:928:VAL:HG23	2:D:1323:MET:HB3	1.82	0.62
3:X:47:HIS:CE1	3:X:181:LYS:HE2	2.35	0.62
1:A:1648:TRP:NE1	1:A:1664:LEU:HD21	2.15	0.61
1:A:442:LEU:HD23	1:A:443:PRO:CD	2.30	0.61
1:A:585:GLY:O	1:A:789:ALA:HB1	2.00	0.61
1:A:779:LEU:HD12	1:A:780:VAL:N	2.15	0.61
2:B:1562:GLN:HB2	2:B:1598:SER:HB3	1.82	0.61
1:A:1102:ASN:HD21	1:C:1162:VAL:H	1.44	0.61
1:C:161:LEU:HD11	1:C:185:PHE:CD1	2.35	0.61
1:C:705:VAL:HA	1:C:739:ARG:CZ	2.30	0.61
1:C:849:ARG:CG	1:C:849:ARG:HH11	2.11	0.61
2:D:380:VAL:CG1	2:D:387:MET:HB3	2.17	0.61
2:D:34:ARG:HD2	2:D:488:LYS:NZ	2.15	0.61
3:X:53:GLU:HB3	3:X:55:PHE:CE2	2.35	0.61
1:A:1076:THR:HG22	1:A:1120:GLU:CD	2.20	0.61
1:A:596:MET:N	1:A:782:ARG:HH11	1.90	0.61
2:B:416:ASN:HA	2:B:425:GLN:NE2	2.14	0.61
2:B:543:THR:OG1	2:B:544:CYS:N	2.31	0.61
1:C:1211:ALA:HA	1:C:1214:ARG:HH11	1.65	0.61
1:C:1381:ILE:O	1:C:1382:ASP:HB3	2.00	0.61
1:C:796:THR:HG23	1:C:818:LYS:CB	2.30	0.61
2:D:1380:THR:HG22	2:D:1381:ILE:H	1.64	0.61
2:D:1610:TRP:CE3	2:D:1628:PHE:CD2	2.87	0.61
2:D:161:VAL:HG21	2:D:180:LEU:CD2	2.28	0.61
2:D:219:TYR:CD1	2:D:220:VAL:N	2.69	0.61
2:D:620:VAL:HG12	2:D:621:PHE:CD2	2.34	0.61
3:X:58:SER:HB2	3:X:125:LYS:HE3	1.82	0.61
1:C:513:GLY:HA2	3:Y:146:LEU:HD13	1.82	0.61
1:A:1219:LYS:HZ3	1:A:1239:VAL:HG11	1.61	0.61
1:A:1504:GLN:HG3	1:A:1505:CYS:CA	2.30	0.61
1:A:393:GLN:HG2	1:A:403:ASP:OD1	2.00	0.61
1:A:576:SER:HB2	1:A:589:SER:CB	2.27	0.61
1:A:653:PHE:CE1	1:A:660:ASP:HB3	2.35	0.61
2:B:120:LEU:HD12	2:B:121:LEU:N	2.11	0.61
2:B:137:TYR:CE2	2:B:143:VAL:HG22	2.35	0.61
2:B:162:ILE:HG21	2:B:202:LYS:HG2	1.81	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1053:MET:SD	1:C:1089:VAL:HG21	2.40	0.61
1:C:586:GLN:O	1:C:586:GLN:HG3	2.00	0.61
1:C:641:ASN:O	1:C:643:ALA:N	2.33	0.61
1:C:23:TYR:CE1	1:C:655:THR:HB	2.35	0.61
2:D:1347:VAL:HG21	2:D:1456:VAL:HG11	1.81	0.61
2:D:1511:GLN:HG2	2:D:1631:PHE:CE1	2.35	0.61
2:D:69:PHE:CD1	2:D:87:ILE:HG22	2.36	0.61
3:Y:166:ASP:CB	3:Y:207:LEU:HD21	2.30	0.61
1:A:1365:VAL:CG2	1:A:1366:HIS:N	2.60	0.61
1:A:270:GLY:HA3	1:A:282:MET:HG2	1.83	0.61
1:A:44:TYR:CE1	1:A:497:THR:HG21	2.35	0.61
1:A:824:PHE:CE2	1:A:846:TYR:HD1	2.19	0.61
2:B:1623:LYS:HA	2:B:1623:LYS:CE	2.30	0.61
2:B:1623:LYS:HA	2:B:1623:LYS:NZ	2.15	0.61
2:B:242:ASN:OD1	2:B:295:LYS:HD2	1.99	0.61
1:A:855:PHE:HA	2:B:904:LEU:CD1	2.28	0.61
1:C:927:LEU:HD23	1:C:928:ARG:N	2.16	0.61
1:C:955:ARG:NH1	1:C:1352:PHE:HA	2.15	0.61
2:D:342:PRO:HG2	2:D:420:LEU:HD13	1.81	0.61
2:D:410:PRO:HA	2:D:431:THR:HG22	1.83	0.61
1:A:868:SER:CA	1:A:1527:CYS:HB2	2.28	0.61
1:A:1641:SER:C	1:A:1643:THR:H	2.02	0.61
2:B:128:LEU:O	2:B:129:PHE:CD1	2.53	0.61
2:B:1344:HIS:O	2:B:1369:THR:HA	2.01	0.61
2:B:237:ILE:O	2:B:306:LEU:HD11	1.99	0.61
1:C:149:ASN:H	1:C:149:ASN:ND2	1.97	0.61
1:C:177:ILE:HG22	1:C:178:ASP:H	1.66	0.61
1:C:317:ASP:C	1:C:319:ASN:H	2.03	0.61
2:D:1344:HIS:O	2:D:1369:THR:HA	2.01	0.61
2:D:964:ILE:O	2:D:964:ILE:HG22	2.00	0.61
3:Y:139:ASN:HD22	3:Y:148:ALA:CB	2.12	0.61
3:Y:139:ASN:HD22	3:Y:148:ALA:HB1	1.66	0.61
3:Y:73:VAL:HG22	3:Y:84:LEU:HB3	1.80	0.61
1:A:1147:PHE:O	1:A:1150:ILE:HB	2.01	0.61
1:A:1163:LYS:NZ	1:C:1109:GLU:CD	2.54	0.61
1:A:871:PRO:HD2	1:A:872:VAL:N	2.15	0.61
1:C:1188:LEU:HD23	1:C:1212:LEU:HD13	1.83	0.61
1:C:20:GLU:O	1:C:20:GLU:CD	2.39	0.61
1:C:481:HIS:HE1	1:C:529:PRO:HB3	1.64	0.61
1:C:742:ILE:HG21	1:C:753:HIS:HA	1.83	0.61
1:C:837:GLU:O	1:C:901:LEU:HD12	2.00	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:581:ASP:O	2:D:582:LYS:C	2.39	0.61
1:A:1033:ILE:HG23	1:A:1034:PHE:N	2.14	0.61
1:A:161:LEU:HD11	1:A:185:PHE:CG	2.36	0.61
1:A:260:VAL:HG12	1:A:261:THR:N	2.15	0.61
1:A:267:ILE:HD12	1:A:299:VAL:HG11	1.83	0.61
1:A:493:ILE:HG23	1:A:495:LYS:HB2	1.82	0.61
2:B:103:TYR:CD2	2:B:120:LEU:HD13	2.35	0.61
2:B:1583:ILE:HG12	2:B:1607:ILE:CG2	2.30	0.61
2:B:384:PHE:O	2:B:385:HIS:C	2.38	0.61
2:B:484:LEU:HD11	2:B:626:LEU:HD11	1.83	0.61
1:C:44:TYR:CE1	1:C:497:THR:HG21	2.35	0.61
1:C:653:PHE:CE1	1:C:660:ASP:HB3	2.35	0.61
2:D:1506:ILE:O	2:D:1508:VAL:N	2.34	0.61
2:D:384:PHE:HD1	2:D:400:LEU:HG	1.60	0.61
3:X:191:ILE:HD12	3:X:199:VAL:HB	1.82	0.61
1:A:1049:LEU:HD11	1:A:1089:VAL:CG1	2.30	0.61
1:A:24:VAL:HG11	1:A:543:TYR:CE2	2.35	0.61
2:B:219:TYR:CD1	2:B:220:VAL:N	2.69	0.61
1:C:153:LYS:HB3	1:C:154:PRO:HD2	1.83	0.61
1:C:1582:LEU:HD11	1:C:1648:TRP:HZ2	1.66	0.61
1:C:489:LYS:CG	1:C:490:SER:H	2.13	0.61
1:C:60:PRO:CD	1:C:61:ASP:N	2.56	0.61
2:D:34:ARG:HD2	2:D:488:LYS:HZ3	1.66	0.61
3:Y:50:TYR:CE2	3:Y:170:ARG:CD	2.81	0.61
1:A:428:VAL:HG22	1:A:429:THR:H	1.65	0.61
1:A:59:TYR:CD1	1:A:60:PRO:HD3	2.36	0.61
2:B:1610:TRP:CD2	2:B:1628:PHE:HD2	2.19	0.61
2:B:599:TRP:CZ3	2:B:602:ILE:HD12	2.36	0.61
1:C:1612:VAL:HB	1:C:1615:ARG:CB	2.26	0.61
2:D:416:ASN:HA	2:D:425:GLN:NE2	2.15	0.61
3:Y:191:ILE:HD12	3:Y:199:VAL:HB	1.83	0.61
1:A:1620:MET:HB2	1:A:1644:TRP:HB3	1.83	0.61
1:A:1667:PHE:O	1:A:1671:ILE:HG22	2.01	0.61
1:A:824:PHE:CE2	1:A:846:TYR:HB2	2.36	0.61
2:B:1447:GLU:HG3	2:B:1447:GLU:O	2.00	0.61
2:B:1544:VAL:HB	2:B:1557:ARG:HA	1.82	0.61
2:B:244:HIS:HB3	2:B:291:LYS:CD	2.29	0.61
2:B:433:ILE:HG22	2:B:434:ALA:O	2.01	0.61
1:C:1147:PHE:O	1:C:1150:ILE:HB	2.00	0.61
1:C:40:VAL:CG2	1:C:512:PHE:HD1	2.14	0.61
2:D:1500:LEU:HD11	2:D:1608:GLU:O	2.01	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:841:ASN:O	2:D:842:GLU:C	2.40	0.61
1:A:119:ILE:O	1:A:119:ILE:HD12	2.01	0.60
1:A:1535:MET:HA	1:A:1645:ILE:HB	1.83	0.60
1:A:658:ASN:OD1	1:A:658:ASN:C	2.40	0.60
2:B:1561:HIS:CE1	2:B:1597:ILE:HD13	2.35	0.60
2:B:342:PRO:HG2	2:B:420:LEU:HD13	1.83	0.60
1:C:1268:ASN:H	1:C:1268:ASN:ND2	1.98	0.60
1:C:502:LEU:HB2	1:C:541:LEU:HD23	1.83	0.60
1:C:824:PHE:CE2	1:C:846:TYR:HD1	2.19	0.60
1:C:822:ASP:HA	1:C:849:ARG:HD2	1.83	0.60
2:D:1391:LEU:HB2	2:D:1417:MET:HE2	1.83	0.60
2:D:829:GLN:NE2	2:D:883:VAL:HG13	2.10	0.60
1:A:1003:LEU:N	1:A:1003:LEU:HD23	2.16	0.60
1:A:1268:ASN:ND2	1:A:1268:ASN:H	1.99	0.60
1:A:1627:ILE:O	1:A:1629:TYR:N	2.34	0.60
1:A:177:ILE:HG22	1:A:178:ASP:H	1.65	0.60
1:A:532:GLN:NE2	1:A:568:GLY:HA2	2.16	0.60
2:B:167:THR:HG23	2:B:171:ILE:H	1.65	0.60
1:C:1054:LEU:HD23	1:C:1057:MET:HE2	1.83	0.60
1:C:1232:LEU:CD1	1:C:1233:GLN:HE21	2.09	0.60
1:C:256:TYR:HD2	1:C:846:TYR:CE1	2.19	0.60
1:C:873:ILE:O	1:C:873:ILE:HD12	2.01	0.60
2:D:133:ASP:OD2	2:D:134:LYS:HG2	2.01	0.60
2:D:1610:TRP:CD2	2:D:1628:PHE:HD2	2.18	0.60
2:D:581:ASP:O	2:D:583:ALA:N	2.34	0.60
2:D:814:PHE:HZ	2:D:846:VAL:HG21	1.66	0.60
3:X:170:ARG:NH2	3:X:206:LYS:HA	2.16	0.60
1:A:1211:ALA:HA	1:A:1214:ARG:HH11	1.66	0.60
1:A:987:ILE:CD1	1:A:1294:ILE:HG23	2.31	0.60
1:A:1323:LEU:HD12	1:A:1324:HIS:N	2.16	0.60
1:A:1427:SER:HB3	1:A:1492:THR:HG23	1.81	0.60
2:B:841:ASN:O	2:B:842:GLU:C	2.38	0.60
2:B:844:ILE:CD1	2:B:872:ILE:HD11	2.32	0.60
1:C:171:VAL:HG11	1:C:1054:LEU:HD11	1.82	0.60
1:C:243:PHE:HE2	1:C:304:GLU:HA	1.66	0.60
1:C:322:TYR:N	1:C:322:TYR:CD2	2.68	0.60
1:C:43:VAL:HG11	1:C:73:LEU:CD1	2.31	0.60
1:C:457:TYR:HE1	1:C:556:SER:O	1.85	0.60
2:D:242:ASN:OD1	2:D:295:LYS:HD2	2.00	0.60
1:A:443:PRO:HG2	1:A:446:ASN:OD1	2.01	0.60
1:A:500:ASN:CB	1:A:543:TYR:CE1	2.61	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:SER:C	1:A:695:VAL:H	2.05	0.60
2:B:269:ILE:HA	2:B:312:HIS:CD2	2.36	0.60
2:B:756:LEU:HD12	2:B:758:LEU:HG	1.84	0.60
1:C:1487:PHE:O	1:C:1488:LEU:C	2.40	0.60
1:C:1549:LYS:HZ2	1:C:1667:PHE:HB3	1.66	0.60
1:C:196:TYR:CE1	1:C:221:GLU:HB2	2.37	0.60
1:C:351:PRO:HG2	1:C:352:TYR:CE2	2.35	0.60
1:A:1042:LYS:NZ	1:C:92:LEU:HD13	2.17	0.60
2:D:196:THR:HG23	2:D:215:ASP:OD1	2.01	0.60
2:D:916:VAL:HG22	2:D:917:PRO:O	2.02	0.60
3:X:88:GLY:HA2	3:X:210:GLU:O	2.01	0.60
1:A:161:LEU:H	1:A:161:LEU:HD12	1.65	0.60
1:A:1585:TYR:HE1	1:A:1671:ILE:HG12	1.66	0.60
2:B:1381:ILE:HG21	2:B:1459:TYR:CE1	2.35	0.60
2:B:1473:HIS:CD2	2:B:1474:PRO:CD	2.84	0.60
2:B:435:TYR:OH	2:B:532:VAL:HG22	2.00	0.60
2:B:738:GLY:O	2:B:901:GLN:HA	2.02	0.60
1:C:1646:GLU:OE2	1:C:1660:PHE:CZ	2.54	0.60
1:C:209:PHE:H	1:C:209:PHE:HD2	1.48	0.60
1:C:531:THR:O	1:C:534:MET:HG3	2.01	0.60
2:D:484:LEU:HD11	2:D:626:LEU:HD11	1.84	0.60
2:D:933:ARG:HG3	2:D:933:ARG:NH1	2.14	0.60
1:A:1213:LYS:HE2	1:A:1266:TYR:CE2	2.37	0.60
1:A:1548:ARG:HD3	1:A:1548:ARG:H	1.66	0.60
1:A:1564:SER:HB2	1:A:1616:GLN:HG3	1.82	0.60
1:A:238:ILE:HB	1:A:347:TYR:HD1	1.67	0.60
1:A:503:ILE:HD11	1:A:540:LEU:HD13	1.83	0.60
1:A:670:LYS:HD2	1:A:671:GLU:HG2	1.84	0.60
2:B:127:PHE:CE2	2:B:602:ILE:HG23	2.37	0.60
2:B:556:ILE:H	2:B:556:ILE:HD12	1.65	0.60
1:C:702:GLY:CA	1:C:728:PHE:CD1	2.84	0.60
2:D:120:LEU:HD12	2:D:121:LEU:N	2.13	0.60
2:D:233:LYS:HG3	2:D:233:LYS:O	2.01	0.60
1:A:101:TYR:CE1	1:A:116:ARG:NH2	2.70	0.60
1:A:690:TYR:CE1	1:A:692:HIS:HA	2.36	0.60
2:B:61:PHE:HB3	2:B:103:TYR:HB2	1.83	0.60
2:B:963:ILE:HD11	2:B:1311:ILE:HG21	1.84	0.60
1:C:931:PRO:HG2	1:C:1366:HIS:NE2	2.16	0.60
1:C:209:PHE:CD2	1:C:209:PHE:N	2.68	0.60
1:C:199:TRP:CD1	1:C:219:VAL:HB	2.37	0.60
2:D:137:TYR:CE2	2:D:143:VAL:HG22	2.36	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1561:HIS:CE1	2:D:1597:ILE:HD13	2.37	0.60
1:A:1053:MET:SD	1:A:1089:VAL:HG21	2.42	0.60
1:A:1128:LYS:C	1:A:1129:LEU:HD23	2.22	0.60
1:A:436:LYS:HA	1:A:448:ALA:O	2.01	0.60
2:B:133:ASP:OD2	2:B:134:LYS:HG2	2.01	0.60
2:B:294:LEU:HD12	2:B:295:LYS:N	2.16	0.60
1:C:1226:ARG:CZ	1:C:1266:TYR:CE1	2.85	0.60
1:C:1259:LEU:HD11	1:C:1300:TYR:HB2	1.84	0.60
1:C:174:VAL:HG22	1:C:175:GLU:N	2.15	0.60
1:C:25:ILE:CD1	1:C:41:ILE:HB	2.31	0.60
1:C:115:LYS:CB	1:C:654:LEU:HD21	2.32	0.60
1:C:820:PHE:O	1:C:821:LYS:HG3	2.00	0.60
1:C:824:PHE:HE2	1:C:846:TYR:HB2	1.65	0.60
2:D:1510:LEU:HD21	2:D:1514:LYS:NZ	2.15	0.60
1:A:931:PRO:HG2	1:A:1366:HIS:NE2	2.17	0.60
1:A:209:PHE:N	1:A:209:PHE:CD2	2.70	0.60
2:B:1380:THR:HG22	2:B:1381:ILE:H	1.67	0.60
2:B:96:THR:HG21	2:B:102:GLN:OE1	2.02	0.60
1:C:1239:VAL:O	1:C:1239:VAL:HG12	2.02	0.60
1:C:154:PRO:O	1:C:155:ALA:CB	2.50	0.60
1:C:165:ASP:O	1:C:167:GLU:N	2.35	0.60
1:A:1231:ASN:HB2	1:A:1235:LYS:HG3	1.83	0.60
1:A:1341:LEU:HB2	1:A:1342:LEU:CD2	2.31	0.60
1:A:1671:ILE:HA	1:A:1675:GLY:H	1.66	0.60
1:A:474:LYS:H	1:A:474:LYS:CD	2.15	0.60
1:A:55:SER:O	1:A:56:ILE:HD13	2.01	0.60
1:A:705:VAL:HA	1:A:739:ARG:CZ	2.31	0.60
2:B:197:TRP:HB2	2:B:214:PHE:CE1	2.36	0.60
2:B:296:ARG:HH11	2:B:296:ARG:HG3	1.66	0.60
2:B:510:ILE:HG23	2:B:514:LEU:HD12	1.84	0.60
2:B:557:GLN:HE21	2:B:563:MET:CE	2.14	0.60
1:C:1150:ILE:CD1	1:C:1193:TYR:CD2	2.85	0.60
1:C:1608:ASN:O	1:C:1610:GLU:N	2.35	0.60
1:C:443:PRO:HG2	1:C:446:ASN:OD1	2.02	0.60
1:C:569:ASN:ND2	1:C:570:GLN:H	2.00	0.60
1:A:443:PRO:HG2	1:A:446:ASN:HB2	1.84	0.59
1:A:429:THR:HA	1:A:456:ALA:HB2	1.84	0.59
1:A:551:THR:O	1:A:552:ALA:HB2	2.00	0.59
1:A:457:TYR:OH	1:A:555:VAL:HG22	2.02	0.59
1:A:362:PHE:HE1	1:A:640:LEU:HB2	1.67	0.59
1:A:25:ILE:HB	1:A:655:THR:HG23	1.84	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:PHE:HD2	1:A:824:PHE:N	1.99	0.59
2:B:523:TYR:HB3	2:B:533:ALA:HB2	1.83	0.59
1:C:1329:THR:H	1:C:1332:ASN:HB2	1.67	0.59
1:C:1560:ALA:HB2	1:C:1620:MET:CG	2.25	0.59
1:C:1585:TYR:CG	1:C:1586:LYS:N	2.69	0.59
1:C:342:ILE:HD12	1:C:345:ILE:HD11	1.84	0.59
2:D:476:ILE:O	2:D:476:ILE:CG2	2.50	0.59
2:D:476:ILE:HD11	2:D:524:TYR:CG	2.36	0.59
1:A:1056:ILE:CD1	1:A:1066:TYR:HE2	2.15	0.59
1:A:504:LEU:HD12	1:A:509:ILE:HG23	1.85	0.59
1:A:612:VAL:HG12	1:A:612:VAL:O	2.01	0.59
1:A:25:ILE:N	1:A:655:THR:HG21	2.12	0.59
2:B:508:LEU:HD12	2:B:509:HIS:N	2.16	0.59
2:B:531:ILE:HD11	2:B:634:LEU:HD23	1.84	0.59
1:C:1152:ILE:HG22	1:C:1168:LEU:HD21	1.82	0.59
1:C:967:LEU:HD12	1:C:968:VAL:H	1.66	0.59
2:D:1486:ILE:HD11	2:D:1591:LEU:HD22	1.85	0.59
2:D:261:ALA:CB	2:D:285:ILE:HD11	2.32	0.59
3:X:179:LEU:HG	3:X:180:TYR:CD2	2.36	0.59
3:X:68:ASN:CG	3:X:69:GLY:N	2.55	0.59
3:Y:101:GLN:HA	3:Y:125:LYS:HB3	1.84	0.59
3:Y:68:ASN:CG	3:Y:69:GLY:N	2.55	0.59
1:A:1113:LEU:CD2	1:A:1114:ASP:H	2.15	0.59
1:A:1381:ILE:O	1:A:1382:ASP:HB3	2.02	0.59
1:A:1559:TYR:HH	1:A:1591:VAL:HA	1.66	0.59
1:A:1612:VAL:HB	1:A:1615:ARG:CB	2.26	0.59
1:A:209:PHE:H	1:A:209:PHE:HD2	1.50	0.59
1:A:199:TRP:CD1	1:A:219:VAL:HB	2.37	0.59
1:A:222:TYR:CD2	1:A:223:VAL:N	2.69	0.59
1:A:838:GLN:HA	1:A:901:LEU:CB	2.29	0.59
1:A:949:ILE:HG22	1:A:950:TYR:CE1	2.37	0.59
2:B:69:PHE:CD1	2:B:87:ILE:HG22	2.37	0.59
2:B:829:GLN:NE2	2:B:883:VAL:HG13	2.13	0.59
1:C:1320:LYS:CE	1:C:1321:GLY:H	2.15	0.59
1:C:493:ILE:HG23	1:C:495:LYS:HB2	1.85	0.59
1:A:623:VAL:HG12	1:A:624:PHE:N	2.18	0.59
2:B:1424:ILE:H	2:B:1424:ILE:CD1	2.14	0.59
2:B:309:LEU:HB3	2:B:338:ILE:HD12	1.84	0.59
1:C:1618:LEU:HD22	1:C:1619:ILE:N	2.16	0.59
1:C:979:VAL:HG21	1:C:1326:TYR:CZ	2.35	0.59
2:D:783:SER:HB2	2:D:787:TRP:HZ2	1.67	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:GLU:O	1:A:1014:SER:HB3	2.02	0.59
1:A:115:LYS:HB2	1:A:654:LEU:HD21	1.85	0.59
1:A:1487:PHE:N	1:A:1487:PHE:CD2	2.68	0.59
1:A:1493:PHE:HD1	1:A:1493:PHE:C	2.06	0.59
1:A:874:ASP:HA	1:A:878:THR:O	2.03	0.59
2:B:813:VAL:HG12	2:B:840:VAL:HG22	1.85	0.59
1:C:1152:ILE:HG21	1:C:1168:LEU:CD2	2.31	0.59
1:C:1615:ARG:NH1	1:C:1647:TYR:CE1	2.70	0.59
1:C:515:ARG:NH1	1:C:526:ILE:HG22	2.16	0.59
1:A:1329:THR:H	1:A:1332:ASN:HB2	1.68	0.59
1:A:356:LEU:HG	1:A:452:TYR:CZ	2.38	0.59
1:A:503:ILE:CB	1:A:511:HIS:HB2	2.33	0.59
2:B:241:GLU:O	2:B:296:ARG:HD3	2.02	0.59
2:B:525:GLN:HA	2:B:530:GLU:O	2.03	0.59
2:B:148:PHE:HB3	2:B:800:ILE:HD11	1.83	0.59
1:C:1487:PHE:CD2	1:C:1487:PHE:N	2.70	0.59
1:C:987:ILE:CD1	1:C:1294:ILE:HG23	2.33	0.59
2:D:1473:HIS:CD2	2:D:1474:PRO:CD	2.79	0.59
2:D:243:PHE:HE1	2:D:336:ILE:HG21	1.67	0.59
2:D:61:PHE:HB3	2:D:103:TYR:HB2	1.83	0.59
2:D:738:GLY:O	2:D:901:GLN:HA	2.03	0.59
1:A:1066:TYR:N	1:A:1079:THR:HG23	2.16	0.59
1:A:1219:LYS:HE2	1:A:1239:VAL:HG21	1.85	0.59
1:A:361:LEU:N	1:A:361:LEU:HD12	2.16	0.59
1:A:936:ARG:NH2	1:A:1284:PHE:CE1	2.71	0.59
2:B:130:ILE:HD13	2:B:199:ILE:HG22	1.83	0.59
2:B:1609:ARG:HG2	2:B:1609:ARG:HH11	1.68	0.59
2:B:26:THR:OG1	2:B:44:GLU:HB2	2.02	0.59
2:B:71:THR:HG23	2:B:72:ARG:N	2.18	0.59
1:C:569:ASN:CG	1:C:570:GLN:H	2.06	0.59
1:C:680:GLN:HG3	1:C:681:LYS:N	2.17	0.59
2:D:745:ILE:HD11	2:D:907:ASP:H	1.66	0.59
3:X:106:VAL:HG22	3:X:163:LYS:CE	2.32	0.59
1:A:24:VAL:HG11	1:A:543:TYR:OH	2.01	0.59
1:A:491:PRO:C	1:A:493:ILE:N	2.51	0.59
1:A:702:GLY:CA	1:A:728:PHE:CD1	2.85	0.59
1:A:752:LEU:HG	1:A:752:LEU:O	2.02	0.59
1:A:774:LEU:HG	1:A:788:PHE:CE1	2.38	0.59
1:A:790:LEU:HB3	1:A:791:PRO:CD	2.32	0.59
1:A:813:ASP:O	1:A:815:VAL:HG23	2.03	0.59
2:B:316:ALA:HB3	2:B:333:GLN:HB3	1.85	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:746:ILE:H	2:B:746:ILE:HD13	1.68	0.59
1:C:1013:MET:CE	1:C:1287:THR:HB	2.32	0.59
1:C:1450:PHE:HZ	1:C:1475:VAL:HB	1.66	0.59
1:C:355:ASN:N	1:C:355:ASN:HD22	2.01	0.59
1:C:474:LYS:CD	1:C:474:LYS:H	2.15	0.59
1:C:617:LYS:HD2	1:C:622:ARG:NH2	2.17	0.59
2:D:922:LYS:HE3	2:D:1329:TYR:CZ	2.38	0.59
2:D:1505:ARG:NE	2:D:1623:LYS:HZ2	2.01	0.59
1:A:505:SER:HB3	1:A:510:ILE:CD1	2.32	0.59
1:A:720:LEU:HD13	1:A:724:CYS:HB3	1.83	0.59
2:B:961:THR:HG22	2:B:1327:THR:CG2	2.32	0.59
1:A:855:PHE:CA	2:B:904:LEU:HD11	2.31	0.59
1:A:78:LYS:HZ1	3:X:144:GLU:HA	1.65	0.59
1:A:1159:CYS:N	1:A:1160:PRO:CD	2.66	0.59
1:A:1352:PHE:HD2	1:A:1352:PHE:N	2.01	0.59
1:A:1493:PHE:HE1	1:A:1495:VAL:HG12	1.67	0.59
1:A:825:LEU:HG	1:A:826:GLU:N	2.18	0.59
1:A:257:ASN:HB2	1:A:848:TYR:CE2	2.37	0.59
1:C:1402:ILE:HG13	1:C:1479:ILE:HD11	1.84	0.59
1:C:182:ILE:HG12	1:C:804:ILE:CD1	2.25	0.59
2:D:103:TYR:CD2	2:D:120:LEU:HD13	2.37	0.59
2:D:309:LEU:HB3	2:D:338:ILE:HD12	1.85	0.59
2:D:476:ILE:CG2	2:D:497:ARG:HD3	2.33	0.59
1:A:322:TYR:CD2	1:A:322:TYR:N	2.70	0.58
1:A:544:TYR:C	1:A:544:TYR:CD2	2.76	0.58
1:A:644:ASN:CG	1:A:648:LEU:HD12	2.23	0.58
1:A:84:ILE:HD12	1:A:84:ILE:H	1.68	0.58
1:A:865:ILE:C	1:A:866:CYS:O	2.41	0.58
1:A:883:CYS:O	1:A:884:VAL:O	2.21	0.58
1:A:944:LEU:N	1:A:944:LEU:HD23	2.18	0.58
1:A:955:ARG:HH12	1:A:1352:PHE:HA	1.66	0.58
5:B:2001:NAG:C3	5:B:2002:NAG:O5	2.51	0.58
2:B:820:MET:HG3	2:B:821:PRO:HD2	1.85	0.58
1:C:1076:THR:HG22	1:C:1120:GLU:CD	2.23	0.58
1:C:1451:THR:O	1:C:1452:ASP:HB3	2.03	0.58
1:C:154:PRO:O	1:C:155:ALA:HB3	2.03	0.58
1:C:267:ILE:HG22	1:C:268:THR:N	2.18	0.58
1:C:975:ARG:NH1	1:C:1340:VAL:HG11	2.18	0.58
2:D:546:GLY:HA3	2:D:570:ASP:OD1	2.02	0.58
2:D:69:PHE:CD2	2:D:69:PHE:C	2.76	0.58
1:A:1065:SER:HB3	1:A:1106:TRP:CD2	2.38	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:863:GLU:H	1:A:863:GLU:CD	2.07	0.58
2:B:481:TYR:CE2	2:B:493:GLY:CA	2.86	0.58
2:B:476:ILE:HD11	2:B:524:TYR:CD2	2.37	0.58
1:C:172:ASP:OD2	1:C:1050:LYS:HD3	2.02	0.58
1:C:1110:ASN:N	1:C:1110:ASN:OD1	2.36	0.58
1:C:1229:LYS:NZ	1:C:1238:SER:OG	2.34	0.58
1:C:1451:THR:O	1:C:1452:ASP:CB	2.51	0.58
1:C:1562:LYS:HD3	1:C:1648:TRP:HE1	1.68	0.58
1:C:838:GLN:HA	1:C:901:LEU:CB	2.28	0.58
1:A:171:VAL:CG1	1:A:172:ASP:N	2.67	0.58
1:A:126:LEU:HD11	1:A:205:TYR:CE2	2.39	0.58
1:A:512:PHE:CD2	1:A:512:PHE:O	2.56	0.58
1:A:680:GLN:HG3	1:A:681:LYS:N	2.19	0.58
1:A:702:GLY:O	1:A:732:CYS:HB2	2.03	0.58
1:A:824:PHE:N	1:A:824:PHE:CD2	2.70	0.58
2:B:1532:GLU:O	2:B:1539:ILE:HD12	2.04	0.58
2:B:243:PHE:HE1	2:B:336:ILE:HG21	1.67	0.58
1:C:1076:THR:HG22	1:C:1120:GLU:OE2	2.02	0.58
1:C:1219:LYS:CD	1:C:1239:VAL:HG21	2.33	0.58
1:C:356:LEU:HG	1:C:452:TYR:CZ	2.38	0.58
1:C:623:VAL:HG12	1:C:624:PHE:N	2.18	0.58
2:D:137:TYR:CE1	2:D:143:VAL:HG22	2.37	0.58
2:D:265:PHE:CE2	2:D:294:LEU:HB2	2.38	0.58
2:D:606:ASP:O	2:D:606:ASP:OD1	2.21	0.58
3:X:166:ASP:CB	3:X:207:LEU:HD21	2.32	0.58
1:A:1572:ASN:O	1:A:1573:VAL:HG23	2.04	0.58
1:A:25:ILE:CD1	1:A:41:ILE:HB	2.33	0.58
1:A:950:TYR:CE2	1:A:1356:LEU:HD11	2.38	0.58
2:B:1563:TYR:HB3	2:B:1601:ILE:HD11	1.86	0.58
2:B:1593:THR:CG2	2:B:1594:LYS:N	2.67	0.58
2:B:183:PHE:CD2	2:B:183:PHE:N	2.70	0.58
2:B:45:ALA:HB3	2:B:81:MET:HE3	1.85	0.58
1:C:362:PHE:HE1	1:C:640:LEU:HB2	1.66	0.58
1:C:813:ASP:O	1:C:815:VAL:HG23	2.02	0.58
2:D:344:GLN:HB2	2:D:367:THR:O	2.03	0.58
2:D:829:GLN:HG2	2:D:885:VAL:CG1	2.34	0.58
1:A:1011:GLU:HG3	1:A:1055:SER:OG	2.03	0.58
1:A:134:VAL:C	1:A:135:TYR:HD2	2.07	0.58
1:A:504:LEU:HD23	1:A:649:ALA:O	2.03	0.58
2:B:1391:LEU:HD12	2:B:1417:MET:HE1	1.84	0.58
1:A:412:ARG:HD2	2:B:458:ASP:OD1	2.03	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1240:PRO:HB2	1:C:1242:THR:HG23	1.84	0.58
1:C:938:SER:OG	1:C:1284:PHE:CZ	2.57	0.58
2:D:887:LEU:CD2	2:D:1490:CYS:HB3	2.34	0.58
1:A:1152:ILE:HG22	1:A:1168:LEU:HD21	1.83	0.58
1:A:1549:LYS:HD3	1:A:1667:PHE:HB3	1.85	0.58
1:A:421:VAL:HG11	2:B:505:THR:HG22	1.86	0.58
1:A:784:LYS:HG2	1:A:785:GLN:N	2.18	0.58
1:A:902:PRO:O	1:A:903:LEU:HD13	2.02	0.58
1:A:907:LEU:HG	1:A:908:HIS:N	2.17	0.58
2:B:28:ILE:HG12	2:B:628:LEU:HD13	1.84	0.58
2:B:61:PHE:CG	2:B:62:PRO:HA	2.38	0.58
2:B:795:THR:HG22	2:B:796:PRO:CD	2.32	0.58
2:B:851:LEU:HD23	2:B:852:TYR:N	2.10	0.58
1:C:309:GLU:HG2	1:C:310:LEU:HD12	1.86	0.58
2:D:1491:ARG:HG3	2:D:1492:CYS:H	1.67	0.58
2:D:1623:LYS:HB3	2:D:1623:LYS:NZ	2.18	0.58
2:D:218:LYS:HD3	2:D:822:TYR:CE2	2.39	0.58
2:D:24:LEU:HB3	2:D:46:HIS:HB2	1.84	0.58
2:D:615:GLN:HB2	2:D:616:ASN:HD22	1.68	0.58
3:X:119:VAL:HG21	3:X:209:PHE:HB3	1.85	0.58
1:A:1527:CYS:O	1:A:1529:GLU:N	2.36	0.58
1:A:534:MET:HB3	1:A:538:SER:OG	2.04	0.58
2:B:1500:LEU:CD1	2:B:1500:LEU:C	2.72	0.58
2:B:1528:LEU:HD13	2:B:1542:MET:HE2	1.84	0.58
2:B:1624:LEU:HG	2:B:1628:PHE:CE1	2.38	0.58
2:B:348:THR:HA	2:B:352:LYS:NZ	2.19	0.58
1:C:1019:PHE:HD2	1:C:1020:TYR:N	2.01	0.58
1:C:1065:SER:HB3	1:C:1106:TRP:CD2	2.39	0.58
1:C:1618:LEU:HD22	1:C:1619:ILE:H	1.67	0.58
1:C:163:PHE:CD2	1:C:188:PHE:CD1	2.91	0.58
1:C:553:GLU:HA	1:C:658:ASN:CB	2.31	0.58
1:C:81:ASN:CG	1:C:82:SER:H	2.07	0.58
1:C:854:GLN:NE2	1:C:854:GLN:H	2.02	0.58
1:A:1333:PHE:CD1	1:A:1334:LEU:HD13	2.39	0.58
1:A:132:LYS:NZ	1:A:139:GLN:HE22	2.01	0.58
1:A:639:GLY:H	1:A:645:VAL:HA	1.68	0.58
1:A:788:PHE:HD2	1:A:788:PHE:N	2.02	0.58
2:B:1278:THR:HB	2:B:1314:THR:HB	1.84	0.58
2:B:1450:PHE:HD1	2:B:1451:ILE:H	1.51	0.58
2:B:1534:GLN:HG3	2:B:1535:ASP:OD2	2.04	0.58
2:B:581:ASP:O	2:B:582:LYS:C	2.42	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:599:TRP:HE3	2:B:599:TRP:HA	1.68	0.58
2:B:746:ILE:HD13	2:B:746:ILE:N	2.18	0.58
2:B:844:ILE:HG13	2:B:872:ILE:CG1	2.34	0.58
1:C:936:ARG:HH12	1:C:1284:PHE:HZ	1.50	0.58
1:C:1411:SER:N	1:C:1414:GLU:HG3	2.19	0.58
1:C:350:SER:OG	1:C:352:TYR:O	2.20	0.58
1:C:361:LEU:N	1:C:361:LEU:HD12	2.18	0.58
1:C:368:PRO:HG3	2:D:505:THR:HB	1.85	0.58
1:C:364:LYS:HE3	1:C:457:TYR:HD1	1.68	0.58
1:C:484:ILE:CD1	1:C:540:LEU:HD21	2.33	0.58
1:C:967:LEU:HD13	1:C:1365:VAL:CG2	2.34	0.58
2:D:71:THR:HG23	2:D:72:ARG:N	2.18	0.58
3:Y:106:VAL:HG22	3:Y:163:LYS:CE	2.33	0.58
1:A:1255:LEU:O	1:A:1255:LEU:HD12	2.03	0.58
1:A:1411:SER:N	1:A:1414:GLU:HG3	2.19	0.58
1:A:1493:PHE:HD1	1:A:1494:THR:H	1.48	0.58
1:A:1496:TYR:CD2	1:A:1496:TYR:N	2.71	0.58
1:A:1496:TYR:N	1:A:1496:TYR:HD2	2.02	0.58
1:A:342:ILE:HG22	1:A:343:PRO:HD2	1.86	0.58
1:A:350:SER:OG	1:A:352:TYR:O	2.20	0.58
2:B:1628:PHE:O	2:B:1629:ALA:C	2.41	0.58
2:B:850:LEU:HD12	2:B:851:LEU:N	2.19	0.58
1:C:1003:LEU:N	1:C:1003:LEU:HD23	2.19	0.58
1:C:161:LEU:HD11	1:C:185:PHE:CG	2.39	0.58
2:D:1528:LEU:HD13	2:D:1542:MET:HE2	1.86	0.58
2:D:283:ILE:HD12	2:D:283:ILE:N	2.18	0.58
1:A:1035:HIS:ND1	1:A:1035:HIS:N	2.52	0.58
1:A:1159:CYS:SG	1:A:1161:LEU:HD23	2.44	0.58
1:A:1408:TYR:CE2	1:A:1410:PRO:HA	2.39	0.58
1:A:1431:GLY:HA2	1:A:1483:PHE:CE1	2.39	0.58
1:A:824:PHE:HE2	1:A:846:TYR:HB2	1.69	0.58
1:A:927:LEU:HD23	1:A:928:ARG:N	2.19	0.58
2:B:239:GLY:H	2:B:296:ARG:NH2	2.02	0.58
2:B:481:TYR:O	2:B:481:TYR:CD2	2.51	0.58
2:B:69:PHE:CD2	2:B:70:GLN:N	2.72	0.58
1:C:1113:LEU:HD22	1:C:1114:ASP:H	1.68	0.58
1:C:1271:ILE:HD13	1:C:1300:TYR:CZ	2.39	0.58
1:C:1536:GLN:HG3	1:C:1536:GLN:O	2.04	0.58
1:C:655:THR:O	1:C:656:ASN:C	2.42	0.58
1:C:720:LEU:HD13	1:C:724:CYS:HB3	1.84	0.58
2:D:460:LEU:O	2:D:460:LEU:HD23	2.04	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:844:ILE:HG13	2:D:872:ILE:CG1	2.34	0.58
2:D:36:ASP:OD1	2:D:90:PRO:HA	2.04	0.58
2:D:825:VAL:HG22	2:D:916:VAL:HG13	1.85	0.58
1:A:1053:MET:CE	1:A:1086:LEU:HD13	2.33	0.57
1:A:1159:CYS:O	1:A:1161:LEU:N	2.37	0.57
1:A:1468:PRO:HD3	1:A:1473:LEU:HD13	1.85	0.57
1:A:1541:LEU:HD21	1:A:1543:ILE:HD12	1.86	0.57
1:A:1560:ALA:HB2	1:A:1620:MET:CG	2.27	0.57
1:A:265:VAL:O	1:A:289:ASN:HA	2.04	0.57
1:A:599:TRP:CD1	1:A:779:LEU:HA	2.39	0.57
2:B:167:THR:HG22	2:B:171:ILE:O	2.03	0.57
2:B:36:ASP:OD1	2:B:90:PRO:HA	2.04	0.57
2:B:964:ILE:O	2:B:964:ILE:CG2	2.51	0.57
1:C:23:TYR:C	1:C:655:THR:HG21	2.24	0.57
1:C:585:GLY:O	1:C:789:ALA:HB1	2.04	0.57
1:C:680:GLN:O	1:C:684:GLU:HG3	2.04	0.57
5:D:2001:NAG:C3	5:D:2002:NAG:O5	2.51	0.57
2:D:362:LEU:HD13	2:D:411:ILE:HD12	1.86	0.57
2:D:508:LEU:HD12	2:D:509:HIS:N	2.18	0.57
3:Y:110:ILE:HG22	3:Y:111:ASP:O	2.04	0.57
1:A:1093:VAL:O	1:A:1093:VAL:HG12	2.03	0.57
1:A:489:LYS:CG	1:A:490:SER:H	2.15	0.57
2:B:1536:GLY:O	2:B:1567:ARG:HG2	2.04	0.57
2:B:449:ILE:HD13	2:B:462:VAL:HG23	1.85	0.57
1:C:1011:GLU:HG3	1:C:1055:SER:OG	2.04	0.57
1:C:55:SER:C	1:C:56:ILE:HD13	2.23	0.57
2:D:481:TYR:HE2	2:D:493:GLY:CA	2.17	0.57
2:D:523:TYR:HB3	2:D:533:ALA:HB2	1.86	0.57
2:D:783:SER:HB2	2:D:787:TRP:CZ2	2.39	0.57
2:D:913:LEU:HD23	2:D:913:LEU:C	2.24	0.57
2:D:916:VAL:HG23	2:D:917:PRO:HD2	1.86	0.57
1:A:512:PHE:CE2	3:X:148:ALA:HB3	2.39	0.57
3:Y:185:LYS:HG2	3:Y:186:TYR:CE2	2.38	0.57
3:Y:194:LYS:NZ	3:Y:197:ASN:HB2	2.10	0.57
1:A:1145:THR:O	1:A:1149:VAL:HG23	2.04	0.57
1:A:190:ILE:HG22	1:A:191:PRO:CD	2.34	0.57
1:A:623:VAL:O	1:A:624:PHE:C	2.38	0.57
2:B:137:TYR:CE1	2:B:143:VAL:HG22	2.40	0.57
2:B:873:LYS:N	2:B:873:LYS:HD2	2.18	0.57
1:C:1053:MET:CE	1:C:1086:LEU:HD22	2.34	0.57
1:C:1159:CYS:SG	1:C:1161:LEU:HD23	2.45	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1468:PRO:HD3	1:C:1473:LEU:HD13	1.86	0.57
1:C:1560:ALA:O	1:C:1561:TYR:HD2	1.86	0.57
1:C:488:PRO:HG3	1:C:499:TYR:OH	2.03	0.57
1:C:687:ALA:O	1:C:690:TYR:HB3	2.04	0.57
2:D:1279:ILE:CG2	2:D:1288:ILE:HB	2.35	0.57
2:D:1346:ASN:HB2	2:D:1368:CYS:HB2	1.86	0.57
3:Y:78:LYS:C	3:Y:78:LYS:HD2	2.25	0.57
2:B:963:ILE:CG1	2:B:1325:ILE:HG12	2.35	0.57
2:B:161:VAL:HG21	2:B:180:LEU:CD2	2.33	0.57
2:B:266:GLY:HA2	2:B:276:ILE:HG13	1.84	0.57
2:B:383:ALA:C	2:B:384:PHE:CD2	2.78	0.57
1:A:1162:VAL:N	1:C:1102:ASN:HD21	2.02	0.57
1:C:503:ILE:CB	1:C:511:HIS:HB2	2.34	0.57
2:D:519:ARG:CZ	2:D:608:GLY:HA3	2.34	0.57
3:X:111:ASP:CG	3:X:112:PRO:HD2	2.24	0.57
1:A:133:PRO:HD2	1:A:609:VAL:HG11	1.86	0.57
1:A:243:PHE:HE2	1:A:304:GLU:HA	1.70	0.57
1:A:455:ILE:HG22	1:A:456:ALA:N	2.20	0.57
1:A:532:GLN:HE21	1:A:568:GLY:HA2	1.69	0.57
1:A:822:ASP:HA	1:A:849:ARG:HD2	1.87	0.57
2:B:1349:VAL:HG22	2:B:1363:LEU:HD12	1.86	0.57
2:B:1498:SER:O	2:B:1573:LEU:HD23	2.04	0.57
2:B:963:ILE:HG13	2:B:1325:ILE:HG12	1.86	0.57
1:C:225:PRO:HG3	1:C:766:ARG:HB2	1.85	0.57
2:D:1443:LEU:N	2:D:1443:LEU:HD13	2.19	0.57
2:D:244:HIS:HB3	2:D:291:LYS:CD	2.28	0.57
2:D:443:ASN:OD1	2:D:469:ASN:HB3	2.05	0.57
2:D:789:VAL:HG23	2:D:806:TYR:O	2.04	0.57
3:X:125:LYS:HA	3:X:127:ASN:H	1.69	0.57
1:A:1075:SER:HB2	1:A:1120:GLU:OE1	2.04	0.57
1:A:457:TYR:HE1	1:A:556:SER:O	1.88	0.57
1:A:512:PHE:HE2	3:X:148:ALA:HB3	1.70	0.57
1:A:481:HIS:HE1	1:A:529:PRO:HB3	1.64	0.57
1:A:742:ILE:HG21	1:A:753:HIS:HA	1.86	0.57
1:A:943:THR:OG1	1:A:1275:SER:OG	2.22	0.57
1:A:980:LYS:HD3	1:A:986:GLU:CA	2.33	0.57
2:B:519:ARG:CZ	2:B:608:GLY:HA3	2.34	0.57
1:C:126:LEU:HD11	1:C:205:TYR:CE2	2.39	0.57
1:C:489:LYS:C	1:C:491:PRO:HD3	2.24	0.57
1:C:358:ALA:H	1:C:672:ILE:CG2	2.18	0.57
2:D:199:ILE:HG22	2:D:199:ILE:O	2.05	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PHE:CG	1:A:112:SER:N	2.73	0.57
1:A:1130:GLN:OE1	1:A:1232:LEU:HD22	2.03	0.57
1:A:196:TYR:CE1	1:A:221:GLU:HB2	2.40	0.57
1:A:274:ASP:HA	1:A:322:TYR:CD2	2.40	0.57
1:A:342:ILE:HD12	1:A:345:ILE:HD11	1.87	0.57
1:A:493:ILE:HG23	1:A:495:LYS:N	2.18	0.57
2:B:168:PRO:HG3	2:B:197:TRP:N	2.20	0.57
1:C:1562:LYS:CD	1:C:1648:TRP:HE1	2.18	0.57
1:C:571:LEU:HD12	1:C:593:ALA:O	2.05	0.57
1:C:599:TRP:O	1:C:803:GLY:CA	2.49	0.57
1:C:457:TYR:CE2	1:C:641:ASN:HA	2.39	0.57
2:D:1371:TYR:CD1	2:D:1377:SER:HB3	2.40	0.57
2:D:556:ILE:H	2:D:556:ILE:CD1	2.14	0.57
2:D:961:THR:HG22	2:D:1327:THR:CG2	2.32	0.57
1:A:1268:ASN:N	1:A:1269:PRO:CD	2.67	0.57
1:A:1526:LYS:C	1:A:1529:GLU:HG3	2.24	0.57
1:A:1552:ALA:HB2	1:A:1620:MET:CE	2.34	0.57
1:A:359:THR:HG23	1:A:359:THR:O	2.03	0.57
1:A:779:LEU:C	1:A:779:LEU:HD12	2.25	0.57
1:A:977:LEU:HD22	1:A:978:SER:N	2.19	0.57
1:A:981:GLY:HA3	1:A:1333:PHE:HB2	1.85	0.57
2:B:484:LEU:HD11	2:B:626:LEU:CD1	2.34	0.57
2:B:825:VAL:HG22	2:B:916:VAL:HG13	1.86	0.57
1:C:23:TYR:O	1:C:655:THR:HB	2.04	0.57
1:C:443:PRO:HG2	1:C:446:ASN:HB2	1.85	0.57
1:C:788:PHE:HD2	1:C:788:PHE:N	2.03	0.57
1:C:805:SER:O	1:C:807:THR:N	2.38	0.57
2:D:1450:PHE:HD1	2:D:1451:ILE:H	1.53	0.57
2:D:1381:ILE:HG21	2:D:1459:TYR:CE1	2.37	0.57
2:D:218:LYS:HD3	2:D:822:TYR:HE2	1.67	0.57
3:X:101:GLN:HA	3:X:125:LYS:HB3	1.86	0.57
1:A:1221:ASN:HA	1:A:1222:PRO:C	2.23	0.57
1:A:492:TYR:CE2	1:A:493:ILE:HB	2.39	0.57
1:A:544:TYR:C	1:A:544:TYR:HD2	2.08	0.57
1:A:571:LEU:HD23	1:A:812:ALA:HB2	1.87	0.57
1:C:610:TYR:N	1:C:610:TYR:CD1	2.71	0.57
3:X:100:GLY:O	3:X:125:LYS:HG2	2.04	0.57
3:X:75:PHE:O	3:X:77:PRO:HD3	2.05	0.57
3:X:78:LYS:HD2	3:X:78:LYS:C	2.25	0.57
1:A:1239:VAL:HG12	1:A:1239:VAL:O	2.04	0.57
1:A:1429:PRO:HB2	1:A:1432:ILE:HG12	1.86	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1451:THR:O	1:A:1452:ASP:CB	2.53	0.57
1:A:1569:THR:O	1:A:1570:VAL:HG23	2.05	0.57
1:A:22:THR:HG22	1:A:23:TYR:CE1	2.40	0.57
1:C:163:PHE:CE2	1:C:188:PHE:CD1	2.93	0.57
2:D:1544:VAL:HB	2:D:1557:ARG:HA	1.87	0.57
2:D:243:PHE:CE1	2:D:336:ILE:HG21	2.40	0.57
2:D:383:ALA:C	2:D:384:PHE:CD2	2.78	0.57
2:D:51:PRO:O	2:D:52:LYS:HG3	2.05	0.57
3:X:129:THR:HG22	3:X:129:THR:O	2.05	0.57
1:A:1213:LYS:HE2	1:A:1266:TYR:HD2	1.69	0.56
1:A:1240:PRO:HB2	1:A:1242:THR:HG23	1.86	0.56
1:A:1226:ARG:O	1:A:1270:VAL:HG22	2.05	0.56
1:A:1333:PHE:O	1:A:1334:LEU:CB	2.51	0.56
1:A:512:PHE:CD2	1:A:512:PHE:C	2.77	0.56
1:A:362:PHE:CE1	1:A:640:LEU:HB2	2.40	0.56
1:A:953:ILE:HD11	1:A:955:ARG:HH21	1.69	0.56
2:B:476:ILE:O	2:B:476:ILE:CG2	2.52	0.56
1:C:1527:CYS:O	1:C:1529:GLU:N	2.38	0.56
1:C:514:THR:HG22	1:C:515:ARG:N	2.19	0.56
1:C:534:MET:HB3	1:C:538:SER:OG	2.05	0.56
1:C:84:ILE:H	1:C:84:ILE:HD12	1.70	0.56
2:D:558:MET:O	2:D:561:ALA:CB	2.53	0.56
2:D:795:THR:HG22	2:D:796:PRO:CD	2.33	0.56
1:A:1271:ILE:O	1:A:1275:SER:HB3	2.05	0.56
1:A:920:LYS:HZ3	2:B:842:GLU:CD	2.08	0.56
1:A:982:LEU:C	1:A:984:VAL:H	2.09	0.56
2:B:1562:GLN:HE22	2:B:1596:LYS:HZ1	1.52	0.56
2:B:840:VAL:HG12	2:B:841:ASN:N	2.11	0.56
2:B:964:ILE:HG22	2:B:964:ILE:O	2.04	0.56
1:C:1056:ILE:CD1	1:C:1066:TYR:CE2	2.88	0.56
1:C:1493:PHE:HE1	1:C:1495:VAL:HG12	1.69	0.56
1:C:153:LYS:HB3	1:C:154:PRO:CD	2.34	0.56
1:C:571:LEU:HD23	1:C:812:ALA:HB2	1.86	0.56
1:C:938:SER:C	1:C:940:SER:N	2.58	0.56
2:D:1424:ILE:CD1	2:D:1424:ILE:H	2.17	0.56
2:D:1631:PHE:CD2	2:D:1632:SER:N	2.73	0.56
2:D:844:ILE:CD1	2:D:872:ILE:HD11	2.35	0.56
3:X:185:LYS:HG2	3:X:186:TYR:CE2	2.40	0.56
3:Y:75:PHE:O	3:Y:77:PRO:HD3	2.05	0.56
1:A:1117:SER:HA	1:A:1145:THR:OG1	2.05	0.56
1:A:309:GLU:HG2	1:A:310:LEU:N	2.21	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLU:HG2	1:A:310:LEU:HD12	1.86	0.56
1:A:550:GLN:HG2	1:A:550:GLN:O	2.04	0.56
2:B:843:ASP:HA	2:B:873:LYS:O	2.06	0.56
1:A:915:GLU:HB2	2:B:905:TRP:CZ2	2.40	0.56
2:B:916:VAL:HG23	2:B:917:PRO:HD2	1.86	0.56
1:C:473:HIS:O	1:C:473:HIS:HD2	1.88	0.56
1:C:511:HIS:CE1	3:Y:149:SER:CB	2.87	0.56
1:C:981:GLY:HA3	1:C:1333:PHE:HB2	1.85	0.56
2:D:1273:LEU:CB	2:D:1319:GLY:HA3	2.31	0.56
2:D:269:ILE:HA	2:D:312:HIS:CD2	2.40	0.56
