



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 01:17 pm GMT

PDB ID : 3KM9  
Title : Structure of complement C5 in complex with the C-terminal beta-grasp domain of SSL7  
Authors : Laursen, N.S.; Gordon, N.; Hermans, S.; Lorenz, N.; Jackson, N.; Wines, B.; Spillner, E.; Christensen, J.B.; Jensen, M.; Fredslund, F.; Bjerre, M.; Sottrup-Jensen, L.; Fraser, J.D.; Andersen, G.R.  
Deposited on : 2009-11-10  
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

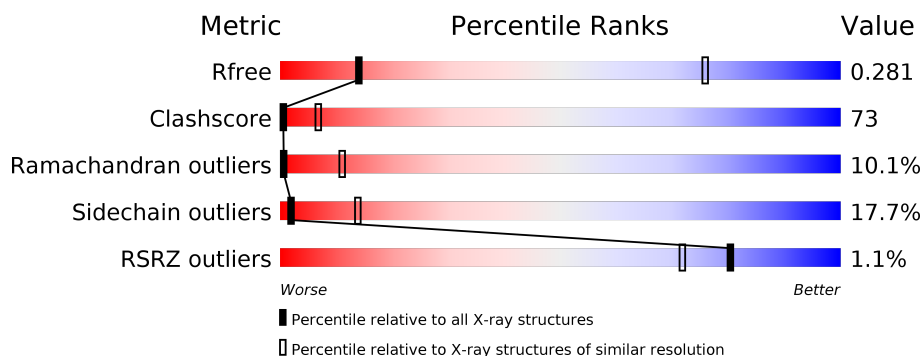
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	1014 (4.70-3.70)
Clashscore	122126	1082 (4.70-3.70)
Ramachandran outliers	120053	1035 (4.70-3.70)
Sidechain outliers	120020	1021 (4.70-3.70)
RSRZ outliers	108989	1179 (4.80-3.60)

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>18%</div> <div>50%</div> <div>18%</div> <div>13%</div> </div>
1	B	1676	<div> <div>18%</div> <div>49%</div> <div>18%</div> <div>13%</div> </div>
2	X	103	<div> <div>9%</div> <div>37%</div> <div>52%</div> <div>10%</div> </div>
2	Y	103	<div> <div>5%</div> <div>38%</div> <div>52%</div> <div>9%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	2002	-	-	-	X
4	NAG	B	2002	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 24809 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	1459	Total	C	N	O	S	0	0	0
			11541	7396	1903	2200	42			
1	B	1459	Total	C	N	O	S	0	0	0
			11541	7396	1903	2200	42			

- Molecule 2 is a protein called Staphylococcal enterotoxin-like toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	102	Total	C	N	O	S	0	0	0
			819	517	138	163	1			
2	Y	102	Total	C	N	O	S	0	0	0
			819	517	138	163	1			

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cd	0	0
			2	2		
3	A	3	Total	Cd	0	0
			3	3		

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

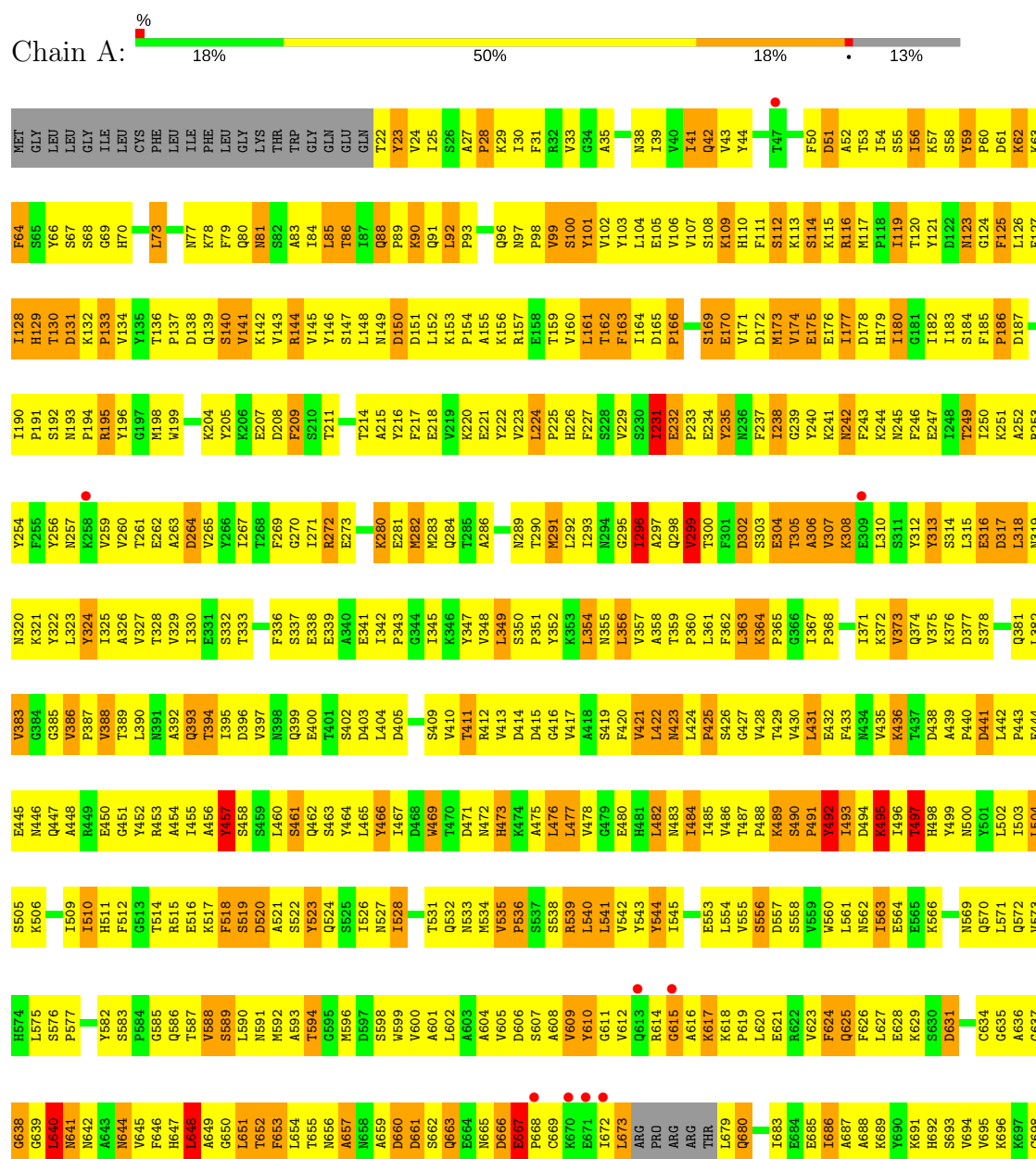


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

### 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

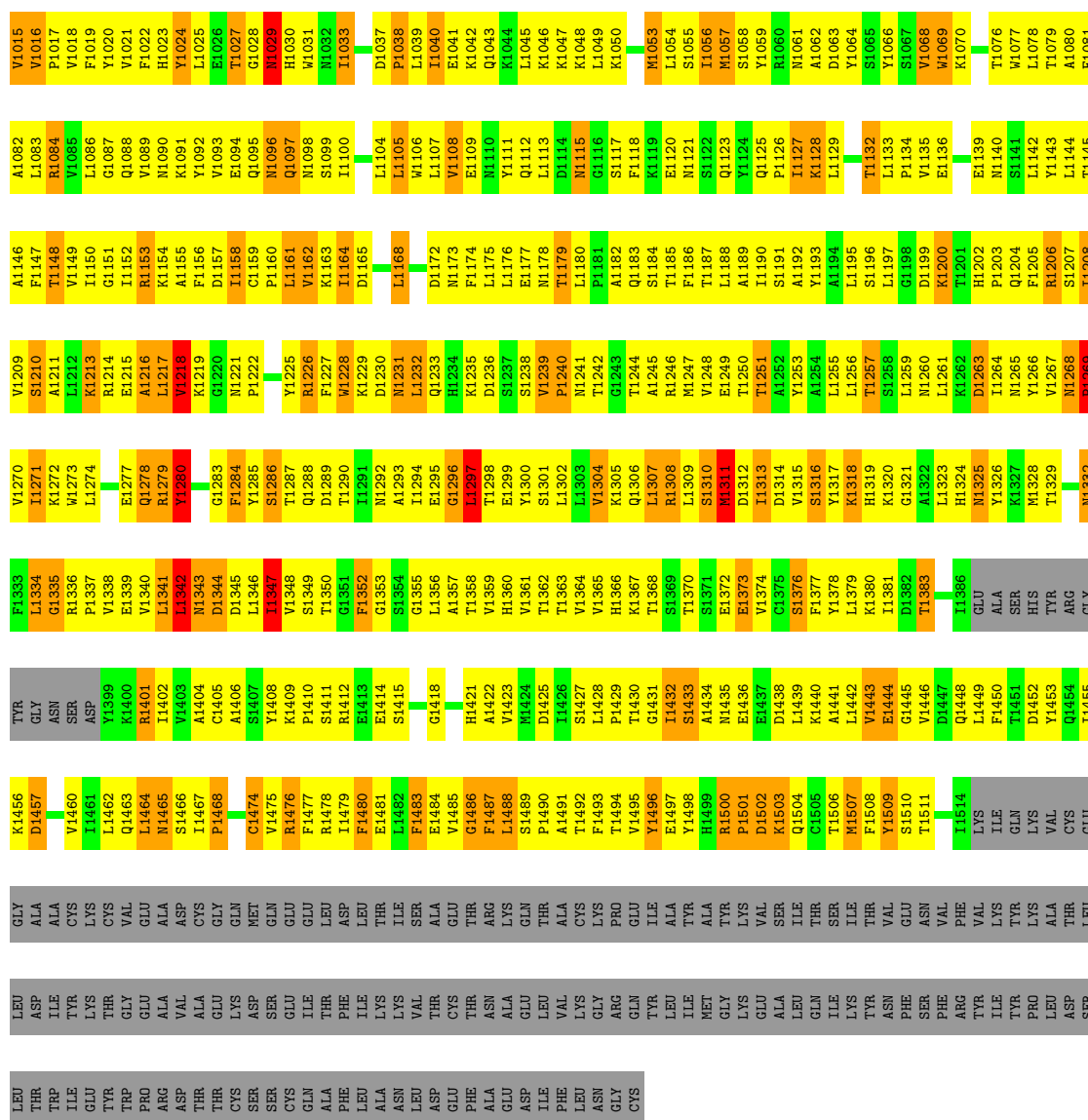


ASP	THR	CYS	Q1454	ARG	M1332	V1270	V1209	V1149	L1086	V1021	K957	L895	F824	S761	C899
SER	LEU	GLU	I1455	GLY	F1333	I1271	S1210	I1150	GL087	F1022	E958	V896	L825	K762	Y700
LEU	ASP	GLY	K1456	TYR	L1334	M1272	A1211	G1151	Q1088	Y1024	F959	T897	I829	E764	G702
THR	ASP	ALA	D1457	GLY	L1334	M1273	A1212	R1152	Q1089	Y1024	P960	F898	P830	G701	G701
TRP	ILE	ALA	G1458	ASN	R1336	S1274	K1213	R1153	M1090	E1025	P961	T899	Y831	T765	A703
ILE	TYR	CYS	H1459	SER	G1336	S1275	K1214	A1154	K1091	E1026	R962	Y900	Y832	C704	C704
GLU	LYS	LYS	H1460	ASP	P1337	E1276	E1216	A1155	V1092	T1027	P963	L901	V833	V705	V705
TYR	THR	CYS	I1461	ASP	V1338	E1277	A1216	A1156	V1093	GL028	P964	P902	V833	N707	N707
TRP	GLY	VAL	L1462	GLU	E1339	Q1278	L1217	D1157	E1094	N1029	L967	E904	V834	D708	D708
PRO	GLU	GLU	Q1463	R1401	E1340	T1279	K1218	I1158	Q1095	W1031	V968	E904	R835	W709	W709
ARG	ALA	ALA	L1464	I1402	L1341	Y1280	K1219	C1159	M1096	W1031	P969	G906	G836	E771	E771
ASP	VAL	ASP	M1465	V1403	L1342	G1281	G1220	Q1097	N1032	N1032	P970	L907	E837	S772	T710
THR	ALA	CYS	S1466	A1404	L1343	G1282	N1221	L1161	Q1098	I1033	K970	H908	Q838	K773	K773
THR	GLY	GLY	I1467	C1405	D1344	G1283	P1222	V1162	S1099	I1033	T971	H908	I839	E712	E712
CYS	LYS	LYS	P1468	A1406	D1345	F1284	P1223	K1163	S1036	S1036	E972	H909	Q840	W775	W775
SER	ASP	MET	G1469	G1407	L1346	T1285	I1224	K1164	C1101	D1037	E973	N910	L841	E776	Q713
SER	GLN	GLN	V1475	Y1408	G1347	S1286	Y1225	D1165	N1102	P1038	K974	N911	I845	A715	A715
CYS	GLU	GLU	R1476	K1409	G1348	T1287	R1226	L1166	S1103	L1039	R975	F912	V846	A716	A716
GLN	ILE	GLU	F1477	P1410	S1349	Q1288	F1227	A1167	L1104	I1040	R976	S913	Y846	R717	R717
ALA	THR	LEU	R1478	S1411	T1350	D1289	W1228	L1168	L1105	E1041	L977	L914	N847	W780	W780
PHE	ASP	ASP	I1479	R1412	G1351	T1290	K1229	I1169	W1106	E1042	S978	E915	N848	S719	S719
LEU	LEU	LEU	F1480	E1413	F1352	I1291	D1230	K1170	L1107	Q1043	W979	T916	R849	W781	W781
ALA	LEU	THR	E1481	E1414	G1353	N1292	N1231	A1171	V1108	K1044	K980	T917	R782	L720	L720
ASN	LYS	ILE	L1482	S1415	S1354	A1293	L1232	D1172	E1109	I1045	C981	N917	I853	G721	G721
LEU	VAL	SER	F1483	G1418	G1355	L1294	Q1233	N1173	N1110	K1046	L982	K920	M853	Q785	Q785
ASP	THR	ALA	E1484	G1418	L1356	E1295	Q1233	F1174	Y1111	K1047	L983	E921	F855	C724	C724
GLU	CYS	GLU	V1485	H1421	A1357	G1296	D1236	L1180	S1117	M1053	R928	L928	E863	R731	R731
THR	THR	THR	G1486	T1358	T1358	L1297	I1237	F1181	L1064	S1055	L992	V929	C732	C732	C732
PHE	ASN	ALA	F1487	A1422	V1359	T1298	S1238	L1119	E1056	S993	T796	W796	C866	W733	W733
ALA	ALA	LYS	L1488	V1423	H1360	E1299	V1239	E1178	E1056	S993	T796	W796	T867	W734	W734
ASP	GLU	GLN	S1489	M1424	V1361	Y1300	P1240	T1179	M1115	S1058	E995	E932	M859	A735	A735
LEU	LEU	THR	P1490	D1425	T1362	S1301	N1241	L1180	S1117	Y1059	G996	G933	S870	S736	S736
ILE	VAL	ALA	A1491	I1426	T1363	L1302	T1242	L1181	F1118	R1060	T997	V934	PRO	Q737	Q737
PHE	LEU	ALA	T1492	S1427	V1364	L1303	G1243	A1189	L1188	M1061	N998	K936	VAL	L738	L738
ASN	GLY	CYS	F1493	L1428	V1365	S1310	T1250	I1190	K1128	D1063	I999	R936	ILE	R802	R802
ARG	ARG	PRO	T1494	P1429	H1366	K1305	A1245	S1184	Y1064	S1065	T1001	S938	ASP	G803	G803
GLY	GLU	GLU	V1495	T1430	K1367	Q1306	R1246	T1185	S1122	S1065	H1002	Y939	HIS	S805	S805
CYS	TYR	ILE	Y1496	G1431	T1368	L1307	M1247	F1186	Q1123	Y1059	G996	G933	GLN	S805	S805
LEU	LEU	ALA	E1497	I1432	S1369	R1308	V1248	T1187	P1126	R1060	T997	V934	GLY	S743	S743
ILE	TYR	ILE	Y1498	S1433	T1370	L1309	E1249	L1188	L1127	M1061	N998	K936	THR	HIS	HIS
MET	ALA	ALA	H1499	A1434	S1371	S1310	T1250	A1189	T1127	D1063	I999	R936	LYS	L738	L738
GLY	TYR	LYS	R1500	N1435	E1372	M1311	T1251	L1190	K1128	D1063	I999	R936	LYS	ASP	ASP
LYS	LYS	VAL	P1501	E1436	E1373	D1312	A1252	S1191	S1065	Y1064	T1001	S938	SER	GLN	GLN
VAL	GLU	VAL	D1502	E1437	V1374	L1313	Y1253	A1192	S1065	Y1064	H1002	Y939	SER	GLN	GLN
ALA	ALA	SER	K1503	D1438	G1375	D1314	A1254	Y1193	T1132	Y1066	L1003	S940	GLY	LEU	LEU
LEU	LEU	ILE	Q1504	L1439	S1376	S1315	L1255	A1194	L1133	S1067	P1004	S941	THR	L751	L751
THR	GLN	THR	C1505	K1440	F1377	S1316	L1256	L1195	P1134	V1068	P1004	S941	LYS	L752	L752
ILE	ILE	SER	T1506	A1441	V1378	Y1317	L1257	S1196	V1135	W1069	S1007	T943	SER	K817	K817
LYS	LYS	ILE	M1507	L1442	L1379	K1318	S1258	L1197	V1135	W1069	S1007	T943	SER	W754	W754
TYR	TYR	THR	F1508	V1443	K1380	H1319	L1259	G1198	E1136	K1070	E1009	T945	GLN	K755	K755
ASN	ASN	VAL	Y1509	E1444	I1381	K1320	L1259	D1199	E1139	T1076	A1010	T945	GLN	F820	F820
PHE	PHE	GLU	S1510	G1445	D1382	G1321	L1261	K1200	N1140	Y1077	E1011	R947	THR	L758	L758
SER	SER	ASN	T1511	V1446	T1383	A1322	K1262	S1141	L1078	L1077	L1012	R948	LYS	P759	P759
VAL	VAL	VAL	D1447	G1447	T1383	L1323	D1263	H1202	S1141	L1078	L1012	R948	ASP	D822	D822
ARG	ARG	PHE	I1514	Q1448	G1386	H1324	I1264	Y1143	F1081	A1080	V1015	Y950	VAL	K755	K755
TYR	TYR	VAL	L1514	L1449	GLU	N1325	N1265	Q1204	F1081	A1080	V1015	Y950	VAL	F820	F820
ILE	ILE	LYS	I1514	L1449	ALA	N1325	N1265	Q1204	F1081	A1080	V1015	Y950	VAL	F820	F820
TYR	TYR	LYS	L1514	L1449	ALA	N1325	N1265	Q1204	F1081	A1080	V1015	Y950	VAL	F820	F820
PRO	PRO	LYS	L1514	L1449	SER	N1325	N1265	Q1204	F1081	A1080	V1015	Y950	VAL	F820	F820
LEU	LEU	ALA	L1514	L1449	HIS	N1325	N1265	Q1204	F1081	A1080	V1015	Y950	VAL	F820	F820
LEU	LEU	ALA	L1514	L1449	TYR	N1325	N1265	Q1204	F1081	A1080	V1015	Y950	VAL	F820	F820

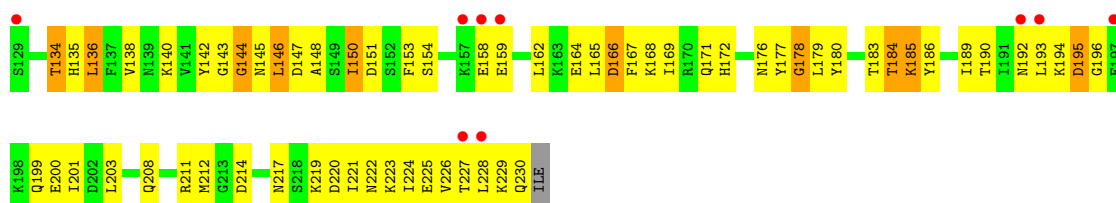
● Molecule 1: Complement C5







• Molecule 2: Staphylococcal enterotoxin-like toxin



• Molecule 2: Staphylococcal enterotoxin-like toxin



E200	L201	D202	L203	Q208	F209	E210	R211	M212	G213	D214	N217	S218	K219	D220	I221	N222	K223	L224	E225	V226	T227	L228	K229	Q230	ILE
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.79Å 144.79Å 245.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.75 – 4.20 49.75 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.75-4.20) 99.8 (49.75-4.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.233 , 0.297 0.215 , 0.281	Depositor DCC
$R_{free}$ test set	2039 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	115.5	Xtriage
Anisotropy	0.855	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.19 , 90.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l 0.397 for h,-h-k,-l 0.045 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	24809	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	205.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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, CD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.53	0/11793	0.77	6/16003 (0.0%)
1	B	0.53	0/11793	0.77	5/16003 (0.0%)
2	X	0.34	0/828	0.54	0/1107
2	Y	0.34	0/828	0.56	1/1107 (0.1%)
All	All	0.52	0/25242	0.75	12/34220 (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	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ASP	CB-CG-OD1	-8.57	110.58	118.30
1	B	640	LEU	CA-CB-CG	7.23	131.94	115.30
1	B	1374	VAL	CB-CA-C	-6.61	98.85	111.40
1	A	640	LEU	CA-CB-CG	6.51	130.28	115.30
1	A	1195	LEU	CA-CB-CG	-5.71	102.17	115.30
1	A	1374	VAL	CB-CA-C	-5.46	101.02	111.40
1	A	1482	LEU	CA-CB-CG	5.38	127.67	115.30
2	Y	175	LYS	CD-CE-NZ	5.25	123.78	111.70
1	B	323	LEU	CA-CB-CG	5.23	127.34	115.30
1	B	1033	ILE	CB-CA-C	-5.14	101.31	111.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1297	LEU	CA-CB-CG	-5.03	103.74	115.30
1	A	471	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	651	LEU	Peptide
1	B	1179	THR	Peptide
1	B	651	LEU	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	11541	0	11511	1721	0
1	B	11541	0	11511	1730	0
2	X	819	0	831	85	0
2	Y	819	0	831	83	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
4	A	42	0	38	2	0
4	B	42	0	38	3	0
All	All	24809	0	24760	3610	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 73.