2:D:348:THR:HA	2:D:352:LYS:NZ	2.20	0.56
1:C:524:GLN:HB2	2:D:401:ASN:OD1	2.05	0.56
2:D:857:CYS:HB3	2:D:885:VAL:HG22	1.87	0.56
1:A:263:ALA:HB3	1:A:292:LEU:HB3	1.86	0.56
1:A:395:ILE:HD12	1:A:395:ILE:O	2.06	0.56
1:A:979:VAL:HG21	1:A:1326:TYR:CZ	2.36	0.56
2:B:173:VAL:HG11	2:B:186:TYR:OH	2.06	0.56
2:B:581:ASP:O	2:B:583:ALA:N	2.38	0.56
1:C:1000:LEU:O	1:C:1001:THR:HG23	2.06	0.56
1:C:128:ILE:HD12	1:C:201:ILE:CG2	2.32	0.56
1:C:543:TYR:CD1	1:C:543:TYR:O	2.57	0.56
1:C:742:ILE:CG2	1:C:753:HIS:HA	2.34	0.56
2:D:1288:ILE:CD1	2:D:1303:VAL:HG21	2.36	0.56
3:X:47:HIS:O	3:X:51:SER:HB2	2.06	0.56
1:A:1094:GLU:H	1:A:1094:GLU:CD	2.07	0.56
1:A:1227:PHE:CD1	1:A:1227:PHE:C	2.78	0.56
1:A:149:ASN:N	1:A:149:ASN:HD22	1.99	0.56
1:A:267:ILE:HG22	1:A:268:THR:N	2.21	0.56
1:A:680:GLN:O	1:A:684:GLU:HG3	2.04	0.56
1:A:587:THR:CG2	1:A:789:ALA:HB2	2.34	0.56
1:C:1352:PHE:HD2	1:C:1352:PHE:N	2.01	0.56
1:C:161:LEU:HD11	1:C:185:PHE:CE1	2.39	0.56
1:C:265:VAL:O	1:C:289:ASN:HA	2.05	0.56
1:C:395:ILE:O	1:C:395:ILE:HD12	2.05	0.56
1:C:512:PHE:HD2	1:C:512:PHE:O	1.89	0.56
1:C:695:VAL:CG1	1:C:724:CYS:HA	2.35	0.56
2:D:235:PHE:HB3	2:D:338:ILE:HG23	1.88	0.56
1:A:1548:ARG:C	1:A:1550:GLN:H	2.09	0.56
1:A:308:LYS:HG3	1:A:309:GLU:N	2.21	0.56
1:A:355:ASN:HD22	1:A:355:ASN:N	2.03	0.56
1:A:617:LYS:HB3	1:A:619:PRO:HD2	1.88	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:MET:SD	1:A:843:GLY:HA3	2.45	0.56
2:B:946:LYS:HA	2:B:1310:ASP:OD1	2.05	0.56
2:B:142:PRO:HB3	2:B:187:ASN:ND2	2.20	0.56
2:B:1562:GLN:NE2	2:B:1596:LYS:HZ2	2.03	0.56
2:B:913:LEU:C	2:B:913:LEU:HD23	2.26	0.56
1:C:1217:LEU:HD13	1:C:1237:SER:HA	1.88	0.56
1:C:22:THR:HG22	1:C:23:TYR:CE1	2.40	0.56
1:C:641:ASN:OD1	1:C:644:ASN:HB2	2.06	0.56
2:D:183:PHE:CD2	2:D:183:PHE:N	2.72	0.56
2:D:39:GLU:OE1	2:D:488:LYS:HB3	2.06	0.56
2:D:435:TYR:OH	2:D:532:VAL:HG22	2.05	0.56
2:D:484:LEU:HD11	2:D:626:LEU:CD1	2.35	0.56
3:X:77:PRO:O	3:X:78:LYS:HB3	2.06	0.56
1:A:25:ILE:CB	1:A:655:THR:HG23	2.36	0.56
2:B:1509:PRO:O	2:B:1512:ILE:HG13	2.06	0.56
1:C:149:ASN:HD22	1:C:149:ASN:N	1.92	0.56
1:C:827:MET:SD	1:C:843:GLY:HA3	2.45	0.56
2:D:1510:LEU:HD21	2:D:1514:LYS:HZ1	1.70	0.56
2:D:494:ARG:CG	2:D:494:ARG:HH11	2.15	0.56
2:D:953:ARG:CZ	2:D:959:ILE:HD11	2.36	0.56
1:A:135:TYR:CD1	1:A:141:VAL:HG22	2.41	0.56
1:A:33:VAL:HG21	1:A:121:TYR:HE1	1.66	0.56
1:A:351:PRO:HG2	1:A:352:TYR:CE2	2.40	0.56
1:A:489:LYS:C	1:A:491:PRO:HD3	2.26	0.56
1:A:655:THR:O	1:A:656:ASN:C	2.43	0.56
1:A:788:PHE:N	1:A:788:PHE:CD2	2.73	0.56
1:A:42:GLN:CA	1:A:80:GLN:HG3	2.35	0.56
2:B:595:GLN:O	2:B:598:ILE:HB	2.05	0.56
1:C:267:ILE:HD12	1:C:299:VAL:HG11	1.88	0.56
1:C:874:ASP:HA	1:C:878:THR:O	2.05	0.56
1:A:1110:ASN:OD1	1:A:1110:ASN:N	2.38	0.56
1:C:1323:LEU:CD1	1:C:1324:HIS:H	2.19	0.56
1:C:135:TYR:CD1	1:C:141:VAL:HG22	2.40	0.56
1:C:1585:TYR:CD1	1:C:1671:ILE:HG12	2.41	0.56
2:D:1384:ILE:HB	2:D:1423:VAL:HG12	1.87	0.56
2:D:167:THR:HG23	2:D:171:ILE:N	2.20	0.56
2:D:518:PHE:CD2	2:D:538:VAL:HB	2.38	0.56
2:D:599:TRP:HA	2:D:599:TRP:HE3	1.70	0.56
2:D:829:GLN:HA	2:D:885:VAL:HG12	1.88	0.56
3:X:110:ILE:HG22	3:X:111:ASP:O	2.05	0.56
1:A:43:VAL:HG11	1:A:73:LEU:CD1	2.36	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:TYR:CE2	1:A:99:VAL:HG21	2.41	0.56
1:A:59:TYR:CE1	1:A:60:PRO:HG3	2.41	0.56
2:B:1288:ILE:CD1	2:B:1303:VAL:HG21	2.36	0.56
2:B:282:ARG:C	2:B:283:ILE:HD12	2.25	0.56
2:B:345:ILE:HD11	2:B:427:THR:N	2.21	0.56
2:B:520:PHE:O	2:B:535:SER:HA	2.06	0.56
1:C:1429:PRO:HB2	1:C:1432:ILE:HG12	1.86	0.56
1:C:1559:TYR:CD1	1:C:1561:TYR:HE2	2.23	0.56
1:C:24:VAL:HG21	1:C:554:LEU:HD11	1.88	0.56
1:C:774:LEU:HG	1:C:788:PHE:CE1	2.41	0.56
2:D:525:GLN:HA	2:D:530:GLU:O	2.05	0.56
2:D:599:TRP:CZ3	2:D:602:ILE:HD12	2.40	0.56
2:D:824:VAL:HG22	2:D:825:VAL:N	2.20	0.56
3:Y:127:ASN:OD1	3:Y:158:GLU:HB3	2.06	0.56
1:A:1095:GLN:O	1:A:1097:GLN:N	2.39	0.56
1:A:115:LYS:HB2	1:A:654:LEU:CD2	2.35	0.56
1:A:1450:PHE:HZ	1:A:1475:VAL:HB	1.70	0.56
1:A:1598:ILE:HG22	1:A:1599:THR:H	1.70	0.56
1:A:78:LYS:HG3	3:X:146:LEU:HB2	1.87	0.56
2:B:69:PHE:C	2:B:69:PHE:CD2	2.79	0.56
2:B:789:VAL:HG23	2:B:806:TYR:O	2.05	0.56
2:B:916:VAL:HG22	2:B:917:PRO:O	2.05	0.56
1:C:1128:LYS:C	1:C:1129:LEU:HD23	2.27	0.56
1:C:1559:TYR:CD1	1:C:1561:TYR:CE2	2.94	0.56
1:C:577:PRO:CD	1:C:588:VAL:HG23	2.36	0.56
2:D:422:ARG:HH12	3:Y:44:ARG:CA	2.18	0.56
2:D:826:LYS:NZ	2:D:1488:ASN:HB3	2.21	0.56
2:D:829:GLN:HE22	2:D:883:VAL:CG1	2.14	0.56
2:D:40:GLN:HG3	2:D:86:THR:HG23	1.88	0.56
2:D:885:VAL:HG23	2:D:885:VAL:O	2.06	0.56
1:A:1132:THR:O	1:A:1134:PRO:N	2.39	0.55
1:A:1585:TYR:CE1	1:A:1671:ILE:HG12	2.40	0.55
1:A:290:THR:O	1:A:291:MET:HB2	2.05	0.55
1:A:489:LYS:HG2	1:A:490:SER:N	2.21	0.55
1:A:610:TYR:CD1	1:A:610:TYR:N	2.73	0.55
1:A:680:GLN:HB2	1:A:684:GLU:OE2	2.06	0.55
1:A:695:VAL:CG1	1:A:724:CYS:HA	2.35	0.55
2:B:1284:ARG:CG	2:B:1285:GLU:N	2.69	0.55
2:B:1621:PHE:O	2:B:1622:GLN:C	2.43	0.55
2:B:1628:PHE:O	2:B:1630:GLN:N	2.39	0.55
2:B:34:ARG:HD2	2:B:488:LYS:NZ	2.21	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:LEU:HD11	1:C:205:TYR:CZ	2.41	0.55
1:C:617:LYS:HB3	1:C:619:PRO:HD2	1.88	0.55
1:C:693:SER:C	1:C:695:VAL:N	2.60	0.55
2:D:1280:GLU:HG2	2:D:1287:PRO:CB	2.33	0.55
2:D:1424:ILE:HG12	2:D:1426:TYR:HE2	1.70	0.55
2:D:1612:HIS:O	2:D:1613:GLU:C	2.44	0.55
2:D:355:LYS:O	2:D:358:MET:CB	2.54	0.55
2:D:595:GLN:O	2:D:598:ILE:HB	2.07	0.55
1:A:1219:LYS:CD	1:A:1239:VAL:HG21	2.36	0.55
1:A:1421:HIS:HD2	1:A:1422:ALA:N	2.03	0.55
1:A:1433:SER:OG	1:A:1482:LEU:HD12	2.06	0.55
2:B:1371:TYR:CD1	2:B:1377:SER:HB3	2.41	0.55
1:C:1108:VAL:HG21	1:C:1167:ALA:CB	2.34	0.55
1:C:1274:LEU:O	1:C:1277:GLU:N	2.37	0.55
1:C:351:PRO:HG3	1:C:442:LEU:HD11	1.88	0.55
2:D:1593:THR:CG2	2:D:1594:LYS:N	2.68	0.55
3:Y:58:SER:HB2	3:Y:125:LYS:HE3	1.87	0.55
3:Y:100:GLY:O	3:Y:125:LYS:HG2	2.05	0.55
3:Y:146:LEU:HD21	3:Y:148:ALA:HB2	1.88	0.55
1:A:1053:MET:CE	1:A:1086:LEU:HD22	2.37	0.55
1:A:1190:ILE:HG22	1:A:1191:SER:N	2.20	0.55
1:A:1453:TYR:O	1:A:1453:TYR:CG	2.59	0.55
1:A:198:MET:SD	1:A:218:GLU:HG3	2.45	0.55
2:B:355:LYS:O	2:B:358:MET:HB3	2.07	0.55
1:C:1083:LEU:HD13	1:C:1104:LEU:HD23	1.89	0.55
1:C:1527:CYS:C	1:C:1529:GLU:H	2.10	0.55
1:C:1562:LYS:O	1:C:1563:VAL:CG1	2.54	0.55
1:C:1627:ILE:O	1:C:1627:ILE:CD1	2.54	0.55
1:C:549:GLU:CD	1:C:550:GLN:N	2.60	0.55
1:C:644:ASN:CG	1:C:648:LEU:HD12	2.26	0.55
2:D:481:TYR:CE2	2:D:493:GLY:HA3	2.41	0.55
1:C:855:PHE:HA	2:D:904:LEU:HD11	1.87	0.55
3:Y:40:LEU:HD11	3:Y:209:PHE:CZ	2.41	0.55
3:Y:41:HIS:O	3:Y:42:ASP:CB	2.54	0.55
1:A:1232:LEU:HG	1:A:1233:GLN:N	2.21	0.55
1:A:428:VAL:HG22	1:A:429:THR:N	2.22	0.55
1:A:364:LYS:HE3	1:A:457:TYR:HD1	1.72	0.55
2:B:42:LEU:HD22	2:B:492:VAL:HG21	1.87	0.55
1:C:1130:GLN:OE1	1:C:1232:LEU:HD22	2.05	0.55
1:C:1611:LEU:HD13	1:C:1617:TYR:CD1	2.41	0.55
1:C:478:VAL:CG1	1:C:566:LYS:HD3	2.37	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ASN:ND2	1:C:81:ASN:HB2	2.22	0.55
1:C:788:PHE:CD2	1:C:788:PHE:N	2.74	0.55
2:D:456:PRO:CG	2:D:515:ILE:HD11	2.37	0.55
1:A:1056:ILE:O	1:A:1056:ILE:HG12	2.05	0.55
1:A:1180:LEU:HG	1:A:1208:ILE:HG12	1.89	0.55
1:A:153:LYS:HB3	1:A:154:PRO:CD	2.35	0.55
1:A:180:ILE:HG22	1:A:181:GLY:N	2.22	0.55
1:A:532:GLN:O	1:A:535:VAL:HG13	2.07	0.55
1:A:923:LEU:HD23	1:A:924:VAL:N	2.22	0.55
1:A:934:VAL:CG2	1:A:1366:HIS:CD2	2.88	0.55
2:B:130:ILE:HG12	2:B:147:VAL:HG23	1.87	0.55
2:B:1606:TRP:C	2:B:1606:TRP:HD1	2.10	0.55
2:B:51:PRO:O	2:B:52:LYS:HG3	2.06	0.55
2:B:558:MET:O	2:B:561:ALA:CB	2.55	0.55
1:C:1108:VAL:CG2	1:C:1167:ALA:HB2	2.36	0.55
1:C:1180:LEU:HG	1:C:1208:ILE:HG12	1.88	0.55
1:C:1287:THR:OG1	1:C:1288:GLN:N	2.39	0.55
1:C:504:LEU:HD21	1:C:651:LEU:HG	1.88	0.55
2:D:1562:GLN:HB2	2:D:1598:SER:HB3	1.88	0.55
2:D:343:TYR:HE1	2:D:420:LEU:HD11	1.72	0.55
2:D:512:PRO:HA	2:D:515:ILE:HD12	1.87	0.55
2:D:76:ASN:HB2	2:D:77:PRO:HD2	1.88	0.55
2:D:826:LYS:HG3	2:D:887:LEU:O	2.05	0.55
3:X:87:LEU:HA	3:X:91:LYS:CD	2.37	0.55
3:Y:146:LEU:HD22	3:Y:146:LEU:C	2.26	0.55
1:A:1228:TRP:N	1:A:1228:TRP:CE3	2.75	0.55
1:A:1272:LYS:O	1:A:1276:GLU:HG3	2.07	0.55
1:A:811:VAL:O	1:A:811:VAL:HG12	2.05	0.55
1:A:851:SER:O	1:A:890:GLY:HA2	2.07	0.55
2:B:233:LYS:HG3	2:B:233:LYS:O	2.05	0.55
2:B:365:TYR:HA	2:B:394:GLY:O	2.07	0.55
1:C:1453:TYR:O	1:C:1453:TYR:CG	2.59	0.55
1:C:1615:ARG:HD2	1:C:1647:TYR:HD1	1.71	0.55
1:C:24:VAL:HA	1:C:655:THR:HG21	1.87	0.55
1:C:256:TYR:HB3	1:C:848:TYR:OH	2.06	0.55
1:C:947:ARG:O	1:C:949:ILE:HG12	2.06	0.55
2:D:1591:LEU:C	2:D:1591:LEU:CD2	2.75	0.55
2:D:28:ILE:HD13	2:D:621:PHE:HE1	1.70	0.55
1:A:1188:LEU:HD23	1:A:1212:LEU:HA	1.89	0.55
2:B:1594:LYS:HA	2:B:1594:LYS:CE	2.18	0.55
2:B:276:ILE:O	2:B:277:PRO:C	2.45	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1132:THR:O	1:C:1134:PRO:N	2.39	0.55
1:C:1327:LYS:O	1:C:1332:ASN:ND2	2.39	0.55
2:D:130:ILE:HD13	2:D:199:ILE:CG2	2.36	0.55
2:D:261:ALA:HB3	2:D:285:ILE:HD11	1.88	0.55
2:D:476:ILE:HG23	2:D:476:ILE:O	2.06	0.55
2:D:481:TYR:HE2	2:D:493:GLY:HA3	1.71	0.55
2:D:838:ASN:OD1	2:D:840:VAL:HG23	2.07	0.55
1:A:1344:ASP:OD1	1:A:1345:ASP:N	2.40	0.55
1:A:1571:GLU:O	1:A:1574:PHE:CD2	2.60	0.55
1:A:569:ASN:ND2	1:A:570:GLN:H	2.04	0.55
1:A:596:MET:H	1:A:782:ARG:NH1	1.92	0.55
1:A:834:VAL:O	1:A:837:GLU:HB2	2.07	0.55
1:A:85:LEU:HD22	1:A:85:LEU:N	2.22	0.55
1:A:873:ILE:HD12	1:A:873:ILE:O	2.06	0.55
1:A:906:GLY:O	1:A:908:HIS:NE2	2.40	0.55
2:B:862:LYS:HD2	2:B:1588:SER:OG	2.06	0.55
2:B:1591:LEU:C	2:B:1591:LEU:CD2	2.75	0.55
2:B:343:TYR:HE1	2:B:420:LEU:HD11	1.71	0.55
2:B:847:ARG:O	2:B:898:ALA:HA	2.07	0.55
2:B:928:VAL:HG23	2:B:1323:MET:HB3	1.87	0.55
1:C:1019:PHE:CD2	1:C:1020:TYR:N	2.75	0.55
1:C:1333:PHE:O	1:C:1334:LEU:CB	2.53	0.55
1:C:1383:THR:HG21	1:C:1511:THR:HG22	1.88	0.55
1:C:510:ILE:HA	3:Y:150:ILE:HG13	1.87	0.55
1:C:539:ARG:HE	1:C:633:GLY:HA3	1.71	0.55
1:C:612:VAL:O	1:C:612:VAL:HG12	2.06	0.55
1:C:599:TRP:CD1	1:C:779:LEU:HA	2.41	0.55
1:C:824:PHE:N	1:C:824:PHE:CD2	2.69	0.55
2:D:1349:VAL:HG22	2:D:1363:LEU:HD12	1.88	0.55
2:D:1602:THR:H	2:D:1605:THR:HB	1.72	0.55
2:D:42:LEU:HD22	2:D:492:VAL:HG21	1.89	0.55
3:Y:134:THR:CG2	3:Y:153:PHE:HB3	2.37	0.55
1:A:1013:MET:HA	1:A:1016:VAL:HG23	1.88	0.55
1:A:614:ARG:C	1:A:614:ARG:HD2	2.24	0.55
2:B:243:PHE:CE1	2:B:336:ILE:HG21	2.42	0.55
2:B:285:ILE:CD1	2:B:285:ILE:N	2.70	0.55
2:B:443:ASN:OD1	2:B:469:ASN:HB3	2.06	0.55
2:B:447:VAL:O	2:B:447:VAL:HG13	2.06	0.55
2:B:923:SER:O	2:B:924:ILE:HD12	2.07	0.55
1:C:1218:VAL:CG1	1:C:1219:LYS:H	2.17	0.55
1:C:145:VAL:HB	1:C:183:ILE:CG1	2.34	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1561:TYR:CD1	1:C:1581:LEU:HD21	2.42	0.55
1:C:1556:GLU:CB	1:C:1622:LYS:HE2	2.30	0.55
1:C:199:TRP:CB	1:C:217:PHE:CE1	2.90	0.55
1:C:290:THR:O	1:C:291:MET:HB2	2.07	0.55
1:C:697:LYS:O	1:C:700:TYR:HB3	2.06	0.55
2:D:1381:ILE:HB	2:D:1459:TYR:CD1	2.42	0.55
2:D:184:TRP:HB2	2:D:185:PRO:CD	2.37	0.55
3:Y:107:GLN:OE1	3:Y:110:ILE:HD11	2.07	0.55
1:A:1474:CYS:HB3	1:A:1476:ARG:NH1	2.22	0.55
1:A:44:TYR:CZ	1:A:497:THR:HG21	2.41	0.55
1:A:773:TRP:HZ3	1:A:788:PHE:CE1	2.25	0.55
1:A:936:ARG:HH12	1:A:1284:PHE:HZ	1.53	0.55
2:B:26:THR:HG22	2:B:630:THR:HG22	1.88	0.55
2:B:523:TYR:HD2	2:B:621:PHE:HZ	1.55	0.55
2:B:965:ILE:HG13	2:B:1301:ARG:CB	2.26	0.55
1:C:1095:GLN:O	1:C:1097:GLN:N	2.41	0.55
1:C:1227:PHE:HB2	1:C:1251:THR:HG21	1.89	0.55
1:C:134:VAL:C	1:C:135:TYR:HD2	2.10	0.55
1:C:171:VAL:CG1	1:C:172:ASP:N	2.70	0.55
1:C:308:LYS:HG3	1:C:309:GLU:N	2.21	0.55
1:C:342:ILE:HG22	1:C:343:PRO:HD2	1.88	0.55
1:C:503:ILE:HD11	1:C:540:LEU:HD13	1.89	0.55
2:D:1530:ARG:HG3	2:D:1530:ARG:HH11	1.72	0.55
3:Y:50:TYR:HE2	3:Y:170:ARG:CZ	2.19	0.55
3:Y:87:LEU:HA	3:Y:91:LYS:CD	2.36	0.55
1:A:1554:LYS:HG3	1:A:1555:PRO:HD2	1.88	0.54
1:A:42:GLN:HE21	1:A:43:VAL:C	2.11	0.54
1:A:662:SER:O	1:A:663:GLN:HG2	2.07	0.54
2:B:126:SER:O	2:B:208:GLU:HG3	2.07	0.54
2:B:1522:TYR:N	2:B:1522:TYR:CD2	2.73	0.54
2:B:1633:TYR:CE1	2:B:1637:GLU:OE1	2.59	0.54
2:B:167:THR:HG23	2:B:171:ILE:N	2.23	0.54
2:B:380:VAL:CG1	2:B:387:MET:HB3	2.27	0.54
2:B:39:GLU:OE1	2:B:488:LYS:HB3	2.07	0.54
1:C:1221:ASN:HA	1:C:1222:PRO:C	2.26	0.54
1:C:127:PHE:HE2	1:C:623:VAL:CG1	2.09	0.54
1:C:1601:ILE:O	1:C:1638:PRO:O	2.25	0.54
1:C:231:ILE:O	1:C:231:ILE:HG23	2.06	0.54
1:C:505:SER:HB3	1:C:510:ILE:CD1	2.37	0.54
1:C:705:VAL:HA	1:C:739:ARG:NH2	2.21	0.54
1:C:587:THR:CG2	1:C:789:ALA:HB2	2.37	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1536:GLY:O	2:D:1567:ARG:HG2	2.07	0.54
2:D:1506:ILE:CD1	2:D:1628:PHE:CE1	2.89	0.54
2:D:96:THR:HG21	2:D:102:GLN:OE1	2.06	0.54
3:Y:111:ASP:CG	3:Y:112:PRO:HD2	2.27	0.54
3:Y:47:HIS:O	3:Y:51:SER:HB2	2.07	0.54
1:A:1013:MET:HE2	1:A:1287:THR:HB	1.88	0.54
1:A:1421:HIS:CD2	1:A:1421:HIS:C	2.78	0.54
1:A:1421:HIS:CE1	1:A:1498:TYR:CD1	2.95	0.54
1:A:316:GLU:HG2	1:A:349:LEU:HD23	1.88	0.54
1:A:494:ASP:CG	1:A:495:LYS:HE2	2.28	0.54
1:A:694:VAL:O	1:A:697:LYS:HE2	2.06	0.54
1:A:824:PHE:CZ	1:A:846:TYR:HD1	2.26	0.54
1:A:854:GLN:NE2	1:A:854:GLN:H	2.05	0.54
1:A:871:PRO:CD	1:A:872:VAL:N	2.68	0.54
2:B:410:PRO:HA	2:B:431:THR:HG22	1.89	0.54
2:B:953:ARG:CZ	2:B:959:ILE:HD11	2.37	0.54
1:C:1562:LYS:O	1:C:1563:VAL:HG13	2.06	0.54
1:C:222:TYR:CD1	1:C:768:TYR:HB2	2.42	0.54
1:C:359:THR:HG23	1:C:359:THR:O	2.08	0.54
1:C:428:VAL:HG22	1:C:429:THR:H	1.72	0.54
1:C:549:GLU:CG	1:C:550:GLN:H	2.19	0.54
1:C:967:LEU:HD13	1:C:1365:VAL:HG22	1.89	0.54
1:A:1611:LEU:HD13	1:A:1617:TYR:CD1	2.43	0.54
1:A:1562:LYS:CD	1:A:1648:TRP:CZ2	2.86	0.54
1:A:472:ASN:O	1:A:473:HIS:HB3	2.07	0.54
1:A:656:ASN:CG	1:A:658:ASN:HB3	2.27	0.54
2:B:1593:THR:CG2	2:B:1594:LYS:H	2.20	0.54
2:B:218:LYS:HD3	2:B:822:TYR:HE2	1.72	0.54
1:C:1013:MET:HA	1:C:1016:VAL:HG23	1.90	0.54
1:C:1011:GLU:O	1:C:1014:SER:HB3	2.08	0.54
1:C:1117:SER:HA	1:C:1145:THR:OG1	2.07	0.54
1:C:1236:ASP:O	1:C:1238:SER:N	2.35	0.54
1:C:455:ILE:HG22	1:C:456:ALA:N	2.22	0.54
1:C:472:ASN:O	1:C:473:HIS:HB3	2.06	0.54
1:C:696:LYS:NZ	1:C:759:PRO:CD	2.64	0.54
2:D:1387:LEU:HD21	2:D:1472:TYR:CE1	2.42	0.54
2:D:1486:ILE:HD11	2:D:1591:LEU:CD2	2.37	0.54
2:D:559:PRO:HG2	2:D:812:LYS:HD2	1.88	0.54
3:X:125:LYS:HA	3:X:126:ASN:C	2.25	0.54
3:X:46:LEU:HD12	3:X:180:TYR:CE1	2.43	0.54
3:Y:166:ASP:HB2	3:Y:207:LEU:HD21	1.89	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1279:ARG:HD3	1:A:1280:TYR:N	2.22	0.54
1:A:1020:TYR:CE1	1:A:1295:GLU:HG3	2.39	0.54
1:A:126:LEU:HD11	1:A:205:TYR:CZ	2.43	0.54
1:A:25:ILE:HD13	1:A:41:ILE:CB	2.37	0.54
1:A:490:SER:N	1:A:491:PRO:CD	2.70	0.54
1:A:44:TYR:CB	1:A:545:ILE:HD12	2.38	0.54
2:B:954:VAL:HG23	2:B:1330:ASN:O	2.07	0.54
2:B:1443:LEU:N	2:B:1443:LEU:HD13	2.23	0.54
2:B:775:THR:HG22	2:B:776:MET:H	1.72	0.54
1:C:1569:THR:O	1:C:1570:VAL:HG23	2.07	0.54
1:C:1582:LEU:HD11	1:C:1648:TRP:CZ2	2.43	0.54
1:C:1562:LYS:HD2	1:C:1648:TRP:CE2	2.42	0.54
1:C:42:GLN:HE21	1:C:43:VAL:C	2.10	0.54
1:C:658:ASN:O	1:C:659:ALA:CB	2.55	0.54
1:C:680:GLN:HG3	1:C:681:LYS:H	1.72	0.54
1:C:779:LEU:HD12	1:C:780:VAL:N	2.22	0.54
2:D:1278:THR:HB	2:D:1314:THR:HB	1.90	0.54
2:D:503:LEU:C	2:D:503:LEU:HD23	2.28	0.54
2:D:775:THR:HG22	2:D:776:MET:H	1.71	0.54
1:A:1084:ARG:HD2	1:A:1154:LYS:HG3	1.90	0.54
1:A:1188:LEU:HD23	1:A:1212:LEU:HD13	1.88	0.54
1:A:1402:ILE:HG13	1:A:1479:ILE:HD13	1.89	0.54
1:A:705:VAL:HA	1:A:739:ARG:NH2	2.22	0.54
1:A:594:THR:O	1:A:782:ARG:HD2	2.07	0.54
1:A:989:SER:O	1:A:993:SER:CB	2.56	0.54
2:B:1274:ASN:OD1	2:B:1291:ARG:NH2	2.41	0.54
1:C:234:GLU:HB3	1:C:246:PHE:HE1	1.72	0.54
1:C:662:SER:O	1:C:663:GLN:HG2	2.07	0.54
1:C:895:LEU:HD12	1:C:896:VAL:N	2.22	0.54
2:D:1636:THR:HG22	2:D:1637:GLU:HG3	1.89	0.54
3:X:119:VAL:HG21	3:X:209:PHE:CB	2.38	0.54
1:A:100:SER:O	1:A:101:TYR:HB2	2.06	0.54
1:A:1133:LEU:HD12	1:A:1133:LEU:N	2.06	0.54
1:A:1440:LYS:O	1:A:1444:GLU:HG3	2.08	0.54
1:A:145:VAL:HB	1:A:183:ILE:CG1	2.33	0.54
1:A:903:LEU:N	1:A:903:LEU:HD22	2.23	0.54
2:B:1288:ILE:HD13	2:B:1303:VAL:HG21	1.90	0.54
2:B:1638:PHE:O	2:B:1639:GLY:O	2.26	0.54
1:C:109:LYS:HD3	1:C:110:HIS:HE1	1.73	0.54
1:C:1084:ARG:HD2	1:C:1154:LYS:HG3	1.88	0.54
1:C:1112:GLN:NE2	1:C:1171:ALA:HB2	2.21	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1188:LEU:HD23	1:C:1212:LEU:CD1	2.37	0.54
1:C:987:ILE:HD11	1:C:1294:ILE:HG23	1.90	0.54
1:C:155:ALA:O	1:C:157:ARG:N	2.40	0.54
1:C:309:GLU:HG2	1:C:310:LEU:N	2.22	0.54
1:C:515:ARG:HG3	1:C:526:ILE:CG2	2.38	0.54
1:C:680:GLN:HB2	1:C:684:GLU:OE2	2.07	0.54
1:C:594:THR:O	1:C:782:ARG:HD2	2.08	0.54
2:D:126:SER:O	2:D:208:GLU:HG3	2.08	0.54
1:A:1549:LYS:HD3	1:A:1667:PHE:CB	2.38	0.54
1:A:154:PRO:O	1:A:155:ALA:CB	2.55	0.54
1:A:199:TRP:CB	1:A:217:PHE:CE1	2.91	0.54
1:A:316:GLU:HG2	1:A:349:LEU:CD2	2.37	0.54
1:A:398:ASN:O	1:A:399:GLN:CB	2.56	0.54
1:A:847:ASN:ND2	1:A:853:MET:HB3	2.23	0.54
1:A:917:TRP:HA	1:A:917:TRP:CE3	2.43	0.54
2:B:1279:ILE:CG2	2:B:1288:ILE:HB	2.35	0.54
2:B:184:TRP:HB2	2:B:185:PRO:CD	2.37	0.54
2:B:861:THR:O	2:B:863:GLY:N	2.41	0.54
1:C:1082:ALA:O	1:C:1086:LEU:HD23	2.07	0.54
1:C:1112:GLN:HB2	1:C:1118:PHE:CE1	2.43	0.54
1:A:1102:ASN:HD21	1:C:1162:VAL:HG22	1.67	0.54
1:C:1278:GLN:NE2	1:C:1293:ALA:HB1	2.22	0.54
1:C:1020:TYR:CE1	1:C:1295:GLU:HG3	2.35	0.54
1:C:23:TYR:HE2	1:C:111:PHE:CD2	2.26	0.54
1:C:489:LYS:HG2	1:C:490:SER:N	2.22	0.54
1:C:614:ARG:HD2	1:C:614:ARG:C	2.24	0.54
1:C:612:VAL:HG21	1:C:769:PHE:HZ	1.72	0.54
2:D:46:HIS:ND1	2:D:525:GLN:HG2	2.22	0.54
2:D:69:PHE:CE1	2:D:87:ILE:HA	2.43	0.54
2:D:861:THR:O	2:D:863:GLY:N	2.41	0.54
3:X:50:TYR:HE2	3:X:170:ARG:CZ	2.21	0.54
3:Y:86:LEU:HG	3:Y:91:LYS:HG3	1.88	0.54
1:A:1108:VAL:CG2	1:A:1167:ALA:HB2	2.38	0.54
1:A:641:ASN:OD1	1:A:644:ASN:HB2	2.08	0.54
1:A:771:GLU:HG3	1:A:772:SER:O	2.08	0.54
2:B:1611:PRO:HD3	2:B:1624:LEU:HD23	1.90	0.54
2:B:28:ILE:HD13	2:B:621:PHE:HE1	1.72	0.54
2:B:941:GLN:HE21	2:B:943:GLU:HG2	1.71	0.54
1:C:1094:GLU:CD	1:C:1094:GLU:H	2.11	0.54
1:C:190:ILE:HD12	1:C:219:VAL:HG21	1.90	0.54
1:C:512:PHE:C	1:C:512:PHE:CD2	2.75	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:656:ASN:CG	1:C:658:ASN:HB3	2.26	0.54
2:D:1509:PRO:O	2:D:1512:ILE:HG13	2.08	0.54
2:D:1562:GLN:HE22	2:D:1596:LYS:HZ2	1.53	0.54
2:D:168:PRO:HG3	2:D:197:TRP:N	2.21	0.54
2:D:595:GLN:OE1	2:D:595:GLN:HA	2.07	0.54
3:X:139:ASN:HD22	3:X:148:ALA:HB1	1.72	0.54
3:Y:163:LYS:HG3	3:Y:212:MET:SD	2.48	0.54
1:A:74:SER:HA	1:A:79:PHE:HE1	1.73	0.54
2:B:175:SER:N	2:B:1300:ALA:HB2	2.20	0.54
2:B:595:GLN:OE1	2:B:595:GLN:HA	2.06	0.54
1:C:1133:LEU:HB2	1:C:1134:PRO:HD3	1.90	0.54
1:C:1286:SER:OG	1:C:1287:THR:N	2.40	0.54
1:C:1548:ARG:C	1:C:1550:GLN:H	2.11	0.54
1:C:497:THR:OG1	1:C:498:HIS:N	2.38	0.54
1:C:753:HIS:O	1:C:754:MET:CB	2.52	0.54
1:C:907:LEU:HG	1:C:908:HIS:N	2.23	0.54
1:C:950:TYR:C	1:C:952:THR:H	2.11	0.54
2:D:57:PHE:HD1	2:D:59:HIS:NE2	2.05	0.54
3:Y:125:LYS:HA	3:Y:127:ASN:H	1.72	0.54
1:A:134:VAL:C	1:A:135:TYR:CD2	2.81	0.54
1:A:1629:TYR:CE1	1:A:1634:ARG:NH2	2.76	0.54
1:A:484:ILE:HG23	1:A:526:ILE:HG13	1.88	0.54
2:B:736:GLU:CD	2:B:737:ASP:H	2.11	0.54
2:B:826:LYS:HG3	2:B:887:LEU:O	2.08	0.54
1:C:430:VAL:HG11	1:C:453:ARG:NH2	2.17	0.54
1:C:44:TYR:CB	1:C:545:ILE:HD12	2.36	0.54
1:C:490:SER:N	1:C:491:PRO:CD	2.71	0.54
1:C:773:TRP:HZ3	1:C:788:PHE:CE1	2.25	0.54
1:C:796:THR:HA	1:C:818:LYS:HA	1.89	0.54
1:C:87:ILE:N	1:C:87:ILE:CD1	2.66	0.54
2:D:1415:ASN:O	2:D:1417:MET:HG3	2.08	0.54
2:D:528:ASN:OD1	2:D:528:ASN:N	2.41	0.54
2:D:585:TYR:CD2	2:D:788:VAL:HG11	2.42	0.54
2:D:820:MET:HG3	2:D:821:PRO:HD2	1.90	0.54
2:D:952:ASP:O	2:D:1331:ALA:HA	2.08	0.54
1:A:1150:ILE:CD1	1:A:1193:TYR:CD2	2.91	0.53
1:A:1623:GLU:HB2	1:A:1638:PRO:CD	2.38	0.53
1:A:287:MET:HG2	1:A:299:VAL:HG21	1.89	0.53
5:B:2001:NAG:H3	5:B:2002:NAG:O5	2.07	0.53
2:B:243:PHE:CD1	2:B:314:LEU:HD23	2.41	0.53
2:B:87:ILE:H	2:B:87:ILE:HD12	1.73	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1190:ILE:HG22	1:C:1191:SER:N	2.22	0.53
1:C:1199:ASP:C	1:C:1201:THR:H	2.10	0.53
1:C:1268:ASN:N	1:C:1269:PRO:CD	2.71	0.53
1:C:1421:HIS:CE1	1:C:1498:TYR:CD1	2.95	0.53
1:C:24:VAL:HG11	1:C:543:TYR:CZ	2.43	0.53
1:C:625:GLN:O	1:C:628:GLU:HB3	2.08	0.53
2:D:130:ILE:HG12	2:D:147:VAL:HG23	1.89	0.53
2:D:1344:HIS:ND1	5:D:2003:NAG:H82	2.23	0.53
2:D:1593:THR:CG2	2:D:1594:LYS:H	2.21	0.53
2:D:476:ILE:HD11	2:D:524:TYR:CD2	2.43	0.53
1:A:149:ASN:O	1:A:151:ASP:N	2.40	0.53
1:A:1631:PHE:N	1:A:1631:PHE:CD2	2.74	0.53
1:A:250:ILE:HD11	1:A:265:VAL:CG1	2.37	0.53
2:B:1345:LEU:HD21	2:B:1456:VAL:HG12	1.90	0.53
2:B:384:PHE:HD1	2:B:400:LEU:HG	1.67	0.53
2:B:546:GLY:HA3	2:B:570:ASP:OD1	2.08	0.53
2:B:606:ASP:OD1	2:B:606:ASP:O	2.26	0.53
1:C:33:VAL:CG2	1:C:121:TYR:HD1	2.20	0.53
1:C:1304:VAL:CG1	1:C:1305:LYS:H	2.21	0.53
1:C:1548:ARG:HE	1:C:1550:GLN:NE2	2.07	0.53
1:C:222:TYR:HE2	1:C:224:LEU:CA	2.21	0.53
1:C:263:ALA:HB3	1:C:292:LEU:HB3	1.90	0.53
1:C:40:VAL:HG23	1:C:41:ILE:H	1.73	0.53
1:C:25:ILE:HD13	1:C:41:ILE:CB	2.36	0.53
1:C:980:LYS:HD3	1:C:986:GLU:CA	2.37	0.53
1:C:982:LEU:C	1:C:984:VAL:N	2.61	0.53
2:D:365:TYR:HA	2:D:394:GLY:O	2.08	0.53
2:D:437:THR:HG23	2:D:444:TYR:CD1	2.43	0.53
2:D:963:ILE:HG13	2:D:1325:ILE:HG12	1.90	0.53
3:X:107:GLN:HB3	3:X:116:LEU:HD22	1.90	0.53
1:A:24:VAL:O	1:A:24:VAL:HG12	2.08	0.53
1:A:77:ASN:ND2	1:A:81:ASN:HB2	2.23	0.53
1:A:81:ASN:CG	1:A:82:SER:H	2.12	0.53
2:B:1384:ILE:HB	2:B:1423:VAL:HG12	1.90	0.53
2:B:1522:TYR:N	2:B:1522:TYR:HD2	2.07	0.53
2:B:218:LYS:HD3	2:B:822:TYR:CE2	2.43	0.53
1:C:1213:LYS:HE2	1:C:1266:TYR:CE2	2.43	0.53
2:D:1386:MET:CE	2:D:1386:MET:HA	2.38	0.53
2:D:1548:ILE:HG23	2:D:1635:LEU:CB	2.39	0.53
1:A:1218:VAL:CG1	1:A:1219:LYS:H	2.20	0.53
1:A:1320:LYS:CE	1:A:1321:GLY:H	2.21	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:TYR:CE1	2:B:424:ARG:HD2	2.43	0.53
2:B:481:TYR:C	2:B:481:TYR:CD2	2.82	0.53
2:B:563:MET:HA	2:B:563:MET:HE3	1.89	0.53
2:B:885:VAL:HG23	2:B:885:VAL:O	2.08	0.53
2:B:952:ASP:N	2:B:952:ASP:OD1	2.33	0.53
1:C:1370:THR:O	1:C:1371:SER:C	2.47	0.53
1:C:149:ASN:O	1:C:150:ASP:C	2.46	0.53
1:C:1581:LEU:HD12	1:C:1592:ALA:HB1	1.91	0.53
1:C:382:LEU:HD13	1:C:415:ASP:O	2.09	0.53
1:C:600:VAL:HA	1:C:802:VAL:O	2.08	0.53
1:C:884:VAL:HG12	1:C:885:ARG:N	2.23	0.53
1:C:917:TRP:CE3	1:C:917:TRP:HA	2.43	0.53
1:C:953:ILE:HD11	1:C:955:ARG:HH21	1.73	0.53
3:X:134:THR:CG2	3:X:153:PHE:HB3	2.38	0.53
3:Y:43:ILE:O	3:Y:44:ARG:C	2.45	0.53
1:A:1180:LEU:CD2	1:A:1208:ILE:HG12	2.38	0.53
1:A:24:VAL:N	1:A:655:THR:HG21	2.23	0.53
1:A:804:ILE:CG2	1:A:809:ILE:HG13	2.36	0.53
2:B:585:TYR:CD2	2:B:788:VAL:HG11	2.44	0.53
1:C:1204:GLN:HA	1:C:1204:GLN:OE1	2.09	0.53
1:C:1620:MET:CB	1:C:1644:TRP:CB	2.85	0.53
1:C:363:LEU:HD12	1:C:456:ALA:HA	1.90	0.53
1:C:493:ILE:HG22	1:C:493:ILE:O	2.08	0.53
1:C:523:TYR:CD1	2:D:359:PRO:HG2	2.43	0.53
1:C:554:LEU:H	1:C:658:ASN:ND2	2.06	0.53
1:C:790:LEU:HB3	1:C:791:PRO:CD	2.38	0.53
1:C:916:THR:C	1:C:918:PHE:H	2.11	0.53
2:D:1400:LEU:HD22	2:D:1406:ARG:HH12	1.73	0.53
2:D:1561:HIS:CD2	2:D:1597:ILE:HD13	2.43	0.53
2:D:1615:GLU:HB3	2:D:1621:PHE:CD1	2.43	0.53
2:D:851:LEU:HD23	2:D:852:TYR:N	2.13	0.53
3:X:217:ASN:HB2	3:X:220:ASP:OD2	2.08	0.53
1:A:1274:LEU:O	1:A:1277:GLU:N	2.42	0.53
1:A:128:ILE:CG2	1:A:145:VAL:HG22	2.28	0.53
1:A:1569:THR:O	1:A:1570:VAL:CG2	2.57	0.53
1:A:1572:ASN:C	1:A:1573:VAL:HG23	2.28	0.53
1:A:600:VAL:HA	1:A:802:VAL:O	2.07	0.53
2:B:1504:GLU:CD	2:B:1504:GLU:H	2.11	0.53
2:B:24:LEU:HB3	2:B:46:HIS:HB2	1.91	0.53
1:C:123:ASN:O	1:C:211:THR:HG21	2.07	0.53
1:C:1320:LYS:HD2	1:C:1321:GLY:N	2.21	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1619:ILE:HG12	1:C:1645:ILE:CD1	2.38	0.53
1:C:250:ILE:HD11	1:C:265:VAL:CG1	2.37	0.53
1:C:655:THR:OG1	1:C:656:ASN:N	2.41	0.53
1:C:720:LEU:HD11	1:C:724:CYS:SG	2.48	0.53
2:D:175:SER:N	2:D:1300:ALA:HB2	2.19	0.53
2:D:345:ILE:HD11	2:D:427:THR:N	2.23	0.53
3:Y:107:GLN:HB3	3:Y:116:LEU:HD22	1.90	0.53
1:A:115:LYS:HB3	1:A:654:LEU:HD21	1.91	0.53
1:C:1056:ILE:CD1	1:C:1066:TYR:HE2	2.22	0.53
1:C:1159:CYS:C	1:C:1161:LEU:H	2.11	0.53
1:C:1142:LEU:HD13	1:C:1187:THR:CG2	2.38	0.53
1:C:1381:ILE:O	1:C:1382:ASP:CB	2.55	0.53
1:C:1496:TYR:N	1:C:1496:TYR:HD2	2.06	0.53
1:C:1598:ILE:HG22	1:C:1599:THR:H	1.73	0.53
1:C:532:GLN:HE21	1:C:568:GLY:CA	2.14	0.53
1:C:955:ARG:HH12	1:C:1352:PHE:HA	1.74	0.53
2:D:954:VAL:HG23	2:D:1330:ASN:O	2.08	0.53
2:D:1593:THR:HB	2:D:1596:LYS:O	2.09	0.53
2:D:204:GLU:O	2:D:205:HIS:HB2	2.08	0.53
2:D:266:GLY:HA2	2:D:276:ILE:HG13	1.90	0.53
2:D:129:PHE:CE2	2:D:598:ILE:HG23	2.44	0.53
2:D:745:ILE:CG2	2:D:897:LYS:HD3	2.39	0.53
3:Y:170:ARG:HD3	3:Y:203:LEU:CD2	2.38	0.53
1:A:1451:THR:O	1:A:1452:ASP:HB3	2.07	0.53
1:A:1615:ARG:NH1	1:A:1647:TYR:CE1	2.77	0.53
1:A:702:GLY:HA3	1:A:728:PHE:CD1	2.44	0.53
1:A:758:LEU:HB3	1:A:759:PRO:HD2	1.91	0.53
1:A:906:GLY:N	1:A:929:VAL:HB	2.21	0.53
2:B:1466:GLU:HA	2:B:1466:GLU:OE1	2.08	0.53
2:B:469:ASN:ND2	2:B:472:SER:H	2.06	0.53
2:B:46:HIS:ND1	2:B:525:GLN:HG2	2.24	0.53
2:B:824:VAL:HG22	2:B:825:VAL:N	2.24	0.53
1:C:1159:CYS:N	1:C:1160:PRO:CD	2.72	0.53
1:C:1228:TRP:N	1:C:1228:TRP:CE3	2.77	0.53
1:C:23:TYR:O	1:C:655:THR:CB	2.56	0.53
1:C:461:SER:C	1:C:463:SER:H	2.12	0.53
1:C:573:VAL:O	1:C:574:HIS:ND1	2.42	0.53
1:C:949:ILE:HG22	1:C:950:TYR:CZ	2.44	0.53
2:D:353:TYR:HA	2:D:433:ILE:O	2.09	0.53
2:D:523:TYR:HD2	2:D:621:PHE:HZ	1.54	0.53
2:D:622:GLU:OE2	2:D:637:LYS:HD3	2.09	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:745:ILE:HG13	2:D:906:SER:HB2	1.90	0.53
3:Y:194:LYS:NZ	3:Y:197:ASN:HD22	2.06	0.53
1:A:1204:GLN:OE1	1:A:1204:GLN:HA	2.09	0.53
1:A:968:VAL:HG22	1:A:1366:HIS:O	2.08	0.53
1:A:1454:GLN:HG3	1:A:1461:ILE:HB	1.90	0.53
1:A:149:ASN:O	1:A:150:ASP:C	2.47	0.53
1:A:702:GLY:HA2	1:A:728:PHE:HE1	1.70	0.53
1:A:979:VAL:HG11	1:A:1326:TYR:HE1	1.73	0.53
2:B:1313:VAL:HG21	2:B:1323:MET:HE2	1.90	0.53
1:A:425:PRO:HG3	2:B:498:ARG:NH1	2.24	0.53
2:B:618:LEU:HD22	2:B:636:THR:HA	1.89	0.53
2:B:622:GLU:OE2	2:B:637:LYS:HD3	2.09	0.53
1:C:1626:GLN:HB2	1:C:1635:TYR:CD1	2.40	0.53
1:C:569:ASN:CG	1:C:570:GLN:N	2.62	0.53
1:C:694:VAL:O	1:C:697:LYS:HE2	2.09	0.53
1:C:771:GLU:HG3	1:C:772:SER:O	2.09	0.53
1:C:824:PHE:CZ	1:C:846:TYR:HD1	2.27	0.53
2:D:1480:LEU:HD12	2:D:1480:LEU:C	2.28	0.53
2:D:285:ILE:CD1	2:D:285:ILE:N	2.67	0.53
3:X:127:ASN:OD1	3:X:158:GLU:HB3	2.07	0.53
3:Y:88:GLY:HA2	3:Y:210:GLU:O	2.08	0.53
1:A:1066:TYR:H	1:A:1079:THR:CG2	2.19	0.53
1:A:1242:THR:OG1	1:A:1243:GLY:N	2.42	0.53
1:A:1559:TYR:CD1	1:A:1561:TYR:HE2	2.27	0.53
1:A:363:LEU:HD12	1:A:456:ALA:HA	1.90	0.53
1:A:612:VAL:HG21	1:A:769:PHE:HZ	1.71	0.53
1:A:655:THR:OG1	1:A:656:ASN:N	2.41	0.53
1:A:599:TRP:NE1	1:A:779:LEU:HA	2.24	0.53
2:B:1281:LEU:HB2	2:B:1283:ASP:HB2	1.89	0.53
2:B:175:SER:O	2:B:1299:LEU:HD12	2.09	0.53
2:B:231:SER:HB3	2:B:244:HIS:HB2	1.90	0.53
2:B:481:TYR:C	2:B:481:TYR:HD2	2.10	0.53
2:B:482:LEU:CD1	2:B:521:VAL:HB	2.39	0.53
2:B:512:PRO:HA	2:B:515:ILE:HD12	1.90	0.53
1:C:1035:HIS:N	1:C:1035:HIS:ND1	2.56	0.53
1:C:111:PHE:HE2	1:C:113:LYS:CB	2.20	0.53
1:C:1549:LYS:HD3	1:C:1667:PHE:CD2	2.44	0.53
1:C:1627:ILE:O	1:C:1629:TYR:N	2.42	0.53
1:C:691:LYS:C	1:C:693:SER:H	2.11	0.53
1:C:689:LYS:O	1:C:691:LYS:N	2.42	0.53
2:D:1534:GLN:HG3	2:D:1535:ASP:OD2	2.09	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:456:PRO:HG3	2:D:515:ILE:HD11	1.91	0.53
3:X:166:ASP:HB2	3:X:207:LEU:HD21	1.90	0.53
1:A:1097:GLN:HG3	1:A:1158:ILE:HG22	1.90	0.52
1:A:1112:GLN:NE2	1:A:1171:ALA:HB2	2.24	0.52
1:A:1226:ARG:CZ	1:A:1266:TYR:CE1	2.92	0.52
1:A:967:LEU:HD13	1:A:1365:VAL:CG2	2.39	0.52
1:A:689:LYS:HG2	1:A:699:CYS:SG	2.48	0.52
1:A:687:ALA:O	1:A:690:TYR:HB3	2.08	0.52
1:A:720:LEU:HD11	1:A:724:CYS:SG	2.49	0.52
1:A:804:ILE:HG22	1:A:809:ILE:CG1	2.37	0.52
2:B:1530:ARG:HH11	2:B:1530:ARG:HG3	1.74	0.52
2:B:1593:THR:HB	2:B:1596:LYS:O	2.09	0.52
2:B:1602:THR:C	2:B:1604:ASN:N	2.63	0.52
2:B:229:GLN:OE1	2:B:229:GLN:HA	2.09	0.52
2:B:357:GLY:HA3	2:B:404:LEU:HD12	1.91	0.52
2:B:780:LEU:HD11	2:B:787:TRP:CD1	2.43	0.52
2:B:39:GLU:O	2:B:87:ILE:HD12	2.08	0.52
1:C:1097:GLN:HG3	1:C:1158:ILE:HG22	1.90	0.52
1:C:1552:ALA:HB1	1:C:1585:TYR:OH	2.09	0.52
1:C:1644:TRP:O	1:C:1645:ILE:HD13	2.08	0.52
1:C:530:VAL:HG23	1:C:534:MET:CE	2.40	0.52
1:C:576:SER:CB	1:C:589:SER:H	2.22	0.52
1:C:24:VAL:HA	1:C:655:THR:CG2	2.39	0.52
1:C:658:ASN:OD1	1:C:658:ASN:C	2.47	0.52
1:C:906:GLY:O	1:C:908:HIS:NE2	2.42	0.52
2:D:736:GLU:CD	2:D:737:ASP:H	2.13	0.52
2:D:941:GLN:HE21	2:D:943:GLU:HG2	1.74	0.52
3:Y:129:THR:HG22	3:Y:129:THR:O	2.09	0.52
1:A:1152:ILE:HG21	1:A:1168:LEU:CD2	2.39	0.52
1:A:680:GLN:HG3	1:A:681:LYS:H	1.75	0.52
1:A:920:LYS:NZ	2:B:842:GLU:CD	2.63	0.52
1:A:938:SER:C	1:A:940:SER:N	2.62	0.52
1:C:1066:TYR:CD1	1:C:1066:TYR:N	2.77	0.52
1:C:1232:LEU:HG	1:C:1233:GLN:N	2.24	0.52
1:C:176:GLU:HB2	1:C:185:PHE:CE1	2.43	0.52
1:C:541:LEU:HD23	1:C:541:LEU:O	2.09	0.52
1:C:610:TYR:N	1:C:610:TYR:HD1	2.06	0.52
1:C:702:GLY:HA2	1:C:728:PHE:HE1	1.67	0.52
2:D:139:PRO:HG2	2:D:218:LYS:HE2	1.91	0.52
2:D:1548:ILE:HG23	2:D:1635:LEU:HB2	1.92	0.52
2:D:234:PHE:CE1	2:D:236:TYR:CE1	2.98	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:469:ASN:ND2	2:D:472:SER:H	2.07	0.52
2:D:481:TYR:CD2	2:D:481:TYR:O	2.52	0.52
3:Y:217:ASN:HB2	3:Y:220:ASP:OD2	2.10	0.52
3:Y:61:SER:O	3:Y:75:PHE:CZ	2.61	0.52
1:A:1082:ALA:O	1:A:1086:LEU:HD23	2.09	0.52
1:A:1076:THR:HG22	1:A:1120:GLU:HA	1.90	0.52
1:A:1381:ILE:O	1:A:1382:ASP:CB	2.57	0.52
1:A:461:SER:C	1:A:463:SER:H	2.13	0.52
1:A:742:ILE:CG2	1:A:753:HIS:HA	2.38	0.52
1:A:696:LYS:NZ	1:A:759:PRO:CD	2.65	0.52
2:B:929:LYS:NZ	2:B:1322:THR:OG1	2.43	0.52
2:B:476:ILE:O	2:B:476:ILE:HG23	2.08	0.52
1:C:1093:VAL:O	1:C:1093:VAL:HG12	2.08	0.52
1:C:24:VAL:HG12	1:C:24:VAL:O	2.09	0.52
1:C:44:TYR:CZ	1:C:497:THR:HG21	2.45	0.52
1:C:59:TYR:CE2	1:C:99:VAL:HG21	2.44	0.52
1:C:779:LEU:C	1:C:779:LEU:HD12	2.30	0.52