All (3610) 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:535:VAL:HG23	1:A:536:PRO:HD3	1.21	1.17
1:A:698:CYS:SG	1:A:724:CYS:CB	2.33	1.16
1:A:698:CYS:SG	1:A:724:CYS:HB2	1.86	1.15
1:A:968:VAL:HG12	1:A:1368:THR:HG22	1.19	1.13

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:VAL:HG23	1:B:536:PRO:HD3	1.29	1.13
1:A:609:VAL:HG23	1:A:610:TYR:H	1.00	1.12
1:B:609:VAL:HG23	1:B:610:TYR:H	1.07	1.12
1:B:968:VAL:HG12	1:B:1368:THR:HG22	1.19	1.12
1:B:440:PRO:HD2	1:B:441:ASP:OD2	1.51	1.10
1:A:855:PHE:CZ	1:A:886:GLN:HB3	1.86	1.09
1:B:66:TYR:HD1	1:B:90:LYS:HE3	1.13	1.09
1:B:855:PHE:CZ	1:B:886:GLN:HB3	1.87	1.09
1:A:994:GLN:HE22	1:A:998:ASN:HB3	1.16	1.08
1:A:195:ARG:HD2	1:A:1058:SER:HA	1.35	1.07
1:A:1068:VAL:HG13	1:A:1069:TRP:H	1.15	1.07
1:A:617:LYS:O	1:A:618:LYS:HG2	1.55	1.07
1:A:66:TYR:HD1	1:A:90:LYS:HE3	1.14	1.06
1:B:940:SER:HB2	1:B:959:PHE:HD1	1.18	1.06
1:B:66:TYR:HE1	1:B:90:LYS:HG3	1.21	1.03
1:B:617:LYS:O	1:B:618:LYS:HG2	1.58	1.03
1:B:1068:VAL:HG13	1:B:1069:TRP:H	1.20	1.03
1:B:120:THR:HG22	1:B:121:TYR:H	1.18	1.02
1:B:38:ASN:O	1:B:39:ILE:HD13	1.60	1.01
1:B:653:PHE:CZ	1:B:660:ASP:HA	1.95	1.01
1:B:195:ARG:HD2	1:B:1058:SER:HA	1.41	1.01
1:B:133:PRO:O	1:B:134:VAL:HG23	1.58	1.01
1:A:1381:ILE:HG13	1:A:1404:ALA:HB2	1.42	1.01
1:A:984:VAL:HG11	1:A:1024:TYR:CE1	1.96	1.01
1:A:386:VAL:HG23	1:A:411:THR:HG21	1.36	1.01
1:B:541:LEU:HB2	1:B:558:SER:HB3	1.41	1.01
2:X:136:LEU:HB3	2:X:224:ILE:HB	1.43	1.01
1:A:120:THR:HG22	1:A:121:TYR:H	1.21	1.00
1:A:59:TYR:HB3	1:A:60:PRO:HD3	1.39	1.00
1:B:1255:LEU:HD21	1:B:1271:ILE:HG22	1.43	1.00
1:A:1435:ASN:HB3	1:A:1438:ASP:HB2	1.40	1.00
1:B:940:SER:HB2	1:B:959:PHE:CD1	1.95	1.00
1:A:386:VAL:H	1:A:411:THR:CG2	1.75	0.99
1:A:698:CYS:HB3	1:A:724:CYS:SG	2.01	0.99
1:B:804:ILE:HG22	1:B:809:ILE:HA	1.41	0.99
1:B:936:ARG:HB2	1:B:1364:VAL:HG22	1.44	0.99
1:A:609:VAL:HG23	1:A:610:TYR:N	1.78	0.99
1:B:840:GLN:HG2	1:B:899:THR:HG22	1.43	0.98
1:A:440:PRO:HD2	1:A:441:ASP:OD2	1.63	0.98
1:B:243:PHE:CZ	1:B:316:GLU:HG2	1.98	0.98
1:A:253:ARG:HH21	1:A:257:ASN:HA	1.29	0.98

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:922:ILE:HD12	4:B:2001:NAG:H82	1.44	0.98
1:B:59:TYR:HB3	1:B:60:PRO:HD3	1.43	0.97
1:B:982:LEU:HD23	1:B:1309:LEU:HD11	1.45	0.97
1:A:973:ILE:HG23	1:A:1365:VAL:HG23	1.46	0.97
1:A:698:CYS:CB	1:A:724:CYS:SG	2.52	0.97
1:B:973:ILE:HG23	1:B:1365:VAL:HG23	1.44	0.97
1:A:1279:ARG:HD3	1:A:1284:PHE:CG	1.99	0.97
1:A:115:LYS:HG2	1:A:117:MET:HE3	1.47	0.96
1:B:618:LYS:CB	1:B:621:GLU:HB3	1.94	0.96
1:A:922:ILE:HD12	4:A:2001:NAG:H82	1.46	0.96
1:B:994:GLN:HE22	1:B:998:ASN:HB3	1.30	0.96
1:A:618:LYS:HG3	1:A:621:GLU:CD	1.86	0.96
1:A:1244:THR:HG22	1:A:1246:ARG:H	1.31	0.95
1:B:66:TYR:CD1	1:B:90:LYS:HE3	2.00	0.95
1:B:96:GLN:O	1:B:98:PRO:HD3	1.65	0.95
1:A:133:PRO:O	1:A:134:VAL:HG23	1.66	0.95
1:A:44:TYR:HE1	1:A:497:THR:HG1	1.00	0.94
1:A:618:LYS:CB	1:A:621:GLU:HB3	1.98	0.94
1:B:635:GLY:HA2	1:B:672:ILE:HG23	1.49	0.94
1:A:984:VAL:HG11	1:A:1024:TYR:HE1	1.30	0.94
1:A:156:LYS:O	1:A:157:ARG:HG3	1.67	0.94
1:A:66:TYR:CD1	1:A:90:LYS:HE3	2.02	0.94
1:A:940:SER:HB2	1:A:959:PHE:CD1	2.03	0.94
1:A:940:SER:HB2	1:A:959:PHE:HD1	1.33	0.94
1:A:1255:LEU:HD22	1:A:1270:VAL:HG12	1.50	0.93
1:A:38:ASN:O	1:A:39:ILE:HD13	1.67	0.93
1:B:1381:ILE:HG13	1:B:1404:ALA:HB2	1.47	0.93
1:A:609:VAL:CG2	1:A:610:TYR:H	1.82	0.93
1:B:618:LYS:HG3	1:B:621:GLU:CD	1.89	0.93
1:B:115:LYS:HG2	1:B:117:MET:HE3	1.49	0.93
1:B:1244:THR:HG22	1:B:1246:ARG:H	1.34	0.93
1:B:1202:HIS:HD2	1:B:1204:GLN:H	1.14	0.93
1:A:1434:ALA:HA	1:A:1479:ILE:HG22	1.49	0.93
1:A:96:GLN:O	1:A:98:PRO:HD3	1.69	0.93
2:Y:136:LEU:HB3	2:Y:224:ILE:HB	1.50	0.93
1:A:940:SER:OG	1:A:1361:VAL:HG12	1.67	0.93
1:B:319:ASN:ND2	1:B:347:TYR:CD1	2.36	0.92
1:B:1348:VAL:HG11	1:B:1359:VAL:HG21	1.49	0.92
1:B:386:VAL:HG23	1:B:411:THR:HG21	1.50	0.92
1:B:253:ARG:HH21	1:B:257:ASN:HA	1.31	0.92
1:B:1206:ARG:HG3	1:B:1206:ARG:HH11	1.31	0.92

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:140:LYS:HG2	2:Y:228:LEU:HD12	1.50	0.92
1:B:1180:LEU:HD21	1:B:1208:ILE:HA	1.49	0.92
1:B:956:ARG:HG3	1:B:1349:SER:HB3	1.50	0.92
1:B:679:LEU:HD13	1:B:742:ILE:HG12	1.50	0.92
1:B:120:THR:CG2	1:B:121:TYR:H	1.82	0.92
1:A:1118:PHE:O	1:A:1144:LEU:HD23	1.69	0.92
1:A:653:PHE:CZ	1:A:660:ASP:HA	2.05	0.91
1:B:66:TYR:CE1	1:B:90:LYS:HG3	2.05	0.91
1:B:835:ARG:HG2	1:B:835:ARG:HH11	1.34	0.91
1:A:986:GLU:HA	1:A:986:GLU:OE2	1.66	0.91
1:A:1090:ASN:HD22	1:A:1158:ILE:HD13	1.35	0.91
1:B:359:THR:HG21	1:B:372:LYS:H	1.34	0.91
1:B:1162:VAL:HG23	1:B:1163:LYS:H	1.35	0.91
1:B:163:PHE:HD1	1:B:163:PHE:H	1.19	0.91
1:B:1217:LEU:O	1:B:1218:VAL:HG13	1.70	0.90
1:B:1251:THR:HG1	1:B:1273:TRP:HZ3	0.94	0.90
1:B:823:VAL:HG22	1:B:847:ASN:HA	1.54	0.90
1:B:1438:ASP:OD2	1:B:1478:ARG:HG3	1.72	0.90
1:B:571:LEU:HD12	1:B:572:GLN:N	1.85	0.90
1:A:1279:ARG:HD3	1:A:1284:PHE:CD2	2.07	0.89
1:B:156:LYS:O	1:B:157:ARG:HG3	1.71	0.89
1:A:1438:ASP:OD2	1:A:1478:ARG:HG3	1.72	0.89
1:B:973:ILE:HG23	1:B:1365:VAL:CG2	2.01	0.89
1:A:1180:LEU:HD21	1:A:1208:ILE:HA	1.52	0.89
1:A:66:TYR:HE1	1:A:90:LYS:HG3	1.35	0.89
1:B:386:VAL:H	1:B:411:THR:CG2	1.85	0.89
1:A:644:ASN:HD21	1:A:648:LEU:HD12	1.37	0.89
1:A:804:ILE:HG22	1:A:809:ILE:HA	1.54	0.89
1:B:1149:VAL:HA	1:B:1152:ILE:HD12	1.55	0.89
1:B:1090:ASN:HD22	1:B:1158:ILE:HD13	1.35	0.89
1:A:412:ARG:HB3	1:A:415:ASP:HB3	1.53	0.89
1:A:635:GLY:HA2	1:A:672:ILE:HG23	1.55	0.89
1:B:319:ASN:O	1:B:320:ASN:ND2	2.06	0.89
1:B:386:VAL:HG12	1:B:387:PRO:HD2	1.55	0.89
1:A:968:VAL:HG12	1:A:1368:THR:CG2	2.03	0.88
1:B:412:ARG:HD2	1:B:415:ASP:HB2	1.55	0.88
1:B:528:ILE:H	1:B:528:ILE:HD12	1.37	0.88
1:B:59:TYR:CB	1:B:60:PRO:HD3	2.03	0.88
1:A:120:THR:CG2	1:A:121:TYR:H	1.85	0.88
1:A:371:ILE:HD11	1:A:422:LEU:HD11	1.55	0.88
1:A:679:LEU:HD13	1:A:742:ILE:HG12	1.53	0.88

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:TYR:CB	1:A:60:PRO:HD3	2.01	0.88
1:B:157:ARG:H	1:B:178:ASP:HB3	1.38	0.88
1:B:249:THR:HG23	1:B:298:GLN:HE21	1.38	0.88
1:A:243:PHE:CZ	1:A:316:GLU:HG2	2.07	0.88
1:B:984:VAL:HG11	1:B:1024:TYR:CE1	2.08	0.88
1:A:1206:ARG:HH11	1:A:1206:ARG:HG3	1.38	0.88
1:A:956:ARG:HG3	1:A:1349:SER:HB3	1.55	0.87
1:A:441:ASP:HA	1:B:443:PRO:HB3	1.55	0.87
2:X:140:LYS:HG2	2:X:228:LEU:HD12	1.55	0.87
1:A:412:ARG:HD2	1:A:415:ASP:HB2	1.54	0.87
1:B:569:ASN:OD1	1:B:596:MET:HB2	1.74	0.87
1:B:120:THR:HG22	1:B:121:TYR:N	1.89	0.87
1:B:609:VAL:HG23	1:B:610:TYR:N	1.89	0.87
1:B:855:PHE:CE1	1:B:886:GLN:HB3	2.08	0.87
1:B:1193:TYR:O	1:B:1196:SER:HB3	1.73	0.87
1:B:242:ASN:HB3	1:B:245:ASN:O	1.74	0.87
1:B:944:LEU:HB2	1:B:1357:ALA:HB3	1.54	0.87
1:B:231:ILE:HG12	1:B:342:ILE:HD11	1.55	0.87
1:A:386:VAL:H	1:A:411:THR:HG23	1.39	0.86
1:A:1244:THR:HB	1:A:1247:MET:HB2	1.55	0.86
1:A:242:ASN:HB3	1:A:245:ASN:O	1.75	0.86
1:B:1318:LYS:HG2	1:B:1319:HIS:CE1	2.10	0.86
1:A:443:PRO:HB3	1:B:441:ASP:HA	1.55	0.86
1:A:936:ARG:HB3	1:A:1364:VAL:HG22	1.55	0.86
1:A:1180:LEU:HD12	1:A:1204:GLN:NE2	1.90	0.86
2:X:146:LEU:HD22	2:X:147:ASP:N	1.89	0.86
1:B:1193:TYR:CE1	1:B:1256:LEU:HB3	2.10	0.86
1:B:412:ARG:HB3	1:B:415:ASP:HB3	1.57	0.86
1:A:1255:LEU:HD21	1:A:1271:ILE:HG22	1.58	0.86
1:A:365:PRO:HD2	1:A:464:TYR:CD2	2.10	0.86
1:B:1193:TYR:HA	1:B:1257:THR:HG23	1.57	0.86
1:A:1090:ASN:HD21	1:A:1158:ILE:HG21	1.38	0.85
1:B:576:SER:OG	1:B:589:SER:HB2	1.76	0.85
1:A:577:PRO:HD2	1:A:588:VAL:HG23	1.58	0.85
1:A:976:ILE:HD12	1:A:1362:THR:HG23	1.59	0.85
1:B:984:VAL:HG11	1:B:1024:TYR:HE1	1.39	0.85
1:A:1348:VAL:HG11	1:A:1359:VAL:HG21	1.57	0.85
1:A:560:TRP:CZ3	1:A:562:ASN:HB2	2.12	0.85
1:B:602:LEU:HD12	1:B:774:LEU:HD22	1.56	0.85
1:A:1193:TYR:HA	1:A:1257:THR:HG23	1.59	0.85
1:A:936:ARG:CB	1:A:1364:VAL:HG22	2.07	0.85

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1209:VAL:O	1:B:1213:LYS:HB2	1.76	0.84
1:A:571:LEU:HD12	1:A:572:GLN:N	1.92	0.84
1:B:1304:VAL:HG12	1:B:1305:LYS:N	1.92	0.84
1:B:1381:ILE:HD13	1:B:1509:TYR:CD1	2.12	0.84
1:A:618:LYS:HG3	1:A:621:GLU:OE1	1.77	0.84
1:A:841:LEU:HD12	1:A:859:MET:HE1	1.59	0.84
1:B:617:LYS:HE3	1:B:625:GLN:HE22	1.43	0.84
1:B:733:VAL:O	1:B:737:GLN:HG2	1.76	0.84
1:B:1304:VAL:HG12	1:B:1305:LYS:H	1.38	0.84
1:B:1118:PHE:O	1:B:1144:LEU:HD23	1.76	0.84
1:B:1435:ASN:HB3	1:B:1438:ASP:HB2	1.58	0.84
1:A:639:GLY:H	1:A:645:VAL:HG22	1.41	0.84
1:B:940:SER:OG	1:B:1361:VAL:HG12	1.77	0.84
1:A:1283:GLY:HA3	1:A:1290:THR:HG23	1.59	0.84
1:B:242:ASN:H	1:B:242:ASN:HD22	1.22	0.84
1:A:1255:LEU:HB2	1:A:1270:VAL:HG11	1.58	0.83
1:B:367:ILE:HD13	1:B:466:TYR:HD2	1.43	0.83
1:B:497:THR:HG23	1:B:498:HIS:H	1.42	0.83
1:B:1132:THR:HB	1:B:1134:PRO:HD2	1.59	0.83
1:B:618:LYS:HB2	1:B:621:GLU:HB3	1.59	0.83
1:B:835:ARG:NH2	1:B:905:ILE:HD11	1.93	0.83
1:B:1255:LEU:CD2	1:B:1271:ILE:HG22	2.07	0.83
1:B:968:VAL:CG1	1:B:1368:THR:HG22	2.07	0.83
1:A:1323:LEU:HD12	1:A:1324:HIS:H	1.43	0.83
1:A:1381:ILE:HG13	1:A:1404:ALA:CB	2.08	0.83
1:A:359:THR:HG21	1:A:372:LYS:H	1.42	0.83
1:B:1255:LEU:HD22	1:B:1270:VAL:HG12	1.58	0.83
1:B:43:VAL:HG12	1:B:79:PHE:HB3	1.58	0.83
1:B:981:GLY:O	1:B:982:LEU:HB2	1.78	0.83
1:A:1304:VAL:HG12	1:A:1305:LYS:H	1.42	0.83
1:A:1068:VAL:HG13	1:A:1069:TRP:N	1.93	0.82
1:A:835:ARG:HG2	1:A:835:ARG:HH11	1.44	0.82
1:B:364:LYS:CD	1:B:364:LYS:H	1.91	0.82
1:B:534:MET:HB3	1:B:538:SER:OG	1.78	0.82
1:B:354:LEU:H	1:B:354:LEU:CD2	1.92	0.82
1:B:618:LYS:HG3	1:B:621:GLU:OE1	1.79	0.82
1:A:120:THR:HG22	1:A:121:TYR:N	1.94	0.82
1:A:386:VAL:HG23	1:A:411:THR:CG2	2.08	0.82
1:B:1279:ARG:HB2	1:B:1284:PHE:HB2	1.62	0.82
1:B:1434:ALA:HA	1:B:1479:ILE:HG22	1.59	0.82
1:A:541:LEU:HB2	1:A:558:SER:HB3	1.60	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1180:LEU:HD12	1:B:1204:GLN:NE2	1.95	0.82
1:B:834:VAL:HG21	1:B:1489:SER:OG	1.78	0.82
1:B:371:ILE:HD11	1:B:422:LEU:HD11	1.60	0.82
2:Y:146:LEU:HD22	2:Y:147:ASP:N	1.94	0.82
1:B:977:LEU:HD12	1:B:1361:VAL:HG21	1.60	0.82
1:B:160:VAL:HG22	1:B:174:VAL:O	1.80	0.82
2:Y:165:LEU:O	2:Y:169:ILE:HG12	1.80	0.82
1:A:1304:VAL:HG12	1:A:1305:LYS:N	1.93	0.82
1:B:494:ASP:O	1:B:496:ILE:HD12	1.77	0.82
1:A:618:LYS:HB2	1:A:621:GLU:HB3	1.61	0.81
1:B:42:GLN:HG3	1:B:80:GLN:HE21	1.44	0.81
1:A:569:ASN:OD1	1:A:596:MET:HB2	1.79	0.81
1:B:639:GLY:H	1:B:645:VAL:HG22	1.43	0.81
1:A:306:ALA:O	1:A:307:VAL:HG23	1.80	0.81
1:B:30:ILE:HG22	1:B:31:PHE:N	1.95	0.81
1:B:841:LEU:HD12	1:B:859:MET:HE1	1.61	0.81
1:B:936:ARG:CB	1:B:1364:VAL:HG22	2.10	0.81
1:A:617:LYS:HE3	1:A:625:GLN:HE22	1.44	0.81
1:A:1372:GLU:HG3	1:A:1373:GLU:H	1.45	0.81
1:A:157:ARG:H	1:A:178:ASP:HB3	1.45	0.81
1:A:330:ILE:HG22	1:A:337:SER:CB	2.10	0.81
1:A:371:ILE:HD12	1:A:390:LEU:HD21	1.63	0.81
1:A:361:LEU:O	1:A:454:ALA:HA	1.80	0.81
1:A:653:PHE:CD2	1:A:653:PHE:N	2.48	0.81
1:B:1244:THR:HG22	1:B:1246:ARG:N	1.95	0.81
1:B:134:VAL:HG22	1:B:218:GLU:HB3	1.63	0.81
1:A:1193:TYR:O	1:A:1196:SER:HB3	1.81	0.81
1:A:364:LYS:CD	1:A:364:LYS:H	1.93	0.81
1:A:492:TYR:HD2	1:A:493:ILE:N	1.79	0.81
1:A:576:SER:OG	1:A:589:SER:HB2	1.81	0.81
1:B:1372:GLU:HG3	1:B:1373:GLU:H	1.46	0.81
1:A:1209:VAL:O	1:A:1213:LYS:HB2	1.81	0.80
1:A:30:ILE:HG22	1:A:31:PHE:N	1.96	0.80
1:A:973:ILE:HG23	1:A:1365:VAL:CG2	2.12	0.80
1:A:115:LYS:HG2	1:A:117:MET:CE	2.11	0.80
1:B:1218:VAL:HG12	1:B:1225:TYR:O	1.81	0.80
1:A:1217:LEU:O	1:A:1218:VAL:HG13	1.82	0.80
1:A:386:VAL:O	1:A:411:THR:HG22	1.81	0.80
1:B:242:ASN:CB	1:B:245:ASN:O	2.29	0.80
1:B:977:LEU:HD12	1:B:1361:VAL:CG2	2.12	0.80
1:A:528:ILE:H	1:A:528:ILE:HD12	1.46	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1429:PRO:HG2	1:B:1511:THR:HB	1.63	0.79
1:B:977:LEU:HA	1:B:1361:VAL:HG23	1.62	0.79
1:A:934:VAL:HG22	1:A:1366:HIS:CD2	2.15	0.79
1:A:134:VAL:HG22	1:A:218:GLU:HB3	1.64	0.79
1:A:1435:ASN:HD22	1:A:1478:ARG:HB2	1.48	0.79
1:A:246:PHE:O	1:A:300:THR:HA	1.82	0.79
1:A:388:VAL:O	1:A:388:VAL:HG12	1.83	0.79
1:B:653:PHE:CD2	1:B:653:PHE:N	2.50	0.79
2:Y:219:LYS:HD2	2:Y:219:LYS:N	1.97	0.79
1:A:395:ILE:HD12	1:A:396:ASP:O	1.82	0.79
1:A:354:LEU:H	1:A:354:LEU:CD2	1.96	0.79
1:A:386:VAL:N	1:A:411:THR:CG2	2.46	0.79
1:B:253:ARG:NH2	1:B:257:ASN:HA	1.98	0.79
1:B:388:VAL:O	1:B:388:VAL:HG12	1.83	0.79
1:B:486:VAL:O	1:B:488:PRO:HD3	1.80	0.79
1:B:560:TRP:CH2	1:B:562:ASN:HB2	2.18	0.78
1:B:560:TRP:CZ3	1:B:562:ASN:HB2	2.18	0.78
1:B:896:VAL:O	1:B:897:THR:HG22	1.82	0.78
1:A:534:MET:HB3	1:A:538:SER:OG	1.84	0.78
1:B:1090:ASN:HD21	1:B:1158:ILE:HG21	1.48	0.78
2:Y:219:LYS:HD2	2:Y:219:LYS:H	1.49	0.78
1:A:535:VAL:CG2	1:A:536:PRO:HD3	2.10	0.78
1:A:824:PHE:CE1	1:A:846:TYR:HD1	2.01	0.78
1:A:160:VAL:HG22	1:A:174:VAL:O	1.84	0.78
1:A:163:PHE:H	1:A:163:PHE:HD1	1.32	0.78
1:B:1206:ARG:CG	1:B:1206:ARG:HH11	1.97	0.78
1:B:1279:ARG:HD3	1:B:1284:PHE:CD2	2.19	0.78
1:B:987:ILE:HD13	1:B:1294:ILE:HG23	1.65	0.78
1:B:1323:LEU:HD12	1:B:1324:HIS:H	1.49	0.78
1:B:92:LEU:N	1:B:93:PRO:HD3	1.99	0.78
1:A:735:ALA:HB1	1:A:754:MET:HE1	1.64	0.78
1:A:92:LEU:N	1:A:93:PRO:HD3	1.99	0.78
1:A:1283:GLY:HA3	1:A:1290:THR:CG2	2.14	0.78
1:A:386:VAL:HG12	1:A:387:PRO:HD2	1.65	0.78
1:B:31:PHE:HZ	1:B:104:LEU:HD22	1.49	0.78
1:B:360:PRO:HA	1:B:636:ALA:HB3	1.65	0.78
1:B:392:ALA:HB3	1:B:404:LEU:HD12	1.66	0.78
1:A:85:LEU:H	1:A:85:LEU:HD22	1.49	0.78
1:B:717:ARG:HD3	1:B:1449:LEU:HA	1.65	0.78
1:A:1162:VAL:HG23	1:A:1163:LYS:H	1.49	0.77
1:A:392:ALA:HB3	1:A:404:LEU:HD12	1.65	0.77