1:C:979:VAL:C	1:C:980:LYS:HG2	2.28	0.52
1:C:986:GLU:HG2	1:C:987:ILE:N	2.25	0.52
1:C:989:SER:O	1:C:993:SER:CB	2.57	0.52
2:D:1522:TYR:CD2	2:D:1522:TYR:N	2.76	0.52
2:D:1529:LEU:O	2:D:1577:VAL:HG13	2.10	0.52
3:X:43:ILE:HG23	3:X:44:ARG:N	2.25	0.52
1:A:1559:TYR:CD1	1:A:1561:TYR:CE2	2.97	0.52
1:A:577:PRO:CD	1:A:588:VAL:HG23	2.39	0.52
1:A:641:ASN:O	1:A:642:ASN:C	2.47	0.52
1:A:753:HIS:O	1:A:754:MET:CB	2.49	0.52
2:B:1595:ASP:OD1	2:B:1595:ASP:N	2.40	0.52
1:C:1130:GLN:NE2	1:C:1230:ASP:HB3	2.25	0.52
1:C:1013:MET:HE3	1:C:1287:THR:HB	1.89	0.52
1:C:1641:SER:O	1:C:1642:LEU:HB2	2.10	0.52
1:C:190:ILE:HG22	1:C:191:PRO:CD	2.39	0.52
1:C:238:ILE:HG23	1:C:242:ASN:HD22	1.75	0.52
1:C:577:PRO:HD2	1:C:588:VAL:HG23	1.92	0.52
1:C:59:TYR:CE1	1:C:60:PRO:HG3	2.44	0.52
1:C:645:VAL:HG12	1:C:646:PHE:N	2.22	0.52
2:D:1284:ARG:CG	2:D:1285:GLU:N	2.72	0.52
2:D:963:ILE:CG1	2:D:1325:ILE:HG12	2.40	0.52
2:D:316:ALA:HB3	2:D:333:GLN:HB3	1.90	0.52
2:D:598:ILE:HD12	2:D:800:ILE:HG21	1.92	0.52
3:X:87:LEU:HD12	3:X:210:GLU:HA	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1287:THR:OG1	1:A:1288:GLN:N	2.40	0.52
1:A:222:TYR:HE2	1:A:224:LEU:CA	2.22	0.52
1:A:239:GLY:O	1:A:241:LYS:N	2.43	0.52
1:A:512:PHE:HD2	1:A:512:PHE:O	1.93	0.52
1:A:837:GLU:O	1:A:901:LEU:HB2	2.10	0.52
2:B:528:ASN:N	2:B:528:ASN:OD1	2.41	0.52
2:B:57:PHE:HD1	2:B:59:HIS:NE2	2.07	0.52
2:B:870:PHE:CD1	2:B:878:ARG:NH2	2.78	0.52
1:C:1279:ARG:HD3	1:C:1280:TYR:N	2.25	0.52
1:C:979:VAL:HG11	1:C:1326:TYR:HE1	1.74	0.52
1:C:25:ILE:HB	1:C:654:LEU:HB2	1.90	0.52
1:C:396:ASP:HB3	1:C:398:ASN:H	1.74	0.52
1:C:702:GLY:HA3	1:C:728:PHE:CD1	2.45	0.52
1:C:599:TRP:NE1	1:C:779:LEU:HA	2.25	0.52
1:C:993:SER:C	1:C:995:GLU:N	2.59	0.52
2:D:1292:ILE:HD12	2:D:1296:ASN:OD1	2.10	0.52
2:D:144:LEU:HD23	2:D:144:LEU:N	2.25	0.52
2:D:343:TYR:CE1	2:D:420:LEU:HD11	2.45	0.52
1:C:421:VAL:HG23	2:D:507:ASN:ND2	2.24	0.52
2:D:966:GLN:HG3	2:D:966:GLN:O	2.09	0.52
3:X:139:ASN:HD22	3:X:148:ALA:CB	2.22	0.52
1:A:1532:CYS:O	1:A:1641:SER:N	2.43	0.52
1:A:161:LEU:HD11	1:A:185:PHE:CZ	2.45	0.52
1:A:610:TYR:HD1	1:A:610:TYR:N	2.08	0.52
2:B:1280:GLU:HB2	2:B:1312:THR:HB	1.91	0.52
2:B:1622:GLN:O	2:B:1625:CYS:HB2	2.10	0.52
2:B:437:THR:HG23	2:B:444:TYR:CD1	2.45	0.52
1:C:125:PHE:CD1	1:C:627:LEU:HD21	2.45	0.52
1:C:1226:ARG:O	1:C:1270:VAL:HG22	2.09	0.52
1:C:500:ASN:O	1:C:542:VAL:HG13	2.09	0.52
1:C:544:TYR:C	1:C:544:TYR:CD2	2.83	0.52
1:C:934:VAL:CG1	1:C:935:LYS:N	2.73	0.52
2:D:175:SER:O	2:D:1299:LEU:HD12	2.09	0.52
2:D:351:PRO:N	2:D:611:ALA:HB3	2.24	0.52
2:D:481:TYR:C	2:D:481:TYR:HD2	2.12	0.52
2:D:484:LEU:HD11	2:D:626:LEU:HG	1.92	0.52
1:A:1019:PHE:HD2	1:A:1020:TYR:N	2.07	0.52
1:A:111:PHE:HE2	1:A:113:LYS:CB	2.23	0.52
1:A:1247:MET:O	1:A:1251:THR:HG23	2.10	0.52
1:A:1527:CYS:O	1:A:1528:VAL:C	2.48	0.52
1:A:161:LEU:HD11	1:A:185:PHE:CD2	2.44	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:VAL:CA	1:A:655:THR:HG21	2.40	0.52
1:A:396:ASP:HB3	1:A:398:ASN:HB2	1.92	0.52
1:A:543:TYR:CD1	1:A:543:TYR:C	2.81	0.52
1:A:934:VAL:CG1	1:A:935:LYS:N	2.73	0.52
2:B:1280:GLU:HG2	2:B:1287:PRO:CB	2.38	0.52
1:C:1496:TYR:N	1:C:1496:TYR:CD2	2.75	0.52
1:C:165:ASP:C	1:C:167:GLU:H	2.12	0.52
2:D:929:LYS:NZ	2:D:1322:THR:OG1	2.42	0.52
2:D:520:PHE:O	2:D:535:SER:HA	2.10	0.52
2:D:531:ILE:HD11	2:D:634:LEU:CD2	2.38	0.52
3:X:150:ILE:C	3:X:150:ILE:HD12	2.30	0.52
3:X:119:VAL:O	3:X:163:LYS:HD2	2.10	0.52
1:A:1161:LEU:HA	1:C:1102:ASN:ND2	2.21	0.52
1:A:1265:ASN:C	1:A:1267:VAL:H	2.12	0.52
1:A:135:TYR:CE1	1:A:141:VAL:HG22	2.44	0.52
1:A:190:ILE:HD12	1:A:219:VAL:HG21	1.92	0.52
1:A:32:ARG:O	1:A:35:ALA:HB3	2.09	0.52
1:A:377:ASP:OD2	1:A:379:LEU:HB2	2.10	0.52
2:B:216:VAL:O	2:B:216:VAL:CG1	2.57	0.52
2:B:452:THR:O	2:B:453:GLU:O	2.28	0.52
2:B:523:TYR:HD1	2:B:523:TYR:C	2.12	0.52
2:B:941:GLN:HE21	2:B:943:GLU:CG	2.22	0.52
1:C:1033:ILE:HG23	1:C:1034:PHE:N	2.24	0.52
1:C:171:VAL:CG1	1:C:1054:LEU:HD11	2.40	0.52
1:A:1163:LYS:HE3	1:C:1109:GLU:HG2	1.92	0.52
1:C:135:TYR:CE1	1:C:141:VAL:HG22	2.45	0.52
1:C:274:ASP:HA	1:C:322:TYR:CD2	2.45	0.52
2:D:1602:THR:C	2:D:1604:ASN:N	2.63	0.52
2:D:965:ILE:HG13	2:D:1301:ARG:CB	2.31	0.52
3:Y:103:VAL:HG22	3:Y:122:VAL:HG22	1.91	0.52
2:B:1450:PHE:HD1	2:B:1451:ILE:N	2.08	0.52
2:B:476:ILE:CG2	2:B:497:ARG:HD3	2.39	0.52
1:C:825:LEU:HG	1:C:826:GLU:N	2.25	0.52
1:C:968:VAL:HG22	1:C:1366:HIS:O	2.10	0.52
2:D:1500:LEU:HD12	2:D:1501:ASN:N	2.20	0.52
2:D:1539:ILE:HG23	2:D:1564:ILE:HG12	1.91	0.52
2:D:433:ILE:CG2	2:D:434:ALA:N	2.72	0.52
2:D:800:ILE:HG23	2:D:801:CYS:N	2.24	0.52
2:D:887:LEU:HD23	2:D:1490:CYS:HB3	1.91	0.52
3:X:103:VAL:HG22	3:X:122:VAL:HG22	1.91	0.52
3:Y:119:VAL:O	3:Y:163:LYS:HD2	2.10	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:61:SER:O	3:Y:75:PHE:HZ	1.92	0.52
1:A:645:VAL:HG12	1:A:646:PHE:N	2.24	0.52
1:A:113:LYS:HE2	1:A:654:LEU:O	2.10	0.52
1:A:222:TYR:CD1	1:A:768:TYR:HB2	2.42	0.52
2:B:1503:GLN:NE2	2:B:1506:ILE:HG12	2.25	0.52
2:B:1593:THR:HG22	2:B:1594:LYS:H	1.73	0.52
2:B:283:ILE:N	2:B:283:ILE:HD12	2.25	0.52
2:B:437:THR:HG21	2:B:443:ASN:N	2.25	0.52
1:C:1098:ASN:O	1:C:1101:CYS:HB2	2.10	0.52
1:C:120:THR:HG22	1:C:121:TYR:N	2.24	0.52
1:C:1408:TYR:CE2	1:C:1410:PRO:HA	2.44	0.52
1:C:1431:GLY:HA2	1:C:1483:PHE:CE1	2.45	0.52
1:C:180:ILE:CB	1:C:599:TRP:CE3	2.93	0.52
2:D:1530:ARG:NH1	2:D:1530:ARG:HG3	2.25	0.52
2:D:558:MET:O	2:D:561:ALA:HB3	2.10	0.52
3:X:86:LEU:HG	3:X:91:LYS:HG3	1.92	0.52
1:A:1021:VAL:HG12	1:A:1022:PHE:N	2.26	0.51
1:A:1199:ASP:C	1:A:1201:THR:H	2.13	0.51
1:A:1013:MET:HE3	1:A:1287:THR:HB	1.91	0.51
1:A:1298:THR:O	1:A:1299:GLU:C	2.49	0.51
1:A:1385:ASP:O	1:A:1386:ILE:HB	2.09	0.51
1:A:1581:LEU:HD12	1:A:1592:ALA:HB1	1.90	0.51
1:A:1612:VAL:HG23	1:A:1617:TYR:OH	2.10	0.51
1:A:1640:ASP:O	1:A:1643:THR:HB	2.11	0.51
1:A:234:GLU:HB3	1:A:246:PHE:HE1	1.74	0.51
2:B:1351:ASN:O	2:B:1352:ILE:HG12	2.09	0.51
2:B:1381:ILE:HB	2:B:1459:TYR:CD1	2.44	0.51
1:C:1226:ARG:NE	1:C:1266:TYR:HE1	2.08	0.51
1:C:1385:ASP:O	1:C:1386:ILE:HB	2.09	0.51
1:C:1559:TYR:HH	1:C:1591:VAL:HA	1.74	0.51
1:C:219:VAL:O	1:C:219:VAL:HG12	2.10	0.51
1:C:40:VAL:CG2	1:C:41:ILE:N	2.73	0.51
1:C:436:LYS:HB2	1:C:449:ARG:CG	2.41	0.51
1:C:914:LEU:HD11	1:C:916:THR:HG22	1.92	0.51
1:C:950:TYR:CE2	1:C:1356:LEU:HD11	2.46	0.51
2:D:1595:ASP:OD1	2:D:1595:ASP:N	2.40	0.51
2:D:216:VAL:CG1	2:D:216:VAL:O	2.58	0.51
2:D:437:THR:HG21	2:D:443:ASN:N	2.25	0.51
2:D:469:ASN:CB	2:D:472:SER:HB2	2.40	0.51
2:D:519:ARG:NH1	2:D:606:ASP:OD2	2.44	0.51
2:D:756:LEU:HD12	2:D:758:LEU:HG	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:LYS:HZ1	3:Y:144:GLU:HA	1.70	0.51
3:Y:43:ILE:HG23	3:Y:44:ARG:N	2.23	0.51
1:A:1093:VAL:HG12	1:A:1095:GLN:HE21	1.74	0.51
1:A:120:THR:HG22	1:A:121:TYR:N	2.24	0.51
1:A:976:ILE:HB	1:A:1362:THR:HG22	1.92	0.51
1:A:1534:GLN:HA	1:A:1608:ASN:HD22	1.75	0.51
1:A:1540:ASP:N	1:A:1660:PHE:CD1	2.78	0.51
1:A:949:ILE:HG22	1:A:949:ILE:O	2.09	0.51
2:B:1275:LEU:HD21	2:B:1319:GLY:O	2.10	0.51
2:B:948:ARG:NH2	2:B:948:ARG:HB2	2.23	0.51
1:C:1227:PHE:CD1	1:C:1227:PHE:C	2.84	0.51
1:C:287:MET:HG2	1:C:299:VAL:HG21	1.92	0.51
1:C:472:ASN:O	1:C:473:HIS:CB	2.57	0.51
1:C:525:SER:H	2:D:401:ASN:ND2	2.06	0.51
2:D:1466:GLU:HA	2:D:1466:GLU:OE1	2.10	0.51
2:D:481:TYR:C	2:D:481:TYR:CD2	2.84	0.51
2:D:523:TYR:C	2:D:523:TYR:HD1	2.14	0.51
2:D:87:ILE:HD12	2:D:87:ILE:H	1.75	0.51
3:Y:187:GLY:C	3:Y:203:LEU:HD12	2.31	0.51
3:Y:77:PRO:O	3:Y:78:LYS:HB3	2.10	0.51
1:A:148:LEU:HG	1:A:153:LYS:O	2.10	0.51
1:A:1560:ALA:O	1:A:1561:TYR:HD2	1.92	0.51
1:A:351:PRO:HG3	1:A:442:LEU:HD11	1.92	0.51
1:A:365:PRO:HG2	1:A:464:TYR:CE2	2.46	0.51
1:A:693:SER:C	1:A:695:VAL:N	2.63	0.51
1:A:698:CYS:HB3	1:A:728:PHE:HB2	1.92	0.51
1:A:985:GLY:O	1:A:986:GLU:C	2.49	0.51
2:B:1390:PHE:CD1	2:B:1442:ILE:HG13	2.44	0.51
2:B:188:LEU:HD13	2:B:216:VAL:HG21	1.93	0.51
2:B:745:ILE:HG13	2:B:906:SER:HB2	1.91	0.51
2:B:745:ILE:CG2	2:B:897:LYS:HD3	2.40	0.51
1:C:1017:PRO:O	1:C:1018:VAL:C	2.48	0.51
1:C:1279:ARG:NH1	1:C:1280:TYR:CD2	2.78	0.51
1:C:161:LEU:HD11	1:C:185:PHE:CD2	2.45	0.51
1:C:465:LEU:HD11	1:C:486:VAL:HG13	1.93	0.51
1:C:689:LYS:HG2	1:C:699:CYS:SG	2.51	0.51
1:C:72:HIS:C	1:C:72:HIS:CD2	2.83	0.51
2:D:946:LYS:HA	2:D:1310:ASP:OD1	2.10	0.51
2:D:1581:TYR:HD1	2:D:1608:GLU:O	1.93	0.51
2:D:239:GLY:N	2:D:296:ARG:NH2	2.59	0.51
2:D:276:ILE:O	2:D:277:PRO:C	2.47	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:146:LEU:C	3:X:146:LEU:HD22	2.31	0.51
3:Y:119:VAL:HG21	3:Y:209:PHE:HB3	1.92	0.51
1:A:1188:LEU:HD23	1:A:1212:LEU:CD1	2.41	0.51
1:A:936:ARG:NH2	1:A:1284:PHE:HE1	2.08	0.51
1:A:154:PRO:O	1:A:155:ALA:HB3	2.10	0.51
1:A:274:ASP:CG	1:A:275:LEU:H	2.14	0.51
2:B:58:VAL:HG12	2:B:104:VAL:CG2	2.40	0.51
2:B:1343:PHE:CD1	2:B:1458:VAL:HG11	2.46	0.51
2:B:1514:LYS:O	2:B:1517:GLU:HB2	2.09	0.51
2:B:565:ILE:O	2:B:776:MET:HB3	2.11	0.51
2:B:563:MET:CG	2:B:780:LEU:HD23	2.30	0.51
2:B:952:ASP:O	2:B:1331:ALA:HA	2.10	0.51
1:C:1229:LYS:HZ3	1:C:1240:PRO:HD2	1.74	0.51
1:C:698:CYS:C	1:C:700:TYR:N	2.62	0.51
2:D:1274:ASN:OD1	2:D:1291:ARG:NH2	2.42	0.51
2:D:1381:ILE:CG2	2:D:1459:TYR:CE1	2.93	0.51
2:D:1438:LEU:O	2:D:1438:LEU:HD13	2.11	0.51
2:D:342:PRO:HG2	2:D:420:LEU:CD1	2.41	0.51
2:D:746:ILE:N	2:D:746:ILE:HD13	2.25	0.51
2:D:89:ILE:HD11	2:D:104:VAL:HG11	1.92	0.51
3:X:113:ASN:ND2	3:X:115:ARG:NH1	2.58	0.51
1:A:165:ASP:HB2	1:A:166:PRO:CD	2.40	0.51
1:A:180:ILE:O	1:A:182:ILE:N	2.44	0.51
1:A:472:ASN:O	1:A:473:HIS:CB	2.58	0.51
1:A:656:ASN:CB	1:A:659:ALA:H	2.23	0.51
1:A:584:PRO:CB	1:A:792:ASP:HA	2.37	0.51
2:B:1273:LEU:CB	2:B:1319:GLY:HA3	2.35	0.51
2:B:1330:ASN:N	2:B:1330:ASN:ND2	2.58	0.51
2:B:1381:ILE:CG2	2:B:1459:TYR:CE1	2.94	0.51
2:B:1391:LEU:HB2	2:B:1417:MET:HE2	1.93	0.51
2:B:1561:HIS:CD2	2:B:1597:ILE:HD13	2.46	0.51
2:B:204:GLU:O	2:B:205:HIS:HB2	2.10	0.51
1:C:1188:LEU:HD23	1:C:1212:LEU:HA	1.92	0.51
1:C:1327:LYS:HG3	1:C:1328:MET:H	1.75	0.51
1:C:1124:TYR:CA	1:C:1465:ASN:OD1	2.50	0.51
2:D:122:SER:OG	2:D:124:GLN:HB3	2.11	0.51
2:D:231:SER:HB3	2:D:244:HIS:HB2	1.91	0.51
2:D:69:PHE:HD2	2:D:69:PHE:C	2.14	0.51
3:X:194:LYS:NZ	3:X:197:ASN:HD22	2.08	0.51
1:C:511:HIS:HE1	3:Y:149:SER:OG	1.92	0.51
1:A:193:ASN:OD1	1:A:1070:LYS:HE2	2.11	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1084:ARG:HG2	1:A:1084:ARG:HH11	1.75	0.51
1:A:1217:LEU:HD13	1:A:1237:SER:HA	1.93	0.51
1:A:1234:HIS:O	1:A:1235:LYS:HB2	2.10	0.51
1:A:40:VAL:CG2	1:A:512:PHE:CD1	2.92	0.51
1:A:625:GLN:O	1:A:628:GLU:HB3	2.11	0.51
1:A:552:ALA:CB	1:A:657:ALA:HB3	2.39	0.51
1:A:875:HIS:HB3	2:B:901:GLN:HE22	1.74	0.51
1:A:914:LEU:HD11	1:A:916:THR:HG22	1.93	0.51
2:B:1530:ARG:NH1	2:B:1530:ARG:HG3	2.26	0.51
2:B:353:TYR:HA	2:B:433:ILE:O	2.11	0.51
2:B:46:HIS:CG	2:B:525:GLN:HG2	2.45	0.51
2:B:573:ALA:HB3	2:B:762:LEU:HD13	1.93	0.51
1:C:1031:TRP:CH2	1:C:1042:LYS:HG3	2.45	0.51
1:C:111:PHE:CG	1:C:112:SER:N	2.78	0.51
1:C:1440:LYS:O	1:C:1444:GLU:HG3	2.11	0.51
1:C:1544:SER:HA	1:C:1547:THR:OG1	2.11	0.51
1:C:20:GLU:C	1:C:21:GLN:CG	2.77	0.51
1:C:492:TYR:CE2	1:C:493:ILE:HB	2.46	0.51
1:C:59:TYR:CD2	1:C:99:VAL:HG21	2.46	0.51
1:C:827:MET:HE2	1:C:912:PHE:CE2	2.46	0.51
2:D:1351:ASN:O	2:D:1352:ILE:HG12	2.10	0.51
2:D:189:PRO:C	2:D:191:LEU:H	2.12	0.51
2:D:795:THR:CG2	2:D:796:PRO:HD2	2.39	0.51
2:D:847:ARG:O	2:D:898:ALA:HA	2.10	0.51
3:X:88:GLY:O	3:X:91:LYS:N	2.38	0.51
1:A:1133:LEU:CD1	1:A:1133:LEU:N	2.71	0.51
1:A:1552:ALA:HB2	1:A:1620:MET:HE1	1.93	0.51
1:A:1601:ILE:O	1:A:1638:PRO:O	2.29	0.51
1:A:33:VAL:CG2	1:A:121:TYR:HD1	2.23	0.51
1:A:361:LEU:HD21	1:A:452:TYR:HB3	1.92	0.51
1:A:459:SER:HG	1:A:461:SER:HB3	1.74	0.51
1:A:689:LYS:HD3	1:A:730:GLU:OE2	2.11	0.51
1:A:257:ASN:ND2	1:A:892:SER:O	2.43	0.51
2:B:343:TYR:CE1	2:B:420:LEU:HD11	2.45	0.51
2:B:870:PHE:HB2	2:B:871:PRO:CD	2.41	0.51
1:C:958:GLU:HA	1:C:1346:LEU:O	2.10	0.51
1:C:1554:LYS:HG3	1:C:1555:PRO:HD2	1.93	0.51
1:C:1571:GLU:O	1:C:1574:PHE:CD2	2.64	0.51
1:C:199:TRP:HB2	1:C:217:PHE:CD1	2.46	0.51
1:C:974:LYS:O	1:C:1364:VAL:HG12	2.11	0.51
2:D:1482:ASN:H	2:D:1495:GLU:HG2	1.76	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1548:ILE:CG2	2:D:1635:LEU:HB3	2.40	0.51
2:D:603:GLU:C	2:D:605:SER:H	2.14	0.51
2:D:902:GLU:HG3	2:D:902:GLU:O	2.11	0.51
1:A:1085:VAL:O	1:A:1089:VAL:HG23	2.10	0.51
1:A:1304:VAL:CG1	1:A:1305:LYS:H	2.23	0.51
1:A:1527:CYS:C	1:A:1529:GLU:N	2.64	0.51
1:A:1536:GLN:O	1:A:1536:GLN:HG3	2.10	0.51
1:A:473:HIS:O	1:A:473:HIS:HD2	1.90	0.51
1:A:59:TYR:CD2	1:A:99:VAL:HG21	2.46	0.51
1:A:974:LYS:O	1:A:1364:VAL:HG12	2.11	0.51
2:B:1386:MET:HA	2:B:1386:MET:CE	2.40	0.51
1:A:849:ARG:HH21	2:B:556:ILE:HD12	1.76	0.51
2:B:745:ILE:HD11	2:B:907:ASP:H	1.75	0.51
2:B:862:LYS:HZ2	2:B:1519:ASN:HB3	1.75	0.51
2:B:89:ILE:HD11	2:B:104:VAL:HG11	1.93	0.51
1:C:123:ASN:OD1	1:C:123:ASN:C	2.49	0.51
1:C:1323:LEU:CG	1:C:1324:HIS:H	2.24	0.51
1:C:1564:SER:CB	1:C:1616:GLN:HG3	2.41	0.51
1:C:1615:ARG:HD2	1:C:1647:TYR:CD1	2.45	0.51
1:C:396:ASP:HB3	1:C:398:ASN:HB2	1.92	0.51
1:C:804:ILE:CG2	1:C:809:ILE:HG13	2.38	0.51
1:C:847:ASN:ND2	1:C:853:MET:HB3	2.26	0.51
3:X:88:GLY:C	3:X:90:ASP:H	2.14	0.51
1:C:513:GLY:CA	3:Y:146:LEU:HD13	2.41	0.51
1:A:1240:PRO:O	1:A:1242:THR:N	2.43	0.51
1:A:1430:THR:O	1:A:1485:VAL:HG11	2.10	0.51
1:A:238:ILE:HG23	1:A:242:ASN:HD22	1.75	0.51
1:A:569:ASN:CG	1:A:570:GLN:H	2.15	0.51
1:A:573:VAL:O	1:A:574:HIS:ND1	2.44	0.51
1:A:945:ASP:C	1:A:945:ASP:OD1	2.47	0.51
1:A:95:GLY:O	1:A:96:GLN:O	2.29	0.51
2:B:1387:LEU:HD21	2:B:1472:TYR:CE1	2.46	0.51
2:B:1457:LYS:HG2	2:B:1469:THR:OG1	2.10	0.51
2:B:280:LEU:HD11	2:B:1379:MET:HG3	1.93	0.51
1:C:62:LYS:HE2	1:C:103:TYR:CE2	2.45	0.51
1:C:1619:ILE:HG12	1:C:1645:ILE:HD13	1.93	0.51
1:C:477:LEU:N	1:C:477:LEU:HD22	2.25	0.51
1:C:961:TYR:C	1:C:961:TYR:CD1	2.83	0.51
2:D:1562:GLN:HE22	2:D:1596:LYS:HZ1	1.57	0.51
2:D:1538:ASP:OD2	2:D:1567:ARG:HD2	2.11	0.51
2:D:1562:GLN:NE2	2:D:1596:LYS:NZ	2.56	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:243:PHE:CD1	2:D:314:LEU:HD23	2.43	0.51
2:D:746:ILE:HD13	2:D:746:ILE:H	1.76	0.51
3:X:106:VAL:HG22	3:X:163:LYS:HE3	1.93	0.51
3:Y:166:ASP:OD2	3:Y:207:LEU:CD2	2.59	0.51
1:A:1033:ILE:HG23	1:A:1034:PHE:H	1.75	0.51
1:A:1232:LEU:CG	1:A:1233:GLN:HG3	2.37	0.51
1:A:977:LEU:HD23	1:A:1361:VAL:HG22	1.93	0.51
1:A:697:LYS:O	1:A:700:TYR:HB3	2.10	0.51
2:B:1526:THR:HA	2:B:1545:LEU:HD13	1.92	0.51
2:B:204:GLU:O	2:B:204:GLU:HG3	2.10	0.51
2:B:54:LEU:HD23	2:B:54:LEU:N	2.26	0.51
2:B:902:GLU:HG3	2:B:902:GLU:O	2.11	0.51
2:B:962:LYS:HD2	2:B:1302:THR:HG21	1.91	0.51
1:C:1031:TRP:CZ3	1:C:1042:LYS:HA	2.46	0.51
1:C:1093:VAL:HG12	1:C:1095:GLN:HE21	1.76	0.51
1:C:1240:PRO:O	1:C:1242:THR:N	2.44	0.51
1:C:1242:THR:OG1	1:C:1243:GLY:N	2.43	0.51
1:C:1421:HIS:C	1:C:1421:HIS:CD2	2.83	0.51
1:C:1569:THR:O	1:C:1570:VAL:CG2	2.59	0.51
1:C:459:SER:HG	1:C:461:SER:HB3	1.75	0.51
1:C:530:VAL:CG2	1:C:563:ILE:HD12	2.40	0.51
1:C:698:CYS:HB3	1:C:728:PHE:HB2	1.93	0.51
3:X:107:GLN:OE1	3:X:110:ILE:HD11	2.10	0.51
3:X:166:ASP:OD2	3:X:207:LEU:CD2	2.57	0.51
3:Y:113:ASN:ND2	3:Y:115:ARG:NH1	2.59	0.51
1:A:220:LYS:HD3	1:A:765:ILE:HG23	1.93	0.50
1:A:614:ARG:N	1:A:614:ARG:HD2	2.26	0.50
2:B:1284:ARG:HG3	2:B:1285:GLU:N	2.26	0.50
2:B:134:LYS:HD2	2:B:584:VAL:HG11	1.93	0.50
2:B:265:PHE:O	2:B:276:ILE:HG13	2.11	0.50
2:B:351:PRO:N	2:B:611:ALA:HB3	2.26	0.50
2:B:923:SER:HB3	2:B:1328:PHE:CE1	2.47	0.50
1:C:1099:SER:O	1:C:1100:ILE:C	2.47	0.50
1:C:1648:TRP:NE1	1:C:1664:LEU:HD21	2.25	0.50
1:C:23:TYR:CD1	1:C:655:THR:CB	2.89	0.50
2:D:1343:PHE:CG	2:D:1458:VAL:HG11	2.46	0.50
2:D:1600:ILE:O	2:D:1600:ILE:HG13	2.11	0.50
2:D:1600:ILE:O	2:D:1602:THR:HG23	2.11	0.50
2:D:410:PRO:CA	2:D:431:THR:HG22	2.41	0.50
1:A:25:ILE:HG13	1:A:106:VAL:HG21	1.92	0.50
1:A:1245:ALA:HB2	1:A:1285:TYR:HB3	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1327:LYS:HG3	1:A:1328:MET:H	1.75	0.50
1:A:375:VAL:O	1:A:383:VAL:HG13	2.11	0.50
1:A:415:ASP:OD1	1:A:415:ASP:N	2.44	0.50
1:A:496:ILE:HG22	1:A:496:ILE:O	2.10	0.50
1:A:541:LEU:HD23	1:A:541:LEU:O	2.10	0.50
1:A:689:LYS:O	1:A:691:LYS:N	2.43	0.50
1:A:698:CYS:C	1:A:700:TYR:N	2.63	0.50
1:A:78:LYS:HZ2	3:X:144:GLU:HA	1.71	0.50
2:B:1330:ASN:N	2:B:1330:ASN:HD22	2.09	0.50
2:B:285:ILE:HD12	2:B:285:ILE:H	1.74	0.50
1:C:1565:ILE:HB	1:C:1614:GLY:H	1.76	0.50
1:C:1622:LYS:CD	1:C:1642:LEU:HB3	2.40	0.50
1:C:365:PRO:HG2	1:C:464:TYR:CE2	2.47	0.50
2:D:1343:PHE:CD1	2:D:1458:VAL:HG11	2.46	0.50
2:D:1624:LEU:O	2:D:1625:CYS:C	2.50	0.50
2:D:208:GLU:OE1	2:D:210:TYR:HB2	2.11	0.50
2:D:236:TYR:CE1	2:D:424:ARG:HD2	2.45	0.50
2:D:44:GLU:OE1	2:D:480:THR:HG21	2.11	0.50
3:X:41:HIS:O	3:X:42:ASP:CB	2.58	0.50
3:X:85:PHE:CD1	3:X:85:PHE:N	2.78	0.50
1:A:1064:TYR:HD2	1:A:1102:ASN:CB	2.25	0.50
1:A:1226:ARG:NE	1:A:1266:TYR:HE1	2.08	0.50
1:A:1227:PHE:HB2	1:A:1251:THR:HG21	1.92	0.50
1:A:1643:THR:CG2	1:A:1644:TRP:N	2.73	0.50
1:A:395:ILE:CG1	1:A:430:VAL:HB	2.42	0.50
2:B:164:GLU:HA	2:B:174:SER:O	2.10	0.50
1:A:470:THR:CG2	2:B:450:THR:HG22	2.29	0.50
1:C:1064:TYR:HD2	1:C:1102:ASN:CB	2.24	0.50
1:C:1153:ARG:CZ	1:C:1168:LEU:HD12	2.42	0.50
1:C:1226:ARG:NE	1:C:1266:TYR:CE1	2.80	0.50
1:C:1474:CYS:HB3	1:C:1476:ARG:NH1	2.26	0.50
1:C:149:ASN:O	1:C:151:ASP:N	2.44	0.50
1:C:1602:LYS:HE3	1:C:1609:ALA:O	2.11	0.50
1:C:1640:ASP:O	1:C:1643:THR:HB	2.12	0.50
1:C:180:ILE:O	1:C:182:ILE:N	2.45	0.50
1:C:54:ILE:HG12	1:C:106:VAL:HG13	1.92	0.50
1:C:784:LYS:HG2	1:C:785:GLN:H	1.75	0.50
1:C:804:ILE:HG22	1:C:809:ILE:CG1	2.39	0.50
1:C:864:GLY:HA3	1:C:907:LEU:HD22	1.92	0.50
2:D:1288:ILE:HD13	2:D:1303:VAL:HG21	1.92	0.50
2:D:1438:LEU:HD22	2:D:1439:HIS:N	2.26	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:45:ALA:HB3	2:D:81:MET:HE3	1.93	0.50
2:D:620:VAL:HG12	2:D:621:PHE:N	2.26	0.50
2:D:962:LYS:HD2	2:D:1302:THR:HG21	1.92	0.50
3:X:43:ILE:O	3:X:44:ARG:C	2.48	0.50
3:Y:58:SER:HB3	3:Y:102:ASN:HD22	1.72	0.50
1:A:1130:GLN:NE2	1:A:1230:ASP:HB3	2.26	0.50
1:A:124:GLY:C	1:A:125:PHE:CG	2.84	0.50
1:A:481:HIS:ND1	1:A:529:PRO:HB3	2.26	0.50
1:A:987:ILE:HD11	1:A:1294:ILE:HG23	1.91	0.50
2:B:942:LEU:HD13	2:B:1314:THR:HG23	1.92	0.50
2:B:503:LEU:HD23	2:B:503:LEU:C	2.32	0.50
2:B:575:VAL:O	2:B:759:THR:HA	2.12	0.50
2:B:40:GLN:HG3	2:B:86:THR:HG23	1.93	0.50
1:C:1320:LYS:CD	1:C:1321:GLY:N	2.72	0.50
1:C:134:VAL:C	1:C:135:TYR:CD2	2.85	0.50
1:C:1408:TYR:O	1:C:1410:PRO:HD3	2.11	0.50
1:C:239:GLY:O	1:C:241:LYS:N	2.44	0.50
1:C:274:ASP:CG	1:C:275:LEU:H	2.15	0.50
1:C:396:ASP:HB2	1:C:400:GLU:H	1.75	0.50
1:C:670:LYS:HD2	1:C:671:GLU:H	1.76	0.50
1:C:923:LEU:HD23	1:C:924:VAL:N	2.26	0.50
2:D:1427:LEU:N	2:D:1427:LEU:HD13	2.26	0.50
2:D:565:ILE:HG22	2:D:806:TYR:HE2	1.77	0.50
3:X:61:SER:N	3:X:75:PHE:HZ	2.09	0.50
1:A:1179:THR:HG22	1:A:1180:LEU:HD23	1.94	0.50
1:A:1540:ASP:HA	1:A:1660:PHE:HD1	1.76	0.50
1:A:396:ASP:HB3	1:A:398:ASN:H	1.76	0.50
1:A:577:PRO:HD2	1:A:588:VAL:HG23	1.93	0.50
1:A:796:THR:HA	1:A:818:LYS:HA	1.93	0.50
1:A:958:GLU:HA	1:A:1346:LEU:O	2.12	0.50
2:B:1438:LEU:HD22	2:B:1439:HIS:N	2.26	0.50
2:B:1589:ASP:HB3	2:B:1600:ILE:HG13	1.94	0.50
2:B:1600:ILE:O	2:B:1602:THR:HG23	2.11	0.50
2:B:484:LEU:HD11	2:B:626:LEU:HG	1.93	0.50
1:C:1456:LYS:HG3	1:C:1457:ASP:OD2	2.11	0.50
1:C:1549:LYS:HD3	1:C:1667:PHE:CG	2.47	0.50
1:C:243:PHE:CE2	1:C:304:GLU:HA	2.45	0.50
1:C:851:SER:O	1:C:890:GLY:HA2	2.10	0.50
1:C:902:PRO:O	1:C:903:LEU:HD13	2.10	0.50
2:D:204:GLU:HG3	2:D:204:GLU:O	2.12	0.50
2:D:54:LEU:N	2:D:54:LEU:HD23	2.25	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:745:ILE:HD11	2:D:907:ASP:N	2.26	0.50
3:X:85:PHE:N	3:X:85:PHE:HD1	2.10	0.50
1:A:1066:TYR:CD1	1:A:1066:TYR:N	2.80	0.50
1:A:1383:THR:HG21	1:A:1511:THR:HG22	1.93	0.50
1:A:1548:ARG:HE	1:A:1550:GLN:NE2	2.09	0.50
1:A:1576:LYS:CG	1:A:1601:ILE:HG22	2.33	0.50
1:A:163:PHE:CE2	1:A:188:PHE:CD1	2.99	0.50
1:A:492:TYR:CD2	1:A:493:ILE:HB	2.46	0.50
1:A:691:LYS:C	1:A:693:SER:H	2.12	0.50
1:A:691:LYS:C	1:A:693:SER:N	2.65	0.50
2:B:1343:PHE:CG	2:B:1458:VAL:HG11	2.46	0.50
2:B:558:MET:O	2:B:561:ALA:HB3	2.11	0.50
2:B:887:LEU:HD23	2:B:1490:CYS:HB3	1.92	0.50
2:B:946:LYS:H	2:B:946:LYS:CD	2.23	0.50
1:C:1056:ILE:HG12	1:C:1056:ILE:O	2.10	0.50
1:C:1433:SER:OG	1:C:1482:LEU:HD12	2.11	0.50
1:C:316:GLU:HG2	1:C:349:LEU:HD23	1.94	0.50
1:C:539:ARG:NE	1:C:633:GLY:HA3	2.27	0.50
1:C:691:LYS:C	1:C:693:SER:N	2.64	0.50
1:C:837:GLU:O	1:C:901:LEU:HB2	2.11	0.50
1:C:856:CYS:HB3	1:C:915:GLU:HG2	1.94	0.50
1:C:95:GLY:O	1:C:96:GLN:O	2.30	0.50
2:D:1610:TRP:CE3	2:D:1628:PHE:CE2	3.00	0.50
2:D:357:GLY:HA3	2:D:404:LEU:HD12	1.94	0.50
2:D:415:THR:O	2:D:425:GLN:CD	2.50	0.50
2:D:846:VAL:HG22	2:D:847:ARG:N	2.26	0.50
1:A:1408:TYR:O	1:A:1410:PRO:HD3	2.12	0.50
2:B:1346:ASN:HB2	2:B:1368:CYS:HB2	1.93	0.50
2:B:338:ILE:C	2:B:339:VAL:HG13	2.32	0.50
2:B:362:LEU:HD13	2:B:411:ILE:HD12	1.94	0.50
1:C:1021:VAL:HG12	1:C:1022:PHE:N	2.27	0.50
1:C:1084:ARG:HA	1:C:1151:GLY:HA2	1.94	0.50
1:C:1365:VAL:CG2	1:C:1366:HIS:H	2.18	0.50
1:C:1430:THR:O	1:C:1485:VAL:HG11	2.11	0.50
1:C:544:TYR:C	1:C:544:TYR:HD2	2.15	0.50
1:C:614:ARG:HD2	1:C:614:ARG:N	2.26	0.50
1:C:661:ASP:OD2	1:C:663:GLN:N	2.45	0.50
1:C:911:ASN:OD1	1:C:924:VAL:HG22	2.12	0.50
1:C:985:GLY:O	1:C:986:GLU:C	2.50	0.50
2:D:1290:TYR:CD2	2:D:1301:ARG:HB3	2.46	0.50
2:D:1593:THR:HG22	2:D:1594:LYS:H	1.72	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1623:LYS:HB3	2:D:1623:LYS:HZ2	1.77	0.50
2:D:476:ILE:HG12	2:D:524:TYR:CD2	2.47	0.50
2:D:565:ILE:O	2:D:776:MET:HB3	2.11	0.50
3:X:229:ASN:N	3:X:229:ASN:OD1	2.45	0.50
1:A:1147:PHE:C	1:A:1147:PHE:CD2	2.85	0.50
1:A:950:TYR:HD1	1:A:1268:ASN:OD1	1.94	0.50
1:A:1347:ILE:CG2	1:A:1347:ILE:O	2.60	0.50
1:A:199:TRP:HB2	1:A:217:PHE:CD1	2.47	0.50
1:A:234:GLU:HB3	1:A:246:PHE:CE1	2.47	0.50
1:A:530:VAL:HG23	1:A:534:MET:CE	2.39	0.50
1:A:23:TYR:O	1:A:655:THR:HB	2.12	0.50
2:B:1292:ILE:CD1	2:B:1301:ARG:HE	2.24	0.50
2:B:206:SER:O	2:B:208:GLU:N	2.45	0.50
2:B:208:GLU:OE1	2:B:210:TYR:HB2	2.12	0.50
2:B:857:CYS:HB3	2:B:885:VAL:HG22	1.93	0.50
1:C:1033:ILE:HD13	1:C:1034:PHE:CE1	2.47	0.50
1:C:33:VAL:HG23	1:C:120:THR:O	2.11	0.50
1:C:1245:ALA:HB2	1:C:1285:TYR:HB3	1.94	0.50
1:C:32:ARG:O	1:C:35:ALA:HB3	2.12	0.50
1:C:523:TYR:CE1	2:D:359:PRO:CG	2.93	0.50
2:D:46:HIS:CG	2:D:525:GLN:HG2	2.46	0.50
2:D:780:LEU:HD11	2:D:787:TRP:CD1	2.47	0.50
2:D:952:ASP:N	2:D:952:ASP:OD1	2.31	0.50
3:Y:107:GLN:CD	3:Y:110:ILE:HD11	2.32	0.50
1:C:78:LYS:HG3	3:Y:146:LEU:HB2	1.92	0.50
3:Y:166:ASP:OD2	3:Y:207:LEU:CG	2.58	0.50
1:A:1012:LEU:HD22	1:A:1085:VAL:CG2	2.25	0.50
1:A:1370:THR:O	1:A:1371:SER:C	2.49	0.50
1:A:1540:ASP:CA	1:A:1660:PHE:HD1	2.25	0.50
1:A:155:ALA:O	1:A:157:ARG:N	2.45	0.50
1:A:1563:VAL:HA	1:A:1582:LEU:H	1.77	0.50
1:A:1582:LEU:O	1:A:1583:ASP:C	2.50	0.50
1:A:1616:GLN:OE1	1:A:1650:ARG:HB3	2.12	0.50
1:A:236:ASN:HD22	1:A:379:LEU:HD21	1.76	0.50
1:A:24:VAL:HA	1:A:655:THR:CB	2.42	0.50
1:A:612:VAL:HG21	1:A:769:PHE:CE2	2.46	0.50
1:A:916:THR:C	1:A:918:PHE:H	2.15	0.50
2:B:1427:LEU:N	2:B:1427:LEU:HD13	2.27	0.50
2:B:1601:ILE:HD12	2:B:1601:ILE:H	1.76	0.50
2:B:1609:ARG:NH1	2:B:1609:ARG:HG2	2.25	0.50
2:B:881:PRO:O	2:B:882:PHE:CD2	2.65	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1240:PRO:C	1:C:1242:THR:N	2.65	0.50
1:C:1263:ASP:O	1:C:1265:ASN:N	2.45	0.50
1:C:1582:LEU:O	1:C:1583:ASP:C	2.50	0.50
1:C:74:SER:HA	1:C:79:PHE:HE1	1.77	0.50
2:D:1381:ILE:HB	2:D:1459:TYR:HD1	1.77	0.50
3:X:61:SER:O	3:X:75:PHE:CZ	2.65	0.50
3:Y:103:VAL:HG22	3:Y:122:VAL:HG13	1.94	0.50
3:Y:104:PHE:CE1	3:Y:164:GLU:HG3	2.47	0.50
1:A:149:ASN:H	1:A:149:ASN:ND2	2.05	0.49
1:A:560:TRP:HH2	1:A:673:LEU:HD22	1.77	0.49
1:A:805:SER:O	1:A:807:THR:N	2.45	0.49
2:B:1539:ILE:HG23	2:B:1564:ILE:HG12	1.94	0.49
2:B:243:PHE:CD2	2:B:243:PHE:C	2.85	0.49
2:B:559:PRO:HG2	2:B:812:LYS:HD2	1.93	0.49
1:C:1147:PHE:CD2	1:C:1147:PHE:C	2.86	0.49
1:C:1365:VAL:CG2	1:C:1366:HIS:N	2.73	0.49
1:C:161:LEU:HD11	1:C:185:PHE:CZ	2.47	0.49
1:C:690:TYR:C	1:C:692:HIS:N	2.66	0.49
1:C:689:LYS:HD3	1:C:730:GLU:OE2	2.12	0.49
1:C:820:PHE:CG	1:C:821:LYS:N	2.80	0.49
2:D:1529:LEU:HD11	2:D:1543:ASP:HB2	1.94	0.49
3:Y:215:VAL:C	3:Y:216:LEU:HD22	2.32	0.49
1:A:1053:MET:HE2	1:A:1086:LEU:CD1	2.42	0.49
1:A:1215:GLU:O	1:A:1217:LEU:HD23	2.12	0.49
1:A:1544:SER:HA	1:A:1547:THR:OG1	2.12	0.49
1:A:1598:ILE:HG22	1:A:1599:THR:N	2.27	0.49
1:A:484:ILE:HD12	1:A:540:LEU:CD2	2.42	0.49
1:A:55:SER:C	1:A:56:ILE:HD13	2.32	0.49
1:A:571:LEU:CD2	1:A:812:ALA:HB2	2.41	0.49
2:B:147:VAL:HG12	2:B:183:PHE:CE1	2.45	0.49
2:B:1480:LEU:C	2:B:1480:LEU:HD12	2.33	0.49
2:B:199:ILE:O	2:B:199:ILE:HG22	2.11	0.49
1:C:1162:VAL:HG23	1:C:1163:LYS:N	2.27	0.49
1:C:42:GLN:HE21	1:C:44:TYR:N	2.10	0.49
1:C:663:GLN:CG	1:C:664:GLU:N	2.74	0.49
1:C:734:VAL:HA	1:C:737:GLN:HG2	1.92	0.49
1:C:998:ASN:HB3	1:C:1000:LEU:HG	1.94	0.49
2:D:923:SER:HB3	2:D:1328:PHE:CE1	2.47	0.49
2:D:1391:LEU:HD12	2:D:1417:MET:HE1	1.92	0.49
3:X:146:LEU:HD21	3:X:148:ALA:HB2	1.94	0.49
3:Y:41:HIS:ND1	3:Y:41:HIS:N	2.60	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1323:LEU:CD1	1:A:1324:HIS:H	2.24	0.49
1:A:658:ASN:O	1:A:659:ALA:HB3	2.11	0.49
1:A:680:GLN:O	1:A:682:LYS:N	2.45	0.49
1:A:983:LEU:HD21	1:A:1271:ILE:HD12	1.94	0.49
2:B:1611:PRO:HG3	2:B:1624:LEU:HB3	1.94	0.49
2:B:218:LYS:HB3	2:B:822:TYR:CE2	2.46	0.49
1:C:1180:LEU:CD2	1:C:1208:ILE:HG12	2.43	0.49
1:C:1537:GLU:O	1:C:1539:LEU:N	2.44	0.49
1:C:398:ASN:O	1:C:399:GLN:HB2	2.13	0.49
1:C:757:LEU:O	1:C:758:LEU:HD23	2.12	0.49
2:D:963:ILE:CD1	2:D:1311:ILE:HG21	2.41	0.49
2:D:1522:TYR:N	2:D:1522:TYR:HD2	2.10	0.49
2:D:167:THR:HG22	2:D:171:ILE:O	2.12	0.49
2:D:563:MET:HA	2:D:563:MET:HE3	1.94	0.49
2:D:756:LEU:HD22	2:D:778:PHE:CD1	2.48	0.49
3:X:61:SER:N	3:X:75:PHE:CZ	2.80	0.49
3:Y:71:ASN:O	3:Y:72:VAL:HG23	2.13	0.49
1:A:1019:PHE:CD2	1:A:1020:TYR:N	2.80	0.49
1:A:1068:VAL:CG1	1:A:1069:TRP:H	2.17	0.49
1:A:196:TYR:HE2	1:A:1070:LYS:NZ	2.10	0.49
1:A:1077:TRP:NE1	1:A:1147:PHE:CD1	2.80	0.49
1:A:1327:LYS:O	1:A:1332:ASN:ND2	2.46	0.49
1:A:1487:PHE:O	1:A:1488:LEU:C	2.50	0.49
1:A:1537:GLU:O	1:A:1539:LEU:N	2.45	0.49
1:A:23:TYR:HA	1:A:43:VAL:HA	1.94	0.49
1:A:987:ILE:HD13	1:A:1294:ILE:HG23	1.94	0.49
1:A:998:ASN:HB3	1:A:1000:LEU:HG	1.93	0.49
2:B:1415:ASN:O	2:B:1417:MET:HG3	2.12	0.49
2:B:1522:TYR:CD2	2:B:1522:TYR:O	2.65	0.49
2:B:1506:ILE:CD1	2:B:1628:PHE:CE1	2.95	0.49
2:B:481:TYR:HE2	2:B:493:GLY:CA	2.24	0.49
2:B:643:LYS:HG3	2:B:644:CYS:N	2.27	0.49
2:B:963:ILE:CD1	2:B:1311:ILE:HG21	2.42	0.49
1:C:1541:LEU:HD21	1:C:1543:ILE:HD12	1.93	0.49
1:C:1643:THR:CG2	1:C:1644:TRP:N	2.74	0.49
1:C:296:ILE:CG2	1:C:297:ALA:N	2.76	0.49
1:C:243:PHE:HE2	1:C:304:GLU:CA	2.25	0.49
1:C:515:ARG:CZ	1:C:526:ILE:HG22	2.42	0.49
1:C:541:LEU:HB2	1:C:558:SER:HB3	1.95	0.49
1:C:613:GLN:O	1:C:615:GLY:N	2.46	0.49
1:C:255:PHE:HB2	1:C:846:TYR:OH	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ILE:H	1:C:87:ILE:HD13	1.73	0.49
1:C:903:LEU:HD22	1:C:903:LEU:N	2.27	0.49
1:C:916:THR:O	1:C:918:PHE:N	2.46	0.49
2:D:1371:TYR:CD1	2:D:1377:SER:CB	2.95	0.49
2:D:322:THR:HG21	2:D:327:ASP:H	1.78	0.49
2:D:564:LYS:HA	2:D:776:MET:O	2.12	0.49
2:D:643:LYS:HG3	2:D:644:CYS:N	2.27	0.49
2:D:916:VAL:CG2	2:D:917:PRO:N	2.76	0.49
3:X:104:PHE:CE1	3:X:164:GLU:HG3	2.47	0.49
3:Y:106:VAL:HG22	3:Y:163:LYS:HE3	1.93	0.49
3:Y:85:PHE:CE1	3:Y:117:SER:HB3	2.47	0.49
3:Y:119:VAL:HG13	3:Y:212:MET:SD	2.52	0.49
1:A:1423:VAL:HG11	1:A:1496:TYR:CZ	2.47	0.49
1:A:23:TYR:HE2	1:A:111:PHE:CD2	2.30	0.49
2:B:1619:GLU:C	2:B:1621:PHE:H	2.15	0.49
2:B:168:PRO:HD3	2:B:197:TRP:CD1	2.47	0.49
2:B:565:ILE:HG22	2:B:806:TYR:HE2	1.77	0.49
2:B:59:HIS:HB3	2:B:64:LYS:HA	1.95	0.49
1:C:1226:ARG:CB	1:C:1269:PRO:HB2	2.42	0.49
1:C:234:GLU:HB3	1:C:246:PHE:CE1	2.47	0.49
1:C:377:ASP:OD2	1:C:379:LEU:HB2	2.12	0.49
1:C:758:LEU:HB3	1:C:759:PRO:HD2	1.93	0.49
1:C:85:LEU:HD22	1:C:85:LEU:N	2.27	0.49
2:D:235:PHE:HB3	2:D:338:ILE:CG2	2.43	0.49
2:D:408:SER:HB3	2:D:410:PRO:HD3	1.95	0.49
2:D:511:THR:O	2:D:513:ASP:N	2.46	0.49
2:D:825:VAL:HB	2:D:828:GLU:CD	2.33	0.49
2:D:942:LEU:HD13	2:D:1314:THR:HG23	1.95	0.49
3:X:71:ASN:O	3:X:72:VAL:HG23	2.12	0.49
1:A:123:ASN:N	1:A:211:THR:HG23	2.27	0.49
1:A:1249:GLU:O	1:A:1253:TYR:HD2	1.96	0.49
1:A:1286:SER:OG	1:A:1287:THR:N	2.46	0.49
1:A:1318:LYS:HB2	1:A:1345:ASP:HB2	1.94	0.49
1:A:1564:SER:CB	1:A:1616:GLN:HG3	2.43	0.49
1:A:719:SER:OG	1:A:1123:GLN:HG3	2.12	0.49
1:A:74:SER:HA	1:A:79:PHE:CE1	2.47	0.49
1:A:820:PHE:CG	1:A:821:LYS:N	2.81	0.49
2:B:1400:LEU:HD22	2:B:1406:ARG:HH12	1.77	0.49
2:B:1347:VAL:HG21	2:B:1456:VAL:HG11	1.94	0.49
2:B:564:LYS:HA	2:B:776:MET:O	2.13	0.49
2:B:560:GLY:HA2	2:B:780:LEU:O	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:916:VAL:CG2	2:B:917:PRO:N	2.74	0.49
1:C:100:SER:O	1:C:101:TYR:HB2	2.11	0.49
1:C:1557:ILE:HD13	1:C:1622:LYS:HG3	1.93	0.49
1:C:423:ASN:HB3	2:D:501:GLN:NE2	2.27	0.49
1:C:682:LYS:HZ2	1:C:686:ILE:CD1	2.26	0.49
1:C:719:SER:OG	1:C:1123:GLN:HG3	2.13	0.49
2:D:280:LEU:HD22	2:D:1462:TYR:HE2	1.76	0.49
2:D:1526:THR:HA	2:D:1545:LEU:HD13	1.95	0.49
2:D:1533:GLU:OE1	2:D:1533:GLU:HA	2.13	0.49
2:D:26:THR:HG22	2:D:630:THR:HG22	1.94	0.49
1:A:100:SER:C	1:A:101:TYR:HD2	2.16	0.49
1:A:1098:ASN:O	1:A:1101:CYS:HB2	2.13	0.49
1:A:1162:VAL:HG23	1:A:1163:LYS:N	2.27	0.49
1:A:514:THR:HG22	1:A:515:ARG:N	2.27	0.49
1:A:766:ARG:H	1:A:766:ARG:HD3	1.78	0.49
1:A:600:VAL:CG2	1:A:780:VAL:HG21	2.42	0.49
2:B:1285:GLU:O	2:B:1287:PRO:HD3	2.13	0.49
2:B:1529:LEU:HD11	2:B:1543:ASP:HB2	1.93	0.49
2:B:494:ARG:CG	2:B:494:ARG:HH11	2.12	0.49
2:B:620:VAL:HG12	2:B:621:PHE:N	2.28	0.49
1:C:1454:GLN:HG3	1:C:1461:ILE:HB	1.94	0.49
1:C:1475:VAL:CG2	1:C:1476:ARG:N	2.75	0.49
1:C:1620:MET:CB	1:C:1644:TRP:HB3	2.27	0.49
1:C:257:ASN:HD21	1:C:892:SER:CA	2.23	0.49