*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	1.99	0.77
1:A:1429:PRO:HG2	1:A:1511:THR:HB	1.66	0.77
1:A:296:ILE:HG22	1:A:297:ALA:H	1.49	0.77
1:B:1248:VAL:HG21	1:B:1277:GLU:HG2	1.64	0.77
1:B:1381:ILE:HG13	1:B:1404:ALA:CB	2.14	0.77
1:B:739:ARG:HB3	1:B:754:MET:SD	2.24	0.77
1:A:1439:LEU:HA	1:A:1442:LEU:HD12	1.66	0.77
1:A:253:ARG:NH2	1:A:257:ASN:HA	2.00	0.77
1:A:249:THR:HG23	1:A:298:GLN:HE21	1.49	0.77
1:B:1090:ASN:ND2	1:B:1158:ILE:HD13	1.98	0.77
1:B:41:ILE:O	1:B:80:GLN:HA	1.84	0.77
1:B:59:TYR:CG	1:B:60:PRO:HD3	2.19	0.77
1:A:115:LYS:HG3	1:A:116:ARG:N	1.99	0.77
1:A:1193:TYR:CE1	1:A:1256:LEU:HB3	2.19	0.77
1:B:1146:ALA:HB1	1:B:1190:ILE:HG22	1.66	0.77
1:B:1229:LYS:HE3	1:B:1231:ASN:OD1	1.85	0.77
1:B:315:LEU:HB2	1:B:318:LEU:HB2	1.67	0.77
1:A:1466:SER:OG	1:A:1468:PRO:HD3	1.85	0.77
1:B:1027:THR:HG22	1:B:1302:LEU:HD21	1.66	0.77
1:A:1435:ASN:HB3	1:A:1438:ASP:CB	2.14	0.76
1:B:1430:THR:O	1:B:1485:VAL:HG11	1.83	0.76
1:B:142:LYS:HD3	1:B:775:TRP:CG	2.20	0.76
2:X:219:LYS:N	2:X:219:LYS:HD2	2.01	0.76
1:A:25:ILE:HB	1:A:654:LEU:HB3	1.68	0.76
1:B:618:LYS:HB3	1:B:621:GLU:HB3	1.65	0.76
1:B:938:SER:OG	1:B:1279:ARG:CZ	2.32	0.76
1:A:1430:THR:O	1:A:1485:VAL:HG11	1.84	0.76
1:B:968:VAL:O	1:B:971:THR:HG23	1.85	0.76
1:A:1434:ALA:HB1	1:A:1477:PHE:CD1	2.20	0.76
1:B:1255:LEU:HB2	1:B:1270:VAL:HG11	1.66	0.76
1:A:1132:THR:HB	1:A:1134:PRO:HD2	1.65	0.76
1:A:232:GLU:OE2	1:A:251:LYS:HE2	1.84	0.76
1:B:1246:ARG:O	1:B:1250:THR:HG23	1.85	0.76
1:B:232:GLU:OE2	1:B:251:LYS:HE2	1.85	0.76
1:A:739:ARG:HB3	1:A:754:MET:SD	2.26	0.76
1:A:849:ARG:HG2	1:A:853:MET:HE1	1.67	0.76
1:A:944:LEU:HB2	1:A:1357:ALA:HB3	1.66	0.76
1:B:161:LEU:HG	1:B:185:PHE:CE1	2.20	0.76
1:A:1146:ALA:HB1	1:A:1190:ILE:HG22	1.66	0.76
1:A:1230:ASP:OD2	1:A:1246:ARG:HD2	1.85	0.76
1:A:1318:LYS:HG2	1:A:1319:HIS:CE1	2.21	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LYS:HE2	1:A:666:ASP:HB3	1.67	0.76
1:A:30:ILE:HG22	1:A:31:PHE:H	1.48	0.76
1:B:115:LYS:HG2	1:B:117:MET:CE	2.15	0.76
1:B:866:CYS:O	1:B:900:VAL:HG12	1.83	0.76
1:A:1030:HIS:NE2	1:A:1306:GLN:NE2	2.34	0.76
1:A:644:ASN:ND2	1:A:648:LEU:HD12	2.00	0.76
1:B:246:PHE:O	1:B:300:THR:HA	1.85	0.76
1:B:386:VAL:HG23	1:B:411:THR:CG2	2.14	0.76
1:A:1211:ALA:O	1:A:1214:ARG:HB3	1.85	0.75
1:B:1283:GLY:HA3	1:B:1290:THR:HG23	1.68	0.75
1:B:1236:ASP:HB2	1:B:1412:ARG:HH22	1.48	0.75
1:A:317:ASP:O	1:A:319:ASN:N	2.18	0.75
1:A:977:LEU:HD12	1:A:1361:VAL:CG2	2.17	0.75
1:A:938:SER:OG	1:A:1279:ARG:CZ	2.35	0.75
1:B:429:THR:OG1	1:B:430:VAL:N	2.14	0.75
1:A:1279:ARG:CG	1:A:1284:PHE:HB2	2.16	0.75
2:X:165:LEU:O	2:X:169:ILE:HG12	1.87	0.75
1:A:820:PHE:HZ	1:A:848:TYR:HB2	1.51	0.75
1:A:85:LEU:O	1:A:86:THR:HB	1.85	0.75
1:B:1229:LYS:HD2	1:B:1239:VAL:HG12	1.67	0.75
1:B:59:TYR:HB3	1:B:60:PRO:CD	2.17	0.75
1:A:1279:ARG:HB2	1:A:1284:PHE:HB2	1.68	0.75
1:B:1205:PHE:CZ	1:B:1261:LEU:HD11	2.20	0.75
1:B:541:LEU:HD12	1:B:645:VAL:HG12	1.69	0.75
1:A:1186:PHE:HD1	1:A:1250:THR:HG22	1.52	0.74
1:B:115:LYS:HG3	1:B:116:ARG:N	2.00	0.74
1:B:1186:PHE:HD1	1:B:1250:THR:HG22	1.52	0.74
1:B:302:ASP:OD2	1:B:304:GLU:HB2	1.86	0.74
1:B:371:ILE:HD12	1:B:390:LEU:HD21	1.69	0.74
1:A:494:ASP:O	1:A:496:ILE:HD12	1.85	0.74
1:B:330:ILE:HG22	1:B:337:SER:CB	2.16	0.74
1:B:963:ILE:HG23	1:B:973:ILE:HD11	1.69	0.74
2:X:219:LYS:H	2:X:219:LYS:HD2	1.51	0.74
1:B:1271:ILE:O	1:B:1271:ILE:HD12	1.87	0.74
1:B:367:ILE:HG21	1:B:466:TYR:HD2	1.52	0.74
1:A:486:VAL:O	1:A:488:PRO:HD3	1.86	0.74
1:B:386:VAL:H	1:B:411:THR:HG23	1.51	0.74
1:A:59:TYR:CG	1:A:60:PRO:HD3	2.22	0.74
1:B:1440:LYS:HD3	1:B:1453:TYR:CE1	2.21	0.74
1:B:829:ILE:HG13	1:B:925:LYS:HG2	1.69	0.74
1:A:1108:VAL:HG13	1:A:1109:GLU:H	1.53	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:TYR:CD2	1:A:60:PRO:HD3	2.22	0.74
2:X:224:ILE:O	2:X:225:GLU:HG3	1.87	0.74
1:A:59:TYR:HB3	1:A:60:PRO:CD	2.16	0.74
1:B:365:PRO:HD2	1:B:464:TYR:CD2	2.23	0.74
1:A:1251:THR:HG1	1:A:1273:TRP:HZ3	1.34	0.73
1:A:363:LEU:O	1:A:363:LEU:HD12	1.88	0.73
1:B:1180:LEU:HD12	1:B:1204:GLN:HE22	1.52	0.73
1:A:1427:SER:HB3	1:A:1492:THR:H	1.53	0.73
1:A:497:THR:HG23	1:A:498:HIS:H	1.52	0.73
1:B:139:GLN:O	1:B:190:ILE:HG12	1.87	0.73
1:A:295:GLY:O	1:A:296:ILE:HD13	1.88	0.73
1:A:386:VAL:CG2	1:A:411:THR:HG21	2.16	0.73
1:B:1283:GLY:HA3	1:B:1290:THR:CG2	2.18	0.73
1:B:297:ALA:O	1:B:298:GLN:HG3	1.88	0.73
1:B:1068:VAL:HG13	1:B:1069:TRP:N	1.99	0.73
1:B:1503:LYS:HD2	1:B:1503:LYS:N	2.02	0.73
1:A:1246:ARG:O	1:A:1250:THR:HG23	1.88	0.73
1:A:1205:PHE:CZ	1:A:1261:LEU:HD11	2.24	0.73
1:A:618:LYS:HB3	1:A:621:GLU:HB3	1.70	0.73
1:A:66:TYR:CE1	1:A:90:LYS:HG3	2.22	0.73
1:B:718:ILE:HG12	1:B:1446:VAL:HG12	1.70	0.73
1:A:1229:LYS:HE3	1:A:1231:ASN:OD1	1.88	0.73
1:A:837:GLU:HG2	1:A:1487:PHE:O	1.88	0.73
1:B:1427:SER:HB3	1:B:1492:THR:H	1.54	0.73
1:B:515:ARG:HH12	1:B:527:ASN:H	1.37	0.73
1:B:59:TYR:CD2	1:B:60:PRO:HD3	2.23	0.73
1:A:1205:PHE:HZ	1:A:1261:LEU:HD11	1.52	0.73
1:A:1440:LYS:HD3	1:A:1453:TYR:CE1	2.23	0.73
1:A:42:GLN:HG3	1:A:80:GLN:HE21	1.53	0.73
1:A:1230:ASP:CG	1:A:1246:ARG:HD2	2.08	0.73
1:A:1236:ASP:HB2	1:A:1412:ARG:HH22	1.53	0.73
1:A:492:TYR:CD2	1:A:493:ILE:N	2.57	0.73
1:B:1193:TYR:CD1	1:B:1256:LEU:HB3	2.23	0.73
1:B:42:GLN:HB2	1:B:80:GLN:HG2	1.68	0.73
1:B:25:ILE:HB	1:B:654:LEU:HB3	1.69	0.73
1:A:43:VAL:HG12	1:A:79:PHE:HB3	1.68	0.73
1:A:913:SER:HB2	1:A:922:ILE:HG12	1.71	0.73
1:B:367:ILE:HD13	1:B:466:TYR:CD2	2.24	0.73
1:A:267:ILE:HG12	1:A:327:VAL:HG13	1.69	0.73
1:B:153:LYS:HB3	1:B:154:PRO:HD2	1.71	0.73
1:A:977:LEU:HD12	1:A:1361:VAL:HG21	1.71	0.72

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ILE:HG22	1:B:31:PHE:H	1.52	0.72
1:B:354:LEU:H	1:B:354:LEU:HD23	1.52	0.72
1:B:700:TYR:HE1	1:B:758:LEU:HB2	1.53	0.72
1:B:1113:LEU:HD12	1:B:1117:SER:OG	1.88	0.72
2:X:146:LEU:HD11	2:X:148:ALA:HB2	1.71	0.72
1:A:976:ILE:HD12	1:A:1362:THR:CG2	2.20	0.72
1:B:849:ARG:HG2	1:B:853:MET:HE1	1.72	0.72
1:A:700:TYR:HE1	1:A:758:LEU:HB2	1.54	0.72
1:B:234:GLU:HG3	1:B:247:GLU:HB3	1.70	0.72
1:B:354:LEU:HD12	1:B:435:VAL:CG1	2.20	0.72
1:A:443:PRO:HG3	1:B:441:ASP:O	1.88	0.72
2:Y:186:TYR:CD2	2:Y:229:LYS:HD3	2.24	0.72
1:A:1229:LYS:HD2	1:A:1239:VAL:HG12	1.71	0.72
1:B:837:GLU:HG2	1:B:1488:LEU:HA	1.72	0.72
1:B:306:ALA:O	1:B:307:VAL:HG23	1.88	0.72
1:B:386:VAL:N	1:B:411:THR:CG2	2.52	0.72
1:B:367:ILE:HG21	1:B:466:TYR:CD2	2.23	0.72
1:B:794:LEU:HD21	1:B:824:PHE:CZ	2.23	0.72
1:A:1334:LEU:N	1:A:1334:LEU:HD22	2.04	0.72
1:B:492:TYR:CD2	1:B:493:ILE:N	2.57	0.72
1:A:1024:TYR:CD2	1:A:1024:TYR:C	2.63	0.72
1:A:157:ARG:HD2	1:A:205:TYR:CE2	2.24	0.72
1:A:367:ILE:HD13	1:A:466:TYR:HD2	1.54	0.72
1:A:638:GLY:HA2	1:A:645:VAL:HG13	1.70	0.72
1:A:915:GLU:OE2	1:A:920:LYS:HE3	1.89	0.72
1:B:1030:HIS:O	1:B:1033:ILE:HG13	1.90	0.72
1:B:1421:HIS:CE1	1:B:1498:TYR:CD2	2.78	0.72
1:B:364:LYS:HD2	1:B:364:LYS:H	1.52	0.72
1:A:1445:GLY:O	1:A:1448:GLN:HB3	1.89	0.72
1:B:242:ASN:ND2	1:B:242:ASN:H	1.86	0.72
1:B:644:ASN:HD21	1:B:648:LEU:HD12	1.53	0.72
1:A:386:VAL:H	1:A:411:THR:HG22	1.54	0.72
1:B:1230:ASP:OD2	1:B:1246:ARG:HD2	1.90	0.72
1:B:585:GLY:HA2	1:B:790:LEU:O	1.89	0.72
1:A:1030:HIS:CE1	1:A:1306:GLN:NE2	2.58	0.72
1:A:1465:ASN:H	1:A:1465:ASN:HD22	1.37	0.72
1:A:441:ASP:O	1:B:443:PRO:HG3	1.90	0.72
1:A:571:LEU:HG	1:A:812:ALA:HB2	1.71	0.72
1:B:1024:TYR:CE2	1:B:1030:HIS:CD2	2.78	0.72
1:B:1274:LEU:HB3	1:B:1297:LEU:HD11	1.71	0.72
1:A:718:ILE:HG12	1:A:1446:VAL:HG12	1.72	0.71