2:D:1502:HIS:ND1	2:D:1503:GLN:N	2.51	0.49
2:D:243:PHE:CD2	2:D:243:PHE:C	2.86	0.49
2:D:361:GLU:HB3	2:D:399:ILE:HD13	1.95	0.49
2:D:63:ARG:HB3	2:D:65:GLN:HG3	1.95	0.49
2:D:218:LYS:HB3	2:D:822:TYR:CE2	2.47	0.49
2:D:948:ARG:HB2	2:D:948:ARG:NH2	2.25	0.49
3:X:88:GLY:C	3:X:90:ASP:N	2.66	0.49
3:Y:86:LEU:HG	3:Y:91:LYS:CG	2.43	0.49
1:A:1204:GLN:O	1:A:1208:ILE:HG13	2.13	0.49
1:A:174:VAL:HG22	1:A:175:GLU:H	1.77	0.49
1:A:191:PRO:O	1:A:194:PRO:HD3	2.13	0.49
1:A:571:LEU:HD12	1:A:593:ALA:O	2.13	0.49
2:B:469:ASN:CB	2:B:472:SER:HB2	2.42	0.49
2:B:519:ARG:NH1	2:B:606:ASP:OD2	2.45	0.49
2:B:825:VAL:HB	2:B:828:GLU:CD	2.32	0.49
2:B:933:ARG:NH1	2:B:933:ARG:HG3	2.18	0.49
1:C:1140:ASN:O	1:C:1143:TYR:HB3	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1265:ASN:C	1:C:1267:VAL:H	2.15	0.49
1:C:1411:SER:H	1:C:1414:GLU:HG3	1.78	0.49
1:C:272:ARG:HG3	1:C:279:GLN:O	2.13	0.49
1:C:296:ILE:HG23	1:C:297:ALA:N	2.26	0.49
1:C:518:PHE:O	1:C:520:ASP:N	2.42	0.49
1:C:571:LEU:CD2	1:C:812:ALA:HB2	2.43	0.49
1:C:682:LYS:NZ	1:C:686:ILE:CD1	2.75	0.49
1:C:862:VAL:O	1:C:863:GLU:C	2.51	0.49
1:C:945:ASP:OD1	1:C:945:ASP:C	2.48	0.49
2:D:1443:LEU:CD1	2:D:1443:LEU:N	2.76	0.49
2:D:1602:THR:O	2:D:1604:ASN:N	2.41	0.49
2:D:1621:PHE:O	2:D:1622:GLN:C	2.50	0.49
2:D:189:PRO:C	2:D:191:LEU:N	2.66	0.49
2:D:322:THR:CG2	2:D:327:ASP:H	2.25	0.49
2:D:463:ASN:OD1	2:D:505:THR:OG1	2.31	0.49
2:D:573:ALA:HB3	2:D:762:LEU:HD13	1.93	0.49
2:D:847:ARG:HG3	2:D:869:GLN:CG	2.36	0.49
1:A:1386:ILE:HG13	1:A:1387:GLU:N	2.27	0.49
1:A:1456:LYS:HG3	1:A:1457:ASP:OD2	2.13	0.49
1:A:757:LEU:O	1:A:758:LEU:HD23	2.12	0.49
1:A:849:ARG:HH11	1:A:849:ARG:CG	2.12	0.49
2:B:1299:LEU:HB3	2:B:1301:ARG:HD3	1.94	0.49
2:B:144:LEU:HD23	2:B:144:LEU:N	2.28	0.49
2:B:531:ILE:O	2:B:617:ASN:ND2	2.39	0.49
2:B:946:LYS:N	2:B:946:LYS:HD3	2.27	0.49
1:C:1423:VAL:HG11	1:C:1496:TYR:CZ	2.48	0.49
1:C:1450:PHE:HB3	1:C:1463:GLN:O	2.12	0.49
1:C:148:LEU:HA	1:C:154:PRO:O	2.12	0.49
1:C:1562:LYS:HD3	1:C:1648:TRP:NE1	2.27	0.49
1:C:165:ASP:C	1:C:167:GLU:N	2.66	0.49
1:C:395:ILE:CG1	1:C:430:VAL:HB	2.43	0.49
2:D:58:VAL:HG12	2:D:104:VAL:CG2	2.41	0.49
2:D:1281:LEU:HB2	2:D:1283:ASP:HB2	1.95	0.49
2:D:1390:PHE:CD1	2:D:1442:ILE:HG13	2.47	0.49
2:D:462:VAL:HG21	2:D:520:PHE:CE2	2.48	0.49
2:D:548:LEU:HD23	2:D:803:ALA:HB2	1.94	0.49
3:Y:87:LEU:HD12	3:Y:210:GLU:HA	1.95	0.49
1:A:1190:ILE:CG1	1:A:1253:TYR:CE1	2.94	0.49
1:A:1069:TRP:HH2	1:A:1465:ASN:ND2	2.10	0.49
1:A:1475:VAL:CG2	1:A:1476:ARG:N	2.76	0.49
1:A:1566:THR:HG23	1:A:1578:LYS:O	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LYS:HG3	1:A:190:ILE:O	2.13	0.49
1:A:123:ASN:C	1:A:211:THR:HG21	2.32	0.49
1:A:515:ARG:NH1	1:A:526:ILE:HG22	2.27	0.49
1:A:682:LYS:NZ	1:A:686:ILE:CD1	2.76	0.49
2:B:1382:ILE:CD1	2:B:1458:VAL:HG22	2.43	0.49
2:B:1381:ILE:HB	2:B:1459:TYR:HD1	1.78	0.49
2:B:239:GLY:N	2:B:296:ARG:NH2	2.61	0.49
1:A:423:ASN:CG	2:B:504:VAL:HG22	2.33	0.49
1:C:1085:VAL:O	1:C:1089:VAL:HG23	2.13	0.49
1:C:1128:LYS:HD3	1:C:1414:GLU:OE1	2.13	0.49
1:C:115:LYS:HB2	1:C:654:LEU:CD2	2.42	0.49
1:C:1255:LEU:C	1:C:1255:LEU:HD12	2.31	0.49
1:C:1318:LYS:HB2	1:C:1345:ASP:HB2	1.95	0.49
1:C:1493:PHE:HD1	1:C:1494:THR:H	1.50	0.49
1:C:1559:TYR:O	1:C:1621:GLY:N	2.46	0.49
1:C:1629:TYR:O	1:C:1630:ASN:HB2	2.13	0.49
1:C:96:GLN:O	1:C:97:ASN:O	2.31	0.49
2:D:1280:GLU:HB2	2:D:1312:THR:HB	1.95	0.49
2:D:1567:ARG:NH1	2:D:1567:ARG:HG3	2.28	0.49
2:D:188:LEU:HD13	2:D:216:VAL:HG21	1.95	0.49
2:D:481:TYR:CE1	2:D:506:MET:SD	2.93	0.49
2:D:889:GLN:HA	2:D:915:VAL:HB	1.95	0.49
3:X:50:TYR:HE2	3:X:170:ARG:HD2	1.72	0.49
3:Y:50:TYR:CE2	3:Y:170:ARG:CZ	2.95	0.49
1:A:1022:PHE:CE2	1:A:1092:TYR:CD1	3.01	0.48
1:A:1278:GLN:NE2	1:A:1293:ALA:HB1	2.28	0.48
1:A:1565:ILE:HB	1:A:1614:GLY:H	1.78	0.48
1:A:354:LEU:HB2	1:A:374:GLN:O	2.13	0.48
1:A:963:ILE:CG2	1:A:967:LEU:HD23	2.41	0.48
2:B:1344:HIS:ND1	5:B:2003:NAG:H82	2.27	0.48
2:B:1610:TRP:CD2	2:B:1628:PHE:CD2	2.99	0.48
2:B:830:VAL:CG2	2:B:831:GLU:N	2.74	0.48
1:C:1234:HIS:O	1:C:1235:LYS:HB2	2.12	0.48
1:C:1559:TYR:CE1	1:C:1587:THR:HA	2.47	0.48
1:C:371:ILE:CG2	1:C:420:PHE:HB2	2.34	0.48
1:C:596:MET:SD	1:C:782:ARG:HG2	2.53	0.48
2:D:1601:ILE:HD12	2:D:1601:ILE:H	1.78	0.48
1:C:523:TYR:CZ	2:D:359:PRO:HD2	2.48	0.48
2:D:945:ILE:N	2:D:945:ILE:HD12	2.28	0.48
3:Y:61:SER:N	3:Y:75:PHE:CZ	2.81	0.48
3:Y:61:SER:N	3:Y:75:PHE:HZ	2.11	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:PRO:O	1:A:1018:VAL:C	2.51	0.48
1:A:1231:ASN:O	1:A:1233:GLN:N	2.46	0.48
1:A:1376:SER:OG	1:A:1503:LYS:HG3	2.13	0.48
1:A:163:PHE:CD2	1:A:188:PHE:CD1	3.00	0.48
1:A:1641:SER:O	1:A:1642:LEU:HB2	2.14	0.48
1:A:24:VAL:HG11	1:A:543:TYR:CZ	2.48	0.48
1:A:272:ARG:HG3	1:A:279:GLN:O	2.13	0.48
1:A:477:LEU:HD23	1:A:480:GLU:OE1	2.14	0.48
1:A:54:ILE:HG12	1:A:106:VAL:HG13	1.94	0.48
1:A:560:TRP:CH2	1:A:673:LEU:CD2	2.96	0.48
1:A:613:GLN:O	1:A:615:GLY:N	2.46	0.48
1:A:689:LYS:CG	1:A:699:CYS:SG	3.01	0.48
1:A:734:VAL:HA	1:A:737:GLN:HG2	1.94	0.48
1:A:853:MET:O	1:A:888:VAL:HG12	2.13	0.48
2:B:1533:GLU:OE1	2:B:1533:GLU:HA	2.12	0.48
2:B:1614:ASP:O	2:B:1616:CYS:N	2.46	0.48
2:B:216:VAL:O	2:B:216:VAL:HG13	2.13	0.48
2:B:580:VAL:CG1	2:B:584:VAL:HG23	2.43	0.48
2:B:615:GLN:HB2	2:B:616:ASN:HD22	1.75	0.48
2:B:598:ILE:HD12	2:B:800:ILE:HG21	1.92	0.48
2:B:925:VAL:HG22	2:B:1326:LEU:CD2	2.39	0.48
1:C:124:GLY:C	1:C:125:PHE:CG	2.86	0.48
1:C:1271:ILE:CD1	1:C:1300:TYR:CZ	2.96	0.48
1:C:136:THR:O	1:C:139:GLN:HG3	2.12	0.48
1:C:1377:PHE:CD2	1:C:1495:VAL:HG22	2.48	0.48
1:C:1622:LYS:HZ2	1:C:1642:LEU:HB3	1.78	0.48
1:C:1562:LYS:CD	1:C:1648:TRP:NE1	2.76	0.48
1:C:248:ILE:HB	1:C:299:VAL:HG13	1.93	0.48
1:C:496:ILE:HG22	1:C:496:ILE:O	2.12	0.48
2:D:853:ASN:C	2:D:853:ASN:OD1	2.52	0.48
3:X:103:VAL:HG22	3:X:122:VAL:HG13	1.94	0.48
3:X:81:ASN:O	3:X:115:ARG:CB	2.53	0.48
3:Y:125:LYS:HA	3:Y:126:ASN:C	2.27	0.48
1:A:1000:LEU:O	1:A:1001:THR:HG23	2.13	0.48
1:A:1240:PRO:C	1:A:1242:THR:N	2.67	0.48
1:A:1671:ILE:CD1	1:A:1676:CYS:SG	3.01	0.48
1:A:284:GLN:H	1:A:310:LEU:HD22	1.78	0.48
1:A:997:ILE:O	1:A:997:ILE:HG13	2.13	0.48
2:B:322:THR:HG21	2:B:327:ASP:H	1.79	0.48
1:C:1077:TRP:NE1	1:C:1147:PHE:CD1	2.79	0.48
1:C:1142:LEU:HD21	1:C:1179:THR:OG1	2.14	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:977:LEU:HD23	1:C:1361:VAL:HG22	1.96	0.48
1:C:222:TYR:HE2	1:C:224:LEU:HA	1.79	0.48
1:C:443:PRO:CD	1:C:446:ASN:HB2	2.42	0.48
1:C:514:THR:CG2	1:C:515:ARG:N	2.77	0.48
1:C:695:VAL:HG12	1:C:727:ALA:CB	2.44	0.48
1:C:43:VAL:HG12	1:C:79:PHE:O	2.13	0.48
2:D:580:VAL:CG1	2:D:584:VAL:HG23	2.43	0.48
2:D:628:LEU:HB3	2:D:636:THR:HG23	1.96	0.48
2:D:850:LEU:HB2	2:D:882:PHE:CD1	2.48	0.48
3:X:187:GLY:C	3:X:203:LEU:HD12	2.33	0.48
3:Y:85:PHE:CD1	3:Y:85:PHE:N	2.81	0.48
1:A:1057:MET:HE2	1:A:1057:MET:HB3	1.77	0.48
1:A:1226:ARG:NE	1:A:1266:TYR:CE1	2.82	0.48
1:A:1320:LYS:HD2	1:A:1321:GLY:N	2.27	0.48
1:A:1431:GLY:HA2	1:A:1483:PHE:HE1	1.78	0.48
1:A:1286:SER:CB	1:A:1499:HIS:HA	2.44	0.48
1:A:493:ILE:O	1:A:493:ILE:HG22	2.12	0.48
1:A:500:ASN:ND2	1:A:543:TYR:CE1	2.77	0.48
1:A:576:SER:CB	1:A:589:SER:H	2.27	0.48
1:A:825:LEU:HB2	1:A:845:VAL:HG23	1.96	0.48
2:B:1611:PRO:CD	2:B:1624:LEU:HD23	2.44	0.48
2:B:628:LEU:HB3	2:B:636:THR:HG23	1.95	0.48
1:C:1231:ASN:O	1:C:1233:GLN:N	2.47	0.48
1:C:132:LYS:NZ	1:C:139:GLN:HE22	2.11	0.48
1:C:1563:VAL:HA	1:C:1582:LEU:H	1.78	0.48
1:C:322:TYR:N	1:C:322:TYR:HD2	2.10	0.48
1:C:236:ASN:HD22	1:C:379:LEU:HD21	1.78	0.48
1:C:494:ASP:OD1	1:C:495:LYS:HE2	2.13	0.48
1:C:481:HIS:ND1	1:C:529:PRO:HB3	2.27	0.48
1:C:950:TYR:HD1	1:C:1268:ASN:OD1	1.96	0.48
1:C:964:PRO:HG2	1:C:1365:VAL:HG11	1.95	0.48
2:D:1285:GLU:O	2:D:1287:PRO:HD3	2.13	0.48
2:D:1525:LYS:HD2	2:D:1610:TRP:CH2	2.48	0.48
2:D:210:TYR:CG	2:D:211:THR:N	2.81	0.48
2:D:32:VAL:HB	2:D:607:PHE:CZ	2.48	0.48
2:D:853:ASN:HA	2:D:854:PRO:HD3	1.58	0.48
2:D:860:SER:OG	2:D:866:TYR:N	2.39	0.48
2:D:941:GLN:HE21	2:D:943:GLU:CG	2.26	0.48
1:A:1084:ARG:HA	1:A:1151:GLY:HA2	1.94	0.48
1:A:1411:SER:H	1:A:1414:GLU:HG3	1.78	0.48
1:A:1563:VAL:HG12	1:A:1581:LEU:HA	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:VAL:CG2	1:A:175:GLU:N	2.74	0.48
1:A:430:VAL:HG11	1:A:453:ARG:NH2	2.14	0.48
1:A:465:LEU:HG	1:A:466:TYR:N	2.28	0.48
1:A:515:ARG:CZ	1:A:526:ILE:HG22	2.43	0.48
1:A:663:GLN:CG	1:A:664:GLU:N	2.76	0.48
1:A:690:TYR:C	1:A:692:HIS:N	2.67	0.48
1:A:911:ASN:OD1	1:A:924:VAL:HG22	2.14	0.48
1:A:92:LEU:HD13	1:C:1026:GLU:OE2	2.13	0.48
2:B:548:LEU:HD23	2:B:803:ALA:HB2	1.96	0.48
2:B:32:VAL:HB	2:B:607:PHE:CZ	2.48	0.48
1:C:1031:TRP:CE2	1:C:1042:LYS:HG3	2.47	0.48
1:C:1204:GLN:O	1:C:1208:ILE:HG13	2.13	0.48
1:C:554:LEU:H	1:C:658:ASN:HD22	1.61	0.48
1:C:545:ILE:HG23	1:C:554:LEU:HD21	1.95	0.48
1:C:682:LYS:NZ	1:C:686:ILE:HD11	2.28	0.48
1:C:856:CYS:HB2	2:D:904:LEU:HD21	1.95	0.48
1:C:883:CYS:O	1:C:884:VAL:C	2.51	0.48
1:A:1042:LYS:HZ1	1:C:92:LEU:HD13	1.77	0.48
2:D:1344:HIS:ND1	5:D:2003:NAG:C8	2.77	0.48
3:X:50:TYR:CE2	3:X:170:ARG:CZ	2.96	0.48
1:A:1142:LEU:HD13	1:A:1187:THR:HG21	1.95	0.48
1:A:981:GLY:HA3	1:A:1333:PHE:CD1	2.49	0.48
1:A:25:ILE:CD1	1:A:41:ILE:HG13	2.43	0.48
1:A:461:SER:CB	1:A:553:GLU:OE2	2.61	0.48
1:A:541:LEU:HB2	1:A:557:ASP:O	2.13	0.48
1:A:859:MET:HB3	1:A:898:PHE:CE1	2.49	0.48
1:A:973:ILE:O	1:A:973:ILE:HG22	2.12	0.48
2:B:1624:LEU:O	2:B:1625:CYS:C	2.52	0.48
2:B:384:PHE:CD2	2:B:384:PHE:N	2.81	0.48
2:B:378:PRO:HB2	2:B:416:ASN:O	2.14	0.48
2:B:795:THR:CG2	2:B:796:PRO:HD2	2.36	0.48
1:C:119:ILE:C	1:C:119:ILE:HD12	2.34	0.48
1:C:1255:LEU:HD13	1:C:1267:VAL:HG13	1.95	0.48
1:C:1421:HIS:HD2	1:C:1422:ALA:N	2.11	0.48
1:C:367:ILE:HD13	1:C:466:TYR:CD2	2.48	0.48
1:C:539:ARG:NH2	1:C:634:CYS:N	2.60	0.48
1:C:971:THR:O	1:C:971:THR:OG1	2.23	0.48
2:D:870:PHE:HB2	2:D:871:PRO:CD	2.42	0.48
3:X:41:HIS:ND1	3:X:41:HIS:N	2.62	0.48
1:A:20:GLU:C	1:A:21:GLN:CG	2.77	0.48
2:B:224:PHE:CE1	2:B:320:VAL:CG1	2.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:570:ASP:O	2:B:573:ALA:HB2	2.14	0.48
1:C:1068:VAL:CG1	1:C:1069:TRP:H	2.18	0.48
1:C:1066:TYR:N	1:C:1079:THR:HG23	2.21	0.48
1:A:1161:LEU:CD1	1:C:1105:LEU:HD13	2.41	0.48
1:C:161:LEU:HD21	1:C:185:PHE:CD2	2.49	0.48
1:C:1622:LYS:NZ	1:C:1642:LEU:HB3	2.29	0.48
1:C:23:TYR:CE2	1:C:111:PHE:CD2	3.01	0.48
1:C:243:PHE:CE2	1:C:304:GLU:CA	2.96	0.48
1:C:361:LEU:HD21	1:C:452:TYR:HB3	1.94	0.48
1:C:627:LEU:HA	1:C:627:LEU:HD23	1.69	0.48
1:C:871:PRO:CD	1:C:872:VAL:N	2.75	0.48
2:D:1631:PHE:HD2	2:D:1632:SER:N	2.11	0.48
2:D:216:VAL:HG13	2:D:216:VAL:O	2.13	0.48
2:D:229:GLN:HA	2:D:229:GLN:OE1	2.14	0.48
2:D:27:LEU:O	2:D:628:LEU:HD12	2.14	0.48
2:D:345:ILE:HG13	2:D:428:LYS:HB3	1.96	0.48
2:D:524:TYR:CE1	2:D:532:VAL:HG12	2.49	0.48
2:D:61:PHE:CD1	2:D:62:PRO:HA	2.48	0.48
3:X:77:PRO:O	3:X:78:LYS:CB	2.61	0.48
1:A:1090:ASN:ND2	1:A:1158:ILE:HG12	2.29	0.48
1:A:1234:HIS:CG	1:A:1235:LYS:H	2.31	0.48
1:A:964:PRO:HG2	1:A:1365:VAL:HG11	1.95	0.48
1:A:30:ILE:HG22	1:A:31:PHE:N	2.29	0.48
1:A:494:ASP:OD2	1:A:495:LYS:HE2	2.14	0.48
1:A:59:TYR:CD2	1:A:60:PRO:HD3	2.49	0.48
2:B:25:TYR:CE2	2:B:113:VAL:HG22	2.48	0.48
2:B:130:ILE:HD13	2:B:199:ILE:CG2	2.44	0.48
2:B:441:SER:HB2	2:B:443:ASN:ND2	2.29	0.48
2:B:462:VAL:HG21	2:B:520:PHE:CE2	2.48	0.48
2:B:575:VAL:HG23	2:B:762:LEU:CD1	2.44	0.48
2:B:853:ASN:C	2:B:853:ASN:OD1	2.52	0.48
2:B:866:TYR:HE2	2:B:868:GLN:OE1	1.96	0.48
1:C:1066:TYR:H	1:C:1079:THR:CG2	2.23	0.48
1:C:1560:ALA:O	1:C:1561:TYR:CD2	2.66	0.48
1:C:1583:ASP:N	1:C:1594:LYS:HZ1	2.11	0.48
1:C:1573:VAL:HG12	1:C:1603:LYS:HD3	1.94	0.48
1:C:30:ILE:HG22	1:C:31:PHE:N	2.28	0.48
1:C:354:LEU:HB2	1:C:374:GLN:O	2.14	0.48
1:C:532:GLN:O	1:C:535:VAL:HG13	2.14	0.48
2:D:1442:ILE:C	2:D:1443:LEU:HD13	2.34	0.48
2:D:59:HIS:HB3	2:D:64:LYS:HA	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LEU:HD11	1:A:486:VAL:HG13	1.95	0.48
1:A:548:GLY:HA3	1:A:550:GLN:OE1	2.14	0.48
2:B:1504:GLU:CD	2:B:1505:ARG:H	2.15	0.48
2:B:1534:GLN:OE1	2:B:1534:GLN:HA	2.13	0.48
2:B:1610:TRP:HA	2:B:1628:PHE:CE2	2.49	0.48
2:B:224:PHE:HE1	2:B:320:VAL:HG11	1.79	0.48
2:B:235:PHE:HB3	2:B:338:ILE:HG23	1.96	0.48
2:B:603:GLU:C	2:B:605:SER:H	2.16	0.48
1:C:999:ILE:HD12	1:C:1001:THR:O	2.14	0.48
1:C:153:LYS:HG2	1:C:806:ASN:O	2.13	0.48
1:C:500:ASN:O	1:C:542:VAL:HA	2.14	0.48
2:D:1345:LEU:HD21	2:D:1456:VAL:HG12	1.96	0.48
2:D:1535:ASP:C	2:D:1537:ASN:H	2.17	0.48
2:D:1628:PHE:O	2:D:1629:ALA:C	2.51	0.48
2:D:285:ILE:HD12	2:D:285:ILE:H	1.71	0.48
3:Y:88:GLY:C	3:Y:90:ASP:N	2.66	0.48
1:A:1022:PHE:O	1:A:1024:TYR:N	2.47	0.48
1:A:1140:ASN:O	1:A:1143:TYR:HB3	2.14	0.48
1:A:1244:THR:HG22	1:A:1246:ARG:H	1.75	0.48
1:A:1323:LEU:CG	1:A:1324:HIS:H	2.27	0.48
1:A:1534:GLN:HG3	1:A:1534:GLN:O	2.14	0.48
1:A:1559:TYR:CE2	1:A:1590:ALA:O	2.67	0.48
1:A:243:PHE:CE2	1:A:304:GLU:HA	2.48	0.48
1:A:274:ASP:HA	1:A:322:TYR:CE2	2.49	0.48
1:A:436:LYS:HB2	1:A:449:ARG:CG	2.43	0.48
1:A:965:LEU:C	1:A:967:LEU:H	2.17	0.48
2:B:370:ASP:N	2:B:370:ASP:OD1	2.46	0.48
2:B:478:TYR:CD1	2:B:478:TYR:O	2.58	0.48
2:B:541:LYS:O	2:B:543:THR:CG2	2.62	0.48
1:C:1376:SER:OG	1:C:1503:LYS:HG3	2.14	0.48
1:C:198:MET:SD	1:C:218:GLU:HG3	2.54	0.48
1:C:397:VAL:O	1:C:399:GLN:NE2	2.46	0.48
1:C:371:ILE:CD1	1:C:433:PHE:CE2	2.93	0.48
1:C:525:SER:CB	2:D:399:ILE:HG21	2.44	0.48
1:C:543:TYR:CD1	1:C:543:TYR:C	2.86	0.48
1:C:576:SER:HB2	1:C:589:SER:H	1.79	0.48
1:C:504:LEU:HD23	1:C:649:ALA:O	2.14	0.48
1:C:680:GLN:O	1:C:684:GLU:CG	2.62	0.48
1:C:733:VAL:O	1:C:737:GLN:HG2	2.14	0.48
1:C:859:MET:HB3	1:C:898:PHE:CE1	2.49	0.48
2:D:1381:ILE:CG2	2:D:1459:TYR:HE1	2.25	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:2001:NAG:H3	5:D:2002:NAG:O5	2.14	0.48
2:D:56:ILE:O	2:D:70:GLN:HA	2.14	0.48
2:D:618:LEU:HD22	2:D:636:THR:HA	1.95	0.48
2:D:760:LYS:HE3	2:D:776:MET:SD	2.54	0.48
3:Y:132:THR:CG2	3:Y:155:ILE:HB	2.41	0.48
1:A:1108:VAL:HG21	1:A:1167:ALA:CB	2.40	0.47
1:A:1113:LEU:HD22	1:A:1114:ASP:H	1.77	0.47
1:A:1379:LEU:HD21	1:A:1495:VAL:HG13	1.95	0.47
1:A:1583:ASP:N	1:A:1594:LYS:HZ1	2.12	0.47
1:A:614:ARG:CD	1:A:614:ARG:N	2.76	0.47
1:A:43:VAL:HG12	1:A:79:PHE:O	2.13	0.47
1:A:986:GLU:HG2	1:A:987:ILE:N	2.29	0.47
2:B:1393:ASP:OD1	2:B:1395:GLU:HB3	2.14	0.47
2:B:63:ARG:HB3	2:B:65:GLN:HG3	1.95	0.47
2:B:69:PHE:CE1	2:B:87:ILE:HA	2.49	0.47
1:A:883:CYS:N	2:B:902:GLU:OE2	2.46	0.47
1:C:1076:THR:HG22	1:C:1120:GLU:HA	1.94	0.47
1:C:1186:PHE:HA	1:C:1250:THR:CG2	2.41	0.47
1:C:1247:MET:O	1:C:1251:THR:HG23	2.14	0.47
1:C:1612:VAL:HG23	1:C:1617:TYR:OH	2.14	0.47
1:C:534:MET:CB	1:C:538:SER:OG	2.62	0.47
1:C:682:LYS:HZ3	1:C:686:ILE:HD11	1.79	0.47
1:C:977:LEU:HD22	1:C:978:SER:H	1.78	0.47
2:D:165:PHE:CZ	2:D:199:ILE:CD1	2.96	0.47
2:D:482:LEU:CD1	2:D:521:VAL:HB	2.44	0.47
2:D:52:LYS:HE3	2:D:111:PRO:O	2.13	0.47
2:D:69:PHE:HD2	2:D:70:GLN:N	2.12	0.47
1:A:1053:MET:HE1	1:A:1086:LEU:HD13	1.95	0.47
1:A:123:ASN:C	1:A:123:ASN:OD1	2.53	0.47
1:A:38:ASN:ND2	3:X:150:ILE:HG12	2.28	0.47
1:A:682:LYS:NZ	1:A:686:ILE:HD11	2.29	0.47
1:A:837:GLU:OE2	1:A:1430:THR:HB	2.14	0.47
2:B:1371:TYR:CD1	2:B:1377:SER:CB	2.98	0.47
2:B:1506:ILE:HB	2:B:1627:ASP:HB3	1.97	0.47
2:B:220:VAL:O	2:B:222:PRO:N	2.47	0.47
2:B:322:THR:CG2	2:B:327:ASP:H	2.27	0.47
2:B:544:CYS:HB3	2:B:546:GLY:O	2.13	0.47
2:B:56:ILE:O	2:B:70:GLN:HA	2.14	0.47
2:B:862:LYS:HZ2	2:B:1519:ASN:CB	2.27	0.47
1:C:1534:GLN:HG3	1:C:1534:GLN:O	2.13	0.47
1:C:1598:ILE:HG22	1:C:1599:THR:N	2.29	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:THR:O	1:C:285:THR:CG2	2.59	0.47
1:C:394:THR:HG23	1:C:402:SER:O	2.14	0.47
1:C:871:PRO:HD2	1:C:872:VAL:N	2.29	0.47
1:C:944:LEU:HD23	1:C:944:LEU:H	1.78	0.47
2:D:237:ILE:HD11	2:D:309:LEU:CB	2.36	0.47
2:D:575:VAL:O	2:D:759:THR:HA	2.14	0.47
1:A:1562:LYS:O	1:A:1563:VAL:CG1	2.62	0.47
1:A:1562:LYS:HD3	1:A:1648:TRP:HE1	1.80	0.47
1:A:42:GLN:HE22	1:A:44:TYR:HB2	1.78	0.47
1:A:569:ASN:CG	1:A:570:GLN:N	2.68	0.47
2:B:1279:ILE:HG22	2:B:1288:ILE:CB	2.43	0.47
2:B:41:ILE:O	2:B:85:PRO:HD2	2.14	0.47
2:B:955:PRO:O	2:B:957:THR:HG23	2.14	0.47
1:C:1003:LEU:HA	1:C:1004:PRO:HD2	1.51	0.47
1:C:1506:THR:HG22	1:C:1507:MET:N	2.29	0.47
1:C:1583:ASP:N	1:C:1594:LYS:NZ	2.63	0.47
1:C:216:TYR:N	1:C:216:TYR:CD2	2.82	0.47
1:C:489:LYS:HG2	1:C:490:SER:OG	2.14	0.47
2:D:25:TYR:CE2	2:D:113:VAL:HG22	2.49	0.47
2:D:1370:ARG:NH1	2:D:1372:LEU:HG	2.29	0.47
2:D:386:SER:O	2:D:398:LEU:HD11	2.14	0.47
2:D:148:PHE:CZ	2:D:792:VAL:HG11	2.48	0.47
3:X:42:ASP:HB3	3:X:45:ASP:HB2	1.95	0.47
3:Y:88:GLY:C	3:Y:90:ASP:H	2.15	0.47
1:A:1018:VAL:HG11	1:A:1048:LYS:HB3	1.95	0.47
1:A:1559:TYR:O	1:A:1621:GLY:N	2.47	0.47
1:A:72:HIS:CD2	1:A:72:HIS:C	2.87	0.47
1:A:87:ILE:CD1	1:A:87:ILE:N	2.55	0.47
2:B:1386:MET:HE2	2:B:1386:MET:HA	1.96	0.47
2:B:1482:ASN:H	2:B:1495:GLU:HG2	1.79	0.47
2:B:1567:ARG:HD2	2:B:1567:ARG:HA	1.63	0.47
2:B:1506:ILE:CD1	2:B:1628:PHE:HE1	2.27	0.47
2:B:575:VAL:CG2	2:B:762:LEU:HD11	2.44	0.47
1:C:1069:TRP:HH2	1:C:1465:ASN:ND2	2.12	0.47
1:C:1637:TYR:N	1:C:1637:TYR:CD2	2.83	0.47
1:C:1663:ASN:O	1:C:1666:GLU:HB3	2.14	0.47
1:C:316:GLU:HG2	1:C:349:LEU:CD2	2.43	0.47
1:C:560:TRP:CH2	1:C:673:LEU:CD2	2.98	0.47
1:C:592:MET:O	1:C:783:ARG:HA	2.15	0.47
1:C:641:ASN:O	1:C:642:ASN:C	2.53	0.47
2:D:1330:ASN:ND2	2:D:1330:ASN:N	2.62	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1399:ARG:HG2	2:D:1399:ARG:HH11	1.79	0.47
2:D:1638:PHE:N	2:D:1638:PHE:CD2	2.82	0.47
2:D:161:VAL:CG2	2:D:180:LEU:HD21	2.38	0.47
2:D:531:ILE:O	2:D:617:ASN:ND2	2.41	0.47
3:X:103:VAL:HA	3:X:121:GLY:O	2.15	0.47
1:A:1271:ILE:HD13	1:A:1300:TYR:CZ	2.50	0.47
1:A:617:LYS:HD2	1:A:622:ARG:NH2	2.22	0.47
1:A:695:VAL:HG12	1:A:727:ALA:CB	2.44	0.47
2:B:120:LEU:HA	2:B:120:LEU:HD13	1.76	0.47
2:B:1446:PHE:C	2:B:1448:VAL:H	2.18	0.47
2:B:1575:LEU:N	2:B:1575:LEU:CD2	2.77	0.47
2:B:1575:LEU:HD13	2:B:1581:TYR:CZ	2.49	0.47
2:B:1614:ASP:C	2:B:1616:CYS:N	2.67	0.47
2:B:148:PHE:CZ	2:B:792:VAL:HG11	2.50	0.47
2:B:173:VAL:HA	2:B:964:ILE:CD1	2.44	0.47
1:C:1572:ASN:O	1:C:1573:VAL:HG23	2.14	0.47
1:C:284:GLN:H	1:C:310:LEU:HD22	1.79	0.47
1:C:968:VAL:HG23	1:C:971:THR:OG1	2.14	0.47
2:D:1482:ASN:HB2	2:D:1495:GLU:HA	1.96	0.47
2:D:778:PHE:N	2:D:778:PHE:CD2	2.83	0.47
2:D:843:ASP:HA	2:D:873:LYS:O	2.14	0.47
2:D:96:THR:HG22	2:D:97:ASP:N	2.30	0.47
1:A:1328:MET:HE2	1:A:1328:MET:HA	1.97	0.47
1:A:231:ILE:HG23	1:A:231:ILE:O	2.14	0.47
1:A:243:PHE:HE2	1:A:304:GLU:CA	2.28	0.47
1:A:443:PRO:CD	1:A:446:ASN:HB2	2.44	0.47
1:A:510:ILE:O	1:A:511:HIS:ND1	2.48	0.47
1:A:20:GLU:HB2	1:A:551:THR:CB	2.44	0.47
1:A:892:SER:HB3	1:A:893:SER:H	1.41	0.47
2:B:35:THR:HB	2:B:91:ALA:HB2	1.97	0.47
1:A:419:SER:CB	2:B:459:ASN:HD22	2.15	0.47
1:C:1079:THR:HB	1:C:1107:LEU:HD11	1.96	0.47
1:C:1427:SER:CB	1:C:1492:THR:HG23	2.44	0.47
1:C:1468:PRO:CD	1:C:1473:LEU:HD13	2.44	0.47
1:C:224:LEU:CD2	1:C:225:PRO:HD2	2.43	0.47
1:C:614:ARG:CD	1:C:614:ARG:N	2.76	0.47
1:C:680:GLN:O	1:C:682:LYS:N	2.48	0.47
1:C:840:GLN:HE21	1:C:897:THR:HG21	1.80	0.47
1:C:963:ILE:HA	1:C:973:ILE:HD11	1.97	0.47
2:D:1438:LEU:C	2:D:1438:LEU:HD13	2.34	0.47
2:D:1517:GLU:O	2:D:1518:THR:C	2.53	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1523:VAL:O	2:D:1548:ILE:HB	2.14	0.47
2:D:280:LEU:HD11	2:D:1379:MET:HG3	1.97	0.47
2:D:433:ILE:HG22	2:D:434:ALA:N	2.28	0.47
2:D:484:LEU:HD11	2:D:626:LEU:CG	2.45	0.47
2:D:543:THR:O	2:D:599:TRP:NE1	2.39	0.47
2:D:794:PHE:C	2:D:794:PHE:CD2	2.88	0.47
2:D:870:PHE:CD1	2:D:878:ARG:NH2	2.83	0.47
3:X:119:VAL:HG13	3:X:212:MET:SD	2.55	0.47
3:Y:136:LEU:HA	3:Y:224:ILE:O	2.14	0.47
1:A:1159:CYS:O	1:A:1161:LEU:HD23	2.14	0.47
1:A:1279:ARG:NH1	1:A:1280:TYR:CD2	2.83	0.47
1:A:1307:LEU:HD22	1:A:1307:LEU:H	1.79	0.47
1:A:394:THR:HG23	1:A:402:SER:O	2.14	0.47
1:A:518:PHE:O	1:A:520:ASP:N	2.43	0.47
2:B:189:PRO:C	2:B:191:LEU:H	2.17	0.47
2:B:511:THR:O	2:B:513:ASP:N	2.48	0.47
2:B:563:MET:HB3	2:B:778:PHE:HE2	1.78	0.47
2:B:83:VAL:C	2:B:85:PRO:HD3	2.35	0.47
2:B:846:VAL:HG22	2:B:847:ARG:N	2.28	0.47
1:C:1249:GLU:O	1:C:1253:TYR:HD2	1.98	0.47
1:C:240:TYR:CD2	1:C:241:LYS:N	2.82	0.47
1:C:383:VAL:O	1:C:383:VAL:CG2	2.62	0.47
1:C:42:GLN:HE22	1:C:44:TYR:HB2	1.80	0.47
1:C:670:LYS:HD2	1:C:671:GLU:N	2.29	0.47
1:C:923:LEU:C	1:C:923:LEU:HD23	2.34	0.47
2:D:143:VAL:O	2:D:143:VAL:HG12	2.14	0.47
2:D:168:PRO:HD3	2:D:197:TRP:CD1	2.49	0.47
2:D:206:SER:O	2:D:208:GLU:N	2.47	0.47
2:D:249:ALA:O	2:D:257:VAL:HB	2.15	0.47
2:D:314:LEU:HD12	2:D:314:LEU:HA	1.71	0.47
2:D:478:TYR:CD1	2:D:478:TYR:O	2.58	0.47
3:X:166:ASP:OD2	3:X:207:LEU:CG	2.62	0.47
1:A:1031:TRP:CZ3	1:A:1042:LYS:HA	2.50	0.47
1:A:1186:PHE:HA	1:A:1250:THR:CG2	2.43	0.47
1:A:1293:ALA:O	1:A:1294:ILE:C	2.51	0.47
1:A:1309:LEU:CD1	1:A:1328:MET:HG3	2.44	0.47
1:A:20:GLU:CB	1:A:551:THR:HG22	2.44	0.47
1:A:506:LYS:HD2	1:A:536:PRO:HG2	1.96	0.47
1:A:59:TYR:CD1	1:A:60:PRO:HG3	2.49	0.47
1:A:656:ASN:OD1	1:A:658:ASN:CB	2.51	0.47
2:B:108:VAL:O	2:B:114:ARG:HA	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:LEU:HD22	2:B:1462:TYR:HE2	1.78	0.47
2:B:34:ARG:HD2	2:B:488:LYS:HZ3	1.79	0.47
2:B:642:ALA:O	2:B:643:LYS:HB3	2.15	0.47
2:B:794:PHE:C	2:B:794:PHE:CD2	2.88	0.47
1:C:1179:THR:HG22	1:C:1180:LEU:HD23	1.97	0.47
1:C:1215:GLU:OE1	1:C:1235:LYS:HD3	2.15	0.47
1:C:1268:ASN:HB2	1:C:1269:PRO:HD3	1.97	0.47
1:C:1309:LEU:O	1:C:1329:THR:HA	2.15	0.47
1:C:1504:GLN:OE1	1:C:1506:THR:OG1	2.28	0.47
1:C:1552:ALA:HB2	1:C:1620:MET:CE	2.45	0.47
1:C:576:SER:CB	1:C:577:PRO:CD	2.91	0.47
1:C:595:GLY:O	1:C:596:MET:C	2.52	0.47
2:D:108:VAL:O	2:D:114:ARG:HA	2.15	0.47
2:D:1387:LEU:O	2:D:1390:PHE:HB2	2.14	0.47
2:D:1506:ILE:HD12	2:D:1628:PHE:CE1	2.49	0.47
2:D:1623:LYS:NZ	2:D:1623:LYS:CB	2.78	0.47
2:D:173:VAL:HG11	2:D:186:TYR:OH	2.13	0.47
2:D:566:LYS:O	2:D:567:LEU:HD23	2.15	0.47
1:A:1047:LYS:O	1:A:1048:LYS:C	2.53	0.47
1:A:1585:TYR:CZ	1:A:1586:LYS:HB3	2.49	0.47
1:A:576:SER:CB	1:A:577:PRO:CD	2.91	0.47
1:A:680:GLN:O	1:A:684:GLU:CG	2.62	0.47
1:A:802:VAL:HG12	1:A:803:GLY:N	2.29	0.47
2:B:1567:ARG:NH1	2:B:1567:ARG:HG3	2.29	0.47
2:B:230:PRO:HG3	2:B:333:GLN:CG	2.44	0.47
2:B:482:LEU:HD11	2:B:521:VAL:HB	1.96	0.47
2:B:79:GLY:O	2:B:81:MET:N	2.47	0.47
1:C:1076:THR:HG23	1:C:1077:TRP:N	2.29	0.47
1:C:1240:PRO:HB2	1:C:1242:THR:CG2	2.45	0.47
1:C:1402:ILE:HG13	1:C:1479:ILE:HD13	1.95	0.47
1:C:532:GLN:O	1:C:534:MET:N	2.47	0.47
1:C:993:SER:O	1:C:995:GLU:N	2.48	0.47
2:D:173:VAL:HG13	2:D:964:ILE:HD11	1.95	0.47
1:C:473:HIS:CE1	2:D:455:LYS:NZ	2.83	0.47
2:D:482:LEU:HD11	2:D:521:VAL:HB	1.97	0.47
2:D:813:VAL:CG1	2:D:840:VAL:HG22	2.43	0.47
3:Y:150:ILE:HD12	3:Y:150:ILE:C	2.34	0.47
3:Y:85:PHE:N	3:Y:85:PHE:HD1	2.13	0.47
1:A:1084:ARG:CA	1:A:1151:GLY:HA2	2.45	0.47
1:A:975:ARG:NH1	1:A:1340:VAL:HG11	2.30	0.47
1:A:161:LEU:HD11	1:A:185:PHE:CE2	2.49	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLY:O	1:A:240:TYR:C	2.52	0.47
1:A:530:VAL:CG2	1:A:563:ILE:HD12	2.45	0.47
1:A:25:ILE:HG12	1:A:655:THR:CG2	2.45	0.47
2:B:1517:GLU:O	2:B:1518:THR:C	2.53	0.47
2:B:341:SER:HA	2:B:342:PRO:HD3	1.72	0.47
2:B:463:ASN:OD1	2:B:505:THR:OG1	2.33	0.47
2:B:466:VAL:HG12	2:B:524:TYR:HE2	1.79	0.47
1:C:25:ILE:HG13	1:C:106:VAL:HG21	1.96	0.47
1:C:1215:GLU:HA	1:C:1215:GLU:OE1	2.15	0.47
1:C:148:LEU:HG	1:C:153:LYS:O	2.14	0.47
1:C:263:ALA:O	1:C:291:MET:HE3	2.14	0.47
1:C:407:SER:O	1:C:420:PHE:HE1	1.98	0.47
1:C:997:ILE:HG13	1:C:997:ILE:O	2.15	0.47
2:D:1593:THR:HG21	2:D:1596:LYS:HE3	1.97	0.47
3:Y:128:LYS:HD3	3:Y:158:GLU:CD	2.35	0.47
3:Y:194:LYS:HZ2	3:Y:197:ASN:HD22	1.63	0.47
3:Y:229:ASN:OD1	3:Y:229:ASN:N	2.46	0.47
1:A:111:PHE:CE2	1:A:113:LYS:CB	2.96	0.47
1:A:1133:LEU:HB2	1:A:1134:PRO:HD3	1.97	0.47
1:A:1637:TYR:N	1:A:1637:TYR:CD2	2.83	0.47
1:A:186:PRO:O	1:A:187:ASP:C	2.53	0.47
1:A:543:TYR:HB3	1:A:556:SER:HB3	1.97	0.47
2:B:433:ILE:CG2	2:B:434:ALA:N	2.78	0.47
2:B:787:TRP:HB2	2:B:808:ILE:HG22	1.97	0.47
2:B:829:GLN:HE22	2:B:883:VAL:CG1	2.19	0.47
1:C:323:LEU:HD22	1:C:324:TYR:N	2.30	0.47
1:C:510:ILE:O	1:C:511:HIS:ND1	2.48	0.47
2:D:1367:ILE:HB	2:D:1438:LEU:CD1	2.45	0.47
2:D:1522:TYR:O	2:D:1522:TYR:CD2	2.68	0.47
2:D:1561:HIS:NE2	2:D:1597:ILE:CD1	2.78	0.47
1:C:525:SER:HB2	2:D:399:ILE:HG21	1.96	0.47
3:X:85:PHE:CE1	3:X:117:SER:HB3	2.50	0.47
3:X:52:SER:OG	3:X:53:GLU:N	2.48	0.47
3:X:86:LEU:HG	3:X:91:LYS:CG	2.45	0.47
3:Y:46:LEU:HD12	3:Y:180:TYR:CE1	2.50	0.47
1:A:1583:ASP:N	1:A:1594:LYS:NZ	2.64	0.46
1:A:497:THR:OG1	1:A:498:HIS:N	2.48	0.46
1:A:515:ARG:HG3	1:A:526:ILE:CG2	2.45	0.46
1:A:24:VAL:HG11	1:A:543:TYR:HE2	1.79	0.46
2:B:1486:ILE:HD11	2:B:1591:LEU:CD2	2.45	0.46
2:B:1602:THR:O	2:B:1604:ASN:N	2.43	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:TYR:C	2:B:238:ASP:H	2.18	0.46
2:B:338:ILE:O	2:B:339:VAL:CG1	2.64	0.46
2:B:342:PRO:HG2	2:B:420:LEU:CD1	2.44	0.46
2:B:563:MET:HA	2:B:563:MET:CE	2.45	0.46
1:C:1083:LEU:HD22	1:C:1104:LEU:HD21	1.96	0.46
1:C:1453:TYR:O	1:C:1453:TYR:CD1	2.67	0.46
1:C:219:VAL:CG1	1:C:219:VAL:O	2.63	0.46
1:C:239:GLY:O	1:C:240:TYR:C	2.53	0.46
1:C:302:ASP:HB3	1:C:305:THR:HB	1.97	0.46
1:C:23:TYR:HA	1:C:43:VAL:HA	1.96	0.46
1:C:481:HIS:HB2	2:D:388:GLY:HA2	1.96	0.46
1:C:461:SER:HB2	1:C:553:GLU:CD	2.34	0.46
1:C:689:LYS:CG	1:C:699:CYS:SG	3.03	0.46
2:D:1371:TYR:HB2	2:D:1377:SER:HB3	1.97	0.46
2:D:1457:LYS:HG2	2:D:1469:THR:OG1	2.15	0.46
2:D:263:VAL:HG21	2:D:292:ALA:CB	2.45	0.46
2:D:319:THR:HG23	2:D:330:VAL:CG1	2.45	0.46
2:D:447:VAL:HG13	2:D:447:VAL:O	2.15	0.46
2:D:750:ASP:OD1	2:D:750:ASP:C	2.53	0.46
2:D:866:TYR:HE2	2:D:868:GLN:OE1	1.99	0.46
3:X:166:ASP:O	3:X:170:ARG:HG3	2.15	0.46
1:A:1031:TRP:CH2	1:A:1042:LYS:HG3	2.51	0.46
1:A:975:ARG:NH2	1:A:1346:LEU:HD22	2.30	0.46
1:A:1453:TYR:CD1	1:A:1453:TYR:O	2.69	0.46
1:A:1506:THR:HG22	1:A:1507:MET:N	2.31	0.46
1:A:152:LEU:HD13	1:A:152:LEU:HA	1.49	0.46
1:A:287:MET:SD	1:A:299:VAL:HG23	2.55	0.46
2:B:961:THR:HG22	2:B:1327:THR:CB	2.45	0.46
2:B:143:VAL:O	2:B:143:VAL:HG12	2.15	0.46
2:B:45:ALA:HB3	2:B:81:MET:CE	2.46	0.46
2:B:52:LYS:HE3	2:B:111:PRO:O	2.14	0.46
2:B:541:LYS:O	2:B:543:THR:HG23	2.15	0.46
2:B:613:SER:HA	2:B:620:VAL:HG23	1.96	0.46
2:B:929:LYS:HD3	2:B:929:LYS:HA	1.74	0.46
1:C:1080:ALA:CB	1:C:1148:THR:HG22	2.44	0.46
1:C:1232:LEU:CG	1:C:1233:GLN:HG3	2.38	0.46
1:C:1616:GLN:OE1	1:C:1650:ARG:HD3	2.15	0.46
1:C:189:LYS:HG3	1:C:190:ILE:O	2.15	0.46
1:C:23:TYR:HE2	1:C:111:PHE:HD2	1.62	0.46
1:C:656:ASN:CB	1:C:659:ALA:H	2.27	0.46
1:C:906:GLY:N	1:C:929:VAL:HB	2.24	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:963:ILE:CG2	1:C:967:LEU:HD23	2.42	0.46
2:D:1299:LEU:HB3	2:D:1301:ARG:HD3	1.96	0.46
2:D:452:THR:O	2:D:453:GLU:O	2.34	0.46
2:D:481:TYR:CE2	2:D:493:GLY:N	2.83	0.46
2:D:39:GLU:O	2:D:87:ILE:HD12	2.15	0.46
1:A:1068:VAL:CG1	1:A:1069:TRP:N	2.78	0.46
1:A:127:PHE:CE1	1:A:626:PHE:CD2	3.04	0.46
1:A:1304:VAL:HG12	1:A:1305:LYS:H	1.80	0.46
1:A:20:GLU:OE2	1:A:20:GLU:O	2.33	0.46
1:A:773:TRP:CE3	1:A:774:LEU:HB2	2.51	0.46
1:A:74:SER:C	1:A:79:PHE:CE1	2.89	0.46
1:A:923:LEU:HD23	1:A:923:LEU:C	2.35	0.46
2:B:1504:GLU:O	2:B:1624:LEU:HD13	2.14	0.46
2:B:1535:ASP:C	2:B:1537:ASN:H	2.18	0.46
2:B:44:GLU:OE1	2:B:480:THR:HG21	2.15	0.46
2:B:953:ARG:CG	2:B:954:VAL:N	2.78	0.46
1:C:1622:LYS:HD2	1:C:1642:LEU:CB	2.44	0.46
1:C:365:PRO:HG2	1:C:464:TYR:HE2	1.79	0.46
1:C:500:ASN:CB	1:C:543:TYR:CE1	2.64	0.46
1:C:554:LEU:N	1:C:658:ASN:HD22	2.13	0.46
1:C:949:ILE:O	1:C:949:ILE:HG22	2.14	0.46
2:D:1294:TYR:O	2:D:1294:TYR:CD2	2.67	0.46
2:D:1589:ASP:HB3	2:D:1600:ILE:HG13	1.97	0.46
2:D:449:ILE:HD13	2:D:462:VAL:HG23	1.97	0.46
2:D:575:VAL:CG2	2:D:762:LEU:HD11	2.46	0.46
2:D:810:VAL:CG1	2:D:811:MET:N	2.79	0.46
3:X:61:SER:O	3:X:75:PHE:HZ	1.97	0.46
3:Y:58:SER:HB3	3:Y:102:ASN:HD21	1.77	0.46
1:A:500:ASN:O	1:A:542:VAL:HG13	2.16	0.46
1:A:680:GLN:O	1:A:681:LYS:C	2.53	0.46
1:A:993:SER:O	1:A:995:GLU:N	2.49	0.46
2:B:130:ILE:HG21	2:B:199:ILE:HG21	1.98	0.46
2:B:1367:ILE:HD13	2:B:1456:VAL:HG21	1.96	0.46
2:B:137:TYR:HB2	2:B:216:VAL:HG23	1.98	0.46
2:B:1399:ARG:HG2	2:B:1399:ARG:HH11	1.79	0.46
2:B:1496:THR:HG23	2:B:1603:LYS:HD2	1.98	0.46
2:B:1499:SER:HA	2:B:1572:ALA:O	2.16	0.46
2:B:129:PHE:CE2	2:B:598:ILE:HG23	2.50	0.46
2:B:69:PHE:C	2:B:69:PHE:HD2	2.19	0.46
2:B:778:PHE:CD2	2:B:778:PHE:N	2.82	0.46
2:B:850:LEU:HB2	2:B:882:PHE:CD1	2.50	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:940:THR:HG22	2:B:940:THR:O	2.15	0.46
1:C:1080:ALA:HB1	1:C:1148:THR:HA	1.97	0.46
1:C:174:VAL:HG22	1:C:175:GLU:H	1.80	0.46
1:C:20:GLU:HG3	1:C:547:THR:CB	2.45	0.46
1:C:241:LYS:NZ	1:C:351:PRO:HB3	2.30	0.46
1:C:428:VAL:HG22	1:C:429:THR:N	2.29	0.46
1:C:489:LYS:NZ	2:D:502:ASN:H	2.13	0.46
1:C:680:GLN:O	1:C:681:LYS:C	2.54	0.46
1:C:811:VAL:O	1:C:811:VAL:HG12	2.16	0.46
1:C:829:ILE:HA	1:C:830:PRO:HD3	1.78	0.46
2:D:296:ARG:HG3	2:D:296:ARG:NH1	2.29	0.46
2:D:466:VAL:HG12	2:D:524:TYR:HE2	1.80	0.46
2:D:787:TRP:HB2	2:D:808:ILE:HG22	1.96	0.46
2:D:920:VAL:O	2:D:1330:ASN:HA	2.15	0.46
2:D:929:LYS:HD3	2:D:929:LYS:HA	1.70	0.46
3:Y:185:LYS:HG2	3:Y:186:TYR:CD2	2.51	0.46
3:Y:119:VAL:HG21	3:Y:209:PHE:CB	2.44	0.46
3:Y:77:PRO:O	3:Y:78:LYS:CB	2.63	0.46
1:A:1159:CYS:C	1:A:1161:LEU:H	2.18	0.46
1:A:1255:LEU:HD13	1:A:1267:VAL:HG13	1.97	0.46
1:A:161:LEU:HD21	1:A:185:PHE:CD2	2.51	0.46
1:A:274:ASP:CG	1:A:275:LEU:N	2.69	0.46
1:A:504:LEU:HD21	1:A:651:LEU:CG	2.44	0.46
1:A:534:MET:CB	1:A:538:SER:OG	2.63	0.46
1:A:787:GLN:O	1:A:788:PHE:HB3	2.15	0.46
2:B:1363:LEU:HD23	2:B:1442:ILE:HG12	1.98	0.46
2:B:1573:LEU:HB3	2:B:1575:LEU:HD23	1.97	0.46
2:B:361:GLU:HB3	2:B:399:ILE:HD13	1.98	0.46
2:B:352:LYS:HG3	2:B:430:MET:HE1	1.98	0.46
2:B:481:TYR:HE2	2:B:493:GLY:HA3	1.81	0.46
2:B:599:TRP:CE3	2:B:602:ILE:HD12	2.51	0.46
2:B:750:ASP:C	2:B:750:ASP:OD1	2.53	0.46
1:C:1022:PHE:CE2	1:C:1092:TYR:CD1	3.04	0.46
1:C:1535:MET:HA	1:C:1645:ILE:HB	1.98	0.46
1:C:42:GLN:CA	1:C:80:GLN:HG3	2.42	0.46
2:D:1534:GLN:OE1	2:D:1534:GLN:HA	2.16	0.46
2:D:1563:TYR:HB3	2:D:1601:ILE:HD11	1.96	0.46
2:D:1567:ARG:HG3	2:D:1567:ARG:HH11	1.80	0.46
2:D:1561:HIS:NE2	2:D:1597:ILE:HD13	2.29	0.46
2:D:825:VAL:HG11	2:D:918:GLU:HB3	1.97	0.46
3:X:136:LEU:HA	3:X:224:ILE:O	2.14	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:179:LEU:HD11	3:X:180:TYR:CE1	2.50	0.46
1:A:119:ILE:C	1:A:119:ILE:HD12	2.36	0.46
1:A:1244:THR:O	1:A:1245:ALA:C	2.54	0.46
1:A:125:PHE:N	1:A:125:PHE:CD1	2.83	0.46
1:A:128:ILE:HD12	1:A:201:ILE:CG2	2.41	0.46
1:A:1671:ILE:HD13	1:A:1676:CYS:SG	2.56	0.46
1:A:216:TYR:CD2	1:A:216:TYR:N	2.82	0.46
1:A:374:GLN:HG2	1:A:382:LEU:CD2	2.45	0.46
1:A:371:ILE:CD1	1:A:433:PHE:CE2	2.96	0.46
1:A:42:GLN:OE1	1:A:500:ASN:ND2	2.48	0.46
1:A:644:ASN:O	1:A:645:VAL:C	2.54	0.46
1:A:86:THR:C	1:A:87:ILE:HD13	2.35	0.46
1:A:982:LEU:C	1:A:984:VAL:N	2.68	0.46
2:B:1424:ILE:HD13	2:B:1424:ILE:N	2.27	0.46
2:B:1500:LEU:HD22	2:B:1607:ILE:HB	1.98	0.46
2:B:398:LEU:HA	2:B:398:LEU:HD23	1.50	0.46
2:B:476:ILE:HG12	2:B:524:TYR:CD2	2.50	0.46
2:B:525:GLN:NE2	2:B:528:ASN:H	2.13	0.46
1:C:1093:VAL:HG12	1:C:1095:GLN:NE2	2.30	0.46
1:C:1426:ILE:O	1:C:1426:ILE:HG22	2.16	0.46
1:C:1572:ASN:C	1:C:1573:VAL:HG23	2.35	0.46
1:C:909:ASN:HD21	4:C:2003:NAG:H83	1.81	0.46
1:C:705:VAL:HA	1:C:739:ARG:HH12	1.80	0.46
1:C:78:LYS:O	1:C:80:GLN:N	2.49	0.46
1:C:853:MET:O	1:C:888:VAL:HG12	2.15	0.46
2:D:1351:ASN:N	2:D:1351:ASN:OD1	2.44	0.46
2:D:1573:LEU:HB3	2:D:1575:LEU:HD23	1.98	0.46
2:D:398:LEU:HA	2:D:398:LEU:HD23	1.53	0.46
2:D:933:ARG:HH11	2:D:933:ARG:CG	2.18	0.46
3:Y:42:ASP:HB3	3:Y:45:ASP:HB2	1.98	0.46
1:A:1025:LEU:HD13	1:A:1031:TRP:CZ3	2.51	0.46
1:A:1227:PHE:HA	1:A:1228:TRP:CE3	2.51	0.46
1:A:938:SER:OG	1:A:1284:PHE:CE2	2.68	0.46
1:A:1561:TYR:CD1	1:A:1581:LEU:HD21	2.50	0.46
1:A:219:VAL:HG12	1:A:219:VAL:O	2.15	0.46
1:A:25:ILE:CG2	1:A:654:LEU:HB2	2.45	0.46
1:A:296:ILE:CG2	1:A:297:ALA:N	2.77	0.46
1:A:248:ILE:HB	1:A:299:VAL:HG13	1.97	0.46
1:A:383:VAL:HG23	1:A:386:VAL:HG23	1.98	0.46
1:A:554:LEU:H	1:A:658:ASN:ND2	2.11	0.46
1:A:827:MET:HE2	1:A:912:PHE:CE2	2.51	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1508:VAL:HG13	2:B:1631:PHE:HB2	1.97	0.46
2:B:267:VAL:HG22	2:B:314:LEU:CD1	2.46	0.46
2:B:338:ILE:O	2:B:339:VAL:HG13	2.16	0.46
2:B:345:ILE:HG13	2:B:428:LYS:HB3	1.98	0.46
2:B:557:GLN:OE1	2:B:557:GLN:CA	2.58	0.46
2:B:582:LYS:O	2:B:583:ALA:C	2.53	0.46
1:C:1133:LEU:N	1:C:1133:LEU:CD1	2.71	0.46
1:C:1246:ARG:HB2	1:C:1246:ARG:CZ	2.46	0.46
1:C:1309:LEU:CD1	1:C:1328:MET:HG3	2.45	0.46
1:C:1406:ALA:O	1:C:1472:PHE:HA	2.16	0.46
1:C:1622:LYS:HZ2	1:C:1642:LEU:HD23	1.80	0.46
1:C:25:ILE:CD1	1:C:41:ILE:HG13	2.46	0.46
1:C:560:TRP:HH2	1:C:673:LEU:HD22	1.80	0.46
5:D:2001:NAG:HO3	5:D:2002:NAG:C5	2.29	0.46
2:D:275:SER:O	2:D:277:PRO:HD3	2.16	0.46
2:D:384:PHE:CD2	2:D:384:PHE:N	2.84	0.46
1:A:1128:LYS:O	1:A:1129:LEU:HD23	2.15	0.46
1:A:1127:ILE:HD11	1:A:1143:TYR:CE2	2.50	0.46
1:A:1641:SER:C	1:A:1643:THR:N	2.69	0.46
1:A:374:GLN:HG2	1:A:382:LEU:HD21	1.96	0.46
1:A:993:SER:C	1:A:995:GLU:N	2.60	0.46
2:B:122:SER:OG	2:B:124:GLN:HB3	2.15	0.46
2:B:148:PHE:CZ	2:B:792:VAL:CG1	2.99	0.46
2:B:1510:LEU:O	2:B:1513:GLU:N	2.48	0.46
2:B:484:LEU:HD11	2:B:626:LEU:CG	2.45	0.46
2:B:953:ARG:CG	2:B:954:VAL:H	2.29	0.46
2:B:96:THR:HG22	2:B:97:ASP:O	2.16	0.46
1:C:1081:PHE:O	1:C:1084:ARG:HB3	2.15	0.46
1:C:1305:LYS:O	1:C:1307:LEU:HD13	2.16	0.46
1:C:1582:LEU:C	1:C:1594:LYS:HZ2	2.19	0.46
1:C:291:MET:HE2	1:C:291:MET:HB3	1.79	0.46
1:C:351:PRO:CG	1:C:442:LEU:HD11	2.45	0.46
1:C:766:ARG:H	1:C:766:ARG:HD3	1.80	0.46
2:D:1284:ARG:HG3	2:D:1285:GLU:N	2.30	0.46
2:D:1506:ILE:HD11	2:D:1628:PHE:CE1	2.43	0.46
2:D:164:GLU:HA	2:D:174:SER:O	2.16	0.46
2:D:511:THR:O	2:D:512:PRO:C	2.54	0.46
2:D:806:TYR:CD1	2:D:806:TYR:C	2.89	0.46
2:D:830:VAL:CG2	2:D:831:GLU:N	2.75	0.46
2:D:191:LEU:HD12	2:D:958:GLU:HG2	1.98	0.46
3:Y:174:VAL:O	3:Y:174:VAL:HG12	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:SER:C	1:A:101:TYR:CD2	2.89	0.46
1:A:1637:TYR:HD2	1:A:1637:TYR:N	2.14	0.46
1:A:164:ILE:HG22	1:A:165:ASP:O	2.16	0.46
1:A:186:PRO:O	1:A:187:ASP:O	2.33	0.46
1:A:296:ILE:HG23	1:A:297:ALA:N	2.30	0.46
1:A:592:MET:O	1:A:783:ARG:HA	2.15	0.46
1:A:909:ASN:HD21	4:A:2003:NAG:C8	2.29	0.46
2:B:1505:ARG:CG	2:B:1505:ARG:HH11	2.07	0.46
2:B:1529:LEU:CD1	2:B:1529:LEU:N	2.79	0.46
2:B:184:TRP:N	2:B:184:TRP:CE3	2.81	0.46
2:B:355:LYS:O	2:B:358:MET:CB	2.63	0.46
2:B:566:LYS:O	2:B:567:LEU:HD23	2.16	0.46
2:B:87:ILE:H	2:B:87:ILE:CD1	2.26	0.46
2:B:954:VAL:O	2:B:957:THR:HG23	2.16	0.46
1:C:1379:LEU:HD21	1:C:1495:VAL:HG13	1.97	0.46
1:C:1436:GLU:HG2	1:C:1453:TYR:HE2	1.81	0.46
1:C:307:VAL:O	1:C:311:SER:HB2	2.16	0.46
1:C:382:LEU:HA	1:C:382:LEU:HD23	1.80	0.46
1:C:477:LEU:HD23	1:C:480:GLU:OE1	2.15	0.46
1:C:493:ILE:CG2	1:C:495:LYS:HB2	2.46	0.46
2:D:1446:PHE:C	2:D:1448:VAL:H	2.19	0.46
2:D:148:PHE:HB2	2:D:800:ILE:HD11	1.95	0.46
3:X:58:SER:HB3	3:X:102:ASN:HD22	1.75	0.46
1:A:1079:THR:HB	1:A:1107:LEU:HD11	1.98	0.46
1:A:22:THR:HG21	1:A:657:ALA:CB	2.39	0.46
1:A:285:THR:CG2	1:A:285:THR:O	2.63	0.46
1:A:322:TYR:N	1:A:322:TYR:HD2	2.13	0.46
1:A:382:LEU:HD22	1:A:416:GLY:HA3	1.97	0.46
1:A:20:GLU:HB2	1:A:551:THR:HG22	1.98	0.46
1:A:690:TYR:CZ	1:A:692:HIS:CB	2.99	0.46
1:A:862:VAL:O	1:A:863:GLU:C	2.53	0.46
2:B:105:VAL:HG12	2:B:118:VAL:HA	1.97	0.46
2:B:139:PRO:HG2	2:B:218:LYS:HE2	1.96	0.46
2:B:1429:LYS:H	2:B:1429:LYS:HE3	1.80	0.46
2:B:1631:PHE:CD2	2:B:1632:SER:N	2.84	0.46
2:B:210:TYR:CG	2:B:211:THR:N	2.84	0.46
2:B:524:TYR:CD1	2:B:524:TYR:C	2.89	0.46
2:B:525:GLN:CD	2:B:525:GLN:O	2.54	0.46
2:B:640:SER:O	2:B:641:ALA:HB2	2.16	0.46
2:B:916:VAL:HG22	2:B:917:PRO:N	2.31	0.46
2:B:96:THR:HG22	2:B:97:ASP:N	2.31	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1068:VAL:CG1	1:C:1069:TRP:N	2.76	0.46
1:C:1156:PHE:O	1:C:1160:PRO:HD3	2.16	0.46
1:C:1298:THR:O	1:C:1299:GLU:C	2.53	0.46
1:C:1332:ASN:O	1:C:1333:PHE:O	2.34	0.46
1:C:1346:LEU:HA	1:C:1346:LEU:HD12	1.48	0.46
1:C:1582:LEU:C	1:C:1594:LYS:NZ	2.70	0.46
1:C:161:LEU:HD11	1:C:185:PHE:CE2	2.50	0.46
1:C:1627:ILE:O	1:C:1627:ILE:HG13	2.16	0.46
1:C:165:ASP:HA	1:C:166:PRO:HD2	1.76	0.46
1:C:545:ILE:HG12	1:C:545:ILE:H	1.41	0.46
1:C:569:ASN:H	1:C:569:ASN:HD22	1.64	0.46
1:C:553:GLU:HA	1:C:658:ASN:HD22	1.81	0.46
2:D:1347:VAL:CG2	2:D:1456:VAL:HG11	2.43	0.46
2:D:1525:LYS:HE3	2:D:1610:TRP:CE2	2.51	0.46
2:D:873:LYS:CD	2:D:873:LYS:N	2.79	0.46
2:D:857:CYS:HB3	2:D:885:VAL:CG2	2.45	0.46
2:D:954:VAL:CG1	2:D:955:PRO:HD2	2.38	0.46
3:X:128:LYS:HD3	3:X:158:GLU:CD	2.36	0.46
3:X:190:ILE:HG12	3:X:190:ILE:O	2.16	0.46
3:Y:215:VAL:O	3:Y:216:LEU:HD13	2.15	0.46
1:A:999:ILE:HD12	1:A:1001:THR:O	2.16	0.45
1:A:148:LEU:HA	1:A:154:PRO:O	2.15	0.45
1:A:364:LYS:HD2	1:A:364:LYS:N	2.32	0.45
1:A:376:LYS:HA	1:A:381:GLN:O	2.15	0.45
1:A:560:TRP:CH2	1:A:562:ASN:HB2	2.51	0.45
1:A:25:ILE:CB	1:A:654:LEU:HB2	2.46	0.45
2:B:1290:TYR:CD2	2:B:1301:ARG:HB3	2.51	0.45
2:B:1382:ILE:HG12	2:B:1427:LEU:HD11	1.98	0.45
2:B:144:LEU:HB3	2:B:185:PRO:HB3	1.97	0.45
2:B:416:ASN:CA	2:B:425:GLN:HE22	2.20	0.45
2:B:518:PHE:H	2:B:518:PHE:HD2	1.64	0.45
1:C:108:SER:OG	1:C:111:PHE:N	2.49	0.45
1:C:114:SER:O	1:C:115:LYS:HE2	2.16	0.45
1:C:1162:VAL:CG2	1:C:1163:LYS:N	2.79	0.45
1:C:1234:HIS:CG	1:C:1235:LYS:H	2.34	0.45
1:C:1317:TYR:CE1	1:C:1342:LEU:HD12	2.51	0.45
1:C:965:LEU:HD23	1:C:1629:TYR:CD1	2.51	0.45
1:C:1641:SER:C	1:C:1643:THR:N	2.69	0.45
1:C:328:THR:HG22	1:C:328:THR:O	2.16	0.45
2:D:1393:ASP:OD1	2:D:1395:GLU:HB3	2.15	0.45
2:D:758:LEU:HD23	2:D:758:LEU:HA	1.70	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:575:VAL:HG23	2:D:762:LEU:CD1	2.46	0.45
2:D:851:LEU:HD21	2:D:865:ARG:HH21	1.81	0.45
3:Y:68:ASN:OD1	3:Y:69:GLY:N	2.40	0.45
1:A:57:LYS:O	1:A:102:VAL:HG22	2.16	0.45
1:A:1022:PHE:HE2	1:A:1092:TYR:CD1	2.34	0.45
1:A:1213:LYS:CG	1:A:1266:TYR:HE2	2.22	0.45
1:A:1562:LYS:O	1:A:1563:VAL:HG13	2.16	0.45
1:A:263:ALA:O	1:A:291:MET:HE3	2.16	0.45
1:A:455:ILE:HG22	1:A:456:ALA:H	1.79	0.45
1:A:705:VAL:HA	1:A:739:ARG:HH12	1.81	0.45
1:A:718:ILE:HD11	1:A:728:PHE:CD2	2.51	0.45
1:A:733:VAL:O	1:A:737:GLN:HG2	2.15	0.45
1:A:76:GLU:O	1:A:76:GLU:CD	2.55	0.45
1:A:871:PRO:HD2	1:A:872:VAL:H	1.78	0.45
1:A:883:CYS:O	1:A:884:VAL:C	2.54	0.45
2:B:132:THR:O	2:B:133:ASP:C	2.55	0.45
2:B:1482:ASN:HB2	2:B:1495:GLU:HA	1.97	0.45
2:B:570:ASP:O	2:B:573:ALA:CB	2.64	0.45
2:B:756:LEU:HD22	2:B:778:PHE:CD1	2.51	0.45
1:C:1525:CYS:C	1:C:1528:VAL:HG22	2.28	0.45
1:C:185:PHE:HD1	1:C:186:PRO:HD2	1.82	0.45
1:C:20:GLU:HG3	1:C:547:THR:HB	1.98	0.45
1:C:465:LEU:HD23	1:C:556:SER:HA	1.98	0.45
1:C:535:VAL:HA	1:C:563:ILE:CD1	2.46	0.45
1:C:690:TYR:CZ	1:C:692:HIS:CB	2.98	0.45
1:C:590:LEU:HD21	1:C:774:LEU:HD11	1.99	0.45
2:D:107:GLN:HG3	2:D:116:GLU:HG3	1.98	0.45
2:D:208:GLU:O	2:D:209:ASN:C	2.55	0.45
2:D:618:LEU:HG	2:D:634:LEU:HD11	1.98	0.45
2:D:79:GLY:O	2:D:81:MET:N	2.50	0.45
3:X:107:GLN:CD	3:X:110:ILE:HD11	2.36	0.45
3:X:119:VAL:HG22	3:X:212:MET:HB2	1.99	0.45
1:A:1249:GLU:HG3	1:A:1289:ASP:CA	2.46	0.45
1:A:1300:TYR:CD2	1:A:1300:TYR:C	2.89	0.45
1:A:1128:LYS:HD3	1:A:1414:GLU:OE1	2.16	0.45
1:A:1646:GLU:HG2	1:A:1660:PHE:CZ	2.51	0.45
1:A:240:TYR:CD2	1:A:241:LYS:N	2.85	0.45
1:A:436:LYS:CB	1:A:449:ARG:HG2	2.45	0.45
1:A:365:PRO:HG2	1:A:464:TYR:HE2	1.80	0.45
1:A:532:GLN:O	1:A:533:ASN:C	2.55	0.45
1:A:506:LYS:HD2	1:A:536:PRO:HD2	1.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:THR:OG1	1:A:713:GLN:HG3	2.16	0.45
1:A:961:TYR:CD1	1:A:961:TYR:C	2.89	0.45
2:B:1371:TYR:HB2	2:B:1377:SER:HB3	1.99	0.45
2:B:760:LYS:HE3	2:B:776:MET:SD	2.55	0.45
2:B:853:ASN:HA	2:B:854:PRO:HD3	1.56	0.45
1:C:1278:GLN:NE2	1:C:1293:ALA:CB	2.79	0.45
1:C:979:VAL:CG2	1:C:1326:TYR:CE1	2.79	0.45
1:C:150:ASP:CG	1:C:151:ASP:N	2.70	0.45
1:C:578:ASP:O	1:C:578:ASP:CG	2.55	0.45
1:C:760:VAL:O	1:C:760:VAL:HG22	2.16	0.45
1:C:96:GLN:HG3	1:C:97:ASN:N	2.31	0.45
2:D:103:TYR:N	2:D:103:TYR:CD2	2.85	0.45
2:D:130:ILE:HG21	2:D:199:ILE:HG21	1.98	0.45
2:D:1380:THR:HG22	2:D:1381:ILE:N	2.31	0.45
2:D:1446:PHE:CD2	2:D:1448:VAL:HG13	2.51	0.45
2:D:1508:VAL:HB	2:D:1509:PRO:CD	2.44	0.45
2:D:63:ARG:CB	2:D:65:GLN:HG3	2.46	0.45
2:D:954:VAL:O	2:D:957:THR:HG23	2.15	0.45
1:A:1215:GLU:HA	1:A:1215:GLU:OE1	2.16	0.45
1:A:1268:ASN:ND2	1:A:1268:ASN:N	2.64	0.45
1:A:1305:LYS:O	1:A:1307:LEU:HD13	2.17	0.45
1:A:224:LEU:CD2	1:A:225:PRO:HD2	2.44	0.45
1:A:61:ASP:O	1:A:62:LYS:CB	2.64	0.45
1:A:661:ASP:OD2	1:A:663:GLN:N	2.50	0.45
1:A:855:PHE:HB2	1:A:914:LEU:HD11	1.98	0.45
1:A:909:ASN:HA	1:A:926:THR:HA	1.98	0.45
1:A:989:SER:O	1:A:993:SER:HB3	2.16	0.45
2:B:962:LYS:HD2	2:B:1302:THR:CG2	2.46	0.45
2:B:178:VAL:HG21	2:B:183:PHE:CD1	2.52	0.45
2:B:531:ILE:HD11	2:B:634:LEU:CD2	2.45	0.45
2:B:778:PHE:N	2:B:778:PHE:HD2	2.13	0.45
1:C:484:ILE:HD13	1:C:540:LEU:HD21	1.96	0.45
1:C:690:TYR:CE1	1:C:696:LYS:HD2	2.52	0.45
1:C:773:TRP:CE3	1:C:774:LEU:HB2	2.52	0.45
1:C:600:VAL:CG2	1:C:780:VAL:HG21	2.46	0.45
2:D:1296:ASN:O	2:D:1297:ALA:C	2.54	0.45
2:D:1313:VAL:HG21	2:D:1323:MET:HE2	1.98	0.45
2:D:1633:TYR:CE1	2:D:1637:GLU:OE1	2.69	0.45
2:D:778:PHE:N	2:D:778:PHE:HD2	2.14	0.45
2:D:953:ARG:CG	2:D:954:VAL:H	2.29	0.45
3:X:60:VAL:O	3:X:60:VAL:HG23	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:HIS:O	1:A:1027:THR:HB	2.15	0.45
1:A:1328:MET:HB2	1:A:1328:MET:HE3	1.85	0.45
1:A:136:THR:O	1:A:139:GLN:HG3	2.17	0.45
1:A:1468:PRO:CD	1:A:1473:LEU:HD13	2.45	0.45
1:A:1557:ILE:HD13	1:A:1622:LYS:HG3	1.99	0.45
1:A:248:ILE:HD13	1:A:325:ILE:HD13	1.99	0.45
1:A:407:SER:O	1:A:420:PHE:HE1	1.99	0.45
2:B:103:TYR:CD2	2:B:103:TYR:N	2.83	0.45
2:B:188:LEU:HD13	2:B:216:VAL:CG2	2.47	0.45
2:B:1344:HIS:ND1	5:B:2003:NAG:C8	2.79	0.45
2:B:162:ILE:HG22	2:B:202:LYS:O	2.16	0.45
1:A:481:HIS:CD2	2:B:387:MET:HG3	2.51	0.45
2:B:456:PRO:CG	2:B:515:ILE:HD11	2.46	0.45
2:B:842:GLU:O	2:B:844:ILE:HG23	2.17	0.45
2:B:922:LYS:NZ	2:B:952:ASP:OD2	2.50	0.45
1:C:1561:TYR:HE1	1:C:1581:LEU:HG	1.82	0.45
1:C:420:PHE:CD2	1:C:420:PHE:N	2.84	0.45
1:C:640:LEU:H	1:C:644:ASN:CB	2.27	0.45
1:C:74:SER:HA	1:C:79:PHE:CE1	2.51	0.45
1:C:970:LYS:C	1:C:971:THR:CG2	2.85	0.45
2:D:105:VAL:HG12	2:D:118:VAL:HA	1.99	0.45
2:D:1529:LEU:N	2:D:1529:LEU:CD1	2.80	0.45
2:D:315:TYR:CD1	2:D:315:TYR:C	2.89	0.45
2:D:44:GLU:OE2	2:D:523:TYR:OH	2.33	0.45
1:C:473:HIS:CE1	2:D:455:LYS:HE3	2.51	0.45
2:D:570:ASP:O	2:D:573:ALA:CB	2.65	0.45
3:X:139:ASN:HB2	3:X:227:THR:HG23	1.98	0.45
1:A:1180:LEU:HD21	1:A:1208:ILE:HA	1.98	0.45
1:A:1488:LEU:HD12	1:A:1488:LEU:C	2.37	0.45
1:A:1570:VAL:HG22	1:A:1575:VAL:HA	1.99	0.45
1:A:1648:TRP:NE1	1:A:1664:LEU:CD2	2.79	0.45
1:A:222:TYR:HE2	1:A:224:LEU:HA	1.81	0.45
1:A:288:GLN:O	1:A:289:ASN:C	2.55	0.45
1:A:419:SER:HB2	2:B:459:ASN:ND2	2.14	0.45
1:A:40:VAL:CG2	1:A:41:ILE:N	2.79	0.45
1:A:554:LEU:N	1:A:658:ASN:HD22	2.13	0.45
1:A:690:TYR:CE1	1:A:696:LYS:HD2	2.52	0.45
1:A:774:LEU:HG	1:A:788:PHE:HE1	1.80	0.45
2:B:1343:PHE:CZ	2:B:1371:TYR:HD1	2.35	0.45
2:B:1391:LEU:HB2	2:B:1417:MET:CE	2.47	0.45
2:B:159:LYS:HE2	2:B:180:LEU:HD12	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:410:PRO:CA	2:B:431:THR:HG22	2.46	0.45
2:B:518:PHE:CD2	2:B:518:PHE:O	2.70	0.45
2:B:613:SER:HA	2:B:620:VAL:CG2	2.46	0.45
2:B:780:LEU:HD11	2:B:787:TRP:HD1	1.82	0.45
2:B:862:LYS:NZ	2:B:1519:ASN:HB3	2.32	0.45
1:C:1113:LEU:HD23	1:C:1114:ASP:H	1.81	0.45
1:C:20:GLU:O	1:C:20:GLU:OE2	2.34	0.45
1:C:224:LEU:HD23	1:C:225:PRO:CD	2.44	0.45
1:C:892:SER:HB3	1:C:893:SER:H	1.41	0.45
2:D:184:TRP:CE3	2:D:184:TRP:N	2.81	0.45
2:D:378:PRO:HA	2:D:389:THR:HA	1.99	0.45
3:Y:222:ARG:HB2	3:Y:222:ARG:HE	1.60	0.45
1:A:1226:ARG:CD	1:A:1266:TYR:HE1	2.29	0.45
1:A:1186:PHE:HD1	1:A:1250:THR:HG22	1.82	0.45
1:A:1332:ASN:O	1:A:1333:PHE:O	2.35	0.45
1:A:532:GLN:HA	1:A:535:VAL:HG13	1.98	0.45
1:A:532:GLN:O	1:A:534:MET:N	2.49	0.45
1:A:256:TYR:HB3	1:A:848:TYR:OH	2.17	0.45
1:A:916:THR:O	1:A:918:PHE:N	2.50	0.45
2:B:1567:ARG:HH11	2:B:1567:ARG:HG3	1.82	0.45
2:B:208:GLU:O	2:B:209:ASN:C	2.55	0.45
2:B:267:VAL:HG22	2:B:314:LEU:HD12	1.99	0.45
2:B:481:TYR:CE1	2:B:506:MET:SD	2.97	0.45
2:B:855:ALA:O	2:B:856:PHE:CD1	2.70	0.45
1:C:1106:TRP:CZ2	1:C:1111:TYR:HE2	2.34	0.45
1:C:274:ASP:OD1	1:C:277:ASP:CG	2.55	0.45
1:C:284:GLN:HG2	1:C:310:LEU:CD1	2.47	0.45
1:C:374:GLN:HG2	1:C:382:LEU:CD2	2.47	0.45
1:C:376:LYS:HA	1:C:381:GLN:O	2.16	0.45
1:C:382:LEU:HD22	1:C:416:GLY:HA3	1.97	0.45
1:C:465:LEU:HG	1:C:466:TYR:N	2.30	0.45
1:C:503:ILE:O	1:C:510:ILE:HG12	2.17	0.45
1:C:612:VAL:HG21	1:C:769:PHE:CE2	2.52	0.45
2:D:1382:ILE:CD1	2:D:1458:VAL:HG22	2.47	0.45
2:D:1524:TYR:HB3	2:D:1544:VAL:HG13	1.98	0.45
2:D:378:PRO:HB2	2:D:416:ASN:O	2.17	0.45
2:D:83:VAL:C	2:D:85:PRO:HD3	2.36	0.45
1:A:1142:LEU:HD13	1:A:1187:THR:CG2	2.47	0.45
1:A:120:THR:CG2	1:A:121:TYR:N	2.80	0.45
1:A:1636:ILE:HG22	1:A:1636:ILE:O	2.16	0.45
1:A:274:ASP:OD1	1:A:277:ASP:CG	2.55	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:SER:O	1:A:506:LYS:C	2.55	0.45
1:A:560:TRP:CH2	1:A:673:LEU:HD22	2.51	0.45
1:A:839:ILE:HA	1:A:839:ILE:HD12	1.71	0.45
1:A:961:TYR:HE1	1:A:963:ILE:HG12	1.82	0.45
2:B:107:GLN:HG3	2:B:116:GLU:HG3	1.98	0.45
2:B:173:VAL:HG13	2:B:964:ILE:HD11	1.98	0.45
2:B:415:THR:O	2:B:425:GLN:CD	2.55	0.45
2:B:44:GLU:OE2	2:B:523:TYR:OH	2.31	0.45
2:B:891:LEU:H	2:B:891:LEU:HG	1.21	0.45
1:C:111:PHE:CE2	1:C:113:LYS:CB	2.94	0.45
1:C:1244:THR:H	1:C:1247:MET:HE3	1.81	0.45
1:C:1272:LYS:O	1:C:1276:GLU:HG3	2.16	0.45
1:C:1304:VAL:HG12	1:C:1305:LYS:H	1.77	0.45
1:C:174:VAL:CG2	1:C:175:GLU:N	2.80	0.45
1:C:356:LEU:HG	1:C:452:TYR:CE2	2.51	0.45
1:C:847:ASN:OD1	1:C:847:ASN:C	2.55	0.45
1:C:977:LEU:HD22	1:C:978:SER:N	2.32	0.45
2:D:615:GLN:CB	2:D:616:ASN:HD22	2.29	0.45
2:D:953:ARG:CG	2:D:954:VAL:N	2.80	0.45
1:A:1053:MET:HE2	1:A:1086:LEU:HD13	1.98	0.45
1:A:1080:ALA:CB	1:A:1148:THR:HG22	2.47	0.45
1:A:1093:VAL:HG12	1:A:1095:GLN:NE2	2.31	0.45
1:A:1127:ILE:HB	1:A:1129:LEU:HD21	1.98	0.45
1:A:1474:CYS:HB3	1:A:1476:ARG:HH12	1.82	0.45
1:A:23:TYR:CE2	1:A:111:PHE:CD2	3.05	0.45
1:A:477:LEU:N	1:A:477:LEU:HD22	2.31	0.45
1:A:481:HIS:CE1	2:B:387:MET:CE	3.00	0.45
1:A:491:PRO:O	1:A:491:PRO:HG2	2.17	0.45
1:A:760:VAL:HG22	1:A:760:VAL:O	2.17	0.45
1:A:96:GLN:O	1:A:97:ASN:O	2.35	0.45
2:B:1561:HIS:NE2	2:B:1597:ILE:CD1	2.80	0.45
2:B:1561:HIS:NE2	2:B:1597:ILE:HD13	2.30	0.45
2:B:297:ASP:N	2:B:297:ASP:OD2	2.49	0.45
2:B:481:TYR:CE2	2:B:493:GLY:HA3	2.51	0.45
2:B:598:ILE:HD13	2:B:800:ILE:HG21	1.95	0.45
1:C:1013:MET:HE2	1:C:1287:THR:HB	1.97	0.45
1:C:1629:TYR:HD2	1:C:1629:TYR:H	1.65	0.45
1:C:491:PRO:O	1:C:493:ILE:N	2.48	0.45
1:C:606:ASP:OD2	1:C:795:THR:HG21	2.17	0.45
2:D:1386:MET:HE2	2:D:1386:MET:HA	1.99	0.45
2:D:1623:LYS:HA	2:D:1623:LYS:HD2	1.68	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:524:TYR:CD1	2:D:524:TYR:C	2.90	0.45
2:D:824:VAL:CG2	2:D:828:GLU:OE1	2.64	0.45
2:D:96:THR:HG22	2:D:97:ASP:O	2.16	0.45
3:Y:191:ILE:O	3:Y:198:LYS:HA	2.17	0.45
1:A:1054:LEU:HD23	1:A:1057:MET:HE1	1.98	0.45
1:A:1560:ALA:O	1:A:1561:TYR:HB3	2.17	0.45
1:A:1638:PRO:HG2	1:A:1639:LEU:H	1.81	0.45
1:A:190:ILE:CG2	1:A:191:PRO:CD	2.95	0.45
1:A:489:LYS:NZ	2:B:502:ASN:H	2.14	0.45
1:A:506:LYS:O	1:A:508:LYS:N	2.49	0.45
1:A:523:TYR:CE2	2:B:465:ASN:CG	2.90	0.45
1:A:596:MET:SD	1:A:782:ARG:HG2	2.57	0.45
1:A:862:VAL:HG12	1:A:863:GLU:OE1	2.16	0.45
1:A:840:GLN:HE21	1:A:897:THR:HG21	1.81	0.45
1:A:950:TYR:C	1:A:952:THR:H	2.20	0.45
1:A:96:GLN:HG3	1:A:97:ASN:N	2.32	0.45
2:B:1347:VAL:CG2	2:B:1367:ILE:HG23	2.43	0.45
2:B:1500:LEU:HD13	2:B:1501:ASN:N	2.32	0.45
2:B:1631:PHE:CD2	2:B:1631:PHE:C	2.90	0.45
2:B:628:LEU:HD12	2:B:629:THR:H	1.81	0.45
2:B:63:ARG:CB	2:B:65:GLN:HG3	2.47	0.45
2:B:133:ASP:CA	2:B:757:TRP:HZ3	2.28	0.45
1:C:1013:MET:O	1:C:1015:VAL:N	2.50	0.45
1:C:1250:THR:O	1:C:1252:ALA:N	2.50	0.45
1:C:1646:GLU:HG2	1:C:1660:PHE:CZ	2.52	0.45
1:C:190:ILE:CG2	1:C:191:PRO:N	2.80	0.45
1:C:259:VAL:HB	1:C:295:GLY:CA	2.46	0.45
1:C:439:ALA:O	1:C:441:ASP:N	2.43	0.45
1:C:473:HIS:CE1	2:D:455:LYS:CE	3.00	0.45
1:C:24:VAL:HG11	1:C:543:TYR:HE2	1.75	0.45
1:C:577:PRO:HD2	1:C:588:VAL:CG2	2.47	0.45
1:C:923:LEU:HD21	1:C:925:LYS:HD3	1.99	0.45
2:D:965:ILE:HD13	2:D:1277:ILE:HD13	1.99	0.45
2:D:176:ASN:HB3	2:D:184:TRP:HZ2	1.82	0.45
2:D:224:PHE:CE1	2:D:320:VAL:CG1	3.01	0.45
2:D:436:GLN:O	2:D:437:THR:C	2.54	0.45
2:D:525:GLN:CD	2:D:525:GLN:O	2.55	0.45
2:D:810:VAL:HG12	2:D:811:MET:N	2.31	0.45
2:D:173:VAL:HA	2:D:964:ILE:CD1	2.47	0.45
1:A:1066:TYR:HD1	1:A:1079:THR:HG23	1.83	0.44
1:A:1156:PHE:O	1:A:1160:PRO:HD3	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1240:PRO:HB2	1:A:1242:THR:CG2	2.47	0.44
1:A:149:ASN:O	1:A:152:LEU:N	2.25	0.44
1:A:476:LEU:HA	1:A:476:LEU:HD23	1.83	0.44
1:A:491:PRO:HB2	1:A:493:ILE:C	2.36	0.44
1:A:60:PRO:CG	1:A:61:ASP:H	2.30	0.44
2:B:1609:ARG:O	2:B:1611:PRO:HD3	2.17	0.44
2:B:1637:GLU:O	2:B:1638:PHE:CG	2.70	0.44
2:B:176:ASN:HB3	2:B:184:TRP:HZ2	1.82	0.44
2:B:189:PRO:C	2:B:191:LEU:N	2.69	0.44
2:B:280:LEU:HG	2:B:280:LEU:O	2.16	0.44
2:B:523:TYR:CB	2:B:533:ALA:HB2	2.47	0.44
2:B:580:VAL:HG13	2:B:584:VAL:CG2	2.47	0.44
2:B:61:PHE:CD1	2:B:62:PRO:HA	2.52	0.44
1:C:1386:ILE:HG13	1:C:1387:GLU:N	2.29	0.44
1:C:506:LYS:O	1:C:508:LYS:N	2.51	0.44
1:C:554:LEU:HB2	1:C:642:ASN:OD1	2.17	0.44
1:C:662:SER:O	1:C:663:GLN:C	2.56	0.44
1:C:77:ASN:O	1:C:78:LYS:C	2.54	0.44
1:C:963:ILE:HA	1:C:964:PRO:HD3	1.72	0.44
2:D:1343:PHE:CZ	2:D:1371:TYR:HD1	2.35	0.44
2:D:1382:ILE:HG12	2:D:1427:LEU:HD11	1.99	0.44
2:D:1425:ILE:HG22	2:D:1427:LEU:HD12	1.98	0.44
2:D:31:ALA:O	2:D:119:VAL:HG12	2.17	0.44
2:D:525:GLN:NE2	2:D:528:ASN:H	2.15	0.44
2:D:640:SER:O	2:D:641:ALA:HB2	2.16	0.44
2:D:946:LYS:N	2:D:946:LYS:HD3	2.32	0.44
3:X:40:LEU:HD11	3:X:209:PHE:CZ	2.52	0.44
1:A:1033:ILE:CG2	1:A:1034:PHE:N	2.80	0.44
1:A:1259:LEU:HD21	1:A:1267:VAL:HG11	1.98	0.44
1:A:134:VAL:HA	1:A:218:GLU:O	2.17	0.44
1:A:356:LEU:HG	1:A:452:TYR:CE2	2.53	0.44
1:A:653:PHE:CE1	1:A:660:ASP:CB	3.00	0.44
1:A:694:VAL:HG12	1:A:694:VAL:O	2.16	0.44
2:B:1284:ARG:CG	2:B:1285:GLU:H	2.29	0.44
2:B:1593:THR:HG21	2:B:1596:LYS:HE3	2.00	0.44
2:B:1597:ILE:HD11	2:B:1599:TYR:CE1	2.53	0.44
2:B:1611:PRO:HA	2:B:1615:GLU:OE1	2.17	0.44
2:B:1617:GLN:HG2	2:B:1617:GLN:H	1.66	0.44
1:C:330:ILE:HG22	1:C:337:SER:HB3	1.99	0.44
1:C:374:GLN:HG2	1:C:382:LEU:HD21	1.98	0.44
1:C:500:ASN:OD1	1:C:514:THR:HG23	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:624:PHE:CD1	1:C:625:GLN:N	2.85	0.44
1:C:639:GLY:HA2	1:C:648:LEU:CD1	2.44	0.44
1:C:700:TYR:O	1:C:703:ALA:N	2.50	0.44
1:C:584:PRO:CB	1:C:792:ASP:HA	2.37	0.44
2:D:111:PRO:O	2:D:113:VAL:HG23	2.18	0.44
2:D:235:PHE:CE2	2:D:299:PHE:CE2	3.05	0.44
2:D:336:ILE:HD13	2:D:336:ILE:HA	1.79	0.44
2:D:739:PHE:CE2	2:D:847:ARG:NE	2.85	0.44
3:X:201:ILE:HD13	3:X:207:LEU:HD23	2.00	0.44
1:A:1153:ARG:CZ	1:A:1168:LEU:HD12	2.47	0.44
1:A:1226:ARG:CD	1:A:1266:TYR:CE1	3.01	0.44
1:A:1525:CYS:N	1:A:1528:VAL:CG1	2.79	0.44
1:A:243:PHE:CE2	1:A:304:GLU:CA	3.00	0.44
1:A:414:ASP:OD1	1:A:414:ASP:N	2.50	0.44
1:A:421:VAL:HG23	2:B:507:ASN:ND2	2.32	0.44
1:A:351:PRO:CG	1:A:442:LEU:HD11	2.48	0.44
1:A:535:VAL:O	1:A:563:ILE:HG12	2.17	0.44
1:A:576:SER:HB2	1:A:589:SER:H	1.81	0.44
1:A:624:PHE:CD1	1:A:625:GLN:N	2.85	0.44
2:B:111:PRO:O	2:B:113:VAL:HG23	2.18	0.44
2:B:345:ILE:HD11	2:B:427:THR:CA	2.47	0.44
1:C:1022:PHE:O	1:C:1024:TYR:N	2.50	0.44
1:C:1286:SER:CB	1:C:1499:HIS:HA	2.46	0.44
1:C:1532:CYS:O	1:C:1641:SER:N	2.51	0.44
1:C:502:LEU:HB2	1:C:541:LEU:HD21	1.97	0.44
1:C:667:GLU:HA	1:C:668:PRO:HD3	1.79	0.44
2:D:1345:LEU:HD12	2:D:1368:CYS:O	2.17	0.44
2:D:148:PHE:CZ	2:D:792:VAL:CG1	3.00	0.44
2:D:1597:ILE:HD11	2:D:1599:TYR:CE1	2.53	0.44
2:D:1610:TRP:CE2	2:D:1628:PHE:HD2	2.35	0.44
2:D:344:GLN:O	2:D:366:VAL:HA	2.17	0.44
2:D:838:ASN:HB2	2:D:844:ILE:HD11	1.98	0.44
3:Y:179:LEU:HD11	3:Y:180:TYR:CE1	2.51	0.44
1:A:977:LEU:CD2	1:A:1361:VAL:HG22	2.48	0.44
1:A:1069:TRP:CH2	1:A:1465:ASN:ND2	2.85	0.44
1:A:1573:VAL:HG12	1:A:1603:LYS:HD3	1.95	0.44
1:A:465:LEU:HD12	1:A:466:TYR:H	1.83	0.44
1:A:493:ILE:CG2	1:A:495:LYS:HB2	2.45	0.44
1:A:632:LEU:N	1:A:632:LEU:CD2	2.68	0.44
1:A:981:GLY:O	1:A:1356:LEU:O	2.35	0.44
2:B:515:ILE:HG21	2:B:599:TRP:CZ2	2.52	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:847:ARG:HG3	2:B:869:GLN:CG	2.42	0.44
2:B:739:PHE:CE2	2:B:847:ARG:NE	2.86	0.44
1:C:1219:LYS:HE2	1:C:1239:VAL:CG2	2.45	0.44
1:C:1268:ASN:N	1:C:1269:PRO:HD2	2.33	0.44
1:C:1298:THR:O	1:C:1301:SER:N	2.51	0.44
1:C:398:ASN:O	1:C:399:GLN:CB	2.64	0.44
1:C:532:GLN:O	1:C:533:ASN:C	2.53	0.44
1:C:854:GLN:NE2	1:C:854:GLN:N	2.65	0.44
1:C:257:ASN:ND2	1:C:892:SER:HA	2.27	0.44
2:D:1371:TYR:CB	2:D:1377:SER:HB3	2.48	0.44
2:D:150:MET:HG3	2:D:602:ILE:HD11	2.00	0.44
2:D:1522:TYR:HD1	2:D:1524:TYR:CE1	2.35	0.44
2:D:1522:TYR:HD1	2:D:1524:TYR:CZ	2.35	0.44
2:D:570:ASP:O	2:D:573:ALA:HB2	2.17	0.44
2:D:642:ALA:O	2:D:643:LYS:HB3	2.17	0.44
3:X:185:LYS:HG2	3:X:186:TYR:CD2	2.53	0.44
3:Y:139:ASN:HB2	3:Y:227:THR:HG23	2.00	0.44
3:Y:88:GLY:O	3:Y:91:LYS:N	2.43	0.44
1:A:1421:HIS:CD2	1:A:1422:ALA:N	2.85	0.44
1:A:1559:TYR:HE2	1:A:1590:ALA:O	1.98	0.44
1:A:1561:TYR:HE1	1:A:1598:ILE:HD11	1.83	0.44
1:A:333:THR:OG1	1:A:334:GLY:N	2.50	0.44
1:A:532:GLN:CA	1:A:532:GLN:OE1	2.57	0.44
1:A:73:LEU:HB2	1:A:79:PHE:HA	1.98	0.44
2:B:257:VAL:CG1	2:B:258:GLU:N	2.80	0.44
2:B:47:GLY:O	2:B:48:ASP:HB2	2.17	0.44
1:A:421:VAL:HG23	2:B:507:ASN:HD22	1.81	0.44
2:B:558:MET:HA	2:B:559:PRO:HD3	1.85	0.44
2:B:830:VAL:HG23	2:B:831:GLU:N	2.32	0.44
1:C:120:THR:CG2	1:C:121:TYR:N	2.81	0.44
1:C:1459:HIS:HD2	1:C:1459:HIS:N	2.15	0.44
1:C:1549:LYS:H	1:C:1549:LYS:HG2	1.41	0.44
1:C:1637:TYR:N	1:C:1637:TYR:HD2	2.15	0.44
1:C:316:GLU:HA	1:C:319:ASN:HB2	1.99	0.44
1:C:909:ASN:HA	1:C:926:THR:HA	1.99	0.44
1:C:930:VAL:HA	1:C:931:PRO:HD3	1.82	0.44
2:D:962:LYS:HD2	2:D:1302:THR:CG2	2.47	0.44
2:D:134:LYS:HD2	2:D:584:VAL:HG11	1.99	0.44
5:D:2001:NAG:O3	5:D:2002:NAG:O5	2.34	0.44
1:C:480:GLU:HG2	2:D:389:THR:HB	2.00	0.44
2:D:445:LEU:HD23	2:D:533:ALA:HA	1.98	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:613:SER:HA	2:D:620:VAL:HG23	1.99	0.44
2:D:41:ILE:O	2:D:85:PRO:HD2	2.18	0.44
2:D:89:ILE:CD1	2:D:104:VAL:HG11	2.48	0.44
2:D:946:LYS:CD	2:D:946:LYS:H	2.29	0.44
3:Y:188:LYS:HD3	3:Y:202:ASP:CA	2.42	0.44
1:A:1003:LEU:HA	1:A:1004:PRO:HD2	1.49	0.44
1:A:1663:ASN:O	1:A:1666:GLU:HB3	2.18	0.44
1:A:284:GLN:HG2	1:A:310:LEU:CD1	2.47	0.44
1:A:569:ASN:HD22	1:A:569:ASN:H	1.64	0.44
1:A:606:ASP:OD2	1:A:795:THR:HG21	2.18	0.44
1:A:60:PRO:CG	1:A:61:ASP:N	2.81	0.44
1:A:671:GLU:HB2	1:A:672:ILE:H	1.66	0.44
1:A:979:VAL:C	1:A:980:LYS:HG2	2.37	0.44
2:B:1282:PRO:O	2:B:1283:ASP:C	2.56	0.44
2:B:1387:LEU:O	2:B:1390:PHE:HB2	2.16	0.44
2:B:1425:ILE:HG22	2:B:1427:LEU:HD12	2.00	0.44
2:B:1438:LEU:HD13	2:B:1438:LEU:C	2.37	0.44
2:B:1523:VAL:O	2:B:1548:ILE:HB	2.18	0.44
2:B:296:ARG:HA	2:B:296:ARG:HD2	1.90	0.44
2:B:386:SER:O	2:B:398:LEU:HD11	2.18	0.44
2:B:930:LEU:HD13	2:B:1315:ALA:HB2	1.99	0.44
1:C:1200:LYS:HE3	1:C:1200:LYS:HB3	1.79	0.44
1:C:1268:ASN:ND2	1:C:1268:ASN:N	2.66	0.44
1:C:1428:LEU:HD11	1:C:1434:ALA:HB2	1.99	0.44
1:C:152:LEU:HA	1:C:152:LEU:HD13	1.48	0.44
1:C:1636:ILE:O	1:C:1636:ILE:HG22	2.17	0.44
1:C:415:ASP:N	1:C:415:ASP:OD1	2.48	0.44
1:C:510:ILE:HA	3:Y:150:ILE:CG1	2.48	0.44
1:C:535:VAL:HA	1:C:563:ILE:HD11	1.99	0.44
1:C:60:PRO:CG	1:C:61:ASP:H	2.30	0.44
1:C:694:VAL:O	1:C:694:VAL:HG12	2.18	0.44
1:C:779:LEU:O	1:C:781:PRO:HD3	2.18	0.44
2:D:1330:ASN:N	2:D:1330:ASN:HD22	2.15	0.44
2:D:1444:LYS:NZ	2:D:1447:GLU:HA	2.32	0.44
2:D:1365:LEU:HD21	2:D:1472:TYR:CE1	2.53	0.44
2:D:1454:GLY:HA3	2:D:1472:TYR:CE2	2.53	0.44
2:D:1525:LYS:HE3	2:D:1610:TRP:NE1	2.32	0.44
2:D:220:VAL:O	2:D:222:PRO:N	2.50	0.44
2:D:518:PHE:HE2	2:D:538:VAL:CG1	2.30	0.44
2:D:818:LEU:HG	2:D:820:MET:HE3	2.00	0.44
2:D:824:VAL:HG21	2:D:830:VAL:CG1	2.41	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:VAL:O	1:A:1020:TYR:HD2	2.01	0.44
1:A:1024:TYR:HB2	1:A:1298:THR:CG2	2.48	0.44
1:A:1066:TYR:CD1	1:A:1079:THR:HG23	2.53	0.44
1:A:1096:ASN:O	1:A:1097:GLN:C	2.55	0.44
1:A:955:ARG:O	1:A:1349:SER:HA	2.18	0.44
1:A:1627:ILE:HD12	1:A:1629:TYR:HB3	2.00	0.44
1:A:1540:ASP:HA	1:A:1660:PHE:CD1	2.53	0.44
1:A:180:ILE:CG2	1:A:181:GLY:N	2.81	0.44
1:A:250:ILE:HG13	1:A:250:ILE:O	2.17	0.44
1:A:273:GLU:O	1:A:274:ASP:HB3	2.17	0.44
1:A:307:VAL:O	1:A:311:SER:HB2	2.18	0.44
1:A:316:GLU:HA	1:A:319:ASN:HB2	1.99	0.44
1:A:383:VAL:HG23	1:A:386:VAL:CG2	2.48	0.44
1:A:42:GLN:HE21	1:A:44:TYR:N	2.10	0.44
1:A:599:TRP:O	1:A:803:GLY:CA	2.58	0.44
2:B:922:LYS:HE3	2:B:1329:TYR:OH	2.18	0.44
2:B:1486:ILE:HG13	2:B:1486:ILE:O	2.18	0.44
2:B:1522:TYR:CE2	2:B:1585:GLY:N	2.79	0.44
1:A:483:ASN:HD21	2:B:399:ILE:HB	1.81	0.44
2:B:518:PHE:CD2	2:B:538:VAL:HB	2.42	0.44
2:B:63:ARG:HD2	2:B:65:GLN:NE2	2.33	0.44
1:C:1180:LEU:HD21	1:C:1208:ILE:HA	2.00	0.44
1:C:1582:LEU:CD2	1:C:1616:GLN:HG2	2.40	0.44
1:C:970:LYS:HD3	1:C:1640:ASP:OD2	2.18	0.44
1:C:180:ILE:HG22	1:C:181:GLY:N	2.32	0.44
1:C:238:ILE:HB	1:C:347:TYR:CE1	2.52	0.44
1:C:33:VAL:HG21	1:C:121:TYR:HE1	1.73	0.44
1:C:41:ILE:HD13	1:C:41:ILE:HG21	1.63	0.44
1:C:40:VAL:HG23	1:C:41:ILE:N	2.32	0.44
1:C:443:PRO:CG	1:C:446:ASN:HB2	2.48	0.44
1:C:436:LYS:CB	1:C:449:ARG:HG2	2.43	0.44
1:C:492:TYR:CD2	1:C:493:ILE:HB	2.53	0.44
1:C:491:PRO:HB2	1:C:493:ILE:C	2.37	0.44
1:C:180:ILE:HG13	1:C:599:TRP:CZ3	2.52	0.44
1:C:59:TYR:CD1	1:C:60:PRO:HG3	2.53	0.44
2:D:1567:ARG:HA	2:D:1567:ARG:HD2	1.65	0.44
2:D:1594:LYS:O	2:D:1596:LYS:HG2	2.17	0.44
2:D:178:VAL:HG21	2:D:183:PHE:CD1	2.53	0.44
2:D:834:ALA:C	2:D:835:ILE:HD13	2.38	0.44
2:D:857:CYS:CB	2:D:885:VAL:CG2	2.95	0.44
2:D:35:THR:HB	2:D:91:ALA:HB2	1.99	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:73:VAL:CG2	3:Y:74:ARG:N	2.78	0.44
1:A:1023:HIS:CD2	1:A:1023:HIS:O	2.70	0.44
1:A:1031:TRP:CE2	1:A:1042:LYS:HG3	2.52	0.44
1:A:1156:PHE:CE1	1:A:1164:ILE:HG13	2.53	0.44
1:A:1234:HIS:CG	1:A:1235:LYS:N	2.85	0.44
1:A:1317:TYR:CE1	1:A:1342:LEU:HD12	2.53	0.44
1:A:132:LYS:HZ1	1:A:139:GLN:HE22	1.65	0.44
1:A:1561:TYR:HE1	1:A:1581:LEU:HG	1.82	0.44
1:A:1644:TRP:O	1:A:1645:ILE:HD13	2.18	0.44
1:A:238:ILE:HB	1:A:347:TYR:CE1	2.53	0.44
1:A:302:ASP:HB3	1:A:305:THR:HB	2.00	0.44
1:A:321:LYS:O	1:A:347:TYR:HB2	2.18	0.44
1:A:804:ILE:HG22	1:A:809:ILE:CB	2.48	0.44
1:A:915:GLU:CB	2:B:905:TRP:CZ2	3.00	0.44
1:A:856:CYS:HB3	1:A:915:GLU:HG2	1.99	0.44
2:B:1404:VAL:O	2:B:1428:ASN:ND2	2.50	0.44
2:B:1438:LEU:HD13	2:B:1438:LEU:O	2.18	0.44
2:B:1443:LEU:CD1	2:B:1443:LEU:N	2.80	0.44
2:B:263:VAL:HG21	2:B:292:ALA:CB	2.47	0.44
2:B:345:ILE:H	2:B:345:ILE:HG12	1.60	0.44
2:B:524:TYR:C	2:B:524:TYR:HD1	2.19	0.44
2:B:949:LYS:H	2:B:949:LYS:HG3	1.54	0.44
1:C:1023:HIS:O	1:C:1027:THR:HB	2.17	0.44
1:A:1163:LYS:CE	1:C:1109:GLU:HG2	2.48	0.44
1:C:1020:TYR:CE1	1:C:1295:GLU:HA	2.52	0.44
1:C:375:VAL:O	1:C:383:VAL:HG13	2.16	0.44
1:C:787:GLN:O	1:C:788:PHE:HB3	2.16	0.44
1:C:839:ILE:HG23	1:C:840:GLN:N	2.31	0.44
1:C:901:LEU:HA	1:C:902:PRO:HD3	1.82	0.44
1:C:917:TRP:HB3	2:D:558:MET:SD	2.58	0.44
2:D:855:ALA:O	2:D:856:PHE:CD1	2.71	0.44
3:X:91:LYS:NZ	3:X:95:LYS:HE3	2.33	0.44
1:A:1007:SER:OG	1:A:1008:ALA:N	2.50	0.44
1:A:1305:LYS:HG3	1:C:101:TYR:OH	2.17	0.44
1:A:1559:TYR:CE1	1:A:1587:THR:HA	2.53	0.44
1:A:1644:TRP:NE1	1:A:1646:GLU:OE1	2.48	0.44
1:A:176:GLU:HB2	1:A:185:PHE:CE1	2.52	0.44
1:A:382:LEU:HD13	1:A:415:ASP:O	2.18	0.44
1:A:383:VAL:CG2	1:A:386:VAL:HG21	2.48	0.44
1:A:42:GLN:HG2	1:A:43:VAL:H	1.83	0.44
1:A:443:PRO:CG	1:A:446:ASN:HB2	2.48	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:GLY:HA2	3:X:146:LEU:HD13	2.00	0.44