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:VAL:HG22	1:A:429:THR:H	1.53	0.71
1:B:1205:PHE:HZ	1:B:1261:LEU:HD11	1.53	0.71
1:A:1084:ARG:HD2	1:A:1154:LYS:HG3	1.72	0.71
1:A:242:ASN:H	1:A:242:ASN:HD22	1.37	0.71
1:A:710:THR:HG23	1:A:713:GLN:CD	2.10	0.71
2:Y:189:ILE:O	2:Y:200:GLU:HA	1.89	0.71
1:A:532:GLN:O	1:A:535:VAL:HG13	1.90	0.71
1:B:1024:TYR:CD2	1:B:1024:TYR:C	2.63	0.71
1:B:363:LEU:HD12	1:B:363:LEU:O	1.91	0.71
1:B:504:LEU:HD21	1:B:651:LEU:HG	1.70	0.71
1:A:1422:ALA:O	1:A:1464:LEU:HD12	1.90	0.71
2:Y:136:LEU:HD21	2:Y:153:PHE:HB2	1.72	0.71
1:A:981:GLY:HA3	1:A:1309:LEU:HD11	1.73	0.71
1:A:499:TYR:O	1:A:514:THR:HG23	1.89	0.71
1:B:1466:SER:OG	1:B:1468:PRO:HD3	1.89	0.71
1:A:123:ASN:HD22	1:A:123:ASN:C	1.94	0.71
1:A:695:VAL:HA	1:A:698:CYS:SG	2.31	0.71
1:B:43:VAL:CG1	1:B:79:PHE:HB3	2.20	0.71
1:A:1488:LEU:O	1:A:1488:LEU:HD12	1.90	0.71
1:A:425:PRO:O	1:A:427:GLY:N	2.23	0.71
1:A:733:VAL:O	1:A:737:GLN:HG2	1.90	0.71
1:A:839:ILE:HG22	1:A:900:VAL:HG23	1.72	0.71
1:B:1053:MET:HE1	1:B:1086:LEU:HD22	1.72	0.71
1:B:1334:LEU:HD22	1:B:1334:LEU:N	2.06	0.71
2:X:140:LYS:HA	2:X:228:LEU:HB2	1.72	0.71
1:B:1239:VAL:O	1:B:1241:ASN:N	2.24	0.71
1:B:1251:THR:HG21	1:B:1273:TRP:CH2	2.25	0.71
1:B:271:ILE:HG21	1:B:313:TYR:CE1	2.25	0.71
1:B:835:ARG:CZ	1:B:905:ILE:HD11	2.20	0.71
1:A:1080:ALA:O	1:A:1083:LEU:N	2.24	0.71
1:A:1296:GLY:O	1:A:1298:THR:N	2.24	0.71
1:A:330:ILE:HG22	1:A:337:SER:OG	1.91	0.71
1:B:1449:LEU:HD12	1:B:1449:LEU:O	1.90	0.71
1:B:1449:LEU:HG	1:B:1450:PHE:CD1	2.26	0.71
1:B:1465:ASN:H	1:B:1465:ASN:HD22	1.38	0.71
1:B:386:VAL:H	1:B:411:THR:HG22	1.56	0.71
1:B:352:TYR:HA	1:B:376:LYS:O	1.91	0.71
1:A:1180:LEU:O	1:A:1182:ALA:N	2.24	0.70
1:A:1421:HIS:CE1	1:A:1498:TYR:CD2	2.79	0.70
1:A:41:ILE:O	1:A:80:GLN:HA	1.90	0.70
1:B:635:GLY:HA2	1:B:672:ILE:CG2	2.20	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1449:LEU:HG	1:A:1450:PHE:CD1	2.26	0.70
1:A:42:GLN:HB2	1:A:80:GLN:HG2	1.72	0.70
1:B:1211:ALA:O	1:B:1214:ARG:HB3	1.90	0.70
1:B:157:ARG:HD2	1:B:205:TYR:CE2	2.27	0.70
1:B:542:VAL:O	1:B:556:SER:HB2	1.91	0.70
1:A:194:PRO:O	1:A:1070:LYS:NZ	2.25	0.70
2:Y:134:THR:HG23	2:Y:153:PHE:HB3	1.73	0.70
1:A:794:LEU:HD21	1:A:824:PHE:CZ	2.26	0.70
1:B:1142:LEU:HD13	1:B:1187:THR:CG2	2.21	0.70
1:A:242:ASN:CB	1:A:245:ASN:O	2.39	0.70
1:A:367:ILE:HG21	1:A:466:TYR:CD2	2.26	0.70
1:B:1008:ALA:HB3	1:B:1078:LEU:HD11	1.71	0.70
1:B:1279:ARG:HD3	1:B:1284:PHE:CG	2.27	0.70
1:B:243:PHE:CE2	1:B:316:GLU:HG2	2.27	0.70
1:A:1202:HIS:HD2	1:A:1204:GLN:H	1.38	0.70
1:B:1377:PHE:CE1	1:B:1467:ILE:HD12	2.27	0.70
1:B:1423:VAL:HG21	1:B:1496:TYR:HE1	1.56	0.70
2:X:183:THR:O	2:X:230:GLN:HA	1.92	0.70
1:A:1449:LEU:HG	1:A:1450:PHE:CE1	2.26	0.70
1:B:1435:ASN:ND2	1:B:1478:ARG:HE	1.90	0.70
1:B:1488:LEU:O	1:B:1488:LEU:HD12	1.92	0.70
1:A:599:TRP:HB2	1:A:804:ILE:O	1.92	0.70
1:B:1219:LYS:HB2	1:B:1225:TYR:HB2	1.72	0.70
1:B:1317:TYR:HB3	1:B:1344:ASP:OD2	1.92	0.70
1:B:354:LEU:N	1:B:354:LEU:CD2	2.53	0.70
1:A:1078:LEU:O	1:A:1078:LEU:HD23	1.92	0.69
1:A:367:ILE:HG21	1:A:466:TYR:HD2	1.56	0.69
1:A:774:LEU:HD11	1:A:788:PHE:CZ	2.27	0.69
1:A:968:VAL:O	1:A:971:THR:HG23	1.92	0.69
1:B:1217:LEU:C	1:B:1218:VAL:HG22	2.11	0.69
1:B:1449:LEU:HG	1:B:1450:PHE:CE1	2.26	0.69
1:B:396:ASP:OD1	1:B:398:ASN:HB2	1.92	0.69
1:B:585:GLY:O	1:B:789:ALA:HB1	1.92	0.69
1:A:244:LYS:HE3	1:A:304:GLU:OE1	1.92	0.69
1:A:560:TRP:CH2	1:A:562:ASN:HB2	2.27	0.69
1:A:717:ARG:HD3	1:A:1449:LEU:HA	1.72	0.69
1:B:577:PRO:HD2	1:B:588:VAL:HG23	1.73	0.69
1:A:554:LEU:HB3	1:A:642:ASN:OD1	1.91	0.69
1:A:1435:ASN:ND2	1:A:1478:ARG:HE	1.90	0.69
1:A:492:TYR:HD2	1:A:493:ILE:H	1.38	0.69
1:A:719:SER:O	1:A:721:GLY:N	2.25	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:PHE:HA	1:A:915:GLU:O	1.91	0.69
1:B:194:PRO:O	1:B:1070:LYS:NZ	2.25	0.69
1:B:191:PRO:HG2	1:B:194:PRO:HB3	1.75	0.69
1:A:1279:ARG:HG3	1:A:1284:PHE:HB2	1.74	0.69
1:B:1069:TRP:HE1	1:B:1463:GLN:NE2	1.89	0.69
1:B:1300:TYR:CZ	1:B:1304:VAL:HG21	2.27	0.69
1:B:1421:HIS:HE1	1:B:1498:TYR:CD2	2.10	0.69
1:B:428:VAL:HG22	1:B:429:THR:H	1.57	0.69
1:B:85:LEU:HD22	1:B:85:LEU:H	1.57	0.69
1:A:1239:VAL:O	1:A:1241:ASN:N	2.26	0.69
1:B:242:ASN:ND2	1:B:242:ASN:N	2.41	0.69
1:B:994:GLN:NE2	1:B:998:ASN:HB3	2.06	0.69
1:A:1180:LEU:HD12	1:A:1204:GLN:HE22	1.55	0.69
1:A:1255:LEU:HD22	1:A:1270:VAL:CG1	2.22	0.69
1:A:180:ILE:HG21	1:A:599:TRP:CE2	2.28	0.69
1:A:1000:LEU:HD12	1:A:1017:PRO:HG3	1.75	0.69
1:B:1218:VAL:HG12	1:B:1226:ARG:HA	1.74	0.69
1:B:1249:GLU:HB2	1:B:1289:ASP:HB3	1.75	0.69
1:B:1348:VAL:HG21	1:B:1359:VAL:HG11	1.75	0.69
1:B:609:VAL:CG2	1:B:610:TYR:H	1.91	0.69
1:B:99:VAL:HB	1:B:121:TYR:OH	1.93	0.69
1:A:1027:THR:HG22	1:A:1302:LEU:HD21	1.74	0.69
1:A:1039:LEU:O	1:A:1042:LYS:HB3	1.93	0.69
1:A:1490:PRO:HB3	1:A:1509:TYR:O	1.92	0.69
1:A:625:GLN:O	1:A:629:LYS:HE2	1.93	0.69
1:A:641:ASN:H	1:A:644:ASN:HB3	1.57	0.69
1:B:1491:ALA:HB3	1:B:1509:TYR:HE2	1.56	0.69
1:B:588:VAL:HG11	1:B:790:LEU:HD11	1.75	0.69
1:B:686:ILE:O	1:B:689:LYS:HG2	1.92	0.69
1:A:1079:THR:HG21	1:A:1106:TRP:CE3	2.27	0.69
1:A:271:ILE:O	1:A:280:LYS:HB2	1.93	0.69
1:A:307:VAL:HG11	1:A:313:TYR:HB2	1.74	0.69
1:A:429:THR:OG1	1:A:430:VAL:N	2.20	0.69
1:B:199:TRP:HB2	1:B:217:PHE:O	1.93	0.69
1:B:488:PRO:O	1:B:491:PRO:HD2	1.93	0.69
1:A:1300:TYR:CZ	1:A:1304:VAL:HG21	2.28	0.68
1:A:977:LEU:HA	1:A:1361:VAL:HG23	1.75	0.68
1:A:1487:PHE:N	1:A:1487:PHE:CD2	2.60	0.68
2:Y:166:ASP:CG	2:Y:201:ILE:HD13	2.13	0.68
1:A:620:LEU:HD13	1:A:811:VAL:H	1.59	0.68
1:B:1104:LEU:HD13	1:B:1164:ILE:HD13	1.75	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1348:VAL:HG11	1:B:1359:VAL:CG2	2.22	0.68
1:B:227:PHE:HB3	1:B:254:TYR:HD2	1.57	0.68
1:B:315:LEU:CB	1:B:318:LEU:HB2	2.24	0.68
1:B:492:TYR:HD2	1:B:493:ILE:N	1.91	0.68
1:B:947:ARG:O	1:B:949:ILE:N	2.25	0.68
2:Y:142:TYR:HB2	2:Y:145:ASN:HB2	1.74	0.68
2:Y:140:LYS:O	2:Y:146:LEU:HD23	1.94	0.68
1:A:628:GLU:C	1:A:629:LYS:HD3	2.14	0.68
1:B:1487:PHE:N	1:B:1487:PHE:CD2	2.61	0.68
1:B:915:GLU:OE2	1:B:920:LYS:HE3	1.93	0.68
1:B:131:ASP:OD1	1:B:132:LYS:N	2.25	0.68
1:B:617:LYS:HE3	1:B:625:GLN:NE2	2.08	0.68
1:A:1334:LEU:HD22	1:A:1334:LEU:H	1.58	0.68
1:A:823:VAL:HG22	1:A:847:ASN:HA	1.76	0.68
1:A:1183:GLN:C	1:A:1232:LEU:HD22	2.14	0.68
1:A:1429:PRO:HB2	1:A:1432:ILE:HG13	1.75	0.68
1:A:297:ALA:O	1:A:298:GLN:HG3	1.93	0.68
1:B:1019:PHE:CE2	1:B:1020:TYR:CE1	2.82	0.68
1:B:1019:PHE:HE2	1:B:1088:GLN:HE21	1.38	0.68
1:B:478:VAL:HG11	1:B:566:LYS:HD3	1.75	0.68
1:B:151:ASP:OD2	1:B:508:LYS:NZ	2.27	0.68
1:A:498:HIS:HB3	1:A:514:THR:CG2	2.24	0.68
1:B:1271:ILE:C	1:B:1271:ILE:HD12	2.14	0.68
1:B:644:ASN:ND2	1:B:648:LEU:HD12	2.09	0.68
1:B:653:PHE:HD2	1:B:653:PHE:N	1.92	0.68
2:X:189:ILE:O	2:X:200:GLU:HA	1.93	0.68
1:A:1029:ASN:O	1:A:1029:ASN:ND2	2.27	0.68
1:A:1219:LYS:HB2	1:A:1225:TYR:HB2	1.74	0.68
1:B:44:TYR:CE1	1:B:497:THR:HG21	2.29	0.68
1:A:29:LYS:O	1:A:30:ILE:HD13	1.94	0.68
1:A:412:ARG:HD2	1:A:415:ASP:CB	2.24	0.68
1:B:820:PHE:CE2	1:B:848:TYR:HD2	2.11	0.68
1:B:986:GLU:OE2	1:B:986:GLU:HA	1.92	0.68
1:A:1132:THR:CB	1:A:1134:PRO:HD2	2.24	0.68
1:A:1378:TYR:CZ	1:A:1409:LYS:HE3	2.29	0.68
1:A:182:ILE:HG12	1:A:804:ILE:HD11	1.74	0.68
1:A:231:ILE:HD13	1:A:342:ILE:HG13	1.76	0.68
1:A:561:LEU:O	1:A:563:ILE:HG22	1.94	0.68
1:B:244:LYS:HE3	1:B:304:GLU:OE1	1.94	0.68
1:B:425:PRO:O	1:B:427:GLY:N	2.27	0.68
1:B:968:VAL:HG12	1:B:1368:THR:CG2	2.11	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:189:ILE:HD11	2:X:203:LEU:HD21	1.76	0.68
1:A:1157:ASP:O	1:A:1160:PRO:HD3	1.94	0.67
1:A:131:ASP:CG	1:A:132:LYS:N	2.48	0.67
1:A:1491:ALA:HB3	1:A:1509:TYR:HE2	1.58	0.67
1:A:488:PRO:O	1:A:491:PRO:HD2	1.94	0.67
1:A:541:LEU:HD12	1:A:645:VAL:HG12	1.76	0.67
1:A:62:LYS:HD3	1:A:105:GLU:OE2	1.92	0.67
1:B:520:ASP:CG	1:B:521:ALA:H	1.97	0.67
1:B:600:VAL:O	1:B:777:VAL:HG13	1.93	0.67
1:B:835:ARG:CG	1:B:835:ARG:HH11	2.06	0.67
1:A:1142:LEU:HD13	1:A:1187:THR:CG2	2.24	0.67
1:A:1494:THR:HB	1:A:1506:THR:HG23	1.77	0.67
1:A:302:ASP:OD2	1:A:304:GLU:HB2	1.93	0.67
1:B:532:GLN:O	1:B:535:VAL:HG13	1.94	0.67
1:A:109:LYS:HD2	1:A:110:HIS:N	2.09	0.67
1:B:1184:SER:HA	1:B:1232:LEU:HB2	1.76	0.67
1:B:249:THR:HG23	1:B:298:GLN:NE2	2.08	0.67
2:X:153:PHE:HE1	2:X:168:LYS:HB3	1.59	0.67
1:A:1150:ILE:HD11	1:A:1190:ILE:HG23	1.74	0.67
1:A:1218:VAL:HG12	1:A:1225:TYR:O	1.95	0.67
1:A:1278:GLN:NE2	1:A:1278:GLN:HA	2.09	0.67
1:A:157:ARG:O	1:A:178:ASP:HB2	1.94	0.67
1:A:316:GLU:O	1:A:317:ASP:C	2.33	0.67
1:A:354:LEU:HD22	1:A:354:LEU:N	2.10	0.67
1:A:504:LEU:HD21	1:A:651:LEU:HG	1.75	0.67
1:A:51:ASP:OD2	1:A:70:HIS:NE2	2.27	0.67
1:B:1183:GLN:C	1:B:1232:LEU:HD22	2.15	0.67
1:B:1244:THR:HB	1:B:1247:MET:CB	2.23	0.67
1:B:271:ILE:O	1:B:280:LYS:HB2	1.93	0.67
1:B:620:LEU:HD13	1:B:811:VAL:H	1.60	0.67
1:B:932:GLU:N	1:B:932:GLU:OE1	2.28	0.67
1:A:1249:GLU:HB2	1:A:1289:ASP:HB3	1.76	0.67
1:A:1323:LEU:CD1	1:A:1324:HIS:H	2.07	0.67
1:B:1111:TYR:CE1	1:B:1121:ASN:HB2	2.30	0.67
2:X:143:GLY:C	2:X:145:ASN:H	1.97	0.67
2:Y:183:THR:O	2:Y:230:GLN:HA	1.94	0.67
1:A:412:ARG:CD	1:A:415:ASP:HB2	2.23	0.67
1:A:99:VAL:HB	1:A:121:TYR:OH	1.94	0.67
1:B:1025:LEU:HD13	1:B:1031:TRP:CZ3	2.30	0.67
1:B:1296:GLY:O	1:B:1298:THR:N	2.27	0.67
1:A:292:LEU:HD13	1:A:293:ILE:N	2.09	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:PHE:CE2	1:A:848:TYR:HD2	2.13	0.67
1:A:859:MET:HB2	1:A:912:PHE:CE1	2.30	0.67
1:B:1019:PHE:CE2	1:B:1020:TYR:HE1	2.13	0.67
1:B:350:SER:CB	1:B:446:ASN:O	2.43	0.67
1:B:528:ILE:N	1:B:528:ILE:HD12	2.08	0.67
2:Y:189:ILE:HD11	2:Y:203:LEU:HD21	1.76	0.67
1:A:227:PHE:O	1:A:338:GLU:HG2	1.95	0.67
1:A:375:VAL:HG12	1:A:383:VAL:HG13	1.77	0.67
1:A:23:TYR:CE1	1:A:656:ASN:HB2	2.30	0.67
2:X:134:THR:HG23	2:X:153:PHE:HB3	1.76	0.67
1:A:354:LEU:CD2	1:A:354:LEU:N	2.57	0.67
1:A:947:ARG:HB2	1:A:949:ILE:HG13	1.77	0.67
1:B:1079:THR:HG21	1:B:1106:TRP:CE3	2.30	0.67
1:B:1323:LEU:CD1	1:B:1324:HIS:H	2.08	0.67
1:B:837:GLU:HG2	1:B:1487:PHE:O	1.95	0.67
1:B:386:VAL:O	1:B:411:THR:HG22	1.94	0.67
1:B:702:GLY:HA2	1:B:728:PHE:CE1	2.30	0.67
1:B:856:CYS:HB3	1:B:915:GLU:HB2	1.76	0.67
1:A:1090:ASN:ND2	1:A:1158:ILE:HD13	2.08	0.66
1:A:1003:LEU:HD13	1:A:1498:TYR:CE1	2.30	0.66
1:A:160:VAL:HG22	1:A:174:VAL:C	2.16	0.66
1:A:855:PHE:CE1	1:A:886:GLN:HB3	2.28	0.66
1:B:700:TYR:CE1	1:B:758:LEU:HB2	2.29	0.66
1:B:859:MET:HB2	1:B:912:PHE:CE1	2.31	0.66
2:X:166:ASP:CG	2:X:201:ILE:HD13	2.14	0.66
2:Y:224:ILE:O	2:Y:225:GLU:HG3	1.95	0.66
1:A:1217:LEU:C	1:A:1218:VAL:HG22	2.14	0.66
1:A:1425:ASP:HB3	1:A:1494:THR:HG23	1.77	0.66
1:A:837:GLU:OE2	1:A:1488:LEU:HB2	1.95	0.66
1:A:617:LYS:HE3	1:A:625:GLN:NE2	2.10	0.66
1:B:719:SER:O	1:B:721:GLY:N	2.28	0.66
1:B:977:LEU:HA	1:B:1361:VAL:CG2	2.24	0.66
1:A:242:ASN:H	1:A:242:ASN:ND2	1.92	0.66
1:A:520:ASP:CG	1:A:521:ALA:H	1.99	0.66
1:A:835:ARG:CZ	1:A:905:ILE:HD11	2.26	0.66
1:B:123:ASN:HD22	1:B:123:ASN:C	1.99	0.66
1:B:1244:THR:HB	1:B:1247:MET:HB2	1.77	0.66
2:Y:167:PHE:O	2:Y:171:GLN:HB2	1.95	0.66
1:A:352:TYR:HA	1:A:376:LYS:O	1.94	0.66
1:A:73:LEU:H	1:A:73:LEU:HD23	1.60	0.66
1:A:1068:VAL:CG1	1:A:1069:TRP:H	1.99	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1115:ASN:ND2	1:A:1117:SER:H	1.94	0.66
1:B:1328:MET:O	1:B:1329:THR:HG23	1.96	0.66
1:B:1334:LEU:HD22	1:B:1334:LEU:H	1.60	0.66
1:A:1054:LEU:O	1:A:1056:ILE:N	2.29	0.66
1:A:1279:ARG:CB	1:A:1284:PHE:HB2	2.25	0.66
1:A:1024:TYR:OH	1:A:1306:GLN:NE2	2.29	0.66
1:B:1379:LEU:HD21	1:B:1495:VAL:HG11	1.75	0.66
1:B:831:TYR:CE1	1:B:1457:ASP:HB3	2.31	0.66
2:Y:162:LEU:CD1	2:Y:165:LEU:HD23	2.26	0.66
1:A:1136:GLU:OE1	1:A:1415:SER:CB	2.43	0.66
1:A:77:ASN:ND2	1:A:81:ASN:ND2	2.43	0.66
1:A:837:GLU:HG2	1:A:1488:LEU:HA	1.77	0.66
1:B:1008:ALA:HB3	1:B:1078:LEU:CD1	2.26	0.66
1:B:109:LYS:HD2	1:B:110:HIS:N	2.10	0.66
1:B:291:MET:O	1:B:293:ILE:HG13	1.95	0.66
1:A:1025:LEU:HD13	1:A:1031:TRP:CZ3	2.31	0.66
1:A:113:LYS:HG3	1:A:114:SER:H	1.61	0.66
1:A:28:PRO:HB2	1:A:30:ILE:O	1.95	0.66
1:A:315:LEU:HB2	1:A:318:LEU:HB2	1.78	0.66
1:B:1144:LEU:O	1:B:1148:THR:HG22	1.96	0.66
1:B:1150:ILE:HD11	1:B:1190:ILE:HG23	1.75	0.66
1:B:415:ASP:CG	1:B:417:VAL:HB	2.16	0.66
1:A:161:LEU:HG	1:A:185:PHE:CE1	2.31	0.66
1:A:308:LYS:HG2	1:A:314:SER:HA	1.78	0.66
1:A:857:VAL:HG21	1:A:896:VAL:HG11	1.78	0.66
1:B:1380:LYS:HG3	1:B:1405:CYS:SG	2.36	0.66
1:B:1245:ALA:HB2	1:B:1501:PRO:HD2	1.77	0.66
1:B:315:LEU:HD12	1:B:318:LEU:HD12	1.76	0.66
1:B:364:LYS:HG2	1:B:465:LEU:O	1.94	0.66
1:B:395:ILE:O	1:B:429:THR:HG23	1.96	0.66
1:B:629:LYS:HD3	1:B:629:LYS:N	2.10	0.66
1:B:839:ILE:CG2	1:B:900:VAL:HG23	2.26	0.66
2:X:143:GLY:O	2:X:145:ASN:N	2.28	0.66
1:A:1104:LEU:HD13	1:A:1164:ILE:HD13	1.77	0.66
1:A:1503:LYS:N	1:A:1503:LYS:HD2	2.10	0.66
1:A:317:ASP:C	1:A:319:ASN:H	1.97	0.66
1:A:350:SER:HB2	1:A:446:ASN:O	1.95	0.66
1:A:927:LEU:HD22	1:A:929:VAL:HG22	1.76	0.66
1:A:946:PRO:HB3	1:A:1352:PHE:O	1.96	0.66
1:B:1203:PRO:O	1:B:1206:ARG:HB2	1.96	0.66
1:B:1422:ALA:O	1:B:1464:LEU:HD12	1.96	0.66