1:A:506:LYS:HD2	1:A:536:PRO:CD	2.48	0.44
1:A:643:ALA:O	1:A:644:ASN:C	2.55	0.44
1:A:949:ILE:HG22	1:A:950:TYR:CZ	2.53	0.44
2:B:1442:ILE:C	2:B:1443:LEU:HD13	2.38	0.44
2:B:243:PHE:C	2:B:243:PHE:HD2	2.20	0.44
2:B:275:SER:O	2:B:277:PRO:HD3	2.17	0.44
2:B:309:LEU:O	2:B:310:VAL:C	2.54	0.44
2:B:889:GLN:HA	2:B:915:VAL:HB	1.99	0.44
1:C:1069:TRP:CH2	1:C:1465:ASN:ND2	2.86	0.44
1:C:1019:PHE:CZ	1:C:1088:GLN:HB3	2.53	0.44
1:C:137:PRO:O	1:C:138:ASP:HB2	2.18	0.44
1:C:1629:TYR:HE1	1:C:1631:PHE:CD1	2.34	0.44
1:C:223:VAL:O	1:C:225:PRO:HD3	2.18	0.44
1:C:317:ASP:O	1:C:319:ASN:N	2.50	0.44
1:C:248:ILE:HD13	1:C:325:ILE:HD13	2.00	0.44
1:C:532:GLN:CA	1:C:532:GLN:OE1	2.59	0.44
1:C:24:VAL:CG2	1:C:554:LEU:HD11	2.48	0.44
1:C:60:PRO:CG	1:C:61:ASP:N	2.81	0.44
1:C:680:GLN:CG	1:C:681:LYS:H	2.31	0.44
1:C:989:SER:O	1:C:993:SER:HB3	2.17	0.44
2:D:966:GLN:OE1	2:D:1298:LEU:HD13	2.17	0.44
2:D:1521:ASP:OD1	2:D:1552:THR:OG1	2.36	0.44
2:D:1539:ILE:HD12	2:D:1539:ILE:N	2.32	0.44
2:D:1637:GLU:C	2:D:1638:PHE:CD2	2.91	0.44
2:D:397:LYS:NZ	2:D:449:ILE:O	2.51	0.44
3:X:215:VAL:O	3:X:216:LEU:HD13	2.18	0.44
1:A:1320:LYS:HA	1:A:1320:LYS:HD2	1.90	0.43
1:A:150:ASP:CG	1:A:151:ASP:N	2.72	0.43
1:A:1627:ILE:O	1:A:1627:ILE:CG1	2.63	0.43
1:A:472:ASN:HA	1:A:474:LYS:HD2	1.99	0.43
1:A:578:ASP:CG	1:A:578:ASP:O	2.56	0.43
1:A:856:CYS:HB2	2:B:904:LEU:HG	1.99	0.43
2:B:783:SER:HB3	2:B:785:THR:HG22	2.00	0.43
2:B:881:PRO:C	2:B:882:PHE:CD2	2.91	0.43
1:C:1090:ASN:ND2	1:C:1158:ILE:HG12	2.33	0.43
1:C:1227:PHE:HA	1:C:1228:TRP:CE3	2.53	0.43
1:C:1257:THR:O	1:C:1261:LEU:HD23	2.17	0.43
1:C:1561:TYR:HE1	1:C:1598:ILE:HD11	1.82	0.43
1:C:535:VAL:O	1:C:563:ILE:HG12	2.18	0.43
1:C:682:LYS:HZ2	1:C:686:ILE:HD12	1.81	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:713:GLN:HG3	1:C:713:GLN:H	1.44	0.43
2:D:137:TYR:HB2	2:D:216:VAL:HG23	2.00	0.43
2:D:1575:LEU:HD13	2:D:1581:TYR:CZ	2.53	0.43
2:D:1610:TRP:CD2	2:D:1628:PHE:CE2	3.06	0.43
2:D:1635:LEU:O	2:D:1636:THR:C	2.55	0.43
2:D:243:PHE:HD2	2:D:243:PHE:C	2.22	0.43
2:D:285:ILE:CD1	2:D:285:ILE:H	2.30	0.43
2:D:283:ILE:O	2:D:285:ILE:HD12	2.18	0.43
2:D:736:GLU:HA	2:D:847:ARG:NH2	2.33	0.43
2:D:850:LEU:CD1	2:D:851:LEU:N	2.81	0.43
2:D:875:LEU:HG	2:D:875:LEU:O	2.18	0.43
2:D:913:LEU:C	2:D:913:LEU:CD2	2.86	0.43
2:D:932:PRO:HB3	2:D:939:GLY:O	2.18	0.43
1:A:1075:SER:OG	1:A:1078:LEU:HB2	2.18	0.43
1:A:23:TYR:HE2	1:A:111:PHE:HD2	1.65	0.43
1:A:108:SER:OG	1:A:111:PHE:N	2.50	0.43
1:A:317:ASP:C	1:A:319:ASN:N	2.71	0.43
1:A:359:THR:CG2	1:A:359:THR:O	2.65	0.43
1:A:387:PRO:HB2	1:A:438:ASP:HB3	2.00	0.43
1:A:475:ALA:O	1:A:476:LEU:HB2	2.18	0.43
1:A:484:ILE:HD13	1:A:540:LEU:HD21	1.98	0.43
1:A:577:PRO:HD2	1:A:588:VAL:CG2	2.48	0.43
1:A:855:PHE:HB2	1:A:914:LEU:CD1	2.48	0.43
2:B:961:THR:HG22	2:B:1327:THR:OG1	2.18	0.43
2:B:234:PHE:CE1	2:B:236:TYR:CE1	3.06	0.43
2:B:326:SER:OG	2:B:327:ASP:N	2.51	0.43
2:B:361:GLU:HB3	2:B:399:ILE:CD1	2.48	0.43
1:C:1084:ARG:CA	1:C:1151:GLY:HA2	2.48	0.43
1:C:1293:ALA:O	1:C:1294:ILE:C	2.56	0.43
1:C:131:ASP:OD2	1:C:132:LYS:HG3	2.18	0.43
1:C:1364:VAL:HG13	1:C:1364:VAL:O	2.18	0.43
1:C:1638:PRO:O	1:C:1639:LEU:CB	2.62	0.43
1:C:273:GLU:O	1:C:274:ASP:HB3	2.17	0.43
1:C:276:LYS:HA	1:C:276:LYS:HD2	1.76	0.43
1:C:419:SER:C	1:C:420:PHE:CD2	2.92	0.43
1:C:955:ARG:O	1:C:1349:SER:HA	2.18	0.43
2:D:142:PRO:HB3	2:D:187:ASN:HD22	1.83	0.43
2:D:930:LEU:HD13	2:D:1315:ALA:HB2	1.99	0.43
2:D:943:GLU:HB2	2:D:1313:VAL:HG23	2.00	0.43
1:A:1112:GLN:HB2	1:A:1118:PHE:CE1	2.54	0.43
1:A:1156:PHE:CE2	1:A:1160:PRO:HB3	2.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1189:ALA:O	1:A:1192:ALA:HB3	2.19	0.43
1:A:1215:GLU:OE1	1:A:1235:LYS:HD3	2.18	0.43
1:A:1249:GLU:O	1:A:1253:TYR:CD2	2.71	0.43
1:A:1257:THR:O	1:A:1261:LEU:HD23	2.19	0.43
1:A:127:PHE:CD1	1:A:127:PHE:N	2.85	0.43
1:A:165:ASP:CB	1:A:166:PRO:CD	2.96	0.43
1:A:231:ILE:HG12	1:A:231:ILE:O	2.18	0.43
1:A:241:LYS:NZ	1:A:351:PRO:HB3	2.34	0.43
1:A:465:LEU:HD12	1:A:487:THR:O	2.19	0.43
1:A:40:VAL:HG12	1:A:509:ILE:HD12	2.01	0.43
1:A:990:ALA:HB1	1:A:1000:LEU:HD11	2.01	0.43
2:B:1296:ASN:O	2:B:1297:ALA:C	2.56	0.43
2:B:1566:GLN:H	2:B:1566:GLN:HG2	1.50	0.43
2:B:1506:ILE:HD11	2:B:1628:PHE:HE1	1.84	0.43
2:B:161:VAL:CG2	2:B:180:LEU:HD21	2.43	0.43
2:B:456:PRO:HG3	2:B:515:ILE:HD11	2.01	0.43
2:B:745:ILE:O	2:B:745:ILE:CG2	2.66	0.43
2:B:736:GLU:HA	2:B:847:ARG:NH2	2.33	0.43
2:B:89:ILE:CD1	2:B:104:VAL:HG11	2.48	0.43
2:B:951:ASP:C	2:B:953:ARG:H	2.13	0.43
1:C:1226:ARG:HD3	1:C:1266:TYR:CE1	2.54	0.43
1:C:1439:LEU:O	1:C:1440:LYS:C	2.57	0.43
1:C:389:THR:OG1	1:C:408:LYS:HE2	2.18	0.43
1:C:504:LEU:HD21	1:C:651:LEU:CG	2.48	0.43
1:C:478:VAL:HG11	1:C:566:LYS:HD3	2.01	0.43
1:C:742:ILE:CG1	1:C:752:LEU:O	2.65	0.43
1:C:862:VAL:HG12	1:C:863:GLU:OE1	2.18	0.43
1:C:990:ALA:HB1	1:C:1000:LEU:HD11	2.00	0.43
2:D:265:PHE:O	2:D:276:ILE:HG13	2.18	0.43
2:D:361:GLU:HB3	2:D:399:ILE:CD1	2.47	0.43
2:D:449:ILE:HG23	2:D:449:ILE:O	2.18	0.43
2:D:358:MET:HE2	2:D:467:LYS:HD2	1.99	0.43
2:D:518:PHE:CE2	2:D:538:VAL:CB	2.71	0.43
2:D:580:VAL:HG13	2:D:584:VAL:HG23	2.00	0.43
2:D:628:LEU:HD12	2:D:629:THR:H	1.82	0.43
3:X:169:ILE:HG21	3:X:189:ILE:HD13	1.99	0.43
3:Y:54:SER:HB2	3:Y:167:PHE:CE1	2.54	0.43
3:Y:81:ASN:O	3:Y:115:ARG:CB	2.53	0.43
1:A:1076:THR:HG23	1:A:1077:TRP:N	2.34	0.43
1:A:1439:LEU:HA	1:A:1439:LEU:HD23	1.64	0.43
1:A:1546:GLU:HG2	1:A:1663:ASN:HD21	1.80	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1573:VAL:HB	1:A:1603:LYS:CD	2.43	0.43
1:A:317:ASP:O	1:A:319:ASN:N	2.51	0.43
1:A:500:ASN:OD1	1:A:514:THR:HG23	2.17	0.43
1:A:484:ILE:HD12	1:A:540:LEU:HD21	1.99	0.43
1:A:595:GLY:O	1:A:596:MET:C	2.57	0.43
2:B:1378:THR:O	2:B:1379:MET:C	2.57	0.43
2:B:1454:GLY:O	2:B:1471:PHE:HD1	2.00	0.43
2:B:269:ILE:HG13	2:B:272:ALA:HB3	2.01	0.43
2:B:224:PHE:HE1	2:B:320:VAL:CG1	2.31	0.43
2:B:319:THR:HG23	2:B:330:VAL:CG1	2.48	0.43
2:B:433:ILE:HG22	2:B:434:ALA:N	2.33	0.43
2:B:851:LEU:HD11	2:B:865:ARG:NH2	2.33	0.43
2:B:191:LEU:HD12	2:B:958:GLU:HG2	1.99	0.43
1:C:1300:TYR:C	1:C:1300:TYR:CD2	2.91	0.43
1:C:1317:TYR:CZ	1:C:1342:LEU:HG	2.53	0.43
1:C:1327:LYS:C	1:C:1332:ASN:HD22	2.22	0.43
1:C:1358:THR:HB	1:C:1360:HIS:HE1	1.77	0.43
1:C:274:ASP:HA	1:C:322:TYR:CE2	2.53	0.43
1:C:433:PHE:N	1:C:433:PHE:CD1	2.87	0.43
1:C:671:GLU:HG2	1:C:671:GLU:H	1.62	0.43
1:C:847:ASN:OD1	1:C:849:ARG:N	2.51	0.43
1:C:949:ILE:HA	1:C:949:ILE:HD13	1.81	0.43
2:D:124:GLN:HG3	2:D:124:GLN:O	2.18	0.43
2:D:1404:VAL:O	2:D:1428:ASN:ND2	2.51	0.43
2:D:1528:LEU:HD11	2:D:1540:TYR:HB3	1.99	0.43
2:D:1614:ASP:O	2:D:1617:GLN:HG2	2.18	0.43
2:D:580:VAL:HG13	2:D:584:VAL:CG2	2.49	0.43
2:D:613:SER:HA	2:D:620:VAL:CG2	2.49	0.43
3:Y:138:VAL:O	3:Y:138:VAL:HG12	2.18	0.43
3:Y:196:GLU:CD	3:Y:196:GLU:N	2.72	0.43
3:Y:201:ILE:HD13	3:Y:207:LEU:HD23	2.00	0.43
1:A:1025:LEU:HD11	1:A:1034:PHE:HZ	1.82	0.43
1:A:1072:GLY:O	1:A:1073:SER:C	2.55	0.43
1:A:109:LYS:HD3	1:A:110:HIS:HE1	1.77	0.43
1:A:33:VAL:CG2	1:A:121:TYR:CD1	2.88	0.43
1:A:1428:LEU:HD11	1:A:1434:ALA:HB2	1.98	0.43
1:A:1589:GLU:O	1:A:1591:VAL:N	2.51	0.43
1:A:1582:LEU:CD2	1:A:1616:GLN:HG2	2.42	0.43
1:A:461:SER:O	1:A:462:GLN:HB2	2.17	0.43
1:A:829:ILE:CG1	1:A:925:LYS:HG2	2.47	0.43
1:A:984:VAL:HG12	1:A:988:LEU:HD12	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1459:TYR:HB3	2:B:1466:GLU:HB3	1.99	0.43
2:B:800:ILE:HG23	2:B:801:CYS:N	2.31	0.43
2:B:954:VAL:CG1	2:B:955:PRO:HD2	2.42	0.43
1:C:987:ILE:HD13	1:C:1294:ILE:HG23	2.00	0.43
1:C:837:GLU:OE2	1:C:1430:THR:HB	2.19	0.43
1:C:1538:GLU:O	1:C:1539:LEU:C	2.57	0.43
1:C:222:TYR:HE2	1:C:224:LEU:N	2.17	0.43
1:C:290:THR:CG2	1:C:297:ALA:HB1	2.48	0.43
1:C:259:VAL:HB	1:C:295:GLY:HA2	2.00	0.43
1:C:916:THR:C	1:C:918:PHE:N	2.71	0.43
2:D:1292:ILE:CD1	2:D:1301:ARG:HE	2.31	0.43
2:D:961:THR:HG22	2:D:1327:THR:CB	2.48	0.43
2:D:1391:LEU:HA	2:D:1392:PRO:HD3	1.85	0.43
2:D:1408:ILE:HD13	2:D:1425:ILE:HA	2.00	0.43
2:D:355:LYS:HE2	2:D:445:LEU:O	2.18	0.43
2:D:56:ILE:HD11	2:D:73:VAL:HG23	2.01	0.43
2:D:830:VAL:HG23	2:D:831:GLU:N	2.33	0.43
2:D:881:PRO:O	2:D:882:PHE:CD2	2.71	0.43
3:X:185:LYS:CG	3:X:186:TYR:CE2	3.01	0.43
1:A:1162:VAL:CG2	1:A:1163:LYS:N	2.82	0.43
1:A:1142:LEU:HD21	1:A:1179:THR:OG1	2.19	0.43
1:A:680:GLN:CG	1:A:681:LYS:N	2.81	0.43
1:A:847:ASN:C	1:A:847:ASN:OD1	2.55	0.43
1:A:96:GLN:CG	1:A:97:ASN:H	2.31	0.43
2:B:249:ALA:O	2:B:257:VAL:HB	2.18	0.43
2:B:763:THR:C	2:B:764:GLU:HG2	2.39	0.43
1:C:1226:ARG:CD	1:C:1266:TYR:CE1	3.01	0.43
1:C:1271:ILE:HD13	1:C:1300:TYR:CE2	2.53	0.43
1:C:131:ASP:OD2	1:C:132:LYS:CG	2.66	0.43
1:C:177:ILE:HD13	1:C:177:ILE:N	2.33	0.43
1:C:23:TYR:HD1	1:C:23:TYR:H	1.31	0.43
1:C:472:ASN:HA	1:C:474:LYS:HD2	2.01	0.43
1:C:113:LYS:HE2	1:C:654:LEU:O	2.19	0.43
1:C:839:ILE:CD1	1:C:1485:VAL:HG12	2.49	0.43
1:C:901:LEU:HD23	1:C:1527:CYS:SG	2.59	0.43
1:C:996:GLY:O	1:C:998:ASN:N	2.52	0.43
2:D:1273:LEU:C	2:D:1273:LEU:HD12	2.39	0.43
2:D:326:SER:OG	2:D:327:ASP:N	2.52	0.43
2:D:476:ILE:O	2:D:497:ARG:HG2	2.18	0.43
2:D:47:GLY:O	2:D:48:ASP:HB2	2.19	0.43
2:D:518:PHE:CD2	2:D:518:PHE:O	2.72	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:618:LEU:CD1	2:D:635:ASN:O	2.65	0.43
3:X:108:GLU:O	3:X:109:LEU:HG	2.18	0.43
3:Y:166:ASP:O	3:Y:170:ARG:HG3	2.18	0.43
3:Y:229:ASN:C	3:Y:230:GLN:HG3	2.39	0.43
1:A:1043:GLN:O	1:A:1044:LYS:C	2.54	0.43
1:A:1106:TRP:CZ2	1:A:1111:TYR:HE2	2.37	0.43
1:A:133:PRO:HD2	1:A:609:VAL:CG1	2.48	0.43
1:A:1646:GLU:HG2	1:A:1660:PHE:HZ	1.84	0.43
1:A:503:ILE:O	1:A:510:ILE:HG12	2.19	0.43
1:A:631:ASP:C	1:A:633:GLY:H	2.22	0.43
1:A:670:LYS:HD2	1:A:671:GLU:H	1.83	0.43
1:A:864:GLY:HA3	1:A:907:LEU:HD22	2.00	0.43
1:A:953:ILE:CD1	1:A:955:ARG:HH21	2.32	0.43
2:B:1367:ILE:HB	2:B:1438:LEU:CD1	2.49	0.43
2:B:1486:ILE:HD11	2:B:1591:LEU:HD21	2.00	0.43
1:A:523:TYR:CE2	2:B:465:ASN:ND2	2.86	0.43
2:B:490:PHE:C	2:B:490:PHE:CD1	2.90	0.43
1:C:1023:HIS:O	1:C:1023:HIS:CD2	2.71	0.43
1:C:1213:LYS:HE2	1:C:1266:TYR:HD2	1.78	0.43
1:C:1249:GLU:O	1:C:1253:TYR:CD2	2.72	0.43
1:C:1665:ASP:O	1:C:1668:ALA:HB3	2.19	0.43
1:C:274:ASP:CG	1:C:275:LEU:N	2.70	0.43
1:C:417:VAL:O	1:C:417:VAL:HG12	2.18	0.43
1:C:365:PRO:CD	1:C:464:TYR:CE2	2.98	0.43
1:C:501:TYR:O	1:C:512:PHE:HA	2.19	0.43
1:C:532:GLN:HA	1:C:535:VAL:HG13	2.00	0.43
1:C:551:THR:HB	1:C:657:ALA:HB1	2.00	0.43
1:C:980:LYS:HB3	1:C:980:LYS:HE2	1.79	0.43
2:D:1430:VAL:HA	2:D:1436:GLU:OE2	2.19	0.43
2:D:551:LYS:HE2	2:D:551:LYS:HB2	1.91	0.43
2:D:828:GLU:O	2:D:886:PRO:HD2	2.18	0.43
2:D:916:VAL:HG22	2:D:917:PRO:N	2.33	0.43
2:D:951:ASP:C	2:D:953:ARG:H	2.19	0.43
3:X:211:ARG:O	3:X:214:ASP:HB2	2.18	0.43
1:A:1037:ASP:HA	1:A:1038:PRO:HD3	1.62	0.43
1:A:33:VAL:HG23	1:A:120:THR:O	2.18	0.43
1:A:1263:ASP:O	1:A:1265:ASN:N	2.52	0.43
1:A:1317:TYR:CZ	1:A:1342:LEU:HG	2.54	0.43
1:A:1426:ILE:O	1:A:1426:ILE:HG22	2.18	0.43
1:A:1403:VAL:HG22	1:A:1476:ARG:HB3	2.01	0.43
1:A:1571:GLU:O	1:A:1574:PHE:N	2.46	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:ARG:HE	1:A:633:GLY:HA3	1.83	0.43
1:A:996:GLY:O	1:A:998:ASN:N	2.51	0.43
2:B:1529:LEU:N	2:B:1529:LEU:HD12	2.34	0.43
2:B:345:ILE:HD11	2:B:426:ALA:C	2.38	0.43
1:C:1053:MET:O	1:C:1056:ILE:HG22	2.19	0.43
1:C:1012:LEU:HD11	1:C:1056:ILE:HG13	2.01	0.43
1:C:938:SER:OG	1:C:1284:PHE:CE2	2.71	0.43
1:C:1566:THR:HG23	1:C:1578:LYS:O	2.18	0.43
1:C:383:VAL:CG2	1:C:386:VAL:HG21	2.49	0.43
1:C:505:SER:HB3	1:C:510:ILE:HD13	2.01	0.43
1:C:587:THR:HA	1:C:789:ALA:HA	2.00	0.43
1:C:64:PHE:HD2	1:C:66:TYR:CE1	2.36	0.43
1:C:258:LYS:HD3	1:C:893:SER:OG	2.17	0.43
2:D:1275:LEU:HD21	2:D:1319:GLY:O	2.19	0.43
2:D:1528:LEU:HD21	2:D:1531:ILE:HD11	2.01	0.43
2:D:144:LEU:HB3	2:D:185:PRO:HB3	2.01	0.43
2:D:384:PHE:CE1	2:D:400:LEU:HG	2.51	0.43
2:D:582:LYS:O	2:D:583:ALA:C	2.56	0.43
2:D:933:ARG:NH1	2:D:933:ARG:CG	2.79	0.43
3:Y:163:LYS:HG3	3:Y:212:MET:CE	2.49	0.43
1:A:1016:VAL:N	1:A:1017:PRO:CD	2.81	0.43
1:A:1208:ILE:HG22	1:A:1208:ILE:O	2.19	0.43
1:A:1309:LEU:O	1:A:1329:THR:HA	2.19	0.43
1:A:931:PRO:CB	1:A:1366:HIS:CD2	3.02	0.43
1:A:1538:GLU:O	1:A:1539:LEU:C	2.54	0.43
1:A:1602:LYS:HE3	1:A:1609:ALA:O	2.18	0.43
1:A:390:LEU:HD23	1:A:420:PHE:CD1	2.54	0.43
1:A:433:PHE:CZ	1:A:452:TYR:HB2	2.54	0.43
1:A:484:ILE:CD1	1:A:540:LEU:CD2	2.97	0.43
1:A:701:ASP:CG	1:A:1446:VAL:HG23	2.39	0.43
2:B:114:ARG:O	2:B:114:ARG:NE	2.51	0.43
2:B:1564:ILE:O	2:B:1601:ILE:HD12	2.19	0.43
2:B:247:ILE:CD1	2:B:318:VAL:HG21	2.49	0.43
2:B:794:PHE:CD2	2:B:795:THR:N	2.86	0.43
2:B:810:VAL:O	2:B:811:MET:HB2	2.19	0.43
1:C:1072:GLY:O	1:C:1073:SER:C	2.57	0.43
1:C:975:ARG:CZ	1:C:1340:VAL:HG11	2.49	0.43
1:C:132:LYS:HZ1	1:C:139:GLN:HE22	1.67	0.43
1:C:492:TYR:CE2	1:C:546:VAL:HG11	2.53	0.43
1:C:653:PHE:CE1	1:C:660:ASP:CB	3.00	0.43
1:C:701:ASP:N	1:C:701:ASP:OD1	2.52	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:802:VAL:HG12	1:C:803:GLY:N	2.34	0.43
1:C:855:PHE:HB2	1:C:914:LEU:HD11	2.00	0.43
2:D:1424:ILE:HD13	2:D:1424:ILE:N	2.29	0.43
2:D:1459:TYR:HB3	2:D:1466:GLU:HB3	1.99	0.43
2:D:146:ARG:CB	2:D:146:ARG:HH11	2.32	0.43
2:D:1482:ASN:HB3	2:D:1493:ALA:CB	2.49	0.43
2:D:1544:VAL:C	2:D:1545:LEU:HD12	2.40	0.43
2:D:1562:GLN:NE2	2:D:1596:LYS:HZ2	2.15	0.43
2:D:222:PRO:HG2	2:D:329:VAL:HG12	1.99	0.43
2:D:341:SER:HA	2:D:342:PRO:HD3	1.72	0.43
2:D:40:GLN:O	2:D:489:ILE:HD12	2.18	0.43
2:D:481:TYR:HE2	2:D:493:GLY:N	2.16	0.43
2:D:780:LEU:HD11	2:D:787:TRP:HD1	1.84	0.43
1:A:1083:LEU:HD13	1:A:1104:LEU:HD23	2.00	0.43
1:A:1084:ARG:HG2	1:A:1084:ARG:NH1	2.33	0.43
1:A:1219:LYS:HB2	1:A:1219:LYS:HE3	1.76	0.43
1:A:1406:ALA:O	1:A:1472:PHE:HA	2.18	0.43
1:A:1556:GLU:HB3	1:A:1622:LYS:CE	2.31	0.43
1:A:373:VAL:CG2	1:A:418:ALA:HB3	2.43	0.43
1:A:582:TYR:O	1:A:819:VAL:HG13	2.18	0.43
2:B:1454:GLY:HA3	2:B:1472:TYR:CE2	2.54	0.43
2:B:315:TYR:CD1	2:B:315:TYR:C	2.91	0.43
2:B:764:GLU:HG3	2:B:772:SER:HB3	2.01	0.43
2:B:840:VAL:CG1	2:B:841:ASN:N	2.77	0.43
2:B:851:LEU:HD21	2:B:865:ARG:HH21	1.83	0.43
2:B:895:GLU:HA	2:B:909:VAL:O	2.19	0.43
1:C:1127:ILE:HD11	1:C:1143:TYR:CE2	2.54	0.43
1:C:1175:LEU:HD23	1:C:1175:LEU:HA	1.88	0.43
1:C:1244:THR:O	1:C:1245:ALA:C	2.57	0.43
1:C:1639:LEU:HA	1:C:1639:LEU:HD22	1.76	0.43
1:C:1643:THR:HG22	1:C:1644:TRP:H	1.84	0.43
1:C:317:ASP:C	1:C:319:ASN:N	2.70	0.43
1:C:487:THR:HA	1:C:488:PRO:HD3	1.83	0.43
1:C:511:HIS:CE1	3:Y:149:SER:HB3	2.54	0.43
1:C:628:GLU:HG3	1:C:628:GLU:O	2.18	0.43
1:C:837:GLU:O	1:C:901:LEU:CD1	2.65	0.43
2:D:1454:GLY:O	2:D:1471:PHE:HD1	2.01	0.43
2:D:1635:LEU:HD23	2:D:1635:LEU:HA	1.70	0.43
2:D:550:VAL:HG22	2:D:567:LEU:HD21	2.01	0.43
3:X:174:VAL:HG12	3:X:174:VAL:O	2.19	0.43
3:X:196:GLU:N	3:X:196:GLU:CD	2.72	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:45:ASP:OD1	3:Y:48:ARG:NH1	2.51	0.43
1:A:1093:VAL:O	1:A:1094:GLU:C	2.57	0.42
1:A:1245:ALA:O	1:A:1246:ARG:C	2.56	0.42
1:A:223:VAL:O	1:A:225:PRO:HD3	2.19	0.42
1:A:40:VAL:HG23	1:A:41:ILE:H	1.83	0.42
1:A:522:SER:HB2	1:A:523:TYR:H	1.54	0.42
1:A:640:LEU:H	1:A:644:ASN:CB	2.28	0.42
1:A:710:THR:N	1:A:713:GLN:OE1	2.50	0.42
1:A:824:PHE:CE2	1:A:846:TYR:CD1	3.05	0.42
1:A:997:ILE:O	1:A:998:ASN:O	2.37	0.42
2:B:1469:THR:O	2:B:1470:LYS:HG2	2.19	0.42
2:B:1522:TYR:HD1	2:B:1524:TYR:CZ	2.36	0.42
2:B:1631:PHE:HD2	2:B:1632:SER:N	2.16	0.42
2:B:235:PHE:CE2	2:B:299:PHE:CE2	3.06	0.42
2:B:247:ILE:HD11	2:B:318:VAL:HG21	2.01	0.42
2:B:345:ILE:HG13	2:B:428:LYS:CB	2.49	0.42
2:B:875:LEU:O	2:B:875:LEU:HG	2.19	0.42
1:C:1075:SER:OG	1:C:1078:LEU:HB2	2.18	0.42
1:A:1163:LYS:NZ	1:C:1109:GLU:HG2	2.34	0.42
1:C:117:MET:HE2	1:C:117:MET:HB2	1.71	0.42
1:C:33:VAL:CG2	1:C:121:TYR:CD1	2.87	0.42
1:C:1402:ILE:CG2	1:C:1403:VAL:N	2.82	0.42
1:C:1562:LYS:C	1:C:1563:VAL:HG13	2.38	0.42
1:C:161:LEU:HD12	1:C:161:LEU:N	2.32	0.42
1:C:515:ARG:HG3	1:C:515:ARG:NH1	2.33	0.42
1:C:569:ASN:HD21	1:C:810:CYS:HB2	1.84	0.42
1:C:869:GLU:HB2	1:C:871:PRO:HG3	2.01	0.42
2:D:1471:PHE:O	2:D:1478:THR:O	2.37	0.42
2:D:267:VAL:HG22	2:D:314:LEU:CD1	2.49	0.42
2:D:63:ARG:HD2	2:D:65:GLN:NE2	2.33	0.42
2:D:878:ARG:HE	2:D:1421:VAL:CG2	2.32	0.42
3:Y:194:LYS:HG2	3:Y:197:ASN:HB3	2.01	0.42
1:A:108:SER:HG	1:A:111:PHE:C	2.22	0.42
1:A:1146:ALA:HB3	1:A:1190:ILE:CG2	2.48	0.42
1:A:1219:LYS:HE2	1:A:1239:VAL:CG2	2.49	0.42
1:A:1560:ALA:O	1:A:1561:TYR:CB	2.67	0.42
1:A:255:PHE:O	1:A:256:TYR:HB2	2.19	0.42
1:A:291:MET:HB3	1:A:291:MET:HE2	1.75	0.42
1:A:364:LYS:HE2	1:A:465:LEU:O	2.18	0.42
1:A:491:PRO:CG	1:A:491:PRO:O	2.67	0.42
1:A:461:SER:HB3	1:A:553:GLU:OE2	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:GLY:HA2	1:A:648:LEU:CD1	2.45	0.42
1:A:689:LYS:CD	1:A:730:GLU:OE2	2.67	0.42
1:A:821:LYS:HB3	1:A:822:ASP:H	1.34	0.42
1:A:862:VAL:O	1:A:865:ILE:HG13	2.19	0.42
1:A:949:ILE:O	1:A:949:ILE:CG2	2.66	0.42
2:B:1538:ASP:OD2	2:B:1567:ARG:HD2	2.19	0.42
2:B:1544:VAL:C	2:B:1545:LEU:HD12	2.40	0.42
2:B:449:ILE:HA	2:B:449:ILE:HD12	1.71	0.42
2:B:967:GLY:O	2:B:969:PRO:HD3	2.18	0.42
1:C:100:SER:C	1:C:101:TYR:HD2	2.22	0.42
1:C:108:SER:HG	1:C:111:PHE:C	2.23	0.42
1:C:1110:ASN:O	1:C:1111:TYR:CD1	2.72	0.42
1:C:1344:ASP:OD1	1:C:1345:ASP:N	2.52	0.42
1:C:1622:LYS:HZ3	1:C:1642:LEU:CD2	2.27	0.42
1:C:1673:LEU:O	1:C:1674:ASN:CB	2.65	0.42
1:C:190:ILE:CG2	1:C:191:PRO:CD	2.97	0.42
1:C:73:LEU:HB2	1:C:79:PHE:HA	2.01	0.42
1:C:871:PRO:O	1:C:873:ILE:N	2.52	0.42
1:C:969:PRO:C	1:C:971:THR:HG23	2.40	0.42
1:C:973:ILE:HG22	1:C:973:ILE:O	2.17	0.42
2:D:126:SER:OG	2:D:152:HIS:HD2	2.02	0.42
2:D:1370:ARG:HG3	2:D:1431:SER:O	2.19	0.42
2:D:1548:ILE:CG2	2:D:1635:LEU:CB	2.95	0.42
2:D:417:HIS:O	2:D:419:ASP:N	2.52	0.42
2:D:820:MET:HA	2:D:821:PRO:HD3	1.73	0.42
3:Y:91:LYS:NZ	3:Y:95:LYS:HE3	2.34	0.42
1:A:1244:THR:N	1:A:1247:MET:HE3	2.33	0.42
1:A:1226:ARG:HD3	1:A:1266:TYR:HE1	1.85	0.42
1:A:1327:LYS:HG3	1:A:1328:MET:N	2.35	0.42
1:A:1348:VAL:HG11	1:A:1359:VAL:HG21	2.01	0.42
1:A:1559:TYR:HB3	1:A:1637:TYR:HE1	1.84	0.42
1:A:185:PHE:HD1	1:A:186:PRO:HD2	1.84	0.42
1:A:290:THR:CG2	1:A:297:ALA:HB1	2.48	0.42
1:A:420:PHE:N	1:A:420:PHE:CD2	2.86	0.42
1:A:489:LYS:HZ3	2:B:501:GLN:HA	1.85	0.42
1:A:949:ILE:O	1:A:950:TYR:CD1	2.72	0.42
1:A:946:PRO:O	1:A:953:ILE:HG13	2.19	0.42
2:B:878:ARG:HE	2:B:1421:VAL:CG2	2.32	0.42
2:B:1583:ILE:CG1	2:B:1607:ILE:HG23	2.42	0.42
1:C:1080:ALA:HB2	1:C:1148:THR:HG22	2.02	0.42
1:C:1468:PRO:HD2	1:C:1473:LEU:HB2	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1644:TRP:O	1:C:1645:ILE:CD1	2.66	0.42
1:C:909:ASN:HD21	4:C:2003:NAG:C8	2.32	0.42
1:C:354:LEU:HD22	1:C:448:ALA:HB1	2.01	0.42
1:C:383:VAL:HG23	1:C:386:VAL:HG23	2.01	0.42
1:C:386:VAL:HA	1:C:387:PRO:HD3	1.83	0.42
2:D:451:SER:O	2:D:452:THR:HG23	2.19	0.42
2:D:482:LEU:CB	2:D:492:VAL:HG23	2.33	0.42
2:D:568:GLU:HA	2:D:772:SER:O	2.19	0.42
3:X:217:ASN:ND2	3:X:220:ASP:OD2	2.48	0.42
3:Y:153:PHE:CE1	3:Y:169:ILE:HD13	2.55	0.42
3:Y:71:ASN:HD22	3:Y:91:LYS:CD	2.33	0.42
1:A:111:PHE:O	1:A:112:SER:OG	2.30	0.42
1:A:1560:ALA:O	1:A:1561:TYR:CD2	2.70	0.42
1:A:1648:TRP:HE1	1:A:1664:LEU:HD21	1.82	0.42
1:A:216:TYR:N	1:A:216:TYR:HD2	2.16	0.42
1:A:243:PHE:O	1:A:303:SER:HB2	2.18	0.42
1:A:315:LEU:HD11	1:A:318:LEU:HG	1.99	0.42
1:A:386:VAL:HA	1:A:387:PRO:HD3	1.82	0.42
1:A:433:PHE:N	1:A:433:PHE:CD1	2.88	0.42
1:A:49:ALA:CB	1:A:74:SER:HB2	2.50	0.42
1:A:662:SER:O	1:A:663:GLN:C	2.57	0.42
1:A:683:ILE:O	1:A:687:ALA:HB3	2.19	0.42
1:A:829:ILE:HD12	1:A:829:ILE:N	2.34	0.42
1:A:968:VAL:CG2	1:A:971:THR:HG21	2.49	0.42
2:B:1626:ASP:O	2:B:1627:ASP:C	2.58	0.42
2:B:1610:TRP:CE3	2:B:1628:PHE:CD2	3.08	0.42
2:B:236:TYR:O	2:B:238:ASP:N	2.52	0.42
2:B:344:GLN:O	2:B:366:VAL:HA	2.18	0.42
2:B:449:ILE:HG23	2:B:449:ILE:O	2.18	0.42
2:B:74:ASP:OD1	2:B:74:ASP:N	2.45	0.42
2:B:563:MET:SD	2:B:808:ILE:HD11	2.60	0.42
1:C:1189:ALA:O	1:C:1192:ALA:HB3	2.19	0.42
1:C:1188:LEU:CD2	1:C:1212:LEU:HA	2.49	0.42
1:C:1328:MET:HE2	1:C:1328:MET:HA	2.01	0.42
1:C:1439:LEU:HA	1:C:1439:LEU:HD23	1.71	0.42
1:C:333:THR:OG1	1:C:334:GLY:N	2.52	0.42
1:C:455:ILE:HG22	1:C:456:ALA:H	1.83	0.42
1:C:969:PRO:O	1:C:971:THR:HG23	2.19	0.42
2:D:964:ILE:HG22	2:D:1324:THR:OG1	2.18	0.42
2:D:1391:LEU:HB2	2:D:1417:MET:CE	2.48	0.42
2:D:1612:HIS:N	2:D:1615:GLU:OE1	2.46	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:174:SER:HA	2:D:1300:ALA:HB2	2.02	0.42
2:D:247:ILE:CD1	2:D:318:VAL:HG21	2.48	0.42
2:D:345:ILE:HD11	2:D:427:THR:CA	2.49	0.42
2:D:616:ASN:OD1	2:D:618:LEU:HB2	2.20	0.42
2:D:781:ARG:HD3	2:D:781:ARG:HA	1.53	0.42
2:D:859:ALA:CB	2:D:866:TYR:CD1	3.00	0.42
3:X:194:LYS:HG2	3:X:197:ASN:HB3	2.00	0.42
3:Y:217:ASN:ND2	3:Y:220:ASP:OD2	2.51	0.42
1:A:114:SER:O	1:A:115:LYS:HE2	2.20	0.42
1:A:571:LEU:HG	1:A:812:ALA:HB2	2.02	0.42
1:A:837:GLU:O	1:A:901:LEU:CD1	2.65	0.42
2:B:1284:ARG:HD2	2:B:1285:GLU:N	2.24	0.42
2:B:1444:LYS:NZ	2:B:1447:GLU:HA	2.34	0.42
2:B:1383:ASP:O	2:B:1456:VAL:HA	2.18	0.42
2:B:781:ARG:HA	2:B:781:ARG:HD3	1.53	0.42
1:C:1161:LEU:O	1:C:1164:ILE:HG12	2.19	0.42
1:C:1267:VAL:O	1:C:1270:VAL:HB	2.19	0.42
1:C:134:VAL:HA	1:C:218:GLU:O	2.19	0.42
1:C:981:GLY:O	1:C:1356:LEU:O	2.38	0.42
1:C:1637:TYR:HB3	1:C:1638:PRO:HD2	2.01	0.42
1:C:191:PRO:O	1:C:194:PRO:HD3	2.20	0.42
1:C:215:ALA:C	1:C:216:TYR:CD2	2.93	0.42
1:C:328:THR:OG1	1:C:339:GLU:HG2	2.19	0.42
1:C:40:VAL:CG2	1:C:512:PHE:CD1	2.99	0.42
1:C:42:GLN:OE1	1:C:500:ASN:ND2	2.52	0.42
1:C:554:LEU:HD23	1:C:554:LEU:HA	1.64	0.42
1:C:693:SER:O	1:C:695:VAL:N	2.53	0.42
1:C:804:ILE:HG22	1:C:809:ILE:CB	2.49	0.42
1:C:997:ILE:O	1:C:998:ASN:O	2.37	0.42
2:D:280:LEU:HD22	2:D:1462:TYR:CE2	2.54	0.42
2:D:147:VAL:HG12	2:D:183:PHE:CE1	2.50	0.42
2:D:188:LEU:HD13	2:D:216:VAL:CG2	2.50	0.42
2:D:224:PHE:HE1	2:D:320:VAL:CG1	2.33	0.42
2:D:455:LYS:O	2:D:458:ASP:CB	2.58	0.42
3:X:153:PHE:CZ	3:X:169:ILE:HD13	2.55	0.42
3:Y:103:VAL:HA	3:Y:121:GLY:O	2.19	0.42
3:Y:125:LYS:HD2	3:Y:126:ASN:HA	2.02	0.42
3:Y:190:ILE:O	3:Y:190:ILE:HG12	2.18	0.42
1:A:1239:VAL:N	1:A:1240:PRO:CD	2.82	0.42
1:A:1298:THR:O	1:A:1301:SER:N	2.53	0.42
1:A:160:VAL:HG11	1:A:204:LYS:HE3	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:TYR:HA	1:A:205:TYR:HD2	1.73	0.42
1:A:545:ILE:HG12	1:A:545:ILE:H	1.44	0.42
1:A:129:HIS:CE1	1:A:620:LEU:HD21	2.54	0.42
1:A:622:ARG:HD3	1:A:622:ARG:HA	1.73	0.42
1:A:905:ILE:O	1:A:905:ILE:HG22	2.19	0.42
2:B:1610:TRP:CE3	2:B:1628:PHE:HD2	2.38	0.42
2:B:164:GLU:HB2	2:B:200:VAL:HG23	2.02	0.42
2:B:296:ARG:NH1	2:B:296:ARG:HG3	2.32	0.42
2:B:599:TRP:O	2:B:600:ASP:C	2.55	0.42
2:B:785:THR:OG1	2:B:786:THR:N	2.51	0.42
2:B:873:LYS:CD	2:B:873:LYS:N	2.82	0.42
2:B:965:ILE:O	2:B:1301:ARG:HG2	2.19	0.42
2:B:968:ASP:O	2:B:1273:LEU:HD23	2.20	0.42
1:C:1283:GLY:HA3	1:C:1290:THR:HG23	2.02	0.42
1:C:1560:ALA:C	1:C:1561:TYR:CD2	2.93	0.42
1:C:1571:GLU:O	1:C:1574:PHE:N	2.49	0.42
1:C:216:TYR:HD2	1:C:216:TYR:N	2.17	0.42
1:C:287:MET:SD	1:C:299:VAL:HG23	2.60	0.42
1:C:383:VAL:HG23	1:C:386:VAL:CG2	2.49	0.42
1:C:40:VAL:HG12	1:C:509:ILE:HD12	2.00	0.42
1:C:461:SER:O	1:C:462:GLN:HB2	2.19	0.42
1:C:680:GLN:CG	1:C:681:LYS:N	2.80	0.42
1:C:718:ILE:HD11	1:C:728:PHE:CD2	2.54	0.42
1:C:752:LEU:CG	1:C:752:LEU:O	2.67	0.42
1:C:74:SER:C	1:C:79:PHE:CE1	2.93	0.42
1:C:582:TYR:O	1:C:819:VAL:HG13	2.20	0.42
1:C:829:ILE:HD12	1:C:829:ILE:N	2.33	0.42
1:C:829:ILE:CD1	1:C:829:ILE:N	2.82	0.42
1:C:839:ILE:HD12	1:C:1485:VAL:HG12	2.01	0.42
1:C:949:ILE:O	1:C:950:TYR:CD1	2.73	0.42
1:C:96:GLN:CG	1:C:97:ASN:H	2.29	0.42
2:D:200:VAL:HG12	2:D:211:THR:HG1	1.80	0.42
2:D:504:VAL:HG12	2:D:504:VAL:O	2.19	0.42
2:D:523:TYR:CB	2:D:533:ALA:HB2	2.48	0.42
2:D:736:GLU:C	2:D:738:GLY:H	2.22	0.42
2:D:80:GLY:O	2:D:81:MET:HB2	2.18	0.42
2:D:838:ASN:CG	2:D:838:ASN:O	2.58	0.42
2:D:952:ASP:O	2:D:1331:ALA:CA	2.67	0.42
2:D:955:PRO:O	2:D:957:THR:HG23	2.20	0.42
3:X:83:GLN:HG2	3:X:85:PHE:HE1	1.85	0.42
3:Y:101:GLN:HB3	3:Y:123:THR:O	2.20	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:119:VAL:HG22	3:Y:212:MET:HB2	2.01	0.42
1:A:1083:LEU:HD22	1:A:1104:LEU:HD21	2.00	0.42
1:A:1147:PHE:HD2	1:A:1147:PHE:C	2.23	0.42
1:A:115:LYS:HB2	1:A:115:LYS:HE2	1.82	0.42
1:A:1639:LEU:HD22	1:A:1639:LEU:HA	1.76	0.42
1:A:259:VAL:HB	1:A:295:GLY:CA	2.49	0.42
1:A:309:GLU:CG	1:A:310:LEU:N	2.83	0.42
1:A:700:TYR:O	1:A:703:ALA:N	2.52	0.42
1:A:255:PHE:HB2	1:A:846:TYR:OH	2.20	0.42
1:A:883:CYS:HB2	2:B:902:GLU:OE2	2.20	0.42
2:B:1371:TYR:CB	2:B:1377:SER:HB3	2.50	0.42
2:B:1423:VAL:CG1	2:B:1423:VAL:O	2.67	0.42
2:B:1491:ARG:HG3	2:B:1492:CYS:N	2.33	0.42
2:B:1521:ASP:OD1	2:B:1552:THR:OG1	2.35	0.42
2:B:1528:LEU:HD21	2:B:1531:ILE:HD11	2.02	0.42
2:B:203:TYR:O	2:B:204:GLU:C	2.57	0.42
2:B:275:SER:C	2:B:277:PRO:HD3	2.40	0.42
2:B:355:LYS:N	2:B:355:LYS:CD	2.82	0.42
2:B:516:PRO:HG2	2:B:603:GLU:HG3	2.00	0.42
2:B:580:VAL:HG13	2:B:584:VAL:HG23	2.00	0.42
2:B:806:TYR:C	2:B:806:TYR:CD1	2.90	0.42
2:B:811:MET:HG3	2:B:812:LYS:N	2.35	0.42
2:B:933:ARG:HH11	2:B:933:ARG:CG	2.21	0.42
1:C:1022:PHE:HE2	1:C:1092:TYR:CD1	2.37	0.42
1:C:1239:VAL:O	1:C:1240:PRO:C	2.58	0.42
1:C:1190:ILE:CG1	1:C:1253:TYR:CE1	2.99	0.42
1:C:1386:ILE:HG22	1:C:1399:TYR:O	2.19	0.42
1:C:1440:LYS:O	1:C:1443:VAL:HG12	2.20	0.42
1:C:123:ASN:N	1:C:211:THR:HG23	2.33	0.42
1:C:506:LYS:HD2	1:C:536:PRO:HG2	2.01	0.42
1:C:821:LYS:HB3	1:C:822:ASP:H	1.31	0.42
2:D:114:ARG:O	2:D:114:ARG:NE	2.52	0.42
2:D:1290:TYR:HD2	2:D:1301:ARG:HB3	1.83	0.42
2:D:1624:LEU:O	2:D:1627:ASP:N	2.53	0.42
2:D:1633:TYR:HE1	2:D:1637:GLU:OE1	2.03	0.42
2:D:159:LYS:HE2	2:D:180:LEU:HD12	2.01	0.42
2:D:764:GLU:O	2:D:765:GLU:C	2.58	0.42
3:Y:194:LYS:HZ2	3:Y:197:ASN:CB	2.15	0.42
1:A:1161:LEU:O	1:A:1164:ILE:HG12	2.20	0.42
1:A:1246:ARG:HG3	1:A:1246:ARG:O	2.18	0.42
1:A:1265:ASN:C	1:A:1267:VAL:N	2.73	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:950:TYR:HE2	1:A:1356:LEU:HD11	1.84	0.42
1:A:1643:THR:HG22	1:A:1644:TRP:H	1.82	0.42
1:A:308:LYS:CG	1:A:309:GLU:N	2.81	0.42
1:A:829:ILE:N	1:A:829:ILE:CD1	2.82	0.42
2:B:121:LEU:HA	2:B:121:LEU:HD12	1.72	0.42
2:B:1594:LYS:O	2:B:1596:LYS:HG2	2.20	0.42
2:B:234:PHE:CD1	2:B:234:PHE:C	2.93	0.42
2:B:513:ASP:OD2	2:B:513:ASP:N	2.52	0.42
2:B:745:ILE:HD11	2:B:907:ASP:N	2.34	0.42
2:B:838:ASN:OD1	2:B:838:ASN:C	2.58	0.42
1:C:1016:VAL:O	1:C:1020:TYR:HD2	2.03	0.42
1:C:1329:THR:HG1	1:C:1331:LYS:HG2	1.85	0.42
1:C:23:TYR:CE1	1:C:655:THR:CB	3.03	0.42
1:C:367:ILE:HD13	1:C:466:TYR:HD2	1.84	0.42
1:C:773:TRP:CZ3	1:C:788:PHE:CE1	3.08	0.42
2:D:1279:ILE:HG22	2:D:1288:ILE:CB	2.44	0.42
2:D:1513:GLU:O	2:D:1516:CYS:N	2.53	0.42
2:D:1522:TYR:HE2	2:D:1585:GLY:C	2.23	0.42
2:D:1575:LEU:CD2	2:D:1575:LEU:N	2.83	0.42
2:D:1598:SER:C	2:D:1599:TYR:HD1	2.23	0.42
3:X:157:LYS:HA	3:X:157:LYS:HD3	1.83	0.42
3:X:215:VAL:C	3:X:216:LEU:HD22	2.40	0.42
3:Y:60:VAL:HG23	3:Y:60:VAL:O	2.19	0.42
1:A:1106:TRP:O	1:A:1110:ASN:OD1	2.38	0.42
1:A:1149:VAL:O	1:A:1153:ARG:HB2	2.19	0.42
1:A:1159:CYS:SG	1:A:1161:LEU:CD2	3.07	0.42
1:A:1297:LEU:CD1	1:A:1297:LEU:H	2.33	0.42
1:A:354:LEU:HD22	1:A:448:ALA:HB1	2.02	0.42
1:A:500:ASN:O	1:A:542:VAL:HA	2.19	0.42
1:A:569:ASN:HD21	1:A:810:CYS:HB2	1.84	0.42
1:A:604:ALA:O	1:A:772:SER:HB3	2.19	0.42
1:A:644:ASN:ND2	1:A:648:LEU:HD12	2.35	0.42
1:A:698:CYS:O	1:A:700:TYR:N	2.52	0.42
1:A:590:LEU:HD21	1:A:774:LEU:HD11	2.01	0.42
1:A:825:LEU:HB2	1:A:845:VAL:CG2	2.50	0.42
1:A:854:GLN:NE2	1:A:854:GLN:N	2.68	0.42
2:B:1294:TYR:O	2:B:1294:TYR:CD2	2.73	0.42
2:B:141:SER:HA	2:B:142:PRO:HD3	1.85	0.42
2:B:618:LEU:HG	2:B:634:LEU:HD11	2.01	0.42
2:B:736:GLU:OE1	2:B:737:ASP:N	2.51	0.42
2:B:56:ILE:HD11	2:B:73:VAL:HG23	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:780:LEU:CD1	2:B:787:TRP:CD1	3.03	0.42
2:B:834:ALA:C	2:B:835:ILE:HD13	2.39	0.42
1:C:1066:TYR:HD1	1:C:1066:TYR:N	2.18	0.42
1:C:1069:TRP:HH2	1:C:1465:ASN:CG	2.24	0.42
1:C:1652:THR:HG22	1:C:1653:THR:N	2.35	0.42
1:C:352:TYR:HE2	1:C:442:LEU:CD1	2.33	0.42
1:C:436:LYS:HG3	1:C:437:THR:N	2.34	0.42
1:C:781:PRO:C	1:C:783:ARG:H	2.20	0.42
1:C:971:THR:O	1:C:972:GLU:C	2.58	0.42
2:D:1511:GLN:O	2:D:1514:LYS:HB2	2.20	0.42
2:D:1555:ASN:O	2:D:1558:ALA:HB3	2.20	0.42
2:D:1520:VAL:HG11	2:D:1584:TRP:CD1	2.55	0.42
2:D:220:VAL:O	2:D:221:LEU:C	2.57	0.42
2:D:869:GLN:O	2:D:870:PHE:HB3	2.20	0.42
1:A:1156:PHE:HZ	1:A:1165:ASP:HB2	1.84	0.42
1:A:1090:ASN:HD22	1:A:1158:ILE:HG12	1.85	0.42
1:A:117:MET:HB2	1:A:117:MET:HE2	1.68	0.42
1:A:1232:LEU:HG	1:A:1233:GLN:H	1.83	0.42
1:A:1245:ALA:O	1:A:1247:MET:N	2.52	0.42
1:A:1548:ARG:C	1:A:1550:GLN:N	2.73	0.42
1:A:177:ILE:N	1:A:177:ILE:HD13	2.35	0.42
1:A:259:VAL:HB	1:A:295:GLY:HA2	2.01	0.42
1:A:417:VAL:HG12	1:A:417:VAL:O	2.20	0.42
1:A:502:LEU:O	1:A:503:ILE:HD13	2.19	0.42
1:A:989:SER:O	1:A:993:SER:HB2	2.19	0.42
2:B:1518:THR:HG23	2:B:1519:ASN:H	1.85	0.42
2:B:341:SER:HB2	2:B:426:ALA:HB2	2.02	0.42
2:B:460:LEU:CD2	2:B:508:LEU:HB3	2.50	0.42
2:B:518:PHE:HE2	2:B:538:VAL:CG1	2.33	0.42
2:B:844:ILE:O	2:B:871:PRO:HA	2.20	0.42
2:B:932:PRO:HB3	2:B:939:GLY:O	2.20	0.42
2:B:946:LYS:N	2:B:946:LYS:CD	2.82	0.42
1:C:977:LEU:CD2	1:C:1361:VAL:HG22	2.49	0.42
1:C:931:PRO:CB	1:C:1366:HIS:CD2	3.00	0.42
1:C:215:ALA:C	1:C:216:TYR:HD2	2.23	0.42
1:C:267:ILE:CG2	1:C:268:THR:N	2.83	0.42
1:C:27:ALA:HB1	1:C:28:PRO:CD	2.50	0.42
1:C:414:ASP:OD1	1:C:414:ASP:N	2.53	0.42
1:C:644:ASN:HD22	1:C:644:ASN:HA	1.59	0.42
1:C:651:LEU:HD23	1:C:651:LEU:HA	1.69	0.42
1:C:698:CYS:O	1:C:700:TYR:N	2.53	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:689:LYS:CD	1:C:730:GLU:OE2	2.68	0.42
1:C:839:ILE:HD12	1:C:839:ILE:HA	1.78	0.42
1:C:835:ARG:HH22	1:C:971:THR:HG22	1.84	0.42
2:D:1282:PRO:O	2:D:1283:ASP:C	2.57	0.42
2:D:1349:VAL:O	2:D:1350:GLU:HB3	2.20	0.42
2:D:1615:GLU:HB3	2:D:1621:PHE:CE1	2.54	0.42
2:D:416:ASN:CA	2:D:425:GLN:HE22	2.22	0.42
2:D:581:ASP:C	2:D:583:ALA:N	2.73	0.42
1:A:1011:GLU:HG3	1:A:1055:SER:CB	2.50	0.41
1:A:1069:TRP:HH2	1:A:1465:ASN:CG	2.23	0.41
1:A:1113:LEU:HD23	1:A:1114:ASP:H	1.85	0.41
1:A:123:ASN:O	1:A:211:THR:CG2	2.66	0.41
1:A:1554:LYS:CG	1:A:1555:PRO:HD2	2.50	0.41
1:A:961:TYR:CE2	1:A:1343:ASN:CA	3.00	0.41
2:B:1331:ALA:O	2:B:1332:GLN:CB	2.55	0.41
2:B:1349:VAL:O	2:B:1350:GLU:HB3	2.20	0.41
5:B:2001:NAG:O3	5:B:2002:NAG:O5	2.38	0.41
2:B:438:GLN:HE22	2:B:530:GLU:HA	1.85	0.41
2:B:632:THR:O	2:B:633:ASN:C	2.56	0.41
1:C:1022:PHE:O	1:C:1023:HIS:C	2.58	0.41
1:C:1108:VAL:CG2	1:C:1167:ALA:CB	2.97	0.41
1:C:1208:ILE:HG22	1:C:1208:ILE:O	2.19	0.41
1:C:1243:GLY:O	1:C:1285:TYR:CE2	2.73	0.41
1:C:1307:LEU:H	1:C:1307:LEU:HD22	1.85	0.41
1:C:1573:VAL:HG12	1:C:1603:LYS:CB	2.45	0.41
1:C:1559:TYR:HE1	1:C:1587:THR:HA	1.85	0.41
1:C:1576:LYS:CG	1:C:1601:ILE:HG22	2.40	0.41
1:C:308:LYS:CG	1:C:309:GLU:N	2.82	0.41
1:C:505:SER:O	1:C:506:LYS:C	2.56	0.41
1:C:943:THR:CG2	1:C:1356:LEU:HD21	2.50	0.41
2:D:1329:TYR:CD2	2:D:1329:TYR:N	2.88	0.41
2:D:276:ILE:HB	2:D:279:SER:OG	2.20	0.41
2:D:946:LYS:CD	2:D:946:LYS:N	2.83	0.41
3:X:113:ASN:HD21	3:X:115:ARG:HG2	1.85	0.41
3:Y:100:GLY:O	3:Y:125:LYS:CG	2.67	0.41
1:C:510:ILE:HG22	3:Y:150:ILE:HD11	2.01	0.41
3:Y:209:PHE:O	3:Y:212:MET:HB2	2.20	0.41
1:A:1084:ARG:HB2	1:A:1151:GLY:HA2	2.00	0.41
1:A:979:VAL:CG2	1:A:1326:TYR:HE1	2.27	0.41
1:A:1423:VAL:HG22	1:A:1496:TYR:HE2	1.85	0.41
1:A:544:TYR:HD2	1:A:544:TYR:O	2.04	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:GLN:C	1:A:615:GLY:N	2.73	0.41
1:A:602:LEU:HA	1:A:801:GLY:HA2	2.02	0.41
1:A:839:ILE:CD1	1:A:1485:VAL:HG12	2.50	0.41
2:B:126:SER:OG	2:B:152:HIS:HD2	2.02	0.41
2:B:1529:LEU:O	2:B:1577:VAL:HG13	2.20	0.41
2:B:1581:TYR:HA	2:B:1608:GLU:O	2.20	0.41
2:B:355:LYS:HA	2:B:356:PRO:HD3	1.85	0.41
2:B:506:MET:O	2:B:506:MET:HG2	2.17	0.41
2:B:816:ILE:HD12	2:B:909:VAL:HG23	2.02	0.41
2:B:966:GLN:HG3	2:B:966:GLN:O	2.20	0.41
1:C:1016:VAL:N	1:C:1017:PRO:CD	2.83	0.41
1:C:1033:ILE:HG23	1:C:1034:PHE:CD1	2.55	0.41
1:C:1342:LEU:H	1:C:1342:LEU:HG	1.50	0.41
1:C:260:VAL:CG1	1:C:261:THR:N	2.82	0.41
1:C:644:ASN:O	1:C:645:VAL:C	2.58	0.41
1:C:984:VAL:HG12	1:C:988:LEU:HD12	2.01	0.41
2:D:961:THR:HG22	2:D:1327:THR:OG1	2.19	0.41
2:D:1410:ARG:HA	2:D:1410:ARG:HD2	1.81	0.41
2:D:203:TYR:O	2:D:204:GLU:C	2.59	0.41
2:D:355:LYS:HA	2:D:356:PRO:HD3	1.85	0.41
2:D:524:TYR:HD1	2:D:524:TYR:C	2.22	0.41
2:D:874:ALA:C	2:D:876:SER:N	2.72	0.41
3:Y:169:ILE:HG21	3:Y:189:ILE:HD13	2.02	0.41
1:A:1153:ARG:NH2	1:A:1172:ASP:OD2	2.53	0.41
1:A:149:ASN:N	1:A:149:ASN:ND2	2.67	0.41
1:A:1571:GLU:O	1:A:1574:PHE:CG	2.73	0.41
1:A:222:TYR:HE2	1:A:224:LEU:N	2.18	0.41
1:A:491:PRO:O	1:A:493:ILE:N	2.52	0.41
1:A:862:VAL:CG1	1:A:863:GLU:OE1	2.68	0.41
2:B:1430:VAL:HA	2:B:1436:GLU:OE2	2.21	0.41
2:B:1476:LYS:HB3	2:B:1476:LYS:HE3	1.90	0.41
2:B:1598:SER:C	2:B:1599:TYR:HD1	2.22	0.41
2:B:358:MET:HE2	2:B:467:LYS:HD2	2.02	0.41
2:B:481:TYR:CE2	2:B:493:GLY:N	2.88	0.41
2:B:76:ASN:CB	2:B:77:PRO:HD2	2.46	0.41
2:B:913:LEU:C	2:B:913:LEU:CD2	2.88	0.41
1:C:1025:LEU:HD11	1:C:1034:PHE:HZ	1.85	0.41
1:C:1226:ARG:CD	1:C:1266:TYR:HE1	2.32	0.41
1:C:981:GLY:HA3	1:C:1333:PHE:CD1	2.55	0.41
1:C:1428:LEU:HA	1:C:1428:LEU:HD23	1.76	0.41
1:C:149:ASN:O	1:C:152:LEU:N	2.23	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1565:ILE:HB	1:C:1614:GLY:N	2.36	0.41
1:C:196:TYR:HA	1:C:219:VAL:HG12	2.02	0.41
1:C:498:HIS:ND1	1:C:516:GLU:HA	2.35	0.41
1:C:504:LEU:HD13	1:C:509:ILE:HG23	1.99	0.41
1:C:604:ALA:O	1:C:772:SER:HB3	2.21	0.41
1:C:621:GLU:HG3	1:C:621:GLU:H	1.32	0.41
1:C:622:ARG:HD3	1:C:622:ARG:HA	1.73	0.41
1:C:76:GLU:O	1:C:76:GLU:CD	2.59	0.41
2:D:235:PHE:CZ	2:D:296:ARG:NE	2.87	0.41
2:D:355:LYS:CD	2:D:355:LYS:N	2.81	0.41
2:D:469:ASN:ND2	2:D:472:SER:N	2.69	0.41
2:D:811:MET:HG3	2:D:812:LYS:N	2.35	0.41
2:D:940:THR:O	2:D:940:THR:HG22	2.19	0.41
2:D:922:LYS:NZ	2:D:952:ASP:OD2	2.53	0.41
3:X:194:LYS:HZ2	3:X:197:ASN:HD22	1.68	0.41
1:A:1175:LEU:HB3	1:A:1195:LEU:HD11	2.02	0.41
1:A:1430:THR:O	1:A:1430:THR:HG22	2.20	0.41
1:A:383:VAL:CG2	1:A:383:VAL:O	2.68	0.41
2:B:1290:TYR:HD2	2:B:1301:ARG:HB3	1.85	0.41
2:B:1524:TYR:HB3	2:B:1544:VAL:HG13	2.01	0.41
2:B:221:LEU:HG	2:B:221:LEU:H	1.66	0.41
2:B:133:ASP:HB3	2:B:757:TRP:CZ3	2.56	0.41
1:C:146:TYR:CD1	1:C:182:ILE:HG23	2.55	0.41
1:C:1534:GLN:HA	1:C:1608:ASN:HD22	1.85	0.41
1:C:1644:TRP:C	1:C:1645:ILE:HG12	2.39	0.41
1:C:162:THR:HB	1:C:173:MET:CE	2.50	0.41
1:C:185:PHE:CB	1:C:186:PRO:HD2	2.50	0.41
1:C:186:PRO:O	1:C:187:ASP:C	2.58	0.41
1:C:905:ILE:O	1:C:905:ILE:HG22	2.18	0.41
1:C:943:THR:OG1	1:C:1275:SER:OG	2.28	0.41
1:C:989:SER:O	1:C:993:SER:HB2	2.20	0.41
2:D:476:ILE:HG23	2:D:497:ARG:HD3	2.03	0.41
2:D:804:GLU:HA	2:D:804:GLU:OE2	2.19	0.41
3:Y:46:LEU:N	3:Y:46:LEU:HD23	2.36	0.41
1:A:1110:ASN:O	1:A:1111:TYR:CD1	2.73	0.41
1:A:1179:THR:HG22	1:A:1208:ILE:HD13	2.00	0.41
1:A:708:ASP:OD2	1:A:1476:ARG:HD3	2.20	0.41
1:A:147:SER:OG	1:A:147:SER:O	2.38	0.41
1:A:1549:LYS:O	1:A:1552:ALA:N	2.46	0.41
1:A:1589:GLU:HB2	1:A:1590:ALA:H	1.69	0.41
1:A:1575:VAL:O	1:A:1601:ILE:HA	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:PHE:CD1	1:A:163:PHE:N	2.88	0.41
1:A:20:GLU:O	1:A:21:GLN:CG	2.69	0.41
1:A:680:GLN:CG	1:A:681:LYS:H	2.32	0.41
2:B:1575:LEU:N	2:B:1575:LEU:HD22	2.34	0.41
2:B:219:TYR:O	2:B:220:VAL:HG13	2.20	0.41
2:B:220:VAL:O	2:B:221:LEU:C	2.59	0.41
2:B:278:ASP:OD1	2:B:278:ASP:N	2.54	0.41
2:B:280:LEU:HD22	2:B:1462:TYR:CE2	2.54	0.41
2:B:423:GLU:CD	2:B:423:GLU:H	2.23	0.41
2:B:511:THR:O	2:B:512:PRO:C	2.58	0.41
2:B:52:LYS:HG2	2:B:111:PRO:HB2	2.01	0.41
2:B:445:LEU:HD23	2:B:533:ALA:HA	2.02	0.41
2:B:150:MET:SD	2:B:800:ILE:HB	2.61	0.41
1:C:1024:TYR:HB2	1:C:1298:THR:CG2	2.50	0.41
1:C:1081:PHE:O	1:C:1084:ARG:N	2.54	0.41
1:C:978:SER:O	1:C:1359:VAL:HA	2.21	0.41
1:C:1560:ALA:O	1:C:1561:TYR:HB3	2.20	0.41
1:C:1610:GLU:C	1:C:1611:LEU:HD23	2.40	0.41
1:C:1629:TYR:CE1	1:C:1631:PHE:CE1	3.08	0.41
1:C:395:ILE:HG22	1:C:401:THR:HG22	2.02	0.41
1:C:439:ALA:HA	1:C:440:PRO:HD3	1.85	0.41
1:C:461:SER:C	1:C:463:SER:N	2.73	0.41
1:C:470:THR:HG22	2:D:450:THR:HA	2.03	0.41
1:C:500:ASN:ND2	1:C:543:TYR:HE1	2.17	0.41
1:C:545:ILE:HG23	1:C:554:LEU:CD2	2.51	0.41
1:C:590:LEU:CD2	1:C:774:LEU:HD11	2.50	0.41
1:C:182:ILE:HG21	1:C:601:ALA:HB2	2.01	0.41
1:C:613:GLN:C	1:C:615:GLY:N	2.73	0.41
1:C:824:PHE:CE2	1:C:846:TYR:CD1	3.04	0.41
2:D:1522:TYR:CE2	2:D:1585:GLY:N	2.77	0.41
2:D:194:LEU:HD22	2:D:194:LEU:N	2.36	0.41
2:D:219:TYR:CG	2:D:220:VAL:N	2.87	0.41
2:D:224:PHE:HE1	2:D:320:VAL:HG11	1.85	0.41
2:D:275:SER:C	2:D:277:PRO:HD3	2.41	0.41
1:A:1080:ALA:HB1	1:A:1148:THR:HA	2.01	0.41
1:A:1156:PHE:CZ	1:A:1165:ASP:HB2	2.56	0.41
1:A:1231:ASN:OD1	1:A:1232:LEU:N	2.53	0.41
1:A:151:ASP:O	1:A:152:LEU:HB2	2.21	0.41
1:A:1652:THR:HG22	1:A:1653:THR:N	2.36	0.41
1:A:238:ILE:HD11	1:A:246:PHE:CD2	2.56	0.41
1:A:23:TYR:CE1	1:A:655:THR:O	2.74	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:SER:O	1:A:313:TYR:N	2.53	0.41
1:A:328:THR:OG1	1:A:339:GLU:HG2	2.20	0.41
1:A:500:ASN:ND2	1:A:543:TYR:HE1	2.15	0.41
1:A:20:GLU:HB2	1:A:551:THR:HB	2.01	0.41
1:A:610:TYR:CE2	1:A:619:PRO:HG3	2.54	0.41
1:A:627:LEU:HD23	1:A:627:LEU:HA	1.69	0.41
2:B:1370:ARG:NH1	2:B:1372:LEU:HG	2.34	0.41
2:B:1500:LEU:C	2:B:1500:LEU:HD12	2.41	0.41
2:B:358:MET:HA	2:B:359:PRO:HD3	1.97	0.41
2:B:436:GLN:O	2:B:437:THR:C	2.57	0.41
2:B:628:LEU:HD12	2:B:629:THR:N	2.35	0.41
2:B:79:GLY:C	2:B:81:MET:H	2.24	0.41
2:B:825:VAL:HG11	2:B:918:GLU:HB3	2.01	0.41
1:C:1179:THR:HG22	1:C:1208:ILE:HD13	1.98	0.41
1:C:1548:ARG:C	1:C:1550:GLN:N	2.74	0.41
1:C:1570:VAL:HG22	1:C:1575:VAL:HG22	2.02	0.41
1:C:286:ALA:O	1:C:287:MET:C	2.58	0.41
1:C:309:GLU:CG	1:C:310:LEU:N	2.84	0.41
1:C:38:ASN:HA	1:C:84:ILE:CG2	2.44	0.41
1:C:525:SER:O	2:D:401:ASN:ND2	2.54	0.41
1:C:705:VAL:CA	1:C:739:ARG:NH2	2.83	0.41
1:C:946:PRO:O	1:C:953:ILE:HG13	2.21	0.41
1:C:958:GLU:HG2	1:C:1347:ILE:HG12	2.01	0.41
1:C:961:TYR:HE1	1:C:963:ILE:HG12	1.86	0.41
2:D:120:LEU:HA	2:D:120:LEU:HD13	1.78	0.41
2:D:965:ILE:HA	2:D:1322:THR:O	2.20	0.41
2:D:1511:GLN:CG	2:D:1631:PHE:CE1	3.04	0.41
2:D:257:VAL:CG1	2:D:258:GLU:N	2.82	0.41
2:D:296:ARG:HA	2:D:296:ARG:HD2	1.93	0.41
2:D:306:LEU:HA	2:D:306:LEU:HD13	1.85	0.41
2:D:59:HIS:HA	2:D:68:LEU:HD22	2.02	0.41
2:D:785:THR:OG1	2:D:786:THR:N	2.52	0.41
2:D:818:LEU:HD23	2:D:911:LYS:HB2	2.01	0.41
1:A:1028:GLY:HA3	1:A:1030:HIS:CE1	2.55	0.41
1:A:1226:ARG:HD3	1:A:1266:TYR:CE1	2.55	0.41
1:A:1267:VAL:O	1:A:1270:VAL:HB	2.21	0.41
1:A:1279:ARG:HD3	1:A:1280:TYR:H	1.85	0.41
1:A:1320:LYS:CD	1:A:1321:GLY:N	2.78	0.41
1:A:1540:ASP:CA	1:A:1660:PHE:CD1	3.03	0.41
2:B:1391:LEU:HA	2:B:1392:PRO:HD3	1.88	0.41
2:B:810:VAL:CG1	2:B:811:MET:N	2.83	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:902:GLU:O	2:B:903:ALA:HB2	2.21	0.41
1:C:1033:ILE:HG23	1:C:1034:PHE:H	1.85	0.41
1:C:1211:ALA:HA	1:C:1214:ARG:NH1	2.34	0.41
1:C:1231:ASN:HB2	1:C:1235:LYS:CG	2.49	0.41
1:C:1445:GLY:O	1:C:1448:GLN:HB3	2.20	0.41
1:C:1563:VAL:HG12	1:C:1581:LEU:HA	2.02	0.41
1:C:433:PHE:N	1:C:433:PHE:HD1	2.19	0.41
2:D:322:THR:HG21	2:D:326:SER:OG	2.21	0.41
2:D:476:ILE:CG1	2:D:524:TYR:CD2	3.03	0.41
2:D:563:MET:HA	2:D:563:MET:CE	2.50	0.41
2:D:610:THR:C	2:D:612:GLY:N	2.72	0.41
2:D:101:ASN:ND2	2:D:641:ALA:HB2	2.36	0.41
1:A:1019:PHE:CZ	1:A:1088:GLN:HB3	2.56	0.41
1:A:1033:ILE:HD13	1:A:1034:PHE:CE1	2.55	0.41
1:A:1145:THR:HG22	1:A:1146:ALA:N	2.35	0.41
1:A:1195:LEU:HD23	1:A:1195:LEU:HA	1.95	0.41
1:A:1435:ASN:O	1:A:1436:GLU:C	2.58	0.41
1:A:1538:GLU:H	1:A:1538:GLU:CD	2.23	0.41
1:A:185:PHE:CB	1:A:186:PRO:HD2	2.51	0.41
1:A:215:ALA:C	1:A:216:TYR:CD2	2.94	0.41
1:A:461:SER:C	1:A:463:SER:N	2.74	0.41
1:A:804:ILE:HA	1:A:809:ILE:HA	2.02	0.41
2:B:1273:LEU:HD12	2:B:1273:LEU:C	2.41	0.41
2:B:965:ILE:HD13	2:B:1277:ILE:HD13	2.03	0.41
2:B:1518:THR:HG23	2:B:1519:ASN:N	2.36	0.41
2:B:1548:ILE:HA	2:B:1636:THR:OG1	2.21	0.41
2:B:276:ILE:HB	2:B:279:SER:OG	2.21	0.41
2:B:345:ILE:O	2:B:428:LYS:HD3	2.21	0.41
2:B:822:TYR:CD1	2:B:822:TYR:O	2.74	0.41
1:C:1093:VAL:O	1:C:1094:GLU:C	2.59	0.41
1:C:1159:CYS:O	1:C:1161:LEU:HD23	2.20	0.41
1:C:1234:HIS:CG	1:C:1235:LYS:N	2.88	0.41
1:C:123:ASN:C	1:C:211:THR:HG21	2.39	0.41
1:C:316:GLU:N	1:C:316:GLU:OE1	2.41	0.41
1:C:465:LEU:HD12	1:C:466:TYR:H	1.85	0.41
1:C:544:TYR:CZ	1:C:555:VAL:HG12	2.55	0.41
1:C:697:LYS:O	1:C:700:TYR:N	2.54	0.41
1:C:710:THR:OG1	1:C:713:GLN:HG3	2.21	0.41
1:C:805:SER:O	1:C:806:ASN:C	2.59	0.41
1:C:953:ILE:CD1	1:C:955:ARG:HH21	2.33	0.41
1:C:965:LEU:C	1:C:967:LEU:H	2.24	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1273:LEU:HD12	2:D:1273:LEU:O	2.20	0.41
2:D:283:ILE:HA	2:D:284:PRO:HD3	1.81	0.41
2:D:417:HIS:CD2	2:D:419:ASP:HB2	2.56	0.41
2:D:541:LYS:O	2:D:543:THR:CG2	2.69	0.41
2:D:748:ARG:NH1	2:D:784:ILE:HG12	2.36	0.41
3:Y:138:VAL:HG11	3:Y:177:TYR:CD2	2.56	0.41
3:Y:52:SER:OG	3:Y:53:GLU:N	2.53	0.41
1:A:1188:LEU:HD23	1:A:1212:LEU:CA	2.51	0.41
1:A:1445:GLY:O	1:A:1448:GLN:HB3	2.21	0.41
1:A:1552:ALA:HB1	1:A:1585:TYR:OH	2.20	0.41
1:A:1560:ALA:C	1:A:1561:TYR:CD2	2.95	0.41
1:A:1565:ILE:HB	1:A:1614:GLY:N	2.36	0.41
1:A:174:VAL:CG2	1:A:175:GLU:H	2.34	0.41
1:A:215:ALA:C	1:A:216:TYR:HD2	2.24	0.41
1:A:49:ALA:HB2	1:A:74:SER:HB2	2.01	0.41
2:B:1424:ILE:HG12	2:B:1426:TYR:HE2	1.80	0.41
2:B:1522:TYR:HD1	2:B:1524:TYR:CE1	2.38	0.41
2:B:1571:GLU:O	2:B:1574:ASN:HB2	2.21	0.41
2:B:1601:ILE:HD12	2:B:1601:ILE:N	2.36	0.41
2:B:173:VAL:HA	2:B:964:ILE:HD11	2.03	0.41
2:B:615:GLN:CB	2:B:616:ASN:HD22	2.34	0.41
2:B:819:GLN:HE21	2:B:819:GLN:HA	1.85	0.41
2:B:857:CYS:CB	2:B:885:VAL:CG2	2.99	0.41
1:C:1047:LYS:O	1:C:1048:LYS:C	2.58	0.41
1:C:1180:LEU:O	1:C:1180:LEU:HD22	2.20	0.41
1:C:1218:VAL:CG1	1:C:1219:LYS:N	2.72	0.41
1:C:1314:ASP:OD2	1:C:1325:ASN:HB3	2.20	0.41
1:C:1342:LEU:HD23	1:C:1342:LEU:N	2.36	0.41
1:C:153:LYS:CB	1:C:154:PRO:CD	2.99	0.41
1:C:1638:PRO:HG2	1:C:1639:LEU:H	1.85	0.41
1:C:1661:LEU:O	1:C:1662:ALA:C	2.59	0.41
1:C:185:PHE:CD1	1:C:186:PRO:HD2	2.56	0.41
1:C:20:GLU:HG3	1:C:547:THR:OG1	2.21	0.41
1:C:560:TRP:CH2	1:C:562:ASN:HB2	2.55	0.41
1:C:999:ILE:O	1:C:1000:LEU:C	2.59	0.41
2:D:1429:LYS:HE3	2:D:1429:LYS:H	1.85	0.41
2:D:338:ILE:C	2:D:339:VAL:HG13	2.41	0.41
2:D:518:PHE:H	2:D:518:PHE:HD2	1.68	0.41
2:D:620:VAL:CG1	2:D:621:PHE:N	2.84	0.41
2:D:819:GLN:HE21	2:D:819:GLN:HA	1.85	0.41
2:D:895:GLU:HA	2:D:909:VAL:O	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:ASN:O	1:A:1092:TYR:N	2.54	0.41
1:A:1246:ARG:HB2	1:A:1246:ARG:CZ	2.51	0.41
1:A:734:VAL:O	1:A:737:GLN:HB2	2.21	0.41
1:A:849:ARG:HH22	2:B:555:LEU:C	2.24	0.41
1:A:958:GLU:HG2	1:A:1347:ILE:HG12	2.03	0.41
2:B:104:VAL:HG12	2:B:121:LEU:HD13	2.02	0.41
2:B:952:ASP:O	2:B:1331:ALA:CA	2.69	0.41
2:B:1444:LYS:HZ1	2:B:1447:GLU:HA	1.86	0.41
2:B:1605:THR:HG22	2:B:1605:THR:O	2.20	0.41
2:B:504:VAL:O	2:B:504:VAL:HG12	2.21	0.41
1:A:856:CYS:N	2:B:904:LEU:HD11	2.36	0.41
1:C:1176:LEU:HD21	1:C:1195:LEU:HD13	2.02	0.41
1:C:1232:LEU:HG	1:C:1233:GLN:H	1.86	0.41
1:C:1644:TRP:NE1	1:C:1646:GLU:OE1	2.52	0.41
1:C:1669:GLU:O	1:C:1673:LEU:HG	2.21	0.41
1:C:354:LEU:H	1:C:354:LEU:HD23	1.85	0.41
1:C:620:LEU:O	1:C:623:VAL:CG2	2.65	0.41
1:C:257:ASN:HB2	1:C:848:TYR:CE2	2.56	0.41
1:C:934:VAL:O	1:C:935:LYS:HE2	2.21	0.41
2:D:1279:ILE:HD13	2:D:1279:ILE:HA	1.86	0.41
2:D:1423:VAL:CG1	2:D:1423:VAL:O	2.68	0.41
2:D:1459:TYR:CB	2:D:1466:GLU:HB3	2.51	0.41
2:D:147:VAL:O	2:D:147:VAL:CG1	2.69	0.41
2:D:1506:ILE:HB	2:D:1627:ASP:HB3	2.02	0.41
2:D:247:ILE:HD11	2:D:318:VAL:HG21	2.03	0.41
2:D:341:SER:HB2	2:D:426:ALA:HB2	2.03	0.41
2:D:438:GLN:HE22	2:D:530:GLU:HA	1.86	0.41
2:D:58:VAL:HG23	2:D:69:PHE:O	2.21	0.41
2:D:751:PHE:N	2:D:751:PHE:CD2	2.88	0.41
2:D:810:VAL:O	2:D:811:MET:HB2	2.20	0.41
2:D:902:GLU:O	2:D:903:ALA:HB2	2.20	0.41
1:C:915:GLU:HG3	2:D:904:LEU:HG	2.03	0.41
1:A:1127:ILE:N	1:A:1127:ILE:HD12	2.28	0.41
1:A:1161:LEU:HD12	1:C:1105:LEU:CD1	2.46	0.41
1:A:1268:ASN:N	1:A:1269:PRO:HD2	2.35	0.41
1:A:131:ASP:OD2	1:A:132:LYS:HG3	2.21	0.41
1:A:149:ASN:HD21	1:A:153:LYS:H	1.67	0.41
1:A:1564:SER:HA	1:A:1616:GLN:HA	2.02	0.41
1:A:161:LEU:HD12	1:A:161:LEU:N	2.35	0.41
1:A:1638:PRO:HG2	1:A:1639:LEU:N	2.36	0.41
1:A:382:LEU:HA	1:A:382:LEU:HD23	1.80	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:SER:HB3	1:A:510:ILE:HD13	2.00	0.41
1:A:535:VAL:HA	1:A:563:ILE:CD1	2.50	0.41
1:A:88:GLN:HA	1:A:89:PRO:HD2	1.88	0.41
1:A:967:LEU:HD12	1:A:968:VAL:H	1.86	0.41
2:B:103:TYR:HD2	2:B:103:TYR:N	2.19	0.41
2:B:1429:LYS:N	2:B:1429:LYS:HE3	2.36	0.41
2:B:1446:PHE:CD2	2:B:1448:VAL:HG13	2.56	0.41
2:B:146:ARG:HH11	2:B:146:ARG:CB	2.34	0.41
2:B:168:PRO:CG	2:B:196:THR:N	2.84	0.41
2:B:101:ASN:ND2	2:B:641:ALA:HB2	2.36	0.41
2:B:811:MET:CE	2:B:839:TYR:HD2	2.35	0.41
2:B:850:LEU:CD1	2:B:851:LEU:N	2.84	0.41
2:B:828:GLU:O	2:B:886:PRO:HD2	2.21	0.41
1:A:1161:LEU:CA	1:C:1102:ASN:HD21	2.26	0.41
1:C:1274:LEU:O	1:C:1275:SER:C	2.59	0.41
1:C:701:ASP:CG	1:C:1446:VAL:HG23	2.41	0.41
1:C:255:PHE:HD1	1:C:255:PHE:O	2.04	0.41
1:C:315:LEU:HD11	1:C:318:LEU:HG	1.98	0.41
1:C:566:LYS:O	1:C:568:GLY:N	2.54	0.41
1:C:734:VAL:O	1:C:737:GLN:HB2	2.21	0.41
1:C:81:ASN:CG	1:C:82:SER:N	2.74	0.41
2:D:1363:LEU:HD23	2:D:1442:ILE:HG12	2.03	0.41
2:D:1378:THR:O	2:D:1379:MET:C	2.59	0.41
2:D:173:VAL:O	2:D:174:SER:HB2	2.20	0.41
2:D:370:ASP:OD1	2:D:370:ASP:N	2.47	0.41
2:D:553:ASP:N	2:D:553:ASP:OD1	2.54	0.41
1:A:1054:LEU:O	1:A:1055:SER:C	2.59	0.40
1:A:25:ILE:HD13	1:A:25:ILE:HA	1.90	0.40
1:A:455:ILE:CG2	1:A:456:ALA:N	2.83	0.40
1:A:367:ILE:HD13	1:A:466:TYR:CD2	2.56	0.40
1:A:46:TYR:HE1	1:A:48:GLU:HB2	1.85	0.40
1:A:531:THR:HG23	1:A:533:ASN:N	2.35	0.40
1:A:23:TYR:CE1	1:A:655:THR:HB	2.55	0.40
1:A:74:SER:CA	1:A:79:PHE:CE1	3.04	0.40
1:A:827:MET:HB3	1:A:829:ILE:CD1	2.52	0.40
2:B:1410:ARG:HD2	2:B:1410:ARG:HA	1.83	0.40
2:B:1494:GLY:O	2:B:1495:GLU:HB2	2.21	0.40
2:B:235:PHE:HB3	2:B:338:ILE:CG2	2.52	0.40
2:B:410:PRO:CB	2:B:431:THR:HG22	2.50	0.40
2:B:464:PHE:O	2:B:503:LEU:HA	2.20	0.40
2:B:620:VAL:CG1	2:B:621:PHE:N	2.84	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:VAL:HG23	2:B:69:PHE:O	2.21	0.40
2:B:148:PHE:HB2	2:B:800:ILE:HD11	2.00	0.40
2:B:816:ILE:CD1	2:B:909:VAL:HG23	2.51	0.40
2:B:253:TYR:HE1	2:B:839:TYR:HE2	1.69	0.40
1:C:100:SER:C	1:C:101:TYR:CD2	2.94	0.40
1:C:54:ILE:HA	1:C:105:GLU:O	2.21	0.40
1:C:1215:GLU:O	1:C:1217:LEU:HD23	2.21	0.40
1:C:1246:ARG:NH1	1:C:1246:ARG:HB2	2.36	0.40
1:C:1267:VAL:HG12	1:C:1267:VAL:O	2.20	0.40
1:C:1305:LYS:HD3	1:C:1305:LYS:HA	1.70	0.40
1:C:1339:GLU:OE1	1:C:1339:GLU:HA	2.21	0.40
1:C:1575:VAL:O	1:C:1601:ILE:HA	2.21	0.40
1:C:404:LEU:HA	1:C:404:LEU:HD22	1.69	0.40
1:C:569:ASN:O	1:C:570:GLN:CB	2.51	0.40
1:C:681:LYS:HD2	1:C:738:LEU:HD21	2.04	0.40
1:C:601:ALA:N	1:C:802:VAL:O	2.48	0.40
1:A:1042:LYS:HZ3	1:C:92:LEU:HD13	1.86	0.40
2:D:1571:GLU:O	2:D:1574:ASN:HB2	2.21	0.40
2:D:490:PHE:C	2:D:490:PHE:CD1	2.91	0.40
2:D:820:MET:HE2	2:D:832:ILE:HG21	2.03	0.40
3:X:100:GLY:O	3:X:125:LYS:CG	2.68	0.40
3:X:153:PHE:CE1	3:X:169:ILE:HD13	2.55	0.40
1:A:1013:MET:O	1:A:1015:VAL:N	2.54	0.40
1:A:1244:THR:HG23	1:A:1502:ASP:CG	2.40	0.40
1:A:1020:TYR:CE1	1:A:1295:GLU:HA	2.56	0.40
1:A:316:GLU:N	1:A:316:GLU:OE1	2.46	0.40
1:A:412:ARG:NE	1:A:415:ASP:OD2	2.54	0.40
1:A:41:ILE:HG21	1:A:41:ILE:HD13	1.68	0.40
1:A:594:THR:O	1:A:782:ARG:CD	2.69	0.40
1:A:705:VAL:CA	1:A:739:ARG:HH22	2.35	0.40
1:A:889:GLU:HB2	1:A:892:SER:HB2	2.04	0.40
1:A:971:THR:O	1:A:972:GLU:C	2.59	0.40
2:B:1292:ILE:HD11	2:B:1301:ARG:HE	1.86	0.40
2:B:1635:LEU:HD23	2:B:1635:LEU:HA	1.60	0.40
2:B:352:LYS:HG3	2:B:430:MET:CE	2.51	0.40
2:B:150:MET:HG3	2:B:602:ILE:HD11	2.02	0.40
1:C:1011:GLU:HG3	1:C:1055:SER:CB	2.51	0.40
1:C:1180:LEU:HA	1:C:1180:LEU:HD23	1.48	0.40
1:C:1320:LYS:HD2	1:C:1320:LYS:HA	1.88	0.40
1:C:1449:LEU:HD12	1:C:1449:LEU:O	2.22	0.40
1:C:162:THR:HG23	1:C:202:LYS:HB2	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:VAL:O	1:C:358:ALA:C	2.60	0.40
1:C:600:VAL:HG11	1:C:602:LEU:HD21	2.02	0.40
1:C:705:VAL:CA	1:C:739:ARG:HH22	2.33	0.40
1:C:604:ALA:HB3	1:C:773:TRP:O	2.21	0.40
1:C:941:GLY:HA2	1:C:1359:VAL:O	2.22	0.40
2:D:1331:ALA:O	2:D:1332:GLN:CB	2.58	0.40
2:D:1367:ILE:HD13	2:D:1456:VAL:HG21	2.02	0.40
2:D:147:VAL:O	2:D:147:VAL:HG13	2.20	0.40
2:D:1491:ARG:HD3	2:D:1491:ARG:HA	1.89	0.40
2:D:1509:PRO:HA	2:D:1512:ILE:CG1	2.51	0.40
2:D:472:SER:O	2:D:475:GLN:HG3	2.22	0.40
2:D:544:CYS:HB3	2:D:546:GLY:O	2.22	0.40
2:D:599:TRP:O	2:D:600:ASP:C	2.58	0.40
2:D:780:LEU:CD1	2:D:787:TRP:CD1	3.05	0.40
2:D:827:ASN:OD1	2:D:1490:CYS:HB2	2.22	0.40
2:D:925:VAL:HG22	2:D:1326:LEU:CD2	2.40	0.40
2:D:967:GLY:O	2:D:969:PRO:HD3	2.21	0.40
3:Y:185:LYS:HB3	3:Y:185:LYS:HE2	1.98	0.40
1:A:1161:LEU:CD1	1:C:1105:LEU:CD1	3.00	0.40
1:A:116:ARG:O	1:A:117:MET:HB3	2.21	0.40
1:A:1220:GLY:O	1:A:1223:PRO:HA	2.21	0.40
1:A:127:PHE:HD2	1:A:623:VAL:HG22	1.85	0.40
1:A:1243:GLY:O	1:A:1285:TYR:CE2	2.74	0.40
1:A:1420:SER:O	1:A:1421:HIS:C	2.58	0.40
1:A:1450:PHE:HB3	1:A:1463:GLN:O	2.21	0.40
1:A:153:LYS:CB	1:A:154:PRO:CD	2.99	0.40
1:A:255:PHE:HD1	1:A:255:PHE:O	2.04	0.40
1:A:284:GLN:HG2	1:A:310:LEU:HD11	2.03	0.40
1:A:510:ILE:HA	3:X:150:ILE:HG13	2.02	0.40
1:A:587:THR:HA	1:A:789:ALA:HA	2.02	0.40
2:B:1539:ILE:N	2:B:1539:ILE:HD12	2.34	0.40
2:B:283:ILE:HA	2:B:284:PRO:HD3	1.81	0.40
2:B:330:VAL:HG23	2:B:330:VAL:O	2.22	0.40
2:B:460:LEU:HD23	2:B:508:LEU:HB3	2.04	0.40
2:B:482:LEU:CB	2:B:492:VAL:HG23	2.35	0.40
2:B:464:PHE:CE2	2:B:506:MET:HE1	2.56	0.40
2:B:476:ILE:CG1	2:B:524:TYR:CD2	3.04	0.40
1:C:1053:MET:CE	1:C:1085:VAL:HG12	2.51	0.40
1:C:1127:ILE:HB	1:C:1129:LEU:HD21	2.03	0.40
1:C:1146:ALA:HB3	1:C:1190:ILE:CG2	2.51	0.40
1:C:602:LEU:HA	1:C:801:GLY:HA2	2.03	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:854:GLN:HE21	1:C:854:GLN:C	2.23	0.40
1:C:914:LEU:O	1:C:914:LEU:HG	2.20	0.40
1:C:92:LEU:HA	1:C:93:PRO:HD3	1.96	0.40
2:D:164:GLU:HB2	2:D:200:VAL:HG23	2.03	0.40
2:D:345:ILE:HD11	2:D:426:ALA:C	2.41	0.40
2:D:352:LYS:HG3	2:D:430:MET:HE1	2.03	0.40
2:D:45:ALA:HB3	2:D:81:MET:CE	2.51	0.40
2:D:468:GLY:O	2:D:469:ASN:C	2.59	0.40
2:D:745:ILE:O	2:D:745:ILE:CG2	2.68	0.40
2:D:943:GLU:CB	2:D:1313:VAL:HG23	2.52	0.40
1:C:78:LYS:NZ	3:Y:143:GLY:O	2.47	0.40
3:Y:40:LEU:HD11	3:Y:209:PHE:HZ	1.85	0.40
3:Y:67:TYR:CD1	3:Y:67:TYR:O	2.74	0.40
3:Y:61:SER:OG	3:Y:99:GLN:HA	2.20	0.40
1:A:1300:TYR:CE2	1:A:1304:VAL:HG21	2.56	0.40
1:A:1358:THR:HB	1:A:1360:HIS:HE1	1.84	0.40
1:A:1440:LYS:O	1:A:1443:VAL:HG12	2.21	0.40
1:A:431:LEU:C	1:A:431:LEU:CD2	2.90	0.40
1:A:718:ILE:HB	1:A:725:ILE:CD1	2.51	0.40
2:B:1292:ILE:HD12	2:B:1296:ASN:OD1	2.21	0.40
2:B:145:TYR:CD1	2:B:145:TYR:C	2.95	0.40
2:B:1534:GLN:HB2	2:B:1539:ILE:HD11	2.04	0.40
2:B:802:VAL:HG12	2:B:802:VAL:O	2.22	0.40
2:B:848:VAL:HG22	2:B:898:ALA:HB2	2.04	0.40
2:B:950:LEU:O	2:B:951:ASP:HB2	2.21	0.40
1:C:1018:VAL:HG11	1:C:1048:LYS:HB3	2.03	0.40
1:C:1231:ASN:OD1	1:C:1232:LEU:N	2.54	0.40
1:C:1217:LEU:CD1	1:C:1237:SER:HA	2.52	0.40
1:C:1248:VAL:H	1:C:1248:VAL:HG23	1.69	0.40
1:C:1430:THR:HG22	1:C:1430:THR:O	2.21	0.40
1:C:243:PHE:O	1:C:303:SER:HB2	2.21	0.40
1:C:492:TYR:HE2	1:C:546:VAL:HG11	1.86	0.40
1:C:531:THR:HG23	1:C:533:ASN:N	2.37	0.40
1:C:22:THR:HG21	1:C:657:ALA:HB2	2.04	0.40
1:C:789:ALA:O	1:C:790:LEU:O	2.40	0.40
1:C:804:ILE:HA	1:C:809:ILE:HA	2.03	0.40
1:C:984:VAL:O	1:C:984:VAL:HG13	2.21	0.40
2:D:121:LEU:HD12	2:D:121:LEU:HA	1.72	0.40
2:D:1383:ASP:O	2:D:1456:VAL:HA	2.22	0.40
2:D:1469:THR:O	2:D:1470:LYS:HG2	2.22	0.40
2:D:1615:GLU:O	2:D:1616:CYS:C	2.60	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:269:ILE:HG13	2:D:272:ALA:HB3	2.02	0.40
2:D:515:ILE:HG21	2:D:599:TRP:CZ2	2.56	0.40
2:D:64:LYS:HG3	2:D:64:LYS:O	2.22	0.40
2:D:76:ASN:CB	2:D:77:PRO:HD2	2.52	0.40
2:D:794:PHE:CD2	2:D:795:THR:N	2.89	0.40
2:D:851:LEU:CD2	2:D:852:TYR:H	2.17	0.40
2:D:878:ARG:HA	2:D:878:ARG:HD2	1.92	0.40
3:X:101:GLN:HB3	3:X:123:THR:O	2.22	0.40
3:Y:113:ASN:HD21	3:Y:115:ARG:HG2	1.87	0.40
1:A:1264:ILE:HD12	1:A:1264:ILE:N	2.36	0.40
1:A:127:PHE:CD2	1:A:623:VAL:HG22	2.56	0.40
1:A:127:PHE:HD1	1:A:127:PHE:N	2.20	0.40
1:A:1309:LEU:CD2	1:A:1355:GLY:HA3	2.52	0.40
1:A:160:VAL:O	1:A:160:VAL:HG12	2.20	0.40
1:A:22:THR:CG2	1:A:23:TYR:CE1	3.04	0.40
1:A:316:GLU:O	1:A:349:LEU:HD21	2.21	0.40
1:A:412:ARG:HG3	1:A:413:VAL:H	1.87	0.40
1:A:644:ASN:O	1:A:647:HIS:N	2.55	0.40
1:A:658:ASN:O	1:A:658:ASN:OD1	2.40	0.40
1:A:984:VAL:HG13	1:A:984:VAL:O	2.21	0.40
2:B:174:SER:HA	2:B:1300:ALA:HB2	2.02	0.40
2:B:1459:TYR:CB	2:B:1466:GLU:HB3	2.52	0.40
2:B:261:ALA:HB2	2:B:285:ILE:HD11	2.01	0.40
2:B:397:LYS:NZ	2:B:449:ILE:O	2.55	0.40
2:B:476:ILE:CD1	2:B:524:TYR:CD2	3.02	0.40
2:B:618:LEU:CD1	2:B:635:ASN:O	2.65	0.40
2:B:751:PHE:CD2	2:B:751:PHE:N	2.90	0.40
2:B:795:THR:CG2	2:B:796:PRO:CD	2.98	0.40
1:C:1008:ALA:O	1:C:1011:GLU:N	2.55	0.40
1:C:1090:ASN:O	1:C:1092:TYR:N	2.54	0.40
1:C:1147:PHE:C	1:C:1147:PHE:HD2	2.25	0.40
1:C:1228:TRP:N	1:C:1228:TRP:HE3	2.20	0.40
1:C:1467:ILE:HA	1:C:1468:PRO:HD3	1.83	0.40
1:C:284:GLN:HG2	1:C:310:LEU:HD11	2.02	0.40
1:C:489:LYS:HZ3	2:D:502:ASN:H	1.69	0.40
1:C:501:TYR:HB3	1:C:542:VAL:HG22	2.03	0.40
1:C:671:GLU:HB2	1:C:672:ILE:H	1.66	0.40
1:C:718:ILE:HB	1:C:725:ILE:CD1	2.51	0.40
1:C:823:VAL:HG23	1:C:846:TYR:O	2.20	0.40
1:C:923:LEU:CD2	1:C:925:LYS:HD3	2.52	0.40
2:D:1296:ASN:HB2	2:D:1299:LEU:HD22	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1486:ILE:O	2:D:1486:ILE:HG13	2.22	0.40
2:D:409:LEU:N	2:D:410:PRO:HD3	2.36	0.40
2:D:23:ALA:CB	2:D:528:ASN:HD22	2.27	0.40
1:C:849:ARG:NH2	2:D:555:LEU:HB2	2.36	0.40
2:D:891:LEU:H	2:D:891:LEU:HG	1.10	0.40
3:Y:83:GLN:O	3:Y:117:SER:HA	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1616/1676 (96%)	1165 (72%)	300 (19%)	151 (9%)	1	14
1	C	1616/1676 (96%)	1179 (73%)	290 (18%)	147 (9%)	1	15
2	B	1203/1642 (73%)	981 (82%)	176 (15%)	46 (4%)	4	34
2	D	1203/1642 (73%)	982 (82%)	177 (15%)	44 (4%)	4	35
3	X	189/231 (82%)	148 (78%)	31 (16%)	10 (5%)	2	27
3	Y	189/231 (82%)	150 (79%)	28 (15%)	11 (6%)	2	25
All	All	6016/7098 (85%)	4605 (76%)	1002 (17%)	409 (7%)	1	21

All (409) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	60	PRO
1	A	89	PRO
1	A	96	GLN
1	A	150	ASP
1	A	154	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	155	ALA
1	A	208	ASP
1	A	274	ASP
1	A	285	THR
1	A	308	LYS
1	A	490	SER
1	A	495	LYS
1	A	507	GLY
1	A	522	SER
1	A	551	THR
1	A	552	ALA
1	A	570	GLN
1	A	634	CYS
1	A	643	ALA
1	A	754	MET
1	A	759	PRO
1	A	790	LEU
1	A	821	LYS
1	A	866	CYS
1	A	873	ILE
1	A	884	VAL
1	A	885	ARG
1	A	948	GLY
1	A	998	ASN
1	A	1004	PRO
1	A	1096	ASN
1	A	1232	LEU
1	A	1242	THR
1	A	1286	SER
1	A	1335	GLY
1	A	1452	ASP
1	A	1538	GLU
1	A	1573	VAL
1	A	1609	ALA
1	A	1628	LYS
1	A	1638	PRO
1	A	1639	LEU
1	A	1674	ASN
2	B	207	PRO
2	B	453	GLU
2	B	490	PHE
2	B	873	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	1529	LEU
2	B	1548	ILE
2	B	1615	GLU
2	B	1639	GLY
1	C	60	PRO
1	C	89	PRO
1	C	96	GLN
1	C	97	ASN
1	C	150	ASP
1	C	155	ALA
1	C	208	ASP
1	C	274	ASP
1	C	285	THR
1	C	308	LYS
1	C	490	SER
1	C	495	LYS
1	C	507	GLY
1	C	522	SER
1	C	570	GLN
1	C	634	CYS
1	C	643	ALA
1	C	669	CYS
1	C	754	MET
1	C	759	PRO
1	C	790	LEU
1	C	821	LYS
1	C	873	ILE
1	C	884	VAL
1	C	885	ARG
1	C	939	TYR
1	C	948	GLY
1	C	998	ASN
1	C	1096	ASN
1	C	1232	LEU
1	C	1242	THR
1	C	1264	ILE
1	C	1286	SER
1	C	1335	GLY
1	C	1452	ASP
1	C	1538	GLU
1	C	1590	ALA
1	C	1609	ALA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	1628	LYS
1	C	1638	PRO
1	C	1639	LEU
1	C	1674	ASN
2	D	51	PRO
2	D	207	PRO
2	D	453	GLU
2	D	490	PHE
2	D	873	LYS
2	D	1507	ASP
2	D	1529	LEU
2	D	1548	ILE
3	X	42	ASP
3	X	72	VAL
3	X	78	LYS
3	Y	42	ASP
3	Y	72	VAL
3	Y	78	LYS
1	A	97	ASN
1	A	133	PRO
1	A	156	LYS
1	A	181	GLY
1	A	187	ASP
1	A	289	ASN
1	A	312	TYR
1	A	318	LEU
1	A	474	LYS
1	A	489	LYS
1	A	519	SER
1	A	520	ASP
1	A	565	GLU
1	A	596	MET
1	A	614	ARG
1	A	623	VAL
1	A	639	GLY
1	A	656	ASN
1	A	659	ALA
1	A	669	CYS
1	A	672	ILE
1	A	690	TYR
1	A	806	ASN
1	A	820	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	850	THR
1	A	870	SER
1	A	939	TYR
1	A	946	PRO
1	A	1133	LEU
1	A	1134	PRO
1	A	1264	ILE
1	A	1333	PHE
1	A	1386	ILE
1	A	1471	ASP
1	A	1528	VAL
1	A	1583	ASP
1	A	1590	ALA
2	B	36	ASP
2	B	48	ASP
2	B	220	VAL
2	B	451	SER
2	B	583	ALA
2	B	604	LYS
2	B	641	ALA
2	B	821	PRO
2	B	842	GLU
2	B	1283	ASP
2	B	1449	GLY
2	B	1493	ALA
2	B	1603	LYS
2	B	1641	PRO
1	C	21	GLN
1	C	133	PRO
1	C	154	PRO
1	C	156	LYS
1	C	166	PRO
1	C	181	GLY
1	C	187	ASP
1	C	255	PHE
1	C	312	TYR
1	C	318	LEU
1	C	474	LYS
1	C	520	ASP
1	C	596	MET
1	C	614	ARG
1	C	623	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	639	GLY
1	C	656	ASN
1	C	671	GLU
1	C	672	ILE
1	C	690	TYR
1	C	793	SER
1	C	806	ASN
1	C	820	PHE
1	C	850	THR
1	C	870	SER
1	C	917	TRP
1	C	946	PRO
1	C	1004	PRO
1	C	1134	PRO
1	C	1333	PHE
1	C	1382	ASP
1	C	1386	ILE
1	C	1573	VAL
1	C	1583	ASP
2	D	36	ASP
2	D	220	VAL
2	D	451	SER
2	D	582	LYS
2	D	583	ALA
2	D	604	LYS
2	D	641	ALA
2	D	821	PRO
2	D	842	GLU
2	D	1283	ASP
2	D	1449	GLY
2	D	1493	ALA
2	D	1603	LYS
3	Y	82	HIS
1	A	171	VAL
1	A	255	PHE
1	A	287	MET
1	A	642	ASN
1	A	671	GLU
1	A	681	LYS
1	A	699	CYS
1	A	791	PRO
1	A	793	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	917	TRP
1	A	931	PRO
1	A	1001	THR
1	A	1023	HIS
1	A	1073	SER
1	A	1122	SER
1	A	1220	GLY
1	A	1235	LYS
1	A	1241	ASN
1	A	1382	ASP
1	A	1589	GLU
2	B	51	PRO
2	B	470	ALA
2	B	582	LYS
2	B	871	PRO
2	B	1379	MET
2	B	1492	CYS
2	B	1558	ALA
1	C	171	VAL
1	C	287	MET
1	C	289	ASN
1	C	441	ASP
1	C	489	LYS
1	C	519	SER
1	C	551	THR
1	C	552	ALA
1	C	565	GLU
1	C	642	ASN
1	C	659	ALA
1	C	681	LYS
1	C	791	PRO
1	C	931	PRO
1	C	997	ILE
1	C	1001	THR
1	C	1014	SER
1	C	1073	SER
1	C	1122	SER
1	C	1133	LEU
1	C	1200	LYS
1	C	1241	ASN
1	C	1471	ASP
1	C	1589	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	48	ASP
2	D	871	PRO
2	D	1379	MET
2	D	1492	CYS
2	D	1558	ALA
2	D	1631	PHE
3	X	82	HIS
3	X	87	LEU
3	X	125	LYS
3	X	185	LYS
3	Y	125	LYS
3	Y	185	LYS
1	A	256	TYR
1	A	441	ASP
1	A	641	ASN
1	A	663	GLN
1	A	822	ASP
1	A	863	GLU
1	A	960	PRO
1	A	997	ILE
1	A	1014	SER
1	A	1160	PRO
1	A	1181	PRO
1	A	1184	SER
1	A	1237	SER
1	A	1284	PHE
1	A	1297	LEU
1	A	1324	HIS
1	A	1488	LEU
1	A	1512	SER
1	A	1653	THR
1	A	1666	GLU
2	B	142	PRO
2	B	310	VAL
2	B	764	GLU
2	B	862	LYS
1	C	137	PRO
1	C	170	GLU
1	C	256	TYR
1	C	641	ASN
1	C	663	GLN
1	C	699	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	752	LEU
1	C	822	ASP
1	C	960	PRO
1	C	1160	PRO
1	C	1181	PRO
1	C	1184	SER
1	C	1220	GLY
1	C	1235	LYS
1	C	1237	SER
1	C	1284	PHE
1	C	1324	HIS
1	C	1352	PHE
1	C	1488	LEU
1	C	1512	SER
1	C	1666	GLU
2	D	142	PRO
2	D	310	VAL
2	D	470	ALA
2	D	764	GLU
2	D	862	LYS
3	Y	68	ASN
3	Y	87	LEU
3	Y	124	LYS
1	A	61	ASP
1	A	475	ALA
1	A	488	PRO
1	A	506	LYS
1	A	694	VAL
1	A	720	LEU
1	A	752	LEU
1	A	994	GLN
1	A	1200	LYS
1	A	1239	VAL
1	A	1352	PHE
1	A	1398	ASP
2	B	193	SER
2	B	1286	VAL
2	B	1592	PRO
2	B	1628	PHE
1	C	61	ASP
1	C	337	SER
1	C	488	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	685	GLU
1	C	694	VAL
1	C	1239	VAL
1	C	1398	ASP
1	C	1653	THR
1	C	1654	CYS
2	D	1435	ASP
2	D	1592	PRO
3	X	68	ASN
3	X	124	LYS
1	A	43	VAL
1	A	137	PRO
1	A	1321	GLY
1	A	1654	CYS
2	B	512	PRO
1	C	41	ILE
1	C	291	MET
1	C	1018	VAL
2	D	418	GLY
2	D	937	VAL
2	D	1286	VAL
1	A	190	ILE
1	A	440	PRO
1	A	645	VAL
1	A	760	VAL
1	A	1296	GLY
2	B	80	GLY
2	B	221	LEU
2	B	339	VAL
2	B	937	VAL
1	C	577	PRO
1	C	760	VAL
1	C	1006	GLY
1	C	1135	VAL
2	D	512	PRO
3	X	76	ASN
3	Y	76	ASN
1	A	406	PRO
1	A	577	PRO
2	B	237	ILE
1	C	43	VAL
1	C	406	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	440	PRO
1	C	872	VAL
2	D	173	VAL
2	D	221	LEU
3	Y	143	GLY
1	A	41	ILE
1	A	231	ILE
1	A	585	GLY
1	A	1018	VAL
1	A	1135	VAL
1	A	1570	VAL
2	B	173	VAL
1	C	231	ILE
1	C	1570	VAL
2	D	47	GLY
2	D	80	GLY
2	D	237	ILE
2	D	339	VAL