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:SER:HB2	1:B:446:ASN:O	1.95	0.66
1:B:708:ASP:OD2	1:B:1401:ARG:NH2	2.29	0.66
1:A:350:SER:CB	1:A:446:ASN:O	2.44	0.65
1:A:563:ILE:HG13	1:A:564:GLU:N	2.10	0.65
1:B:1020:TYR:HD2	1:B:1294:ILE:HG22	1.60	0.65
1:B:1024:TYR:OH	1:B:1306:GLN:NE2	2.29	0.65
1:B:182:ILE:HG12	1:B:804:ILE:HD11	1.76	0.65
1:B:249:THR:CG2	1:B:298:GLN:HE21	2.09	0.65
1:B:503:ILE:HG12	1:B:540:LEU:HB3	1.78	0.65
2:X:162:LEU:CD1	2:X:165:LEU:HD23	2.26	0.65
1:A:700:TYR:CE1	1:A:758:LEU:HB2	2.31	0.65
1:B:1202:HIS:CD2	1:B:1204:GLN:HB3	2.31	0.65
1:B:243:PHE:CE1	1:B:316:GLU:HG2	2.31	0.65
1:B:364:LYS:HD2	1:B:364:LYS:N	2.11	0.65
1:B:987:ILE:HD11	1:B:1294:ILE:HD13	1.77	0.65
1:A:1239:VAL:HG23	1:A:1239:VAL:O	1.95	0.65
1:A:1020:TYR:HD2	1:A:1294:ILE:HG22	1.61	0.65
1:A:156:LYS:O	1:A:157:ARG:CG	2.41	0.65
1:A:617:LYS:CE	1:A:625:GLN:HE22	2.09	0.65
1:B:1028:GLY:O	1:B:1029:ASN:C	2.33	0.65
1:B:1378:TYR:CZ	1:B:1409:LYS:HE3	2.31	0.65
1:B:492:TYR:HD2	1:B:493:ILE:H	1.41	0.65
2:X:189:ILE:HG23	2:X:226:VAL:HG22	1.76	0.65
1:A:952:THR:OG1	1:A:953:ILE:N	2.29	0.65
1:B:1213:LYS:HE3	1:B:1266:TYR:CE2	2.32	0.65
1:B:1320:LYS:HD2	1:B:1321:GLY:H	1.62	0.65
1:B:583:SER:OG	1:B:586:GLN:HB2	1.97	0.65
2:Y:143:GLY:C	2:Y:145:ASN:H	1.99	0.65
1:A:1221:ASN:HA	1:A:1222:PRO:C	2.17	0.65
1:A:1379:LEU:HD21	1:A:1495:VAL:HG11	1.78	0.65
1:A:394:THR:HG22	1:A:402:SER:OG	1.96	0.65
1:A:968:VAL:O	1:A:968:VAL:HG23	1.95	0.65
1:B:1263:ASP:O	1:B:1265:ASN:N	2.30	0.65
1:B:242:ASN:HB3	1:B:245:ASN:OD1	1.96	0.65
1:B:238:ILE:HG12	1:B:246:PHE:CE1	2.32	0.65
1:A:1008:ALA:HB2	1:A:1059:TYR:CD2	2.31	0.65
1:A:1076:THR:CG2	1:A:1120:GLU:HA	2.27	0.65
1:A:856:CYS:O	1:A:914:LEU:HA	1.97	0.65
1:B:1003:LEU:HD13	1:B:1498:TYR:CE1	2.31	0.65
1:B:1115:ASN:HD22	1:B:1115:ASN:C	1.99	0.65
1:B:1445:GLY:O	1:B:1448:GLN:HB3	1.96	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:146:LEU:O	2:X:146:LEU:HD13	1.96	0.65
1:A:712:GLU:HA	1:A:715:ALA:HB3	1.78	0.65
1:A:43:VAL:CG1	1:A:79:PHE:HB3	2.26	0.65
1:B:934:VAL:HG22	1:B:1366:HIS:CD2	2.32	0.65
1:B:227:PHE:HZ	1:B:329:VAL:O	1.80	0.65
1:B:628:GLU:C	1:B:629:LYS:HD3	2.16	0.65
1:B:683:ILE:HD13	1:B:735:ALA:HB2	1.77	0.65
2:Y:146:LEU:HD11	2:Y:148:ALA:HB2	1.78	0.65
1:A:1227:PHE:HA	1:A:1228:TRP:CE3	2.32	0.65
1:A:160:VAL:HG23	1:A:175:GLU:HB3	1.79	0.65
1:A:360:PRO:HA	1:A:636:ALA:HB3	1.79	0.65
1:A:987:ILE:HD13	1:A:1294:ILE:HG23	1.77	0.65
1:B:163:PHE:CD1	1:B:163:PHE:N	2.65	0.65
1:B:160:VAL:HG22	1:B:174:VAL:C	2.17	0.65
1:A:1465:ASN:ND2	1:A:1465:ASN:H	1.95	0.65
1:A:157:ARG:H	1:A:178:ASP:CB	2.10	0.65
1:A:307:VAL:CG1	1:A:313:TYR:HB2	2.27	0.65
1:B:1148:THR:O	1:B:1152:ILE:HG13	1.97	0.65
1:B:1279:ARG:CB	1:B:1284:PHE:HB2	2.27	0.65
1:B:1284:PHE:HD2	1:B:1285:TYR:CE1	2.15	0.65
1:A:1342:LEU:C	1:A:1343:ASN:HD22	2.01	0.64
1:B:1047:LYS:O	1:B:1049:LEU:N	2.30	0.64
1:B:1007:SER:HA	1:B:1069:TRP:CD1	2.32	0.64
1:B:1105:LEU:HA	1:B:1108:VAL:CG1	2.27	0.64
1:B:1218:VAL:CG1	1:B:1226:ARG:HA	2.27	0.64
1:B:1239:VAL:HG23	1:B:1239:VAL:O	1.96	0.64
1:B:123:ASN:ND2	1:B:150:ASP:H	1.95	0.64
1:B:498:HIS:HD2	1:B:516:GLU:HA	1.61	0.64
1:A:982:LEU:HD23	1:A:1309:LEU:HD11	1.78	0.64
1:A:536:PRO:HG3	1:A:624:PHE:HE2	1.61	0.64
1:B:1029:ASN:ND2	1:B:1029:ASN:O	2.30	0.64
1:B:1255:LEU:HD21	1:B:1271:ILE:CG2	2.24	0.64
2:Y:189:ILE:HG23	2:Y:226:VAL:HG22	1.78	0.64
2:Y:140:LYS:HA	2:Y:228:LEU:HB2	1.79	0.64
1:A:1000:LEU:HD12	1:A:1017:PRO:CG	2.27	0.64
1:A:1274:LEU:HB3	1:A:1297:LEU:HD11	1.78	0.64
1:A:169:SER:O	1:A:170:GLU:O	2.15	0.64
1:A:835:ARG:NH2	1:A:905:ILE:HD11	2.13	0.64
1:B:976:ILE:HD12	1:B:1362:THR:CG2	2.27	0.64
1:B:975:ARG:HG3	1:B:1340:VAL:HB	1.79	0.64
1:A:1213:LYS:HE3	1:A:1266:TYR:CE2	2.33	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ARG:HB2	1:B:253:ARG:CZ	2.27	0.64
1:B:62:LYS:HD3	1:B:105:GLU:OE2	1.98	0.64
1:B:838:GLN:O	1:B:1486:GLY:N	2.30	0.64
1:B:906:GLY:O	1:B:908:HIS:CE1	2.51	0.64
1:B:1019:PHE:HE2	1:B:1020:TYR:HE1	1.46	0.64
1:B:515:ARG:HH22	1:B:527:ASN:N	1.96	0.64
1:B:554:LEU:HB3	1:B:642:ASN:OD1	1.97	0.64
1:A:1053:MET:CE	1:A:1086:LEU:HD13	2.26	0.64
1:A:1079:THR:HG21	1:A:1106:TRP:HE3	1.62	0.64
1:A:517:LYS:HA	1:A:524:GLN:HE22	1.62	0.64
1:A:598:SER:HA	1:A:805:SER:OG	1.98	0.64
1:B:1104:LEU:HD22	1:B:1152:ILE:HG23	1.79	0.64
1:B:1161:LEU:HB3	1:B:1164:ILE:HG23	1.79	0.64
1:A:1083:LEU:HD11	1:A:1107:LEU:HD11	1.80	0.64
1:B:364:LYS:CD	1:B:364:LYS:N	2.60	0.64
1:B:956:ARG:HG3	1:B:1349:SER:CB	2.27	0.64
2:X:169:ILE:HG21	2:X:189:ILE:HD13	1.79	0.64
1:A:1090:ASN:HD22	1:A:1158:ILE:CD1	2.08	0.64
1:A:1379:LEU:HD13	1:A:1493:PHE:CE2	2.33	0.64
1:A:835:ARG:HD3	1:A:903:LEU:O	1.98	0.64
1:A:839:ILE:CG2	1:A:900:VAL:HG23	2.28	0.64
1:A:906:GLY:O	1:A:908:HIS:CE1	2.50	0.64
1:B:1316:SER:O	1:B:1346:LEU:HD12	1.98	0.64
1:B:160:VAL:HG23	1:B:175:GLU:HB3	1.78	0.64
1:B:319:ASN:ND2	1:B:347:TYR:CG	2.65	0.64
1:B:653:PHE:H	1:B:653:PHE:HD2	1.43	0.64
1:B:679:LEU:HD22	1:B:738:LEU:HD11	1.80	0.64
1:A:31:PHE:HB2	1:A:119:ILE:HB	1.79	0.64
1:A:50:PHE:CG	1:A:109:LYS:HE2	2.33	0.64
1:A:686:ILE:O	1:A:689:LYS:HG2	1.97	0.64
1:B:31:PHE:CZ	1:B:104:LEU:HD13	2.33	0.64
1:B:1162:VAL:HG23	1:B:1163:LYS:N	2.10	0.64
1:B:1142:LEU:HD13	1:B:1187:THR:HG22	1.79	0.64
1:B:1379:LEU:HD22	1:B:1493:PHE:CE2	2.32	0.64
1:B:50:PHE:CG	1:B:109:LYS:HE2	2.32	0.64
1:B:835:ARG:NH1	1:B:835:ARG:HG2	2.12	0.64
1:A:1105:LEU:HA	1:A:1108:VAL:CG1	2.28	0.64
1:B:119:ILE:HG13	1:B:120:THR:N	2.13	0.64
1:B:1213:LYS:HE3	1:B:1266:TYR:CD2	2.33	0.64
1:B:363:LEU:HD23	1:B:454:ALA:HB3	1.77	0.64
1:B:412:ARG:HD2	1:B:415:ASP:CB	2.27	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:LEU:O	1:B:540:LEU:HA	1.98	0.64
1:B:641:ASN:O	1:B:644:ASN:N	2.31	0.64
1:A:159:THR:HG22	1:A:160:VAL:N	2.14	0.63
1:A:544:TYR:HD1	1:A:544:TYR:H	1.45	0.63
1:B:490:SER:O	1:B:491:PRO:C	2.34	0.63
1:B:493:ILE:HG23	1:B:494:ASP:N	2.13	0.63
1:A:1381:ILE:HD12	1:A:1493:PHE:HB2	1.81	0.63
1:B:85:LEU:O	1:B:86:THR:HB	1.97	0.63
1:A:583:SER:OG	1:A:586:GLN:HB2	1.98	0.63
1:A:856:CYS:HB3	1:A:915:GLU:HB2	1.80	0.63
1:B:1132:THR:CB	1:B:1134:PRO:HD2	2.28	0.63
1:B:717:ARG:CD	1:B:1449:LEU:HA	2.29	0.63
1:B:42:GLN:HB2	1:B:80:GLN:CG	2.28	0.63
1:A:1232:LEU:O	1:A:1233:GLN:HG2	1.99	0.63
1:A:263:ALA:HB3	1:A:292:LEU:HB3	1.81	0.63
1:B:113:LYS:HG3	1:B:114:SER:N	2.13	0.63
1:B:441:ASP:OD2	1:B:441:ASP:N	2.30	0.63
1:A:1202:HIS:O	1:A:1203:PRO:C	2.37	0.63
1:A:1255:LEU:HD21	1:A:1271:ILE:CG2	2.28	0.63
1:A:23:TYR:HE1	1:A:656:ASN:HB2	1.62	0.63
1:A:491:PRO:O	1:A:493:ILE:N	2.32	0.63
1:B:1378:TYR:O	1:B:1406:ALA:HA	1.99	0.63
1:B:180:ILE:HG21	1:B:599:TRP:CE2	2.34	0.63
1:A:1113:LEU:HD12	1:A:1117:SER:OG	1.98	0.63
1:A:386:VAL:C	1:A:410:VAL:HG13	2.19	0.63
1:A:493:ILE:HG23	1:A:494:ASP:N	2.12	0.63
1:B:839:ILE:HD11	1:B:1483:PHE:CZ	2.34	0.63
1:B:491:PRO:O	1:B:493:ILE:N	2.32	0.63
1:B:653:PHE:CZ	1:B:660:ASP:CA	2.79	0.63
1:A:1128:LYS:NZ	1:A:1415:SER:HB3	2.14	0.63
1:A:1263:ASP:O	1:A:1265:ASN:N	2.31	0.63
1:A:857:VAL:HA	1:A:913:SER:O	1.98	0.63
1:B:1143:TYR:HE1	1:B:1186:PHE:CZ	2.16	0.63
1:B:710:THR:N	1:B:713:GLN:OE1	2.29	0.63
1:B:911:ASN:CG	1:B:924:VAL:HG13	2.19	0.63
2:Y:153:PHE:HE1	2:Y:168:LYS:HB3	1.64	0.63
1:A:101:TYR:HE1	1:A:116:ARG:CZ	2.12	0.63
1:A:1380:LYS:HG3	1:A:1405:CYS:SG	2.39	0.63
1:A:451:GLY:C	1:A:452:TYR:CD2	2.73	0.63
1:A:710:THR:N	1:A:713:GLN:OE1	2.29	0.63
1:A:906:GLY:H	1:A:929:VAL:HB	1.64	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1156:PHE:CD1	1:B:1164:ILE:HD11	2.34	0.63
1:B:1429:PRO:HB2	1:B:1432:ILE:HG13	1.81	0.63
1:B:295:GLY:C	1:B:296:ILE:HG12	2.19	0.63
1:B:571:LEU:HD21	1:B:600:VAL:HG13	1.81	0.63
1:A:1050:LYS:O	1:A:1053:MET:HB3	1.98	0.63
2:X:166:ASP:OD2	2:X:201:ILE:HG21	1.99	0.63
1:A:467:ILE:HD12	1:A:484:ILE:CD1	2.29	0.62
1:B:1315:VAL:HG22	1:B:1346:LEU:HD11	1.81	0.62
1:B:267:ILE:HG12	1:B:327:VAL:HG13	1.81	0.62
1:B:679:LEU:HB3	1:B:738:LEU:HD11	1.81	0.62
1:B:905:ILE:HD13	1:B:931:PRO:HG3	1.80	0.62
2:X:142:TYR:HB2	2:X:145:ASN:HB2	1.80	0.62
1:A:1205:PHE:O	1:A:1209:VAL:HG23	1.99	0.62
1:A:1273:TRP:CE3	1:A:1274:LEU:HD23	2.34	0.62
1:A:1378:TYR:O	1:A:1406:ALA:HA	2.00	0.62
1:A:730:GLU:O	1:A:734:VAL:HG23	1.99	0.62
1:B:269:PHE:HB2	1:B:283:MET:HE3	1.81	0.62
1:B:330:ILE:HG22	1:B:337:SER:OG	1.99	0.62
1:A:1218:VAL:HG12	1:A:1226:ARG:HA	1.79	0.62
1:A:295:GLY:C	1:A:296:ILE:HG12	2.19	0.62
1:A:307:VAL:HG12	1:A:313:TYR:O	1.98	0.62
1:A:796:THR:HA	1:A:818:LYS:HA	1.81	0.62
1:A:840:GLN:HG2	1:A:899:THR:HG22	1.82	0.62
1:A:92:LEU:N	1:A:93:PRO:CD	2.62	0.62
1:B:386:VAL:N	1:B:411:THR:HG23	2.14	0.62
1:B:610:TYR:CB	1:B:614:ARG:HD2	2.30	0.62
2:Y:146:LEU:HD13	2:Y:146:LEU:O	2.00	0.62
1:A:701:ASP:O	1:A:704:CYS:HB2	2.00	0.62
1:B:835:ARG:HD3	1:B:903:LEU:O	1.99	0.62
2:X:162:LEU:HD12	2:X:165:LEU:HD23	1.80	0.62
1:A:1162:VAL:HG23	1:A:1163:LYS:N	2.13	0.62
1:A:1248:VAL:HG21	1:A:1277:GLU:HG2	1.82	0.62
1:A:315:LEU:CB	1:A:318:LEU:HB2	2.30	0.62
1:A:1003:LEU:HD22	1:A:1004:PRO:HD2	1.80	0.62
1:A:315:LEU:O	1:A:316:GLU:O	2.17	0.62
1:B:133:PRO:O	1:B:134:VAL:CG2	2.43	0.62
1:B:375:VAL:HG12	1:B:383:VAL:HG13	1.81	0.62
1:B:361:LEU:O	1:B:454:ALA:HA	1.99	0.62
1:B:942:VAL:HG21	1:B:957:LYS:HB3	1.82	0.62
1:A:367:ILE:HG23	1:A:368:PRO:HD2	1.81	0.62
1:A:717:ARG:CD	1:A:1449:LEU:HA	2.30	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:PRO:HG3	1:B:624:PHE:HE2	1.63	0.62
1:A:1081:PHE:CE1	1:A:1288:GLN:NE2	2.66	0.62
1:A:1316:SER:O	1:A:1346:LEU:HD12	1.99	0.62
1:A:640:LEU:H	1:A:644:ASN:HB3	1.65	0.62
1:A:909:ASN:H	1:A:926:THR:HG22	1.65	0.62
1:B:1097:GLN:O	1:B:1099:SER:N	2.33	0.62
1:B:1202:HIS:O	1:B:1203:PRO:C	2.37	0.62
1:B:1279:ARG:CG	1:B:1284:PHE:HB2	2.30	0.62
2:X:140:LYS:O	2:X:146:LEU:HD23	2.00	0.62
1:A:364:LYS:HD2	1:A:364:LYS:H	1.62	0.62
1:A:490:SER:O	1:A:491:PRO:C	2.36	0.62
1:A:932:GLU:N	1:A:932:GLU:OE1	2.33	0.62
1:A:124:GLY:O	1:A:125:PHE:CD2	2.53	0.62
1:A:1255:LEU:CD2	1:A:1271:ILE:HG22	2.29	0.62
1:A:354:LEU:H	1:A:354:LEU:HD23	1.64	0.62
1:A:73:LEU:N	1:A:73:LEU:HD23	2.14	0.62
1:B:1050:LYS:O	1:B:1053:MET:HB3	1.99	0.62
1:B:829:ILE:CG1	1:B:925:LYS:HG2	2.29	0.62
2:X:153:PHE:CD2	2:X:154:SER:N	2.68	0.62
1:A:1127:ILE:HD12	1:A:1127:ILE:H	1.64	0.61
1:A:119:ILE:HG13	1:A:120:THR:N	2.15	0.61
1:A:1245:ALA:HB2	1:A:1501:PRO:HD2	1.82	0.61
1:B:1076:THR:CG2	1:B:1120:GLU:HA	2.30	0.61
1:B:131:ASP:CG	1:B:132:LYS:N	2.53	0.61
1:A:1379:LEU:HD22	1:A:1493:PHE:CE2	2.35	0.61
1:A:364:LYS:HG2	1:A:465:LEU:O	2.00	0.61
1:A:59:TYR:CB	1:A:60:PRO:CD	2.76	0.61
1:A:635:GLY:HA2	1:A:672:ILE:CG2	2.30	0.61
1:A:718:ILE:HG12	1:A:1446:VAL:O	2.01	0.61
1:B:1079:THR:HG21	1:B:1106:TRP:HE3	1.64	0.61
1:B:1337:PRO:O	1:B:1338:VAL:HG23	2.00	0.61
1:B:1432:ILE:O	1:B:1432:ILE:HG22	2.00	0.61
1:B:214:THR:HG22	1:B:215:ALA:N	2.15	0.61
1:B:947:ARG:HB2	1:B:949:ILE:HG13	1.82	0.61
1:A:1313:ILE:HG22	1:A:1314:ASP:N	2.16	0.61
1:A:1434:ALA:HB1	1:A:1477:PHE:HD1	1.63	0.61
1:A:866:CYS:O	1:A:900:VAL:HG12	2.00	0.61
1:A:994:GLN:HE22	1:A:998:ASN:CB	2.02	0.61
1:B:1146:ALA:O	1:B:1150:ILE:HG13	2.00	0.61
1:B:1425:ASP:HB3	1:B:1494:THR:HG23	1.82	0.61
1:B:30:ILE:CG2	1:B:31:PHE:N	2.64	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:GLY:N	1:B:411:THR:HG23	2.16	0.61
1:B:563:ILE:HG13	1:B:564:GLU:N	2.14	0.61
1:B:641:ASN:H	1:B:644:ASN:HB3	1.64	0.61
2:Y:178:GLY:O	2:Y:184:THR:HG21	1.99	0.61
1:B:1080:ALA:O	1:B:1083:LEU:N	2.33	0.61
1:B:1380:LYS:HE3	1:B:1405:CYS:SG	2.41	0.61
1:B:59:TYR:CB	1:B:60:PRO:CD	2.77	0.61
1:B:628:GLU:O	1:B:628:GLU:HG3	2.01	0.61
1:B:855:PHE:HA	1:B:915:GLU:O	1.99	0.61
1:B:909:ASN:HA	1:B:925:LYS:O	2.00	0.61
1:A:1161:LEU:HD12	1:A:1162:VAL:N	2.15	0.61
1:A:1226:ARG:CZ	1:A:1266:TYR:CE1	2.84	0.61
1:A:265:VAL:HG23	1:A:292:LEU:H	1.66	0.61
1:A:362:PHE:HA	1:A:455:ILE:H	1.64	0.61
1:A:629:LYS:HD3	1:A:629:LYS:N	2.14	0.61
1:B:599:TRP:HB2	1:B:804:ILE:O	2.01	0.61
1:A:1019:PHE:HE2	1:A:1020:TYR:HE1	1.48	0.61
1:A:1161:LEU:HD12	1:A:1162:VAL:HG22	1.81	0.61
1:A:1213:LYS:HE3	1:A:1266:TYR:CD2	2.36	0.61
1:A:1290:THR:O	1:A:1294:ILE:HG12	1.99	0.61
1:A:1434:ALA:HB1	1:A:1477:PHE:CE1	2.35	0.61
1:A:153:LYS:HB3	1:A:154:PRO:HD2	1.83	0.61
1:B:101:TYR:HE1	1:B:116:ARG:NE	1.97	0.61
1:B:322:TYR:N	1:B:322:TYR:HD2	1.98	0.61
1:B:464:TYR:H	1:B:491:PRO:HD3	1.65	0.61
1:B:92:LEU:N	1:B:93:PRO:CD	2.63	0.61
2:X:146:LEU:C	2:X:146:LEU:HD22	2.18	0.61
1:A:1104:LEU:HD22	1:A:1152:ILE:HG23	1.82	0.61
1:A:1435:ASN:O	1:A:1438:ASP:N	2.30	0.61
1:A:352:TYR:O	1:A:448:ALA:HB2	2.00	0.61
1:A:85:LEU:N	1:A:85:LEU:HD22	2.16	0.61
1:B:100:SER:O	1:B:101:TYR:HB2	2.01	0.61
1:B:1157:ASP:O	1:B:1160:PRO:HD3	2.01	0.61
1:B:1423:VAL:HG21	1:B:1496:TYR:CE1	2.35	0.61
1:B:1423:VAL:CG2	1:B:1496:TYR:CE1	2.83	0.61
1:B:161:LEU:HD11	1:B:185:PHE:CD1	2.35	0.61
1:B:362:PHE:HB3	1:B:455:ILE:O	2.00	0.61
1:B:73:LEU:HD12	1:B:79:PHE:HD2	1.65	0.61
1:B:92:LEU:H	1:B:93:PRO:HD3	1.65	0.61
2:Y:166:ASP:OD2	2:Y:201:ILE:HG21	2.01	0.61
1:A:1019:PHE:CE2	1:A:1020:TYR:CE1	2.88	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LYS:N	1:A:364:LYS:CD	2.61	0.61
1:B:1279:ARG:O	1:B:1280:TYR:C	2.38	0.61
1:B:610:TYR:HB3	1:B:614:ARG:HD2	1.83	0.61
1:A:106:VAL:HG12	1:A:107:VAL:N	2.16	0.61
1:A:131:ASP:OD1	1:A:132:LYS:N	2.33	0.61
1:A:1401:ARG:HB2	1:A:1478:ARG:HG2	1.83	0.61
1:A:1496:TYR:HD1	1:A:1496:TYR:O	1.83	0.61
1:A:293:ILE:N	1:A:296:ILE:O	2.22	0.61
1:A:386:VAL:N	1:A:411:THR:HG23	2.11	0.61
1:A:946:PRO:HD2	1:A:947:ARG:H	1.66	0.61
1:B:349:LEU:HD22	1:B:349:LEU:C	2.20	0.61
1:B:535:VAL:CG2	1:B:536:PRO:HD3	2.17	0.61
1:B:820:PHE:HZ	1:B:848:TYR:HB2	1.64	0.61
2:X:179:LEU:HD12	2:X:180:TYR:H	1.66	0.61
1:A:103:TYR:HA	1:A:115:LYS:O	2.01	0.61
1:A:113:LYS:HG3	1:A:114:SER:N	2.15	0.61
1:A:271:ILE:HG21	1:A:313:TYR:CE1	2.36	0.61
1:A:73:LEU:HD12	1:A:79:PHE:HD2	1.65	0.61
1:B:361:LEU:HB3	1:B:453:ARG:O	2.01	0.61
1:B:352:TYR:O	1:B:448:ALA:HB2	2.01	0.61
1:B:730:GLU:O	1:B:734:VAL:HG23	2.00	0.61
2:X:183:THR:HB	2:X:230:GLN:HB3	1.83	0.61
1:A:243:PHE:CE1	1:A:316:GLU:HG2	2.35	0.60