1	A	618	LYS
2	B	418	GLY
1	C	618	LYS
1	C	645	VAL
1	C	1296	GLY
2	B	598	ILE
1	C	1321	GLY

### 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	1445/1484 (97%)	1090 (75%)	355 (25%)	1	6
1	C	1445/1484 (97%)	1098 (76%)	347 (24%)	1	6
2	B	1084/1435 (76%)	849 (78%)	235 (22%)	1	8
2	D	1084/1435 (76%)	855 (79%)	229 (21%)	1	9
3	X	175/205 (85%)	143 (82%)	32 (18%)	2	14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Y	175/205 (85%)	142 (81%)	33 (19%)	2	13
All	All	5408/6248 (87%)	4177 (77%)	1231 (23%)	1	8

All (1231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	21	GLN
1	A	22	THR
1	A	23	TYR
1	A	24	VAL
1	A	40	VAL
1	A	42	GLN
1	A	43	VAL
1	A	46	TYR
1	A	55	SER
1	A	58	SER
1	A	63	LYS
1	A	64	PHE
1	A	73	LEU
1	A	84	ILE
1	A	85	LEU
1	A	87	ILE
1	A	89	PRO
1	A	90	LYS
1	A	91	GLN
1	A	102	VAL
1	A	106	VAL
1	A	114	SER
1	A	125	PHE
1	A	126	LEU
1	A	128	ILE
1	A	131	ASP
1	A	136	THR
1	A	144	ARG
1	A	147	SER
1	A	149	ASN
1	A	152	LEU
1	A	157	ARG
1	A	161	LEU
1	A	162	THR
1	A	169	SER

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	170	GLU
1	A	176	GLU
1	A	182	ILE
1	A	183	ILE
1	A	184	SER
1	A	195	ARG
1	A	200	THR
1	A	209	PHE
1	A	211	THR
1	A	212	THR
1	A	214	THR
1	A	216	TYR
1	A	219	VAL
1	A	222	TYR
1	A	223	VAL
1	A	224	LEU
1	A	228	SER
1	A	230	SER
1	A	240	TYR
1	A	242	ASN
1	A	249	THR
1	A	251	LYS
1	A	255	PHE
1	A	261	THR
1	A	264	ASP
1	A	268	THR
1	A	276	LYS
1	A	279	GLN
1	A	287	MET
1	A	289	ASN
1	A	291	MET
1	A	292	LEU
1	A	294	ASN
1	A	296	ILE
1	A	315	LEU
1	A	321	LYS
1	A	322	TYR
1	A	323	LEU
1	A	328	THR
1	A	333	THR
1	A	342	ILE
1	A	353	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	354	LEU
1	A	355	ASN
1	A	363	LEU
1	A	371	ILE
1	A	373	VAL
1	A	375	VAL
1	A	380	ASP
1	A	383	VAL
1	A	388	VAL
1	A	389	THR
1	A	394	THR
1	A	404	LEU
1	A	414	ASP
1	A	415	ASP
1	A	422	LEU
1	A	426	SER
1	A	431	LEU
1	A	433	PHE
1	A	435	VAL
1	A	436	LYS
1	A	442	LEU
1	A	455	ILE
1	A	457	TYR
1	A	458	SER
1	A	467	ILE
1	A	469	TRP
1	A	471	ASP
1	A	474	LYS
1	A	483	ASN
1	A	487	THR
1	A	492	TYR
1	A	493	ILE
1	A	494	ASP
1	A	495	LYS
1	A	497	THR
1	A	504	LEU
1	A	506	LYS
1	A	509	ILE
1	A	510	ILE
1	A	512	PHE
1	A	522	SER
1	A	526	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	532	GLN
1	A	534	MET
1	A	535	VAL
1	A	541	LEU
1	A	543	TYR
1	A	544	TYR
1	A	545	ILE
1	A	547	THR
1	A	549	GLU
1	A	550	GLN
1	A	559	VAL
1	A	561	LEU
1	A	563	ILE
1	A	565	GLU
1	A	569	ASN
1	A	570	GLN
1	A	583	SER
1	A	599	TRP
1	A	605	VAL
1	A	613	GLN
1	A	614	ARG
1	A	620	LEU
1	A	621	GLU
1	A	627	LEU
1	A	628	GLU
1	A	630	SER
1	A	632	LEU
1	A	640	LEU
1	A	644	ASN
1	A	648	LEU
1	A	652	THR
1	A	654	LEU
1	A	658	ASN
1	A	669	CYS
1	A	679	LEU
1	A	684	GLU
1	A	700	TYR
1	A	701	ASP
1	A	710	THR
1	A	711	CYS
1	A	713	GLN
1	A	720	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	732	CYS
1	A	754	MET
1	A	756	THR
1	A	766	ARG
1	A	774	LEU
1	A	777	VAL
1	A	779	LEU
1	A	782	ARG
1	A	786	LEU
1	A	787	GLN
1	A	788	PHE
1	A	793	SER
1	A	795	THR
1	A	800	GLN
1	A	805	SER
1	A	813	ASP
1	A	824	PHE
1	A	825	LEU
1	A	833	VAL
1	A	838	GLN
1	A	844	THR
1	A	845	VAL
1	A	848	TYR
1	A	849	ARG
1	A	850	THR
1	A	854	GLN
1	A	856	CYS
1	A	857	VAL
1	A	859	MET
1	A	865	ILE
1	A	871	PRO
1	A	876	GLN
1	A	887	LYS
1	A	895	LEU
1	A	899	THR
1	A	901	LEU
1	A	905	ILE
1	A	916	THR
1	A	917	TRP
1	A	928	ARG
1	A	935	LYS
1	A	936	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	942	VAL
1	A	944	LEU
1	A	945	ASP
1	A	952	THR
1	A	955	ARG
1	A	965	LEU
1	A	972	GLU
1	A	975	ARG
1	A	979	VAL
1	A	980	LYS
1	A	983	LEU
1	A	984	VAL
1	A	988	LEU
1	A	999	ILE
1	A	1001	THR
1	A	1002	HIS
1	A	1003	LEU
1	A	1007	SER
1	A	1011	GLU
1	A	1012	LEU
1	A	1013	MET
1	A	1015	VAL
1	A	1018	VAL
1	A	1021	VAL
1	A	1029	ASN
1	A	1033	ILE
1	A	1049	LEU
1	A	1054	LEU
1	A	1055	SER
1	A	1056	ILE
1	A	1061	ASN
1	A	1067	SER
1	A	1070	LYS
1	A	1079	THR
1	A	1098	ASN
1	A	1105	LEU
1	A	1110	ASN
1	A	1113	LEU
1	A	1123	GLN
1	A	1125	GLN
1	A	1127	ILE
1	A	1128	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1132	THR
1	A	1133	LEU
1	A	1140	ASN
1	A	1142	LEU
1	A	1144	LEU
1	A	1147	PHE
1	A	1150	ILE
1	A	1166	THR
1	A	1179	THR
1	A	1180	LEU
1	A	1184	SER
1	A	1190	ILE
1	A	1196	SER
1	A	1200	LYS
1	A	1201	THR
1	A	1202	HIS
1	A	1207	SER
1	A	1230	ASP
1	A	1232	LEU
1	A	1246	ARG
1	A	1264	ILE
1	A	1268	ASN
1	A	1275	SER
1	A	1280	TYR
1	A	1284	PHE
1	A	1286	SER
1	A	1301	SER
1	A	1302	LEU
1	A	1303	LEU
1	A	1307	LEU
1	A	1309	LEU
1	A	1313	ILE
1	A	1315	VAL
1	A	1323	LEU
1	A	1326	TYR
1	A	1329	THR
1	A	1331	LYS
1	A	1334	LEU
1	A	1336	ARG
1	A	1341	LEU
1	A	1342	LEU
1	A	1346	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1347	ILE
1	A	1348	VAL
1	A	1350	THR
1	A	1352	PHE
1	A	1356	LEU
1	A	1358	THR
1	A	1360	HIS
1	A	1363	THR
1	A	1366	HIS
1	A	1372	GLU
1	A	1376	SER
1	A	1401	ARG
1	A	1416	SER
1	A	1423	VAL
1	A	1430	THR
1	A	1446	VAL
1	A	1455	ILE
1	A	1459	HIS
1	A	1464	LEU
1	A	1470	SER
1	A	1475	VAL
1	A	1476	ARG
1	A	1479	ILE
1	A	1480	PHE
1	A	1483	PHE
1	A	1487	PHE
1	A	1492	THR
1	A	1493	PHE
1	A	1494	THR
1	A	1496	TYR
1	A	1500	ARG
1	A	1502	ASP
1	A	1503	LYS
1	A	1507	MET
1	A	1525	CYS
1	A	1532	CYS
1	A	1535	MET
1	A	1539	LEU
1	A	1542	THR
1	A	1548	ARG
1	A	1549	LYS
1	A	1556	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1557	ILE
1	A	1559	TYR
1	A	1566	THR
1	A	1569	THR
1	A	1573	VAL
1	A	1580	THR
1	A	1581	LEU
1	A	1583	ASP
1	A	1585	TYR
1	A	1589	GLU
1	A	1602	LYS
1	A	1604	VAL
1	A	1606	CYS
1	A	1618	LEU
1	A	1620	MET
1	A	1626	GLN
1	A	1629	TYR
1	A	1631	PHE
1	A	1632	SER
1	A	1634	ARG
1	A	1636	ILE
1	A	1637	TYR
1	A	1639	LEU
1	A	1654	CYS
1	A	1664	LEU
2	B	43	VAL
2	B	54	LEU
2	B	56	ILE
2	B	58	VAL
2	B	68	LEU
2	B	69	PHE
2	B	71	THR
2	B	74	ASP
2	B	82	LEU
2	B	86	THR
2	B	87	ILE
2	B	105	VAL
2	B	114	ARG
2	B	119	VAL
2	B	120	LEU
2	B	121	LEU
2	B	124	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	146	ARG
2	B	147	VAL
2	B	161	VAL
2	B	167	THR
2	B	177	SER
2	B	178	VAL
2	B	179	ASP
2	B	183	PHE
2	B	191	LEU
2	B	196	THR
2	B	198	ARG
2	B	199	ILE
2	B	206	SER
2	B	211	THR
2	B	214	PHE
2	B	219	TYR
2	B	220	VAL
2	B	221	LEU
2	B	226	VAL
2	B	243	PHE
2	B	264	LEU
2	B	274	LYS
2	B	278	ASP
2	B	280	LEU
2	B	291	LYS
2	B	296	ARG
2	B	297	ASP
2	B	299	PHE
2	B	306	LEU
2	B	317	SER
2	B	320	VAL
2	B	328	MET
2	B	338	ILE
2	B	341	SER
2	B	344	GLN
2	B	345	ILE
2	B	349	LYS
2	B	390	THR
2	B	398	LEU
2	B	400	LEU
2	B	404	LEU
2	B	411	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	422	ARG
2	B	435	TYR
2	B	437	THR
2	B	450	THR
2	B	458	ASP
2	B	460	LEU
2	B	469	ASN
2	B	472	SER
2	B	477	LYS
2	B	478	TYR
2	B	481	TYR
2	B	482	LEU
2	B	488	LYS
2	B	492	VAL
2	B	497	ARG
2	B	498	ARG
2	B	504	VAL
2	B	505	THR
2	B	506	MET
2	B	507	ASN
2	B	511	THR
2	B	513	ASP
2	B	518	PHE
2	B	519	ARG
2	B	520	PHE
2	B	521	VAL
2	B	523	TYR
2	B	524	TYR
2	B	525	GLN
2	B	526	VAL
2	B	528	ASN
2	B	531	ILE
2	B	543	THR
2	B	544	CYS
2	B	555	LEU
2	B	556	ILE
2	B	563	MET
2	B	567	LEU
2	B	574	ARG
2	B	582	LYS
2	B	584	VAL
2	B	588	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	593	ILE
2	B	594	SER
2	B	599	TRP
2	B	606	ASP
2	B	620	VAL
2	B	629	THR
2	B	634	LEU
2	B	638	GLN
2	B	643	LYS
2	B	740	ILE
2	B	742	ASP
2	B	743	SER
2	B	745	ILE
2	B	746	ILE
2	B	747	SER
2	B	769	GLN
2	B	778	PHE
2	B	780	LEU
2	B	783	SER
2	B	784	ILE
2	B	789	VAL
2	B	793	SER
2	B	800	ILE
2	B	802	VAL
2	B	804	GLU
2	B	808	ILE
2	B	812	LYS
2	B	813	VAL
2	B	816	ILE
2	B	817	ASP
2	B	819	GLN
2	B	829	GLN
2	B	830	VAL
2	B	836	LEU
2	B	851	LEU
2	B	857	CYS
2	B	867	ARG
2	B	870	PHE
2	B	872	ILE
2	B	873	LYS
2	B	875	LEU
2	B	880	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	884	ILE
2	B	889	GLN
2	B	891	LEU
2	B	893	ASP
2	B	913	LEU
2	B	914	LYS
2	B	916	VAL
2	B	918	GLU
2	B	920	VAL
2	B	926	THR
2	B	946	LYS
2	B	948	ARG
2	B	952	ASP
2	B	960	GLU
2	B	963	ILE
2	B	964	ILE
2	B	1278	THR
2	B	1279	ILE
2	B	1281	LEU
2	B	1283	ASP
2	B	1291	ARG
2	B	1292	ILE
2	B	1293	ASN
2	B	1298	LEU
2	B	1303	VAL
2	B	1305	THR
2	B	1308	ASN
2	B	1313	VAL
2	B	1324	THR
2	B	1326	LEU
2	B	1329	TYR
2	B	1330	ASN
2	B	1332	GLN
2	B	1344	HIS
2	B	1350	GLU
2	B	1351	ASN
2	B	1365	LEU
2	B	1372	LEU
2	B	1378	THR
2	B	1380	THR
2	B	1401	SER
2	B	1404	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	1406	ARG
2	B	1423	VAL
2	B	1424	ILE
2	B	1425	ILE
2	B	1427	LEU
2	B	1429	LYS
2	B	1433	SER
2	B	1437	CYS
2	B	1438	LEU
2	B	1442	ILE
2	B	1443	LEU
2	B	1445	HIS
2	B	1448	VAL
2	B	1459	TYR
2	B	1465	ASP
2	B	1475	ASP
2	B	1480	LEU
2	B	1481	LEU
2	B	1490	CYS
2	B	1491	ARG
2	B	1492	CYS
2	B	1495	GLU
2	B	1496	THR
2	B	1497	CYS
2	B	1500	LEU
2	B	1503	GLN
2	B	1504	GLU
2	B	1505	ARG
2	B	1516	CYS
2	B	1522	TYR
2	B	1526	THR
2	B	1529	LEU
2	B	1535	ASP
2	B	1539	ILE
2	B	1561	HIS
2	B	1566	GLN
2	B	1584	TRP
2	B	1591	LEU
2	B	1594	LYS
2	B	1597	ILE
2	B	1598	SER
2	B	1604	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	1605	THR
2	B	1606	TRP
2	B	1607	ILE
2	B	1612	HIS
2	B	1616	CYS
2	B	1617	GLN
2	B	1623	LYS
2	B	1631	PHE
1	C	20	GLU
1	C	21	GLN
1	C	22	THR
1	C	23	TYR
1	C	24	VAL
1	C	40	VAL
1	C	42	GLN
1	C	43	VAL
1	C	46	TYR
1	C	55	SER
1	C	58	SER
1	C	63	LYS
1	C	64	PHE
1	C	73	LEU
1	C	84	ILE
1	C	85	LEU
1	C	87	ILE
1	C	89	PRO
1	C	90	LYS
1	C	91	GLN
1	C	102	VAL
1	C	106	VAL
1	C	114	SER
1	C	125	PHE
1	C	126	LEU
1	C	128	ILE
1	C	131	ASP
1	C	134	VAL
1	C	136	THR
1	C	143	VAL
1	C	144	ARG
1	C	147	SER
1	C	149	ASN
1	C	152	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	157	ARG
1	C	161	LEU
1	C	162	THR
1	C	165	ASP
1	C	169	SER
1	C	170	GLU
1	C	176	GLU
1	C	182	ILE
1	C	183	ILE
1	C	184	SER
1	C	195	ARG
1	C	200	THR
1	C	209	PHE
1	C	211	THR
1	C	212	THR
1	C	214	THR
1	C	216	TYR
1	C	219	VAL
1	C	222	TYR
1	C	223	VAL
1	C	224	LEU
1	C	228	SER
1	C	230	SER
1	C	240	TYR
1	C	242	ASN
1	C	246	PHE
1	C	249	THR
1	C	251	LYS
1	C	255	PHE
1	C	261	THR
1	C	264	ASP
1	C	268	THR
1	C	276	LYS
1	C	279	GLN
1	C	287	MET
1	C	289	ASN
1	C	291	MET
1	C	292	LEU
1	C	294	ASN
1	C	296	ILE
1	C	315	LEU
1	C	321	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	322	TYR
1	C	323	LEU
1	C	328	THR
1	C	333	THR
1	C	342	ILE
1	C	353	LYS
1	C	354	LEU
1	C	355	ASN
1	C	363	LEU
1	C	371	ILE
1	C	373	VAL
1	C	375	VAL
1	C	383	VAL
1	C	388	VAL
1	C	389	THR
1	C	394	THR
1	C	404	LEU
1	C	414	ASP
1	C	415	ASP
1	C	422	LEU
1	C	426	SER
1	C	431	LEU
1	C	433	PHE
1	C	435	VAL
1	C	436	LYS
1	C	442	LEU
1	C	455	ILE
1	C	457	TYR
1	C	458	SER
1	C	459	SER
1	C	467	ILE
1	C	469	TRP
1	C	471	ASP
1	C	474	LYS
1	C	483	ASN
1	C	487	THR
1	C	492	TYR
1	C	493	ILE
1	C	494	ASP
1	C	495	LYS
1	C	497	THR
1	C	504	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	506	LYS
1	C	509	ILE
1	C	510	ILE
1	C	512	PHE
1	C	522	SER
1	C	526	ILE
1	C	532	GLN
1	C	534	MET
1	C	535	VAL
1	C	541	LEU
1	C	543	TYR
1	C	544	TYR
1	C	545	ILE
1	C	547	THR
1	C	553	GLU
1	C	559	VAL
1	C	561	LEU
1	C	563	ILE
1	C	565	GLU
1	C	569	ASN
1	C	570	GLN
1	C	573	VAL
1	C	583	SER
1	C	599	TRP
1	C	605	VAL
1	C	613	GLN
1	C	614	ARG
1	C	620	LEU
1	C	621	GLU
1	C	627	LEU
1	C	628	GLU
1	C	632	LEU
1	C	640	LEU
1	C	644	ASN
1	C	648	LEU
1	C	652	THR
1	C	654	LEU
1	C	658	ASN
1	C	669	CYS
1	C	679	LEU
1	C	684	GLU
1	C	700	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	701	ASP
1	C	710	THR
1	C	713	GLN
1	C	720	LEU
1	C	754	MET
1	C	756	THR
1	C	766	ARG
1	C	774	LEU
1	C	777	VAL
1	C	779	LEU
1	C	782	ARG
1	C	786	LEU
1	C	787	GLN
1	C	788	PHE
1	C	795	THR
1	C	800	GLN
1	C	805	SER
1	C	813	ASP
1	C	824	PHE
1	C	825	LEU
1	C	833	VAL
1	C	838	GLN
1	C	845	VAL
1	C	849	ARG
1	C	850	THR
1	C	854	GLN
1	C	856	CYS
1	C	857	VAL
1	C	859	MET
1	C	865	ILE
1	C	876	GLN
1	C	887	LYS
1	C	895	LEU
1	C	899	THR
1	C	901	LEU
1	C	905	ILE
1	C	916	THR
1	C	917	TRP
1	C	928	ARG
1	C	935	LYS
1	C	936	ARG
1	C	942	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	944	LEU
1	C	945	ASP
1	C	952	THR
1	C	955	ARG
1	C	965	LEU
1	C	972	GLU
1	C	975	ARG
1	C	977	LEU
1	C	979	VAL
1	C	980	LYS
1	C	983	LEU
1	C	984	VAL
1	C	988	LEU
1	C	1001	THR
1	C	1002	HIS
1	C	1007	SER
1	C	1011	GLU
1	C	1012	LEU
1	C	1013	MET
1	C	1015	VAL
1	C	1018	VAL
1	C	1021	VAL
1	C	1029	ASN
1	C	1033	ILE
1	C	1049	LEU
1	C	1054	LEU
1	C	1055	SER
1	C	1056	ILE
1	C	1061	ASN
1	C	1067	SER
1	C	1070	LYS
1	C	1079	THR
1	C	1098	ASN
1	C	1105	LEU
1	C	1113	LEU
1	C	1125	GLN
1	C	1127	ILE
1	C	1128	LYS
1	C	1132	THR
1	C	1133	LEU
1	C	1140	ASN
1	C	1142	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	1144	LEU
1	C	1150	ILE
1	C	1159	CYS
1	C	1166	THR
1	C	1179	THR
1	C	1180	LEU
1	C	1184	SER
1	C	1190	ILE
1	C	1196	SER
1	C	1200	LYS
1	C	1201	THR
1	C	1202	HIS
1	C	1207	SER
1	C	1230	ASP
1	C	1232	LEU
1	C	1246	ARG
1	C	1264	ILE
1	C	1275	SER
1	C	1280	TYR
1	C	1284	PHE
1	C	1286	SER
1	C	1301	SER
1	C	1302	LEU
1	C	1307	LEU
1	C	1309	LEU
1	C	1313	ILE
1	C	1315	VAL
1	C	1323	LEU
1	C	1326	TYR
1	C	1329	THR
1	C	1331	LYS
1	C	1334	LEU
1	C	1336	ARG
1	C	1338	VAL
1	C	1341	LEU
1	C	1342	LEU
1	C	1346	LEU
1	C	1347	ILE
1	C	1348	VAL
1	C	1350	THR
1	C	1352	PHE
1	C	1356	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	1358	THR
1	C	1360	HIS
1	C	1363	THR
1	C	1366	HIS
1	C	1372	GLU
1	C	1376	SER
1	C	1401	ARG
1	C	1416	SER
1	C	1423	VAL
1	C	1430	THR
1	C	1446	VAL
1	C	1455	ILE
1	C	1459	HIS
1	C	1464	LEU
1	C	1470	SER
1	C	1475	VAL
1	C	1476	ARG
1	C	1479	ILE
1	C	1480	PHE
1	C	1483	PHE
1	C	1487	PHE
1	C	1492	THR
1	C	1493	PHE
1	C	1494	THR
1	C	1496	TYR
1	C	1500	ARG
1	C	1502	ASP
1	C	1503	LYS
1	C	1507	MET
1	C	1525	CYS
1	C	1531	ASP
1	C	1532	CYS
1	C	1535	MET
1	C	1539	LEU
1	C	1548	ARG
1	C	1549	LYS
1	C	1556	GLU
1	C	1557	ILE
1	C	1559	TYR
1	C	1566	THR
1	C	1569	THR
1	C	1573	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	1580	THR
1	C	1581	LEU
1	C	1583	ASP
1	C	1585	TYR
1	C	1589	GLU
1	C	1602	LYS
1	C	1604	VAL
1	C	1606	CYS
1	C	1618	LEU
1	C	1620	MET
1	C	1626	GLN
1	C	1627	ILE
1	C	1631	PHE
1	C	1635	TYR
1	C	1636	ILE
1	C	1637	TYR
1	C	1639	LEU
1	C	1654	CYS
1	C	1664	LEU
2	D	40	GLN
2	D	43	VAL
2	D	54	LEU
2	D	56	ILE
2	D	58	VAL
2	D	68	LEU
2	D	69	PHE
2	D	71	THR
2	D	74	ASP
2	D	82	LEU
2	D	86	THR
2	D	87	ILE
2	D	105	VAL
2	D	114	ARG
2	D	119	VAL
2	D	120	LEU
2	D	121	LEU
2	D	124	GLN
2	D	146	ARG
2	D	147	VAL
2	D	150	MET
2	D	161	VAL
2	D	167	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	177	SER
2	D	178	VAL
2	D	179	ASP
2	D	183	PHE
2	D	191	LEU
2	D	196	THR
2	D	198	ARG
2	D	199	ILE
2	D	206	SER
2	D	209	ASN
2	D	211	THR
2	D	219	TYR
2	D	220	VAL
2	D	221	LEU
2	D	226	VAL
2	D	243	PHE
2	D	264	LEU
2	D	274	LYS
2	D	278	ASP
2	D	280	LEU
2	D	291	LYS
2	D	297	ASP
2	D	299	PHE
2	D	306	LEU
2	D	317	SER
2	D	320	VAL
2	D	328	MET
2	D	338	ILE
2	D	341	SER
2	D	344	GLN
2	D	345	ILE
2	D	349	LYS
2	D	390	THR
2	D	398	LEU
2	D	400	LEU
2	D	404	LEU
2	D	411	ILE
2	D	422	ARG
2	D	435	TYR
2	D	437	THR
2	D	450	THR
2	D	458	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	460	LEU
2	D	469	ASN
2	D	472	SER
2	D	477	LYS
2	D	478	TYR
2	D	481	TYR
2	D	482	LEU
2	D	488	LYS
2	D	492	VAL
2	D	497	ARG
2	D	498	ARG
2	D	504	VAL
2	D	505	THR
2	D	506	MET
2	D	507	ASN
2	D	511	THR
2	D	513	ASP
2	D	518	PHE
2	D	519	ARG
2	D	520	PHE
2	D	521	VAL
2	D	523	TYR
2	D	524	TYR
2	D	525	GLN
2	D	526	VAL
2	D	528	ASN
2	D	531	ILE
2	D	543	THR
2	D	544	CYS
2	D	555	LEU
2	D	556	ILE
2	D	563	MET
2	D	567	LEU
2	D	574	ARG
2	D	582	LYS
2	D	584	VAL
2	D	588	ASN
2	D	593	ILE
2	D	594	SER
2	D	606	ASP
2	D	620	VAL
2	D	629	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	634	LEU
2	D	638	GLN
2	D	643	LYS
2	D	740	ILE
2	D	742	ASP
2	D	743	SER
2	D	745	ILE
2	D	746	ILE
2	D	747	SER
2	D	769	GLN
2	D	778	PHE
2	D	780	LEU
2	D	783	SER
2	D	784	ILE
2	D	789	VAL
2	D	793	SER
2	D	800	ILE
2	D	802	VAL
2	D	804	GLU
2	D	808	ILE
2	D	812	LYS
2	D	813	VAL
2	D	816	ILE
2	D	817	ASP
2	D	819	GLN
2	D	829	GLN
2	D	830	VAL
2	D	836	LEU
2	D	851	LEU
2	D	857	CYS
2	D	867	ARG
2	D	870	PHE
2	D	872	ILE
2	D	873	LYS
2	D	875	LEU
2	D	880	VAL
2	D	884	ILE
2	D	889	GLN
2	D	891	LEU
2	D	913	LEU
2	D	914	LYS
2	D	916	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	918	GLU
2	D	920	VAL
2	D	926	THR
2	D	946	LYS
2	D	948	ARG
2	D	952	ASP
2	D	960	GLU
2	D	963	ILE
2	D	964	ILE
2	D	1278	THR
2	D	1279	ILE
2	D	1281	LEU
2	D	1283	ASP
2	D	1291	ARG
2	D	1292	ILE
2	D	1293	ASN
2	D	1298	LEU
2	D	1303	VAL
2	D	1305	THR
2	D	1308	ASN
2	D	1313	VAL
2	D	1324	THR
2	D	1326	LEU
2	D	1329	TYR
2	D	1330	ASN
2	D	1332	GLN
2	D	1344	HIS
2	D	1350	GLU
2	D	1351	ASN
2	D	1365	LEU
2	D	1367	ILE
2	D	1372	LEU
2	D	1378	THR
2	D	1401	SER
2	D	1404	VAL
2	D	1406	ARG
2	D	1423	VAL
2	D	1424	ILE
2	D	1425	ILE
2	D	1427	LEU
2	D	1429	LYS
2	D	1433	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	1437	CYS
2	D	1438	LEU
2	D	1442	ILE
2	D	1443	LEU
2	D	1445	HIS
2	D	1448	VAL
2	D	1459	TYR
2	D	1465	ASP
2	D	1475	ASP
2	D	1480	LEU
2	D	1481	LEU
2	D	1490	CYS
2	D	1491	ARG
2	D	1492	CYS
2	D	1495	GLU
2	D	1496	THR
2	D	1497	CYS
2	D	1504	GLU
2	D	1522	TYR
2	D	1526	THR
2	D	1529	LEU
2	D	1535	ASP
2	D	1539	ILE
2	D	1561	HIS
2	D	1566	GLN
2	D	1584	TRP
2	D	1591	LEU
2	D	1594	LYS
2	D	1597	ILE
2	D	1598	SER
2	D	1604	ASN
2	D	1605	THR
2	D	1607	ILE
2	D	1612	HIS
2	D	1616	CYS
2	D	1632	SER
2	D	1634	THR
2	D	1638	PHE
3	X	41	HIS
3	X	43	ILE
3	X	46	LEU
3	X	50	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	X	51	SER
3	X	65	GLU
3	X	66	ASN
3	X	67	TYR
3	X	75	PHE
3	X	78	LYS
3	X	80	GLN
3	X	85	PHE
3	X	94	TYR
3	X	105	VAL
3	X	111	ASP
3	X	113	ASN
3	X	117	SER
3	X	119	VAL
3	X	123	THR
3	X	130	SER
3	X	132	THR
3	X	136	LEU
3	X	146	LEU
3	X	175	ASN
3	X	185	LYS
3	X	190	ILE
3	X	191	ILE
3	X	196	GLU
3	X	209	PHE
3	X	210	GLU
3	X	225	SER
3	X	229	ASN
3	Y	41	HIS
3	Y	43	ILE
3	Y	46	LEU
3	Y	50	TYR
3	Y	51	SER
3	Y	63	LYS
3	Y	65	GLU
3	Y	66	ASN
3	Y	67	TYR
3	Y	75	PHE
3	Y	78	LYS
3	Y	80	GLN
3	Y	85	PHE
3	Y	94	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	Y	105	VAL
3	Y	111	ASP
3	Y	113	ASN
3	Y	115	ARG
3	Y	117	SER
3	Y	119	VAL
3	Y	123	THR
3	Y	132	THR
3	Y	136	LEU
3	Y	146	LEU
3	Y	175	ASN
3	Y	185	LYS
3	Y	190	ILE
3	Y	191	ILE
3	Y	196	GLU
3	Y	209	PHE
3	Y	210	GLU
3	Y	225	SER
3	Y	229	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	42	GLN
1	A	77	ASN
1	A	80	GLN
1	A	97	ASN
1	A	139	GLN
1	A	149	ASN
1	A	236	ASN
1	A	242	ASN
1	A	257	ASN
1	A	289	ASN
1	A	294	ASN
1	A	355	ASN
1	A	391	ASN
1	A	473	HIS
1	A	481	HIS
1	A	569	ASN
1	A	706	ASN
1	A	785	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	787	GLN
1	A	800	GLN
1	A	838	GLN
1	A	854	GLN
1	A	875	HIS
1	A	876	GLN
1	A	909	ASN
1	A	1023	HIS
1	A	1029	ASN
1	A	1030	HIS
1	A	1095	GLN
1	A	1102	ASN
1	A	1112	GLN
1	A	1123	GLN
1	A	1202	HIS
1	A	1233	GLN
1	A	1241	ASN
1	A	1260	ASN
1	A	1268	ASN
1	A	1306	GLN
1	A	1360	HIS
1	A	1448	GLN
1	A	1550	GLN
1	A	1608	ASN
1	A	1658	GLN
1	A	1663	ASN
2	B	40	GLN
2	B	65	GLN
2	B	124	GLN
2	B	152	HIS
2	B	176	ASN
2	B	187	ASN
2	B	333	GLN
2	B	344	GLN
2	B	417	HIS
2	B	459	ASN
2	B	469	ASN
2	B	507	ASN
2	B	525	GLN
2	B	615	GLN
2	B	819	GLN
2	B	829	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	869	GLN
2	B	889	GLN
2	B	901	GLN
2	B	921	GLN
2	B	1330	ASN
2	B	1341	ASN
2	B	1473	HIS
2	B	1501	ASN
2	B	1503	GLN
2	B	1562	GLN
1	C	38	ASN
1	C	42	GLN
1	C	77	ASN
1	C	80	GLN
1	C	97	ASN
1	C	110	HIS
1	C	149	ASN
1	C	236	ASN
1	C	242	ASN
1	C	257	ASN
1	C	289	ASN
1	C	294	ASN
1	C	355	ASN
1	C	391	ASN
1	C	473	HIS
1	C	481	HIS
1	C	511	HIS
1	C	550	GLN
1	C	569	ASN
1	C	658	ASN
1	C	706	ASN
1	C	785	GLN
1	C	787	GLN
1	C	800	GLN
1	C	838	GLN
1	C	854	GLN
1	C	875	HIS
1	C	876	GLN
1	C	909	ASN
1	C	1023	HIS
1	C	1029	ASN
1	C	1030	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	1095	GLN
1	C	1102	ASN
1	C	1112	GLN
1	C	1123	GLN
1	C	1202	HIS
1	C	1233	GLN
1	C	1241	ASN
1	C	1260	ASN
1	C	1268	ASN
1	C	1306	GLN
1	C	1360	HIS
1	C	1448	GLN
1	C	1550	GLN
1	C	1608	ASN
1	C	1658	GLN
2	D	40	GLN
2	D	65	GLN
2	D	124	GLN
2	D	152	HIS
2	D	176	ASN
2	D	187	ASN
2	D	333	GLN
2	D	344	GLN
2	D	417	HIS
2	D	459	ASN
2	D	465	ASN
2	D	469	ASN
2	D	507	ASN
2	D	525	GLN
2	D	615	GLN
2	D	819	GLN
2	D	829	GLN
2	D	869	GLN
2	D	889	GLN
2	D	921	GLN
2	D	1308	ASN
2	D	1330	ASN
2	D	1341	ASN
2	D	1473	HIS
2	D	1503	GLN
2	D	1511	GLN
2	D	1562	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	X	47	HIS
3	X	59	ASN
3	X	80	GLN
3	X	83	GLN
3	X	113	ASN
3	X	139	ASN
3	X	142	ASN
3	X	197	ASN
3	Y	47	HIS
3	Y	59	ASN
3	Y	71	ASN
3	Y	80	GLN
3	Y	83	GLN
3	Y	113	ASN
3	Y	139	ASN
3	Y	142	ASN
3	Y	197	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 ⓘ

8 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	B	2001	2,5	14,14,15	0.99	1 (7%)	15,19,21	2.11	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	B	2002	5	14,14,15	1.02	1 (7%)	15,19,21	2.45	4 (26%)
5	NAG	B	2003	2,5	14,14,15	2.07	7 (50%)	15,19,21	3.37	7 (46%)
5	NAG	B	2004	5	14,14,15	1.70	1 (7%)	15,19,21	2.11	5 (33%)
5	NAG	D	2001	2,5	14,14,15	0.90	1 (7%)	15,19,21	2.09	6 (40%)
5	NAG	D	2002	5	14,14,15	1.08	1 (7%)	15,19,21	1.76	4 (26%)
5	NAG	D	2003	2,5	14,14,15	2.00	6 (42%)	15,19,21	3.55	7 (46%)
5	NAG	D	2004	5	14,14,15	1.59	1 (7%)	15,19,21	2.25	5 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	2001	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2002	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2003	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2004	5	-	0/6/23/26	0/1/1/1
5	NAG	D	2001	2,5	-	0/6/23/26	0/1/1/1
5	NAG	D	2002	5	-	0/6/23/26	0/1/1/1
5	NAG	D	2003	2,5	-	0/6/23/26	0/1/1/1
5	NAG	D	2004	5	-	0/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2003	NAG	C3-C2	2.11	1.57	1.52
5	B	2003	NAG	C2-N2	2.12	1.50	1.46
5	B	2002	NAG	C3-C2	2.22	1.57	1.52
5	D	2003	NAG	C3-C2	2.35	1.57	1.52
5	D	2003	NAG	C4-C5	2.44	1.58	1.53
5	D	2001	NAG	C1-C2	2.49	1.55	1.52
5	D	2002	NAG	C1-C2	2.51	1.55	1.52
5	B	2003	NAG	O4-C4	2.55	1.48	1.43
5	D	2003	NAG	O5-C1	2.61	1.48	1.43
5	B	2003	NAG	C4-C5	2.72	1.58	1.53
5	D	2003	NAG	O4-C4	2.74	1.49	1.43
5	B	2003	NAG	C4-C3	2.78	1.59	1.52
5	D	2003	NAG	C4-C3	2.98	1.59	1.52
5	B	2001	NAG	C1-C2	3.00	1.56	1.52
5	B	2003	NAG	O5-C1	3.06	1.48	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	2003	NAG	C1-C2	3.58	1.57	1.52
5	B	2003	NAG	C1-C2	4.09	1.58	1.52
5	D	2004	NAG	C1-C2	5.30	1.59	1.52
5	B	2004	NAG	C1-C2	5.47	1.60	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2004	NAG	O5-C1-C2	-3.35	106.82	111.47
5	D	2004	NAG	O5-C1-C2	-3.23	106.97	111.47
5	D	2001	NAG	O3-C3-C2	-2.70	103.61	109.39
5	D	2004	NAG	O7-C7-C8	-2.50	117.50	122.06
5	B	2004	NAG	O7-C7-C8	-2.28	117.91	122.06
5	D	2003	NAG	O3-C3-C2	-2.26	104.54	109.39
5	D	2001	NAG	C3-C4-C5	-2.17	106.39	110.22
5	D	2001	NAG	C4-C3-C2	-2.11	107.92	111.02
5	B	2001	NAG	O3-C3-C2	-2.02	105.05	109.39
5	B	2003	NAG	C8-C7-N2	-2.00	112.50	116.11
5	D	2002	NAG	O7-C7-N2	2.05	125.87	121.92
5	D	2003	NAG	O3-C3-C4	2.15	115.04	110.36
5	D	2003	NAG	O5-C1-C2	2.34	114.73	111.47
5	B	2003	NAG	O3-C3-C4	2.38	115.53	110.36
5	D	2002	NAG	C1-O5-C5	2.44	115.53	112.17
5	D	2004	NAG	O3-C3-C2	2.45	114.63	109.39
5	B	2001	NAG	O3-C3-C4	2.56	115.92	110.36
5	B	2002	NAG	O4-C4-C3	2.64	116.10	110.36
5	B	2002	NAG	C2-N2-C7	2.79	127.01	122.94
5	B	2004	NAG	C2-N2-C7	2.82	127.06	122.94
5	B	2004	NAG	O3-C3-C2	2.83	115.45	109.39
5	B	2003	NAG	O7-C7-N2	2.84	127.38	121.92
5	D	2002	NAG	C2-N2-C7	3.14	127.52	122.94
5	D	2001	NAG	C1-C2-N2	3.22	115.99	110.49
5	B	2001	NAG	C1-C2-N2	3.26	116.05	110.49
5	B	2003	NAG	O5-C1-C2	3.30	116.07	111.47
5	D	2003	NAG	O4-C4-C3	3.40	117.75	110.36
5	D	2001	NAG	C1-O5-C5	3.55	117.06	112.17
5	B	2001	NAG	C1-O5-C5	3.62	117.16	112.17
5	D	2004	NAG	C2-N2-C7	3.74	128.40	122.94
5	D	2001	NAG	O5-C1-C2	3.83	116.81	111.47
5	D	2002	NAG	C4-C3-C2	3.93	116.77	111.02
5	B	2002	NAG	C1-O5-C5	4.09	117.81	112.17
5	B	2003	NAG	C4-C3-C2	4.16	117.11	111.02

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2001	NAG	O5-C1-C2	4.39	117.58	111.47
5	B	2003	NAG	C2-N2-C7	5.23	130.58	122.94
5	D	2003	NAG	C2-N2-C7	5.24	130.58	122.94
5	D	2003	NAG	C4-C3-C2	5.29	118.77	111.02
5	B	2004	NAG	C1-C2-N2	5.45	119.79	110.49
5	D	2004	NAG	C1-C2-N2	5.47	119.84	110.49
5	B	2002	NAG	C4-C3-C2	6.58	120.66	111.02
5	B	2003	NAG	C1-O5-C5	9.15	124.78	112.17
5	D	2003	NAG	C1-O5-C5	9.93	125.86	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2001	NAG	3	0
5	B	2002	NAG	3	0
5	B	2003	NAG	3	0
5	D	2001	NAG	4	0
5	D	2002	NAG	4	0
5	D	2003	NAG	3	0

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	2003	1	14,14,15	1.86	5 (35%)	15,19,21	3.49	12 (80%)
4	NAG	C	2003	1	14,14,15	2.06	4 (28%)	15,19,21	2.60	9 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	2003	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2003	1	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2003	NAG	O5-C5	2.05	1.47	1.43
4	A	2003	NAG	C4-C5	2.16	1.57	1.53
4	A	2003	NAG	C4-C3	2.22	1.58	1.52
4	C	2003	NAG	O4-C4	2.22	1.48	1.43
4	A	2003	NAG	O4-C4	2.49	1.48	1.43
4	C	2003	NAG	C4-C5	3.07	1.59	1.53
4	C	2003	NAG	C3-C2	3.87	1.60	1.52
4	A	2003	NAG	C3-C2	4.25	1.61	1.52
4	C	2003	NAG	C1-C2	4.72	1.59	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2003	NAG	O7-C7-C8	-5.21	112.57	122.06
4	C	2003	NAG	O7-C7-C8	-3.61	115.49	122.06
4	A	2003	NAG	C3-C4-C5	-3.54	103.97	110.22
4	A	2003	NAG	O3-C3-C4	-3.36	103.06	110.36
4	C	2003	NAG	C1-C2-N2	-2.77	105.75	110.49
4	A	2003	NAG	C1-C2-N2	-2.71	105.86	110.49
4	A	2003	NAG	O7-C7-N2	2.01	125.79	121.92
4	C	2003	NAG	O7-C7-N2	2.27	126.30	121.92
4	C	2003	NAG	C4-C3-C2	2.30	114.38	111.02
4	C	2003	NAG	O4-C4-C3	2.73	116.30	110.36
4	C	2003	NAG	C1-O5-C5	3.02	116.33	112.17
4	A	2003	NAG	O3-C3-C2	3.04	115.91	109.39
4	A	2003	NAG	C8-C7-N2	3.06	121.64	116.11
4	C	2003	NAG	C2-N2-C7	3.06	127.41	122.94
4	A	2003	NAG	O4-C4-C5	3.31	117.64	109.28
4	C	2003	NAG	O4-C4-C5	3.42	117.91	109.28
4	A	2003	NAG	C1-O5-C5	3.92	117.58	112.17
4	C	2003	NAG	O3-C3-C2	4.26	118.53	109.39
4	A	2003	NAG	O4-C4-C3	4.48	120.10	110.36
4	A	2003	NAG	C4-C3-C2	4.83	118.10	111.02
4	A	2003	NAG	C2-N2-C7	5.13	130.43	122.94



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2003	NAG	1	0
4	C	2003	NAG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	1626/1676 (97%)	-0.04	19 (1%)	79 72	72, 150, 260, 469	0
1	C	1626/1676 (97%)	0.03	43 (2%)	56 47	60, 153, 277, 515	0
2	B	1215/1642 (73%)	0.02	22 (1%)	69 61	73, 160, 235, 335	0
2	D	1215/1642 (73%)	-0.03	16 (1%)	77 69	85, 155, 241, 362	0
3	X	191/231 (82%)	0.68	26 (13%)	3 5	99, 230, 333, 437	0
3	Y	191/231 (82%)	0.41	14 (7%)	16 13	95, 195, 300, 385	0
All	All	6064/7098 (85%)	0.03	140 (2%)	61 53	60, 157, 264, 515	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	X	112	PRO	11.7
3	Y	114	GLY	6.7
1	C	1651	ASP	5.6
3	X	113	ASN	5.6
3	X	114	GLY	5.5
3	Y	113	ASN	5.3
1	C	1592	ALA	5.0
1	C	1585	TYR	4.6
2	D	1272	ASP	4.4
3	X	70	SER	4.2
3	Y	115	ARG	4.1
3	X	95	LYS	4.1
3	Y	59	ASN	3.9
2	D	100	GLN	3.9
2	D	98	SER	3.8
3	Y	71	ASN	3.4
3	Y	92	GLU	3.4
2	D	1318	ASP	3.4
1	A	874	ASP	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	1319	GLY	3.4
2	D	97	ASP	3.3
1	A	1002	HIS	3.3
1	C	1622	LYS	3.3
1	C	1537	GLU	3.2
1	A	94	GLY	3.2
1	C	1586	LYS	3.2
1	C	1593	GLU	3.1
2	B	1272	ASP	3.1
1	C	1525	CYS	3.1
1	C	1002	HIS	3.1
1	C	882	LYS	3.1
1	C	273	GLU	3.1
2	D	1273	LEU	3.0
3	Y	195	ASP	3.0
3	X	90	ASP	3.0
1	C	1538	GLU	3.0
2	B	1320	LYS	3.0
1	C	874	ASP	3.0
3	X	108	GLU	3.0
3	Y	95	LYS	3.0
1	A	879	LYS	2.9
1	C	278	ASP	2.9
1	C	712	GLU	2.8
2	B	639	ARG	2.8
3	X	104	PHE	2.8
2	B	1435	ASP	2.8
1	A	1545	ALA	2.7
2	D	940	THR	2.7
3	X	76	ASN	2.7
2	B	1273	LEU	2.7
3	X	93	GLN	2.7
1	C	1609	ALA	2.6
3	X	71	ASN	2.6
2	D	99	ARG	2.6
1	C	1596	SER	2.6
3	X	127	ASN	2.6
1	A	1398	ASP	2.6
3	X	111	ASP	2.6
1	C	93	PRO	2.6
1	C	1557	ILE	2.6
1	C	1597	GLU	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	X	126	ASN	2.6
1	C	159	THR	2.6
1	A	817	ALA	2.5
1	A	1622	LYS	2.5
1	C	1594	LYS	2.5
2	D	941	GLN	2.5
2	B	1344	HIS	2.5
3	X	128	LYS	2.5
3	Y	159	GLU	2.4
1	A	1399	TYR	2.4
1	C	94	GLY	2.4
1	C	1598	ILE	2.4
2	B	1370	ARG	2.4
2	D	765	GLU	2.4
1	C	1544	SER	2.4
3	X	74	ARG	2.4
3	X	79	ASP	2.4
2	B	1376	ASP	2.4
3	X	92	GLU	2.4
1	C	403	ASP	2.3
2	D	1354	LEU	2.3
3	X	120	GLY	2.3
1	C	446	ASN	2.3
2	B	1434	GLU	2.3
1	A	1526	LYS	2.3
1	C	255	PHE	2.3
3	X	101	GLN	2.3
1	A	273	GLU	2.3
1	C	1241	ASN	2.3
3	X	195	ASP	2.3
2	B	640	SER	2.3
2	B	1374	GLU	2.3
3	Y	196	GLU	2.3
2	B	1371	TYR	2.3
1	A	691	LYS	2.3
2	D	66	LYS	2.3
3	Y	90	ASP	2.2
3	Y	89	LYS	2.2
1	A	240	TYR	2.2
2	B	99	ARG	2.2
2	B	1375	VAL	2.2
3	X	159	GLU	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	1233	GLN	2.2
2	B	369	PRO	2.2
1	C	817	ALA	2.2
2	B	344	GLN	2.2
1	A	692	HIS	2.2
1	C	879	LYS	2.1
1	C	95	GLY	2.1
2	B	61	PHE	2.1
1	A	271	ILE	2.1
1	C	1595	ASP	2.1
2	D	967	GLY	2.1
1	C	314	SER	2.1
2	D	951	ASP	2.1
2	D	337	HIS	2.1
1	C	393	GLN	2.1
2	B	1537	ASN	2.1
3	Y	64	VAL	2.1
3	X	73	VAL	2.1
1	C	240	TYR	2.1
1	A	1380	LYS	2.1
1	C	313	TYR	2.1
1	A	1651	ASP	2.1
2	B	23	ALA	2.1
1	C	274	ASP	2.0
3	Y	72	VAL	2.0
1	A	1546	GLU	2.0
2	B	52	LYS	2.0
2	D	764	GLU	2.0
1	C	1548	ARG	2.0
1	C	312	TYR	2.0
3	X	99	GLN	2.0
3	X	41	HIS	2.0
3	X	82	HIS	2.0
1	A	311	SER	2.0
1	C	1650	ARG	2.0
1	C	1545	ALA	2.0
2	B	1271	LYS	2.0

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

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

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	B	2002	14/15	0.72	0.69	-	228,239,253,257	0
5	NAG	D	2001	14/15	0.88	0.41	-	228,253,282,288	0
5	NAG	D	2002	14/15	0.66	0.60	-	228,239,251,252	0
5	NAG	B	2001	14/15	0.74	0.55	-	278,305,319,322	0
5	NAG	D	2004	14/15	0.72	0.84	-	271,274,277,278	0
5	NAG	D	2003	14/15	0.54	0.53	-	246,253,258,265	0
5	NAG	B	2003	14/15	0.24	0.77	-	225,233,240,245	0
5	NAG	B	2004	14/15	0.56	0.77	-	297,301,307,310	0

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	C	2003	14/15	0.74	0.39	0.84	177,180,183,183	0
4	NAG	A	2003	14/15	0.78	0.29	0.34	166,169,171,172	0

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

There are no such residues in this entry.