1:A:976:ILE:HG21	1:A:1280:TYR:HE1	1.65	0.60
1:B:1063:ASP:O	1:B:1064:TYR:HB2	2.01	0.60
1:B:982:LEU:CD2	1:B:1309:LEU:HD11	2.26	0.60
1:B:1381:ILE:HD13	1:B:1509:TYR:CE1	2.36	0.60
1:B:321:LYS:C	1:B:322:TYR:HD2	2.05	0.60
1:B:386:VAL:C	1:B:410:VAL:HG13	2.21	0.60
2:Y:143:GLY:O	2:Y:145:ASN:N	2.33	0.60
1:B:1313:ILE:HG22	1:B:1314:ASP:N	2.16	0.60
1:B:371:ILE:HD12	1:B:390:LEU:CD2	2.31	0.60
1:A:1076:THR:HG21	1:A:1120:GLU:HA	1.83	0.60
1:A:1278:GLN:CA	1:A:1278:GLN:HE21	2.13	0.60
1:B:1202:HIS:CD2	1:B:1204:GLN:H	2.06	0.60
1:B:307:VAL:HG11	1:B:313:TYR:HB2	1.83	0.60
1:B:438:ASP:O	1:B:439:ALA:C	2.39	0.60
1:A:498:HIS:HB3	1:A:514:THR:HG21	1.83	0.60
1:A:948:GLY:HA2	1:A:952:THR:O	2.01	0.60
1:B:113:LYS:HG3	1:B:114:SER:H	1.66	0.60
1:B:29:LYS:O	1:B:30:ILE:HD13	2.02	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:GLY:C	1:B:452:TYR:CD2	2.75	0.60
1:B:835:ARG:HH21	1:B:905:ILE:HD11	1.64	0.60
2:Y:179:LEU:HD12	2:Y:180:TYR:H	1.67	0.60
1:A:250:ILE:HG13	1:A:250:ILE:O	2.01	0.60
1:A:505:SER:HB3	1:A:510:ILE:HD11	1.82	0.60
1:A:855:PHE:CZ	1:A:886:GLN:CB	2.73	0.60
1:B:243:PHE:CE2	1:B:316:GLU:CG	2.85	0.60
1:B:840:GLN:HG2	1:B:899:THR:CG2	2.25	0.60
1:A:1023:HIS:O	1:A:1027:THR:HB	2.01	0.60
1:A:1146:ALA:O	1:A:1150:ILE:HG13	2.01	0.60
1:A:242:ASN:ND2	1:A:242:ASN:N	2.49	0.60
1:A:352:TYR:HD1	1:A:375:VAL:CG1	2.14	0.60
1:A:802:ILE:HD11	1:A:804:ILE:HG23	1.84	0.60
1:A:857:VAL:HG12	1:A:914:LEU:HB3	1.84	0.60
1:B:308:LYS:HG2	1:B:314:SER:HA	1.83	0.60
1:B:354:LEU:HD12	1:B:435:VAL:HG11	1.82	0.60
1:B:735:ALA:HB1	1:B:754:MET:HE1	1.81	0.60
1:B:982:LEU:HD23	1:B:1309:LEU:CD1	2.25	0.60
2:X:178:GLY:O	2:X:184:THR:HG21	2.01	0.60
1:A:653:PHE:H	1:A:653:PHE:HD2	1.41	0.60
1:B:185:PHE:HB3	1:B:186:PRO:CD	2.31	0.60
1:B:392:ALA:CB	1:B:404:LEU:HD12	2.32	0.60
1:B:511:HIS:HE2	1:B:531:THR:HG21	1.66	0.60
1:B:605:VAL:HG12	1:B:606:ASP:N	2.16	0.60
1:B:903:LEU:N	1:B:903:LEU:HD22	2.16	0.60
1:A:1028:GLY:O	1:A:1029:ASN:C	2.40	0.60
1:A:269:PHE:HB2	1:A:283:MET:CE	2.32	0.60
1:A:394:THR:HG23	1:A:395:ILE:N	2.16	0.60
1:A:653:PHE:N	1:A:653:PHE:HD2	1.94	0.60
1:B:29:LYS:HE2	1:B:666:ASP:HB3	1.83	0.60
1:B:571:LEU:HG	1:B:812:ALA:HB2	1.84	0.60
1:A:137:PRO:O	1:A:138:ASP:HB2	2.01	0.60
1:A:257:ASN:OD1	1:A:893:SER:O	2.20	0.60
1:A:385:GLY:N	1:A:411:THR:HG23	2.16	0.60
1:A:450:GLU:HB3	1:A:452:TYR:CE2	2.37	0.60
1:A:362:PHE:HB3	1:A:455:ILE:O	2.02	0.60
1:A:927:LEU:HD22	1:A:929:VAL:CG2	2.32	0.60
1:B:157:ARG:H	1:B:178:ASP:CB	2.12	0.60
1:B:23:TYR:CE1	1:B:656:ASN:HB2	2.37	0.60
1:B:354:LEU:N	1:B:354:LEU:HD22	2.16	0.60
1:B:829:ILE:HG22	1:B:830:PRO:HD2	1.83	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:166:ASP:OD1	2:X:201:ILE:HD13	2.01	0.60
1:A:1144:LEU:O	1:A:1148:THR:HG22	2.02	0.60
1:A:249:THR:HG23	1:A:298:GLN:NE2	2.16	0.60
1:A:679:LEU:HB3	1:A:738:LEU:HD11	1.83	0.60
1:A:837:GLU:OE2	1:A:1488:LEU:HA	2.02	0.60
1:B:1250:THR:O	1:B:1253:TYR:N	2.35	0.60
1:B:961:TYR:OH	1:B:1343:ASN:ND2	2.35	0.60
1:B:349:LEU:HD22	1:B:349:LEU:O	2.02	0.60
1:B:412:ARG:HD3	1:B:414:ASP:OD1	2.02	0.60
1:A:936:ARG:HB2	1:A:1364:VAL:HG22	1.83	0.59
1:A:968:VAL:CG1	1:A:1368:THR:HG22	2.12	0.59
1:A:464:TYR:H	1:A:491:PRO:HD3	1.67	0.59
1:B:1180:LEU:O	1:B:1182:ALA:N	2.34	0.59
1:B:373:VAL:HG23	1:B:374:GLN:N	2.17	0.59
1:B:457:TYR:CD2	1:B:457:TYR:C	2.76	0.59
1:B:66:TYR:CE1	1:B:90:LYS:CG	2.84	0.59
1:B:906:GLY:H	1:B:929:VAL:HB	1.66	0.59
1:A:238:ILE:HG12	1:A:246:PHE:CE1	2.37	0.59
1:A:647:HIS:O	1:A:649:ALA:N	2.34	0.59
1:B:1232:LEU:O	1:B:1233:GLN:HG2	2.02	0.59
1:B:244:LYS:C	1:B:302:ASP:HA	2.23	0.59
1:B:322:TYR:N	1:B:322:TYR:CD2	2.70	0.59
1:A:888:VAL:HG12	1:A:894:HIS:HB2	1.84	0.59
1:B:1024:TYR:HD2	1:B:1025:LEU:N	2.01	0.59
1:B:1206:ARG:CG	1:B:1206:ARG:NH1	2.61	0.59
1:B:1465:ASN:H	1:B:1465:ASN:ND2	1.98	0.59
1:B:1434:ALA:HB1	1:B:1477:PHE:CD1	2.37	0.59
1:B:239:GLY:O	1:B:241:LYS:N	2.36	0.59
1:B:588:VAL:CG1	1:B:790:LEU:HD11	2.31	0.59
2:X:136:LEU:HD21	2:X:153:PHE:HB2	1.84	0.59
1:A:1379:LEU:HD13	1:A:1493:PHE:CD2	2.38	0.59
1:A:1421:HIS:HE1	1:A:1498:TYR:CD2	2.20	0.59
1:A:244:LYS:C	1:A:302:ASP:HA	2.23	0.59
1:B:1221:ASN:HA	1:B:1222:PRO:C	2.21	0.59
1:B:1401:ARG:HB2	1:B:1478:ARG:HG2	1.83	0.59
1:B:163:PHE:CD2	1:B:188:PHE:CD2	2.91	0.59
1:B:250:ILE:HG21	1:B:327:VAL:HG21	1.83	0.59
1:A:1093:VAL:HG12	1:A:1095:GLN:NE2	2.17	0.59
1:B:101:TYR:HE1	1:B:116:ARG:CZ	2.15	0.59
1:B:1054:LEU:O	1:B:1056:ILE:N	2.36	0.59
1:B:54:ILE:HG23	1:B:106:VAL:HG22	1.84	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ASP:O	1:B:209:PHE:HB2	2.01	0.59
1:B:855:PHE:CE1	1:B:886:GLN:CB	2.84	0.59
1:B:994:GLN:HE22	1:B:998:ASN:CB	2.11	0.59
1:A:1278:GLN:HE21	1:A:1278:GLN:N	2.00	0.59
1:A:199:TRP:HB2	1:A:217:PHE:O	2.02	0.59
1:A:249:THR:CG2	1:A:298:GLN:HE21	2.15	0.59
1:A:859:MET:HB2	1:A:912:PHE:HE1	1.67	0.59
1:B:1196:SER:HB2	1:B:1257:THR:HG23	1.83	0.59
1:A:1053:MET:HE3	1:A:1086:LEU:HD13	1.85	0.59
1:A:1495:VAL:O	1:A:1495:VAL:HG13	2.03	0.59
1:A:185:PHE:HB3	1:A:186:PRO:CD	2.31	0.59
1:A:361:LEU:HB3	1:A:453:ARG:O	2.01	0.59
1:A:457:TYR:C	1:A:457:TYR:HD2	2.06	0.59
1:A:979:VAL:HG13	1:A:1359:VAL:HG22	1.84	0.59
1:B:1145:THR:O	1:B:1149:VAL:HG23	2.03	0.59
1:B:1090:ASN:ND2	1:B:1158:ILE:HG21	2.18	0.59
1:B:976:ILE:O	1:B:1361:VAL:HG22	2.02	0.59
1:A:1132:THR:CG2	1:A:1134:PRO:HD2	2.33	0.59
1:A:324:TYR:C	1:A:324:TYR:CD2	2.75	0.59
1:A:786:LEU:N	1:A:786:LEU:HD23	2.17	0.59
1:A:994:GLN:NE2	1:A:998:ASN:HB3	2.02	0.59
1:B:837:GLU:OE2	1:B:1488:LEU:HB2	2.02	0.59
1:B:41:ILE:HG22	1:B:81:ASN:O	2.02	0.59
1:A:1304:VAL:CG1	1:A:1305:LYS:N	2.66	0.59
1:A:610:TYR:CB	1:A:614:ARG:HD2	2.32	0.59
1:A:838:GLN:O	1:A:1486:GLY:N	2.34	0.59
1:B:269:PHE:HB2	1:B:283:MET:CE	2.32	0.59
1:B:271:ILE:HD11	1:B:307:VAL:HG22	1.83	0.59
1:B:639:GLY:N	1:B:645:VAL:HG22	2.16	0.59
1:B:902:PRO:C	1:B:903:LEU:HD13	2.23	0.59
1:A:30:ILE:CG2	1:A:31:PHE:N	2.65	0.59
1:A:44:TYR:CE1	1:A:497:THR:HG21	2.38	0.59
1:A:902:PRO:C	1:A:903:LEU:HD13	2.23	0.59
1:B:988:LEU:HD23	1:B:1021:VAL:HG13	1.84	0.59
1:B:1255:LEU:O	1:B:1255:LEU:HD12	2.01	0.59
1:B:485:ILE:CG2	1:B:487:THR:HG23	2.33	0.59
1:B:553:GLU:OE1	1:B:555:VAL:HG23	2.03	0.59
1:A:100:SER:O	1:A:101:TYR:HB2	2.03	0.58
1:A:1105:LEU:O	1:A:1109:GLU:HG3	2.03	0.58
1:A:1228:TRP:N	1:A:1228:TRP:CE3	2.71	0.58
1:A:348:VAL:HG12	1:A:349:LEU:N	2.18	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1304:VAL:CG1	1:B:1305:LYS:N	2.66	0.58
1:B:161:LEU:CG	1:B:185:PHE:CE1	2.86	0.58
1:B:263:ALA:HB3	1:B:292:LEU:HB3	1.84	0.58
1:B:293:ILE:N	1:B:296:ILE:O	2.28	0.58
1:B:227:PHE:O	1:B:338:GLU:HG2	2.03	0.58
1:B:98:PRO:HB2	1:B:99:VAL:HG23	1.85	0.58
1:A:936:ARG:NH1	1:A:1002:HIS:CE1	2.71	0.58
1:A:1226:ARG:NE	1:A:1266:TYR:CE1	2.71	0.58
1:A:1255:LEU:HD12	1:A:1255:LEU:O	2.03	0.58
1:A:1401:ARG:HB2	1:A:1478:ARG:HA	1.84	0.58
1:A:239:GLY:O	1:A:241:LYS:N	2.36	0.58
1:A:835:ARG:NE	1:A:905:ILE:HD11	2.17	0.58
1:A:975:ARG:HG3	1:A:1340:VAL:HB	1.84	0.58
1:B:947:ARG:C	1:B:949:ILE:H	2.05	0.58
1:A:571:LEU:C	1:A:571:LEU:HD12	2.22	0.58
1:B:1108:VAL:HG13	1:B:1109:GLU:H	1.68	0.58
1:B:265:VAL:HG23	1:B:292:LEU:H	1.68	0.58
1:B:491:PRO:C	1:B:493:ILE:N	2.55	0.58
1:A:1143:TYR:HE1	1:A:1186:PHE:CZ	2.20	0.58
1:A:457:TYR:C	1:A:457:TYR:CD2	2.77	0.58
1:A:594:THR:O	1:A:782:ARG:HG2	2.03	0.58
1:A:52:ALA:HB2	1:A:73:LEU:HD21	1.86	0.58
1:A:981:GLY:O	1:A:982:LEU:HB2	2.03	0.58
1:B:1008:ALA:HB2	1:B:1059:TYR:CD2	2.39	0.58
1:B:635:GLY:O	1:B:673:LEU:HB2	2.03	0.58
1:A:1432:ILE:O	1:A:1432:ILE:HG22	2.03	0.58
1:A:330:ILE:HG22	1:A:337:SER:HA	1.85	0.58
1:A:475:ALA:C	1:A:476:LEU:HD23	2.24	0.58
1:A:641:ASN:O	1:A:644:ASN:N	2.36	0.58
1:B:124:GLY:HA3	1:B:148:LEU:O	2.03	0.58
1:A:1007:SER:HA	1:A:1069:TRP:CD1	2.39	0.58
1:A:315:LEU:HD12	1:A:318:LEU:HD12	1.85	0.58
1:A:498:HIS:HD2	1:A:516:GLU:HA	1.66	0.58
1:A:758:LEU:C	1:A:760:VAL:H	2.07	0.58
1:B:1003:LEU:N	1:B:1003:LEU:HD23	2.19	0.58
1:B:1255:LEU:HD22	1:B:1270:VAL:CG1	2.30	0.58
1:B:42:GLN:CG	1:B:80:GLN:HE21	2.13	0.58
1:B:444:GLU:O	1:B:445:GLU:C	2.39	0.58
1:B:23:TYR:HE1	1:B:656:ASN:H	1.50	0.58
1:B:768:TYR:CE2	1:B:770:PRO:HA	2.38	0.58
2:Y:192:ASN:O	2:Y:221:ILE:HG23	2.02	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1228:TRP:N	1:A:1228:TRP:HE3	2.01	0.58
1:A:1279:ARG:O	1:A:1280:TYR:C	2.41	0.58
1:A:160:VAL:HG23	1:A:175:GLU:CB	2.33	0.58
1:A:290:THR:HG22	1:A:290:THR:O	2.04	0.58
1:A:505:SER:HB3	1:A:510:ILE:CD1	2.34	0.58
1:A:628:GLU:O	1:A:629:LYS:HD3	2.04	0.58
1:B:1226:ARG:CZ	1:B:1266:TYR:CE1	2.87	0.58
1:B:457:TYR:HD2	1:B:457:TYR:C	2.07	0.58
1:B:702:GLY:HA2	1:B:728:PHE:CD1	2.37	0.58
1:A:1368:THR:O	1:A:1508:PHE:HE2	1.87	0.58
1:A:161:LEU:HD11	1:A:185:PHE:CD1	2.39	0.58
1:A:576:SER:CB	1:A:577:PRO:HD3	2.33	0.58
1:A:794:LEU:O	1:A:795:THR:HG23	2.03	0.58
1:B:940:SER:HG	1:B:1361:VAL:HG12	1.66	0.58
1:B:140:SER:OG	1:B:187:ASP:HB3	2.04	0.58
1:B:123:ASN:O	1:B:211:THR:HG21	2.04	0.58
1:B:307:VAL:CG1	1:B:313:TYR:HB2	2.33	0.58
1:A:1080:ALA:HA	1:A:1083:LEU:HD12	1.86	0.58
1:A:129:HIS:HD2	1:A:130:THR:O	1.87	0.58
1:A:502:LEU:O	1:A:540:LEU:HA	2.04	0.58
1:B:1438:ASP:O	1:B:1441:ALA:HB3	2.04	0.58
1:B:1244:THR:HG23	1:B:1502:ASP:OD2	2.03	0.58
1:B:256:TYR:O	1:B:257:ASN:ND2	2.37	0.58
1:B:27:ALA:O	1:B:28:PRO:O	2.22	0.58
1:B:494:ASP:O	1:B:496:ILE:N	2.31	0.58
1:A:1255:LEU:HB2	1:A:1270:VAL:CG1	2.30	0.58
1:B:156:LYS:O	1:B:157:ARG:CG	2.48	0.58
1:B:30:ILE:CG2	1:B:31:PHE:H	2.17	0.58
2:X:153:PHE:CE1	2:X:168:LYS:HB3	2.39	0.58
1:A:31:PHE:HZ	1:A:104:LEU:HD22	1.69	0.57
1:A:363:LEU:HD21	1:A:431:LEU:HB2	1.86	0.57
1:B:141:VAL:HG23	1:B:190:ILE:HD11	1.84	0.57
1:B:952:THR:OG1	1:B:953:ILE:N	2.37	0.57
1:A:1047:LYS:O	1:A:1049:LEU:N	2.37	0.57
1:A:290:THR:CG2	1:A:290:THR:O	2.51	0.57
1:A:319:ASN:C	1:A:320:ASN:HD22	2.08	0.57
1:A:823:VAL:HG13	1:A:846:TYR:O	2.04	0.57
1:B:1019:PHE:CD2	1:B:1020:TYR:CD1	2.92	0.57
1:B:284:GLN:NE2	1:B:310:LEU:HD22	2.18	0.57
1:A:1096:ASN:C	1:A:1096:ASN:HD22	2.08	0.57
1:A:24:VAL:HG11	1:A:543:TYR:OH	2.04	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1334:LEU:CD2	1:B:1334:LEU:H	2.17	0.57
1:B:1370:THR:HG22	1:B:1370:THR:O	2.03	0.57
1:B:1408:TYR:CD1	1:B:1409:LYS:N	2.72	0.57
1:B:814:THR:OG1	1:B:815:VAL:N	2.36	0.57
1:B:86:THR:HG23	1:B:86:THR:O	2.05	0.57
1:A:1083:LEU:CD1	1:A:1107:LEU:HD11	2.34	0.57
1:A:271:ILE:HD11	1:A:307:VAL:HG22	1.85	0.57
1:A:30:ILE:CG2	1:A:31:PHE:H	2.17	0.57
1:A:443:PRO:HG2	1:A:446:ASN:OD1	2.04	0.57
1:B:1049:LEU:CD2	1:B:1089:VAL:HG13	2.35	0.57
1:B:1183:GLN:O	1:B:1232:LEU:HD22	2.04	0.57
1:B:1495:VAL:O	1:B:1495:VAL:HG13	2.05	0.57
1:B:154:PRO:HB3	1:B:180:ILE:O	2.04	0.57
1:A:1320:LYS:HD2	1:A:1321:GLY:H	1.70	0.57
1:A:41:ILE:HG22	1:A:81:ASN:O	2.04	0.57
1:A:388:VAL:O	1:A:420:PHE:HZ	1.88	0.57
1:A:528:ILE:HD12	1:A:528:ILE:N	2.15	0.57
1:A:686:ILE:CG2	1:A:689:LYS:HE3	2.35	0.57
1:B:1024:TYR:C	1:B:1024:TYR:HD2	2.08	0.57
1:B:478:VAL:CG1	1:B:566:LYS:HD3	2.35	0.57
1:B:786:LEU:N	1:B:786:LEU:HD23	2.19	0.57
1:A:124:GLY:C	1:A:125:PHE:CG	2.78	0.57
1:A:128:ILE:HG13	1:A:215:ALA:HB2	1.85	0.57
1:A:1323:LEU:HD12	1:A:1324:HIS:N	2.16	0.57
1:A:1069:TRP:HE1	1:A:1463:GLN:NE2	2.03	0.57
1:A:1465:ASN:ND2	1:A:1465:ASN:N	2.53	0.57
1:A:1423:VAL:CG2	1:A:1496:TYR:CE1	2.87	0.57
1:A:284:GLN:N	1:A:284:GLN:OE1	2.37	0.57
1:A:367:ILE:HD13	1:A:466:TYR:CD2	2.39	0.57
1:A:415:ASP:CG	1:A:417:VAL:HB	2.25	0.57
1:A:503:ILE:HG12	1:A:540:LEU:HB3	1.85	0.57
1:A:634:CYS:SG	1:A:635:GLY:N	2.78	0.57
1:B:1342:LEU:HD23	1:B:1342:LEU:N	2.19	0.57
1:B:1381:ILE:HD12	1:B:1493:PHE:HB2	1.87	0.57
1:B:412:ARG:CD	1:B:415:ASP:HB2	2.31	0.57
1:B:415:ASP:OD2	1:B:417:VAL:HB	2.03	0.57
1:B:576:SER:CB	1:B:577:PRO:HD3	2.34	0.57
1:B:589:SER:HB2	1:B:785:GLN:HE21	1.68	0.57
1:B:823:VAL:HG13	1:B:846:TYR:O	2.04	0.57
2:Y:153:PHE:CD2	2:Y:154:SER:N	2.72	0.57
1:A:1076:THR:HG22	1:A:1120:GLU:OE2	2.03	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:CYS:SG	1:A:672:ILE:HG22	2.44	0.57
1:A:693:SER:O	1:A:696:LYS:HB3	2.05	0.57
1:B:1133:LEU:HD12	1:B:1133:LEU:N	2.19	0.57
1:A:1100:ILE:O	1:A:1103:SER:HB2	2.03	0.57
1:A:719:SER:HB2	1:A:1123:GLN:NE2	2.20	0.57
1:A:1279:ARG:CD	1:A:1284:PHE:CG	2.81	0.57
1:A:208:ASP:O	1:A:209:PHE:CB	2.53	0.57
1:A:364:LYS:N	1:A:364:LYS:HD2	2.17	0.57
1:A:24:VAL:HA	1:A:655:THR:OG1	2.04	0.57
1:B:1039:LEU:O	1:B:1042:LYS:HB3	2.05	0.57
1:B:1056:ILE:O	1:B:1058:SER:N	2.38	0.57
1:B:1490:PRO:HB3	1:B:1509:TYR:O	2.04	0.57
1:B:157:ARG:O	1:B:178:ASP:HB2	2.05	0.57
1:B:27:ALA:O	1:B:652:THR:O	2.23	0.57
1:B:774:LEU:HD11	1:B:788:PHE:CZ	2.40	0.57
1:B:77:ASN:ND2	1:B:81:ASN:ND2	2.52	0.57
1:A:132:LYS:NZ	1:A:139:GLN:HE22	2.03	0.57
1:A:173:MET:O	1:A:174:VAL:HB	2.05	0.57
1:A:604:ALA:O	1:A:772:SER:HB3	2.04	0.57
1:A:61:ASP:O	1:A:63:LYS:N	2.36	0.57
1:A:829:ILE:CG1	1:A:925:LYS:HG2	2.35	0.57
1:B:1379:LEU:HD13	1:B:1493:PHE:CD2	2.39	0.57
1:B:1435:ASN:HB3	1:B:1438:ASP:CB	2.33	0.57
1:B:1423:VAL:CG2	1:B:1496:TYR:HE1	2.18	0.57
1:B:386:VAL:CG2	1:B:411:THR:HG21	2.31	0.57
1:A:1008:ALA:N	1:A:1068:VAL:O	2.37	0.57
1:A:1274:LEU:O	1:A:1276:GLU:N	2.38	0.57
1:A:1370:THR:O	1:A:1370:THR:HG22	2.04	0.57
1:A:222:TYR:OH	1:A:224:LEU:HD22	2.05	0.57
1:A:227:PHE:HZ	1:A:329:VAL:O	1.88	0.57
1:A:834:VAL:HG11	1:A:1489:SER:OG	2.05	0.57
1:A:98:PRO:HB2	1:A:99:VAL:HG23	1.86	0.57
1:B:367:ILE:HG23	1:B:368:PRO:HD2	1.86	0.57
1:B:707:ASN:HB3	1:B:739:ARG:HH12	1.69	0.57
1:B:602:LEU:HB2	1:B:774:LEU:O	2.05	0.57
1:A:1156:PHE:CD1	1:A:1164:ILE:HD11	2.39	0.56
1:A:1186:PHE:CD1	1:A:1250:THR:HG22	2.37	0.56
1:A:1307:LEU:O	1:A:1308:ARG:C	2.43	0.56
1:A:298:GLN:O	1:A:299:VAL:HG13	2.04	0.56
1:A:304:GLU:O	1:A:305:THR:O	2.22	0.56
1:A:814:THR:OG1	1:A:815:VAL:N	2.38	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ILE:HD13	2:X:135:HIS:CD2	2.40	0.56
1:B:1027:THR:HG22	1:B:1028:GLY:N	2.20	0.56
1:B:234:GLU:HB2	1:B:247:GLU:H	1.69	0.56
1:B:303:SER:HB3	1:B:347:TYR:OH	2.05	0.56
1:B:422:LEU:H	1:B:422:LEU:HD12	1.70	0.56
1:B:451:GLY:O	1:B:452:TYR:CD2	2.58	0.56
1:B:42:GLN:CD	1:B:543:TYR:HH	2.09	0.56
1:B:758:LEU:C	1:B:760:VAL:H	2.07	0.56
1:A:1206:ARG:HG3	1:A:1206:ARG:NH1	2.15	0.56
1:A:465:LEU:HD13	1:A:544:TYR:CE1	2.40	0.56
1:A:614:ARG:NH2	1:A:798:GLU:OE2	2.38	0.56
1:A:829:ILE:HG13	1:A:925:LYS:HG2	1.87	0.56
1:B:1202:HIS:HD2	1:B:1204:GLN:N	1.93	0.56
1:B:1320:LYS:HG2	1:B:1342:LEU:HD12	1.86	0.56
1:B:1509:TYR:CD2	1:B:1509:TYR:O	2.58	0.56
1:B:169:SER:O	1:B:170:GLU:O	2.23	0.56
1:B:393:GLN:O	1:B:431:LEU:HD23	2.05	0.56
1:B:592:MET:HB3	1:B:780:VAL:HG11	1.87	0.56
1:B:835:ARG:NH1	1:B:835:ARG:CG	2.67	0.56
1:A:1080:ALA:HA	1:A:1083:LEU:HB2	1.86	0.56
1:A:123:ASN:ND2	1:A:150:ASP:H	2.02	0.56
1:A:544:TYR:HE1	1:A:555:VAL:HG12	1.70	0.56
1:B:1016:VAL:HG12	1:B:1017:PRO:N	2.20	0.56
1:B:1370:THR:HG21	1:B:1506:THR:O	2.05	0.56
1:B:153:LYS:HB3	1:B:154:PRO:CD	2.35	0.56
1:B:242:ASN:HB2	1:B:245:ASN:O	2.04	0.56
1:B:28:PRO:HB2	1:B:30:ILE:O	2.05	0.56
1:B:466:TYR:HD1	1:B:467:ILE:N	2.03	0.56
1:A:1056:ILE:O	1:A:1057:MET:C	2.43	0.56
1:A:1100:ILE:HG21	1:A:1158:ILE:HD12	1.86	0.56
1:A:1193:TYR:CD1	1:A:1256:LEU:HB3	2.41	0.56
1:A:1216:ALA:C	1:A:1217:LEU:HG	2.25	0.56
1:A:1278:GLN:CA	1:A:1278:GLN:NE2	2.68	0.56
1:A:1278:GLN:HE21	1:A:1278:GLN:HA	1.70	0.56
1:A:364:LYS:H	1:A:364:LYS:HD3	1.68	0.56
1:B:1320:LYS:HD2	1:B:1321:GLY:N	2.20	0.56
1:B:1465:ASN:ND2	1:B:1465:ASN:N	2.52	0.56
1:B:208:ASP:O	1:B:209:PHE:CB	2.53	0.56
1:B:456:ALA:O	1:B:458:SER:N	2.38	0.56
1:B:686:ILE:CG2	1:B:689:LYS:HE3	2.35	0.56
1:B:909:ASN:H	1:B:926:THR:HG22	1.68	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:158:GLU:HG3	2:Y:159:GLU:OE1	2.06	0.56
1:A:1063:ASP:O	1:A:1064:TYR:HB2	2.06	0.56
1:A:644:ASN:C	1:A:644:ASN:HD22	2.07	0.56
1:A:702:GLY:HA2	1:A:728:PHE:CE1	2.41	0.56
1:B:1323:LEU:HD12	1:B:1324:HIS:N	2.20	0.56
1:B:1401:ARG:HB2	1:B:1478:ARG:HA	1.87	0.56
1:B:394:THR:HG23	1:B:395:ILE:N	2.19	0.56
1:B:485:ILE:HG22	1:B:487:THR:HG23	1.86	0.56
1:B:641:ASN:ND2	1:B:644:ASN:HB2	2.20	0.56
2:Y:169:ILE:HG21	2:Y:189:ILE:HD13	1.88	0.56
1:A:1449:LEU:O	1:A:1449:LEU:HD12	2.06	0.56
1:A:215:ALA:C	1:A:216:TYR:CD2	2.79	0.56
1:B:1117:SER:HA	1:B:1145:THR:HG21	1.87	0.56
1:B:103:TYR:HA	1:B:115:LYS:O	2.06	0.56
1:B:348:VAL:HG12	1:B:349:LEU:N	2.21	0.56
1:B:373:VAL:HG23	1:B:374:GLN:H	1.71	0.56
1:B:240:TYR:CZ	1:B:443:PRO:CD	2.88	0.56
1:B:52:ALA:HB2	1:B:73:LEU:HD21	1.87	0.56
1:A:1024:TYR:CE2	1:A:1030:HIS:CD2	2.93	0.56
1:A:1500:ARG:C	1:A:1502:ASP:H	2.08	0.56
1:A:478:VAL:HG11	1:A:566:LYS:HD3	1.88	0.56
1:A:765:ILE:O	1:A:765:ILE:HG23	2.05	0.56
1:B:54:ILE:HG23	1:B:105:GLU:O	2.06	0.56
1:B:1244:THR:O	1:B:1285:TYR:HD2	1.88	0.56
1:B:165:ASP:HB3	1:B:171:VAL:HG21	1.86	0.56
1:B:42:GLN:HA	1:B:79:PHE:O	2.06	0.56
1:A:1090:ASN:ND2	1:A:1158:ILE:HG21	2.15	0.56
1:A:976:ILE:HG21	1:A:1280:TYR:CE1	2.41	0.56
1:A:451:GLY:O	1:A:452:TYR:CD2	2.58	0.56
1:A:531:THR:HG23	1:A:533:ASN:HB2	1.87	0.56
1:A:54:ILE:HG23	1:A:106:VAL:HG22	1.86	0.56
1:A:963:ILE:HG23	1:A:973:ILE:HD11	1.88	0.56
1:B:42:GLN:CB	1:B:80:GLN:HG2	2.35	0.56
1:B:430:VAL:HG22	1:B:455:ILE:HG12	1.87	0.56
1:B:743:SER:OG	1:B:752:LEU:HD13	2.05	0.56
1:A:1191:SER:O	1:A:1195:LEU:HG	2.05	0.56
1:A:1218:VAL:CG1	1:A:1226:ARG:HA	2.35	0.56
1:A:1317:TYR:HB3	1:A:1344:ASP:OD2	2.06	0.56
1:A:1372:GLU:HG3	1:A:1373:GLU:N	2.19	0.56
1:A:243:PHE:CE2	1:A:316:GLU:HG2	2.38	0.56
1:A:42:GLN:HB2	1:A:80:GLN:CG	2.35	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ASP:O	1:A:439:ALA:C	2.43	0.56
1:A:55:SER:HB2	1:A:67:SER:O	2.04	0.56
1:B:1143:TYR:CE1	1:B:1186:PHE:CZ	2.94	0.56
1:B:226:HIS:CD2	1:B:336:PHE:CE2	2.93	0.56
1:B:576:SER:HG	1:B:589:SER:HB2	1.67	0.56
1:A:1023:HIS:CD2	1:A:1092:TYR:OH	2.59	0.56
1:A:1238:SER:C	1:A:1240:PRO:HD3	2.26	0.56
1:A:1250:THR:O	1:A:1253:TYR:N	2.39	0.56
1:A:1315:VAL:HG22	1:A:1346:LEU:HD11	1.88	0.56
1:A:190:ILE:HG22	1:A:194:PRO:HG3	1.88	0.56
1:A:24:VAL:HA	1:A:655:THR:HG1	1.71	0.56
1:A:600:VAL:O	1:A:777:VAL:HG13	2.06	0.56
1:A:835:ARG:HG2	1:A:835:ARG:NH1	2.19	0.56
1:A:903:LEU:N	1:A:903:LEU:HD22	2.21	0.56
1:B:123:ASN:HD22	1:B:124:GLY:N	2.03	0.56
2:Y:162:LEU:HD12	2:Y:165:LEU:HD23	1.87	0.56
1:A:1206:ARG:HH11	1:A:1206:ARG:CG	2.12	0.56
1:A:1307:LEU:HD13	1:A:1356:LEU:HD12	1.88	0.56
1:A:208:ASP:O	1:A:209:PHE:HB2	2.06	0.56
1:A:291:MET:O	1:A:293:ILE:HG13	2.06	0.56
1:A:503:ILE:HB	1:A:511:HIS:HB2	1.88	0.56
1:B:1435:ASN:O	1:B:1438:ASP:N	2.38	0.56
1:B:1496:TYR:HB3	1:B:1504:GLN:HG3	1.87	0.56
1:B:707:ASN:HB3	1:B:739:ARG:NH1	2.21	0.56
1:B:707:ASN:OD1	1:B:707:ASN:N	2.39	0.56
1:A:1008:ALA:HA	1:A:1059:TYR:CE2	2.41	0.55
1:A:1244:THR:HB	1:A:1247:MET:CB	2.30	0.55
1:A:1259:LEU:CD1	1:A:1300:TYR:HB2	2.36	0.55
1:A:1304:VAL:CG1	1:A:1305:LYS:H	2.17	0.55
1:A:833:VAL:HA	1:A:1430:THR:HG21	1.86	0.55
1:A:838:GLN:HB3	1:A:1486:GLY:HA3	1.88	0.55
1:B:1019:PHE:CD2	1:B:1020:TYR:CE1	2.95	0.55
1:B:352:TYR:HD1	1:B:375:VAL:CG1	2.18	0.55
2:X:186:TYR:CD2	2:X:229:LYS:HD3	2.41	0.55
2:Y:166:ASP:OD1	2:Y:201:ILE:HD13	2.04	0.55
1:A:1225:TYR:CE1	1:A:1272:LYS:CG	2.89	0.55
1:A:486:VAL:O	1:A:486:VAL:HG12	2.05	0.55
1:B:1304:VAL:CG1	1:B:1305:LYS:H	2.16	0.55
1:B:477:LEU:HA	1:B:564:GLU:HG2	1.88	0.55
1:B:497:THR:HG23	1:B:498:HIS:N	2.17	0.55
1:B:915:GLU:HG3	1:B:920:LYS:HG3	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:968:VAL:O	1:B:968:VAL:HG23	2.04	0.55
1:A:1020:TYR:CD2	1:A:1294:ILE:HG22	2.40	0.55
1:A:1024:TYR:HD2	1:A:1024:TYR:C	2.08	0.55
1:A:1023:HIS:HD2	1:A:1092:TYR:OH	1.89	0.55
1:A:269:PHE:HB2	1:A:283:MET:HE3	1.88	0.55
1:A:295:GLY:O	1:A:296:ILE:CD1	2.55	0.55
1:A:444:GLU:O	1:A:445:GLU:C	2.44	0.55
1:B:1491:ALA:HB3	1:B:1509:TYR:CE2	2.40	0.55
1:A:1248:VAL:CG2	1:A:1277:GLU:HG2	2.37	0.55
1:A:1502:ASP:C	1:A:1503:LYS:HD2	2.27	0.55
1:A:905:ILE:HD13	1:A:931:PRO:HG3	1.87	0.55
1:B:113:LYS:NZ	1:B:656:ASN:HD21	2.05	0.55
1:B:1290:THR:O	1:B:1294:ILE:CG1	2.54	0.55
1:B:163:PHE:CE2	1:B:188:PHE:CD2	2.95	0.55
1:B:824:PHE:CE1	1:B:846:TYR:HD1	2.25	0.55
1:A:1108:VAL:HG13	1:A:1109:GLU:N	2.21	0.55
1:A:124:GLY:HA3	1:A:148:LEU:O	2.06	0.55
1:B:1056:ILE:O	1:B:1057:MET:C	2.44	0.55
1:B:330:ILE:HG22	1:B:337:SER:HA	1.87	0.55
1:B:950:TYR:CE1	1:B:1271:ILE:HD11	2.41	0.55
1:A:330:ILE:HG22	1:A:337:SER:CA	2.35	0.55
1:A:432:GLU:OE2	1:A:453:ARG:NH2	2.40	0.55
1:A:647:HIS:O	1:A:650:GLY:N	2.38	0.55
1:A:92:LEU:H	1:A:93:PRO:HD3	1.72	0.55
1:B:106:VAL:HG12	1:B:107:VAL:N	2.22	0.55
1:B:1143:TYR:CE1	1:B:1186:PHE:CE2	2.94	0.55
1:B:1184:SER:HA	1:B:1232:LEU:CB	2.36	0.55
1:B:442:LEU:O	1:B:443:PRO:C	2.41	0.55
1:B:24:VAL:HA	1:B:655:THR:HG1	1.71	0.55
1:B:981:GLY:O	1:B:982:LEU:CB	2.49	0.55
2:Y:146:LEU:HD22	2:Y:146:LEU:C	2.27	0.55
1:A:1277:GLU:OE2	1:A:1277:GLU:HA	2.06	0.55
1:A:1259:LEU:HD11	1:A:1300:TYR:HB2	1.89	0.55
1:A:829:ILE:HG13	1:A:925:LYS:CG	2.37	0.55
1:B:1112:GLN:HB2	1:B:1118:PHE:CE1	2.42	0.55
1:B:33:VAL:HB	1:B:209:PHE:HE2	1.72	0.55
1:B:481:HIS:CE1	1:B:529:PRO:HG3	2.41	0.55
1:B:686:ILE:HG22	1:B:689:LYS:HE3	1.88	0.55
1:B:838:GLN:H	1:B:1486:GLY:HA3	1.71	0.55
1:A:1066:TYR:CD1	1:A:1066:TYR:N	2.74	0.55
1:A:1115:ASN:HD22	1:A:1115:ASN:C	2.10	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1221:ASN:ND2	1:A:1222:PRO:HA	2.22	0.55
1:A:834:VAL:HG21	1:A:1489:SER:OG	2.06	0.55
1:A:829:ILE:HG22	1:A:830:PRO:HD2	1.89	0.55
1:A:896:VAL:O	1:A:897:THR:HG22	2.06	0.55
1:A:957:LYS:HG3	1:A:958:GLU:N	2.21	0.55
1:B:1216:ALA:C	1:B:1217:LEU:HG	2.27	0.55
1:B:1272:LYS:O	1:B:1272:LYS:HG3	2.05	0.55
1:B:1279:ARG:HG3	1:B:1284:PHE:HB2	1.89	0.55
1:B:498:HIS:HB3	1:B:514:THR:CG2	2.36	0.55
1:B:465:LEU:HD13	1:B:544:TYR:CE1	2.42	0.55
1:B:606:ASP:O	1:B:608:ALA:N	2.40	0.55
1:A:1429:PRO:HB3	1:A:1488:LEU:HD22	1.88	0.55
1:A:515:ARG:HH12	1:A:527:ASN:H	1.55	0.55
1:A:561:LEU:O	1:A:563:ILE:CG2	2.55	0.55
1:B:50:PHE:CD1	1:B:109:LYS:HE2	2.42	0.55
1:B:1432:ILE:HG21	1:B:1479:ILE:HD12	1.89	0.55
1:B:1379:LEU:HD13	1:B:1493:PHE:CE2	2.41	0.55
1:B:348:VAL:CG1	1:B:349:LEU:N	2.70	0.55
1:A:768:TYR:CE2	1:A:770:PRO:HA	2.42	0.55
1:B:1012:LEU:O	1:B:1015:VAL:HG13	2.07	0.55
1:B:1024:TYR:HB2	1:B:1298:THR:CG2	2.37	0.55
1:B:1230:ASP:CG	1:B:1246:ARG:HD2	2.26	0.55
1:B:306:ALA:O	1:B:307:VAL:CG2	2.55	0.55
1:B:628:GLU:O	1:B:629:LYS:HD3	2.07	0.55
1:B:707:ASN:HB3	1:B:739:ARG:NH2	2.22	0.55
2:X:194:LYS:HG3	2:X:195:ASP:H	1.72	0.55
2:Y:208:GLN:O	2:Y:212:MET:HG3	2.07	0.55
1:A:1401:ARG:HH11	1:A:1403:VAL:CG2	2.20	0.54
1:A:395:ILE:O	1:A:429:THR:HG23	2.06	0.54
1:A:42:GLN:CB	1:A:80:GLN:HG2	2.37	0.54
1:B:1028:GLY:O	1:B:1029:ASN:O	2.25	0.54
1:B:1244:THR:HG22	1:B:1245:ALA:N	2.21	0.54
1:B:1300:TYR:C	1:B:1300:TYR:CD2	2.80	0.54
1:B:182:ILE:HD12	1:B:777:VAL:HG11	1.89	0.54
1:B:489:LYS:O	1:B:490:SER:HB2	2.08	0.54
1:B:707:ASN:HB3	1:B:739:ARG:HH22	1.71	0.54
2:Y:153:PHE:CE1	2:Y:168:LYS:HB3	2.42	0.54
1:A:123:ASN:O	1:A:211:THR:HG21	2.08	0.54
1:A:1408:TYR:O	1:A:1410:PRO:HD3	2.06	0.54
1:B:1083:LEU:CD1	1:B:1107:LEU:HD11	2.38	0.54
1:B:1196:SER:HB2	1:B:1257:THR:CG2	2.37	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ILE:HG22	1:B:194:PRO:HG3	1.89	0.54
1:B:235:TYR:CD2	1:B:235:TYR:N	2.74	0.54
1:A:1204:GLN:OE1	1:A:1204:GLN:HA	2.07	0.54
1:A:160:VAL:HG13	1:A:161:LEU:O	2.07	0.54
1:A:226:HIS:CD2	1:A:336:PHE:CE2	2.96	0.54
1:A:373:VAL:HG23	1:A:374:GLN:N	2.22	0.54
1:A:556:SER:OG	1:A:557:ASP:N	2.40	0.54
1:A:477:LEU:HA	1:A:564:GLU:HG2	1.89	0.54
1:A:703:ALA:HB1	1:A:735:ALA:HB3	1.90	0.54
1:B:1238:SER:C	1:B:1240:PRO:HD3	2.28	0.54
1:B:617:LYS:CE	1:B:625:GLN:HE22	2.17	0.54
1:B:700:TYR:CE1	1:B:758:LEU:HD12	2.43	0.54
1:B:765:ILE:O	1:B:765:ILE:HG23	2.07	0.54
1:A:1066:TYR:HD1	1:A:1066:TYR:N	2.06	0.54
1:A:1136:GLU:OE1	1:A:1415:SER:HB2	2.06	0.54
1:A:1320:LYS:HG2	1:A:1342:LEU:HD12	1.88	0.54
1:B:1076:THR:HG22	1:B:1120:GLU:OE2	2.08	0.54
1:B:1104:LEU:HD13	1:B:1164:ILE:CD1	2.38	0.54
1:B:1278:GLN:NE2	1:B:1278:GLN:HA	2.22	0.54
1:B:373:VAL:CG2	1:B:374:GLN:N	2.70	0.54
1:B:387:PRO:HA	1:B:410:VAL:HG22	1.90	0.54
1:B:73:LEU:N	1:B:73:LEU:HD23	2.23	0.54
1:B:796:THR:HA	1:B:818:LYS:HA	1.88	0.54
1:B:856:CYS:O	1:B:914:LEU:HA	2.08	0.54
2:X:158:GLU:HG3	2:X:159:GLU:OE1	2.07	0.54
1:A:1311:MET:HE2	1:A:1354:SER:O	2.08	0.54
1:A:489:LYS:O	1:A:490:SER:HB2	2.07	0.54
1:A:511:HIS:NE2	1:A:531:THR:HG21	2.22	0.54
1:A:831:TYR:CE1	1:A:1457:ASP:HB3	2.42	0.54
1:A:835:ARG:CG	1:A:835:ARG:HH11	2.18	0.54
1:B:292:LEU:HD22	1:B:296:ILE:O	2.08	0.54
1:B:457:TYR:CD2	1:B:457:TYR:O	2.61	0.54
1:B:541:LEU:HB2	1:B:558:SER:CB	2.26	0.54
1:B:947:ARG:HB2	1:B:949:ILE:CG1	2.37	0.54
1:A:628:GLU:HG3	1:A:628:GLU:O	2.06	0.54
1:A:915:GLU:HG3	1:A:920:LYS:HG3	1.88	0.54
1:B:1228:TRP:HZ3	1:B:1270:VAL:HG22	1.73	0.54
1:B:1186:PHE:CD1	1:B:1250:THR:HG22	2.38	0.54
1:B:1500:ARG:C	1:B:1502:ASP:H	2.11	0.54
1:B:160:VAL:HG13	1:B:161:LEU:O	2.06	0.54
1:B:394:THR:HG22	1:B:402:SER:OG	2.08	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:TRP:CD1	1:B:482:LEU:HD21	2.43	0.54
1:B:640:LEU:H	1:B:644:ASN:HB3	1.73	0.54
1:B:823:VAL:HA	1:B:846:TYR:O	2.06	0.54
1:A:1290:THR:HG22	1:A:1290:THR:O	2.07	0.54
1:A:987:ILE:HG12	1:A:1294:ILE:HD12	1.90	0.54
1:A:1325:ASN:O	1:A:1325:ASN:ND2	2.41	0.54
1:A:743:SER:OG	1:A:752:LEU:HD13	2.08	0.54
1:B:1066:TYR:HD1	1:B:1066:TYR:N	2.05	0.54
1:B:544:TYR:HE1	1:B:555:VAL:HG12	1.73	0.54
1:B:739:ARG:HB2	1:B:752:LEU:HD21	1.88	0.54
1:A:961:TYR:OH	1:A:1343:ASN:ND2	2.41	0.54
1:A:1423:VAL:HG21	1:A:1496:TYR:CE1	2.43	0.54
1:A:144:ARG:HG2	1:A:775:TRP:CZ2	2.43	0.54
1:A:1456:LYS:O	1:A:1457:ASP:C	2.46	0.54
1:A:491:PRO:C	1:A:493:ILE:N	2.60	0.54
1:A:56:ILE:HG13	1:A:66:TYR:HD2	1.73	0.54
1:A:142:LYS:HD3	1:A:775:TRP:CG	2.43	0.54
1:B:1115:ASN:HD22	1:B:1117:SER:H	1.56	0.54
1:B:362:PHE:HA	1:B:455:ILE:H	1.72	0.54
1:B:509:ILE:HD11	1:B:651:LEU:HD21	1.90	0.54
1:B:839:ILE:HG22	1:B:900:VAL:HG23	1.88	0.54
1:A:1043:GLN:O	1:A:1046:LYS:HB2	2.08	0.54
1:A:1381:ILE:CG1	1:A:1404:ALA:HB2	2.28	0.54
1:A:942:VAL:HG21	1:A:957:LYS:HB3	1.89	0.54
1:B:101:TYR:CE1	1:B:116:ARG:NE	2.75	0.54
1:B:1341:LEU:HB3	1:B:1342:LEU:HD23	1.89	0.54
1:B:1236:ASP:HB2	1:B:1412:ARG:NH2	2.20	0.54
1:B:235:TYR:N	1:B:235:TYR:HD2	2.05	0.54
1:B:493:ILE:HG23	1:B:494:ASP:H	1.72	0.54
1:B:948:GLY:HA2	1:B:952:THR:O	2.08	0.54
1:A:1307:LEU:HB2	1:A:1355:GLY:HA2	1.90	0.54
1:A:235:TYR:CD2	1:A:235:TYR:N	2.76	0.54
1:A:968:VAL:HG23	1:A:971:THR:HG21	1.91	0.54
1:B:35:ALA:HA	1:B:150:ASP:OD1	2.07	0.54
1:B:647:HIS:O	1:B:650:GLY:N	2.41	0.54
1:A:1161:LEU:HB3	1:A:1164:ILE:HG23	1.90	0.53
1:A:1273:TRP:CZ3	1:A:1274:LEU:HD23	2.43	0.53
1:A:1381:ILE:HD13	1:A:1509:TYR:CD1	2.43	0.53
1:A:195:ARG:HH11	1:A:195:ARG:CG	2.22	0.53
1:A:25:ILE:O	1:A:654:LEU:N	2.38	0.53
1:A:718:ILE:HG21	1:A:725:ILE:HG12	1.89	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1082:ALA:O	1:B:1083:LEU:C	2.46	0.53
1:B:1205:PHE:HA	1:B:1208:ILE:HG13	1.90	0.53
1:B:138:ASP:H	1:B:190:ILE:HB	1.73	0.53
1:B:794:LEU:O	1:B:795:THR:HG23	2.08	0.53
2:X:167:PHE:O	2:X:171:GLN:HB2	2.09	0.53
2:Y:162:LEU:O	2:Y:166:ASP:HB2	2.08	0.53
1:A:59:TYR:CD1	1:A:103:TYR:HE1	2.25	0.53
1:A:1225:TYR:CE1	1:A:1272:LYS:HG2	2.43	0.53
1:A:161:LEU:C	1:A:162:THR:HG22	2.28	0.53
1:A:371:ILE:HD12	1:A:390:LEU:CD2	2.35	0.53
1:A:605:VAL:HG12	1:A:606:ASP:N	2.22	0.53
1:A:610:TYR:HB2	1:A:614:ARG:HD2	1.90	0.53
1:B:1334:LEU:CD2	1:B:1334:LEU:N	2.71	0.53
1:B:160:VAL:HG23	1:B:175:GLU:CB	2.38	0.53
1:B:23:TYR:HE1	1:B:656:ASN:HB2	1.72	0.53
1:B:608:ALA:O	1:B:609:VAL:C	2.47	0.53
1:B:686:ILE:C	1:B:688:ALA:N	2.58	0.53
1:B:614:ARG:NH2	1:B:798:GLU:OE2	2.39	0.53
1:A:1053:MET:O	1:A:1056:ILE:HG23	2.08	0.53
1:A:195:ARG:HG2	1:A:195:ARG:NH1	2.23	0.53
1:A:541:LEU:HB2	1:A:558:SER:CB	2.35	0.53
1:A:823:VAL:HA	1:A:846:TYR:O	2.09	0.53
1:B:1190:ILE:HG12	1:B:1253:TYR:CE1	2.44	0.53
1:B:124:GLY:C	1:B:125:PHE:CG	2.81	0.53
1:B:231:ILE:HB	1:B:250:ILE:HG22	1.89	0.53
1:B:292:LEU:HD13	1:B:293:ILE:N	2.22	0.53
1:B:718:ILE:HG21	1:B:725:ILE:HG12	1.89	0.53
1:B:781:PRO:O	1:B:782:ARG:HB2	2.08	0.53
1:B:855:PHE:CZ	1:B:886:GLN:CB	2.77	0.53
2:Y:150:ILE:O	2:Y:150:ILE:HG13	2.09	0.53
1:A:1184:SER:HA	1:A:1232:LEU:HB2	1.90	0.53
1:A:154:PRO:HB3	1:A:180:ILE:O	2.08	0.53
1:A:172:ASP:OD2	1:A:173:MET:N	2.38	0.53
1:A:493:ILE:HG23	1:A:494:ASP:H	1.72	0.53
1:A:593:ALA:HA	1:A:782:ARG:O	2.08	0.53
1:A:739:ARG:HB2	1:A:752:LEU:HD21	1.91	0.53
1:A:911:ASN:CG	1:A:924:VAL:HG13	2.29	0.53
1:A:988:LEU:HD23	1:A:1021:VAL:HG13	1.89	0.53
1:B:1008:ALA:O	1:B:1009:GLU:C	2.47	0.53
1:B:137:PRO:O	1:B:138:ASP:HB2	2.08	0.53
1:B:326:ALA:HA	1:B:341:GLU:HA	1.91	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:VAL:HG23	1:B:610:TYR:CD2	2.43	0.53
1:A:1020:TYR:HD2	1:A:1294:ILE:CG2	2.21	0.53
1:A:1148:THR:OG1	1:A:1152:ILE:HD11	2.08	0.53
1:A:1337:PRO:O	1:A:1338:VAL:HG23	2.09	0.53
1:A:1348:VAL:HG11	1:A:1359:VAL:CG2	2.35	0.53
1:A:1377:PHE:CE1	1:A:1467:ILE:HD12	2.43	0.53
1:A:1467:ILE:N	1:A:1468:PRO:HD3	2.23	0.53
1:A:639:GLY:N	1:A:645:VAL:HG22	2.16	0.53
1:A:42:GLN:HA	1:A:79:PHE:O	2.08	0.53
1:A:85:LEU:O	1:A:86:THR:CB	2.54	0.53
1:B:1090:ASN:O	1:B:1090:ASN:OD1	2.27	0.53
1:B:635:GLY:C	1:B:673:LEU:HA	2.28	0.53
1:A:1030:HIS:CE1	1:A:1306:GLN:HE22	2.25	0.53
1:A:1145:THR:O	1:A:1149:VAL:HG23	2.08	0.53
1:A:1429:PRO:HG2	1:A:1511:THR:CB	2.36	0.53
1:A:229:VAL:HG22	1:A:252:ALA:HB2	1.90	0.53
1:A:308:LYS:HA	1:A:313:TYR:O	2.08	0.53
1:A:467:ILE:HD12	1:A:484:ILE:HD12	1.90	0.53
1:B:1080:ALA:HA	1:B:1083:LEU:HB2	1.91	0.53
1:B:1153:ARG:CZ	1:B:1168:LEU:HD22	2.39	0.53
1:B:1257:THR:O	1:B:1260:ASN:HB2	2.08	0.53
1:B:169:SER:O	1:B:171:VAL:HG23	2.08	0.53
1:B:922:ILE:CD1	4:B:2001:NAG:H82	2.28	0.53
1:B:284:GLN:OE1	1:B:284:GLN:N	2.42	0.53
1:B:290:THR:O	1:B:290:THR:CG2	2.57	0.53
1:B:598:SER:HA	1:B:805:SER:OG	2.08	0.53
1:B:625:GLN:O	1:B:629:LYS:HE2	2.08	0.53
1:A:1003:LEU:HD13	1:A:1498:TYR:CD1	2.43	0.53
1:A:951:GLY:HA3	1:A:1224:ILE:HG23	1.91	0.53
1:A:141:VAL:HG23	1:A:190:ILE:HD11	1.91	0.53
1:A:456:ALA:O	1:A:458:SER:N	2.42	0.53
1:A:754:MET:O	1:A:755:LYS:HG2	2.09	0.53
1:A:841:LEU:HD12	1:A:859:MET:CE	2.36	0.53
1:B:983:LEU:HD11	1:B:1356:LEU:HD22	1.91	0.53
1:B:243:PHE:CZ	1:B:316:GLU:CG	2.85	0.53
1:B:296:ILE:HG22	1:B:297:ALA:H	1.73	0.53
1:B:56:ILE:HG13	1:B:66:TYR:HD2	1.74	0.53
1:B:710:THR:HG23	1:B:713:GLN:CD	2.29	0.53
1:B:857:VAL:HG21	1:B:896:VAL:HG11	1.90	0.53
2:X:136:LEU:HD23	2:X:136:LEU:N	2.24	0.53
1:A:1090:ASN:O	1:A:1090:ASN:OD1	2.26	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:THR:HG22	1:A:215:ALA:N	2.23	0.53
1:A:73:LEU:HB2	1:A:79:PHE:HA	1.89	0.53
1:B:1043:GLN:HA	1:B:1043:GLN:OE1	2.09	0.53
1:B:298:GLN:O	1:B:299:VAL:HG13	2.09	0.53
1:B:515:ARG:NH1	1:B:527:ASN:H	2.04	0.53
1:B:837:GLU:C	1:B:901:LEU:HD12	2.30	0.53
1:A:1142:LEU:HD13	1:A:1187:THR:HG22	1.90	0.53
1:A:240:TYR:CZ	1:A:443:PRO:CD	2.92	0.53
1:A:313:TYR:CZ	1:A:321:LYS:HD2	2.43	0.53
1:A:435:VAL:CG1	1:A:436:LYS:N	2.72	0.53
1:A:531:THR:CG2	1:A:533:ASN:HB2	2.38	0.53
1:A:707:ASN:N	1:A:707:ASN:OD1	2.41	0.53
1:A:907:LEU:HD12	1:A:908:HIS:H	1.73	0.53
1:A:979:VAL:C	1:A:980:LYS:HD2	2.29	0.53
1:B:1096:ASN:HD22	1:B:1099:SER:H	1.56	0.53
1:B:1150:ILE:HD11	1:B:1190:ILE:CG2	2.38	0.53
1:B:1290:THR:O	1:B:1294:ILE:HG12	2.09	0.53
1:B:1439:LEU:HA	1:B:1442:LEU:HD12	1.90	0.53
1:B:1475:VAL:HG22	1:B:1476:ARG:N	2.22	0.53
1:B:27:ALA:HB2	1:B:39:ILE:HD12	1.91	0.53
1:B:430:VAL:HA	1:B:454:ALA:O	2.09	0.53
1:B:240:TYR:OH	1:B:443:PRO:HD3	2.09	0.53
1:B:606:ASP:C	1:B:608:ALA:H	2.12	0.53
1:B:653:PHE:CE1	1:B:660:ASP:HB3	2.44	0.53
1:B:700:TYR:C	1:B:702:GLY:N	2.60	0.53
1:B:838:GLN:HB3	1:B:1486:GLY:HA3	1.89	0.53
1:B:835:ARG:NE	1:B:905:ILE:HD11	2.24	0.53
1:A:1115:ASN:ND2	1:A:1115:ASN:C	2.63	0.53
1:A:1257:THR:O	1:A:1260:ASN:HB2	2.09	0.53
1:A:1491:ALA:HB3	1:A:1509:TYR:CE2	2.42	0.53
1:A:306:ALA:O	1:A:307:VAL:CG2	2.56	0.53
1:A:284:GLN:NE2	1:A:310:LEU:HD22	2.24	0.53
1:B:1105:LEU:HD22	1:B:1109:GLU:OE1	2.09	0.53
1:B:1383:THR:HG22	1:B:1402:ILE:HG12	1.91	0.53
1:B:1467:ILE:N	1:B:1468:PRO:HD3	2.23	0.53
1:B:499:TYR:O	1:B:514:THR:HG23	2.09	0.53
1:B:561:LEU:O	1:B:563:ILE:CG2	2.57	0.53
1:B:61:ASP:O	1:B:63:LYS:N	2.37	0.53
1:A:319:ASN:O	1:A:320:ASN:ND2	2.43	0.52
1:A:686:ILE:C	1:A:688:ALA:H	2.12	0.52
1:B:1028:GLY:O	1:B:1030:HIS:CD2	2.62	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1053:MET:O	1:B:1056:ILE:HG23	2.08	0.52
1:B:1129:LEU:HD13	1:B:1139:GLU:HB3	1.91	0.52
1:B:1136:GLU:OE1	1:B:1415:SER:CB	2.57	0.52
1:B:177:ILE:HD11	1:B:179:HIS:HB2	1.91	0.52
1:B:50:PHE:CE2	1:B:79:PHE:CE2	2.97	0.52
1:A:1003:LEU:N	1:A:1003:LEU:HD23	2.23	0.52
1:A:1019:PHE:CD2	1:A:1020:TYR:CD1	2.98	0.52
1:A:1452:ASP:O	1:A:1462:LEU:HA	2.08	0.52
1:A:505:SER:O	1:A:506:LYS:HB2	2.10	0.52
1:A:661:ASP:OD2	1:A:663:GLN:NE2	2.43	0.52
1:A:127:PHE:CE2	1:A:809:ILE:HD12	2.44	0.52
1:A:992:LEU:HD21	1:A:1045:LEU:HD11	1.90	0.52
1:B:1105:LEU:HA	1:B:1108:VAL:HG11	1.91	0.52
1:B:1210:SER:OG	1:B:1211:ALA:N	2.40	0.52
1:B:1456:LYS:O	1:B:1457:ASP:C	2.48	0.52
1:B:328:THR:OG1	1:B:339:GLU:HG2	2.08	0.52
1:B:363:LEU:HD23	1:B:454:ALA:CB	2.40	0.52
1:B:531:THR:HG23	1:B:533:ASN:H	1.74	0.52
2:X:222:ASN:O	2:X:223:LYS:HG3	2.07	0.52
1:A:1408:TYR:HD2	1:A:1418:GLY:HA2	1.74	0.52
1:A:363:LEU:HD23	1:A:454:ALA:HB3	1.91	0.52
1:A:792:ASP:O	1:A:793:SER:HB2	2.10	0.52
1:A:957:LYS:HG3	1:A:958:GLU:H	1.73	0.52
1:B:719:SER:HB2	1:B:1123:GLN:NE2	2.25	0.52
1:B:1288:GLN:O	1:B:1292:ASN:ND2	2.43	0.52
1:B:349:LEU:HD22	1:B:446:ASN:HD22	1.75	0.52
1:B:571:LEU:CD2	1:B:600:VAL:HG13	2.39	0.52
1:B:142:LYS:HD3	1:B:775:TRP:CD2	2.43	0.52
1:A:1113:LEU:N	1:A:1117:SER:O	2.43	0.52
1:A:348:VAL:CG1	1:A:349:LEU:N	2.72	0.52
1:A:720:LEU:HD11	1:A:1446:VAL:HG22	1.91	0.52
1:A:838:GLN:HA	1:A:901:LEU:HB2	1.92	0.52
1:B:1226:ARG:NE	1:B:1266:TYR:CE1	2.77	0.52
1:B:1432:ILE:CG2	1:B:1479:ILE:HD12	2.39	0.52
1:B:27:ALA:CB	1:B:39:ILE:HD12	2.39	0.52
2:X:162:LEU:O	2:X:166:ASP:HB2	2.10	0.52
2:X:192:ASN:O	2:X:221:ILE:HG23	2.08	0.52
1:A:173:MET:O	1:A:174:VAL:CB	2.57	0.52
1:A:322:TYR:CD2	1:A:322:TYR:N	2.78	0.52
1:A:460:LEU:C	1:A:462:GLN:H	2.13	0.52
1:A:466:TYR:HD1	1:A:467:ILE:N	2.08	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LYS:HD2	1:A:105:GLU:OE1	2.10	0.52
1:A:814:THR:O	1:A:815:VAL:HG23	2.10	0.52
1:B:1016:VAL:HG12	1:B:1017:PRO:HD3	1.92	0.52
1:B:1045:LEU:HD23	1:B:1045:LEU:N	2.25	0.52
1:B:198:MET:HE1	1:B:218:GLU:HB2	1.91	0.52
1:B:362:PHE:CE1	1:B:638:GLY:O	2.62	0.52
1:B:517:LYS:HA	1:B:524:GLN:HE22	1.75	0.52
1:B:916:THR:HG22	1:B:917:TRP:N	2.25	0.52
1:A:1236:ASP:HB2	1:A:1412:ARG:NH2	2.24	0.52
1:A:1128:LYS:O	1:A:1246:ARG:NH2	2.42	0.52
1:A:1196:SER:HB2	1:A:1257:THR:CG2	2.39	0.52
1:A:944:LEU:HD13	1:A:1350:THR:HB	1.90	0.52
1:A:977:LEU:HA	1:A:1361:VAL:CG2	2.38	0.52
1:A:250:ILE:HG21	1:A:327:VAL:HG21	1.91	0.52
1:B:386:VAL:N	1:B:410:VAL:HG13	2.25	0.52
1:A:1249:GLU:HG2	1:A:1253:TYR:HE2	1.75	0.52
1:A:1431:GLY:C	1:A:1432:ILE:HG12	2.30	0.52
1:A:1440:LYS:O	1:A:1444:GLU:HB2	2.09	0.52
1:A:196:TYR:CZ	1:A:221:GLU:HB2	2.45	0.52
1:A:267:ILE:HG23	1:A:327:VAL:HG22	1.91	0.52
1:A:431:LEU:C	1:A:431:LEU:CD2	2.78	0.52
1:A:901:LEU:HD23	1:A:901:LEU:O	2.10	0.52
1:B:1022:PHE:HD2	1:B:1092:TYR:CD2	2.27	0.52
1:B:987:ILE:CD1	1:B:1294:ILE:HD13	2.39	0.52
1:B:24:VAL:HA	1:B:655:THR:OG1	2.09	0.52
1:A:132:LYS:HZ1	1:A:139:GLN:HE22	1.58	0.52
1:A:1432:ILE:CG2	1:A:1479:ILE:HD12	2.40	0.52
1:A:244:LYS:HE3	1:A:304:GLU:CD	2.30	0.52
1:A:686:ILE:HG22	1:A:689:LYS:HE3	1.92	0.52
1:B:1066:TYR:CD1	1:B:1066:TYR:N	2.75	0.52
1:B:1115:ASN:ND2	1:B:1117:SER:H	2.07	0.52
1:B:1153:ARG:HD2	1:B:1197:LEU:O	2.10	0.52
1:B:1411:SER:O	1:B:1414:GLU:HB2	2.10	0.52
1:B:1423:VAL:HG22	1:B:1496:TYR:CD1	2.45	0.52
1:B:661:ASP:OD2	1:B:663:GLN:NE2	2.42	0.52
1:B:85:LEU:HD22	1:B:85:LEU:N	2.23	0.52
1:B:948:GLY:O	1:B:950:TYR:N	2.42	0.52
1:A:1334:LEU:N	1:A:1334:LEU:CD2	2.72	0.52
1:A:172:ASP:O	1:A:173:MET:HB2	2.09	0.52
1:A:227:PHE:HB3	1:A:254:TYR:HD2	1.75	0.52
1:A:243:PHE:CZ	1:A:316:GLU:HA	2.45	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ALA:HA	1:A:341:GLU:HA	1.90	0.52
1:A:435:VAL:HG12	1:A:436:LYS:N	2.25	0.52
1:B:1003:LEU:HD13	1:B:1498:TYR:CD1	2.45	0.52
1:B:222:TYR:OH	1:B:224:LEU:HD22	2.09	0.52
2:Y:190:THR:HG22	2:Y:200:GLU:HG2	1.92	0.52
1:A:1022:PHE:HE2	1:A:1092:TYR:CG	2.28	0.52
1:A:1421:HIS:CE1	1:A:1498:TYR:CG	2.97	0.52
1:A:1435:ASN:O	1:A:1438:ASP:HB2	2.10	0.52
1:A:1511:THR:HG23	1:A:1511:THR:O	2.10	0.52
1:A:163:PHE:N	1:A:163:PHE:CD1	2.73	0.52
1:A:621:GLU:O	1:A:625:GLN:HG3	2.10	0.52
1:A:362:PHE:CE1	1:A:638:GLY:O	2.63	0.52
1:A:680:GLN:HG2	1:A:680:GLN:O	2.10	0.52
1:A:840:GLN:HG2	1:A:899:THR:CG2	2.40	0.52
1:B:1025:LEU:HD13	1:B:1031:TRP:HZ3	1.74	0.52
1:B:1313:ILE:HG22	1:B:1314:ASP:H	1.75	0.52
1:B:138:ASP:OD1	1:B:192:SER:HA	2.10	0.52
1:B:1408:TYR:HD2	1:B:1418:GLY:HA2	1.75	0.52
1:B:169:SER:O	1:B:170:GLU:C	2.49	0.52
1:B:269:PHE:CB	1:B:283:MET:CE	2.88	0.52
1:B:44:TYR:HE1	1:B:497:THR:OG1	1.92	0.52
1:B:626:PHE:O	1:B:628:GLU:N	2.44	0.52
1:B:686:ILE:C	1:B:688:ALA:H	2.10	0.52
1:A:1016:VAL:HG12	1:A:1017:PRO:N	2.25	0.51
1:A:101:TYR:HE1	1:A:116:ARG:NE	2.08	0.51
1:A:1045:LEU:N	1:A:1045:LEU:HD23	2.24	0.51
1:A:1228:TRP:HZ3	1:A:1270:VAL:HG22	1.73	0.51
1:A:1411:SER:O	1:A:1414:GLU:HB2	2.10	0.51
1:A:328:THR:OG1	1:A:339:GLU:HG2	2.10	0.51
1:A:415:ASP:OD2	1:A:417:VAL:HB	2.09	0.51
1:B:1019:PHE:HE2	1:B:1088:GLN:NE2	2.07	0.51
1:B:1133:LEU:H	1:B:1133:LEU:HD12	1.74	0.51
1:B:128:ILE:HG23	1:B:145:VAL:CG2	2.39	0.51
1:B:1030:HIS:CE1	1:B:1306:GLN:NE2	2.78	0.51
1:B:1434:ALA:HB1	1:B:1477:PHE:CE1	2.45	0.51
1:B:1435:ASN:HD22	1:B:1478:ARG:HB2	1.74	0.51
1:B:295:GLY:O	1:B:296:ILE:HD13	2.10	0.51
2:X:183:THR:CB	2:X:230:GLN:HB3	2.40	0.51
1:A:1133:LEU:N	1:A:1134:PRO:CD	2.73	0.51
1:A:1272:LYS:HG3	1:A:1272:LYS:O	2.09	0.51
1:A:1284:PHE:HD2	1:A:1285:TYR:CE1	2.28	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1320:LYS:HD2	1:A:1321:GLY:N	2.25	0.51
1:A:162:THR:OG1	1:A:162:THR:O	2.27	0.51
1:A:253:ARG:HB2	1:A:253:ARG:CZ	2.40	0.51
1:A:839:ILE:HD11	1:A:1483:PHE:CE1	2.44	0.51
1:B:100:SER:O	1:B:101:TYR:HD2	1.94	0.51
1:B:1172:ASP:O	1:B:1175:LEU:HB2	2.10	0.51
1:B:215:ALA:C	1:B:216:TYR:CD2	2.83	0.51
1:B:227:PHE:CZ	1:B:329:VAL:O	2.63	0.51
1:B:250:ILE:O	1:B:250:ILE:HG13	2.10	0.51
1:B:754:MET:O	1:B:755:LYS:HG2	2.11	0.51
1:B:594:THR:O	1:B:782:ARG:HG2	2.09	0.51
1:B:829:ILE:HG13	1:B:925:LYS:CG	2.38	0.51
1:A:106:VAL:HG12	1:A:107:VAL:H	1.74	0.51
1:A:269:PHE:CB	1:A:283:MET:CE	2.89	0.51
1:A:322:TYR:N	1:A:322:TYR:HD2	2.07	0.51
1:A:585:GLY:HA2	1:A:790:LEU:O	2.10	0.51
1:B:1018:VAL:O	1:B:1021:VAL:N	2.44	0.51
1:B:1023:HIS:O	1:B:1027:THR:HB	2.11	0.51
1:B:1076:THR:HG22	1:B:1120:GLU:HA	1.92	0.51
1:B:1193:TYR:CA	1:B:1257:THR:HG23	2.36	0.51
1:B:330:ILE:HG22	1:B:337:SER:CA	2.40	0.51
1:B:701:ASP:O	1:B:704:CYS:HB2	2.11	0.51
1:A:1429:PRO:CG	1:A:1511:THR:HB	2.39	0.51
1:A:1401:ARG:HA	1:A:1478:ARG:HA	1.93	0.51
1:A:165:ASP:HB3	1:A:171:VAL:HG21	1.91	0.51
1:B:491:PRO:O	1:B:492:TYR:C	2.49	0.51
1:B:544:TYR:H	1:B:544:TYR:HD1	1.57	0.51
1:B:573:VAL:O	1:B:815:VAL:HG21	2.09	0.51
1:B:647:HIS:O	1:B:649:ALA:N	2.43	0.51
1:B:712:GLU:HA	1:B:715:ALA:HB3	1.92	0.51
1:A:1161:LEU:HD12	1:A:1162:VAL:CG2	2.41	0.51
1:A:1210:SER:O	1:A:1214:ARG:N	2.38	0.51
1:A:1296:GLY:O	1:A:1299:GLU:N	2.42	0.51
1:A:1334:LEU:CD2	1:A:1334:LEU:H	2.21	0.51
1:B:1043:GLN:O	1:B:1046:LYS:HB2	2.10	0.51
1:B:1049:LEU:O	1:B:1050:LYS:C	2.47	0.51
1:B:1076:THR:HG21	1:B:1120:GLU:HA	1.93	0.51
1:B:1157:ASP:C	1:B:1160:PRO:HD3	2.31	0.51
1:B:1259:LEU:CD1	1:B:1300:TYR:HB2	2.40	0.51
1:B:799:ILE:O	1:B:799:ILE:HG12	2.10	0.51
1:B:849:ARG:CG	1:B:853:MET:HE1	2.38	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1080:ALA:O	1:A:1081:PHE:C	2.47	0.51
1:A:1432:ILE:O	1:A:1433:SER:C	2.49	0.51
1:A:1460:VAL:O	1:A:1460:VAL:HG12	2.10	0.51
1:A:169:SER:O	1:A:170:GLU:C	2.49	0.51
1:A:586:GLN:O	1:A:790:LEU:HD12	2.11	0.51
1:A:80:GLN:HB3	1:A:512:PHE:HE1	1.76	0.51
1:A:913:SER:HA	1:A:921:GLU:O	2.11	0.51
1:B:1008:ALA:O	1:B:1011:GLU:N	2.44	0.51
1:B:1096:ASN:ND2	1:B:1099:SER:H	2.08	0.51
1:B:1127:ILE:HD12	1:B:1127:ILE:H	1.74	0.51
1:B:1307:LEU:O	1:B:1308:ARG:C	2.48	0.51
1:B:981:GLY:HA3	1:B:1309:LEU:HD11	1.92	0.51
1:B:342:ILE:CG2	1:B:343:PRO:HD2	2.41	0.51
1:B:494:ASP:C	1:B:496:ILE:H	2.14	0.51
1:B:571:LEU:HD12	1:B:572:GLN:H	1.68	0.51
1:A:1229:LYS:HB3	1:A:1231:ASN:OD1	2.10	0.51
1:A:582:TYR:HB2	1:A:819:VAL:HG12	1.93	0.51
1:A:626:PHE:O	1:A:629:LYS:HG2	2.10	0.51
1:B:1022:PHE:CE2	1:B:1092:TYR:CG	2.99	0.51
1:B:847:ASN:O	1:B:848:TYR:CD1	2.63	0.51
1:A:1025:LEU:HD13	1:A:1031:TRP:HZ3	1.74	0.51
1:A:1290:THR:HA	1:A:1293:ALA:HB3	1.93	0.51
1:A:1311:MET:HG2	1:A:1350:THR:OG1	2.11	0.51
1:A:269:PHE:CD1	1:A:286:ALA:HB1	2.46	0.51
1:A:27:ALA:HB2	1:A:39:ILE:HD12	1.92	0.51
1:A:493:ILE:CG2	1:A:494:ASP:N	2.73	0.51
1:A:50:PHE:CD1	1:A:109:LYS:HE2	2.45	0.51
1:A:700:TYR:C	1:A:702:GLY:N	2.62	0.51
1:B:1100:ILE:HG21	1:B:1158:ILE:HD12	1.92	0.51
1:B:1251:THR:HG21	1:B:1273:TRP:HH2	1.73	0.51
1:B:269:PHE:CB	1:B:283:MET:HE3	2.41	0.51
1:B:323:LEU:HB3	1:B:345:ILE:HB	1.92	0.51
1:B:575:LEU:HG	1:B:815:VAL:HG11	1.93	0.51
1:B:73:LEU:H	1:B:73:LEU:HD23	1.76	0.51
1:B:592:MET:HE2	1:B:784:LYS:HB3	1.93	0.51
1:B:833:VAL:HA	1:B:1430:THR:HG21	1.92	0.51
1:A:1316:SER:O	1:A:1347:ILE:HG13	2.11	0.51
1:A:146:TYR:CE1	1:A:182:ILE:HG23	2.46	0.51
1:A:316:GLU:O	1:A:319:ASN:N	2.43	0.51
1:A:330:ILE:HB	1:A:336:PHE:O	2.11	0.51
1:A:395:ILE:HG13	1:A:429:THR:OG1	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ARG:HD3	1:A:414:ASP:OD1	2.11	0.51
1:A:27:ALA:O	1:A:652:THR:O	2.29	0.51
1:A:701:ASP:OD1	1:A:702:GLY:N	2.44	0.51
1:B:1030:HIS:NE2	1:B:1306:GLN:NE2	2.59	0.51
1:B:1372:GLU:HG3	1:B:1373:GLU:N	2.20	0.51
1:B:1440:LYS:HD3	1:B:1453:TYR:CZ	2.45	0.51
1:B:155:ALA:O	1:B:156:LYS:C	2.49	0.51
1:B:165:ASP:C	1:B:165:ASP:OD1	2.49	0.51
1:B:515:ARG:HH22	1:B:527:ASN:C	2.14	0.51
1:B:73:LEU:HB2	1:B:79:PHE:HA	1.92	0.51
1:B:142:LYS:HD3	1:B:775:TRP:CD1	2.46	0.51
1:B:961:TYR:HD2	1:B:1344:ASP:O	1.94	0.51
1:B:976:ILE:HG21	1:B:1280:TYR:HE1	1.76	0.51
2:Y:192:ASN:HB2	2:Y:223:LYS:H	1.76	0.51
1:A:296:ILE:HG22	1:A:297:ALA:N	2.23	0.51
1:A:354:LEU:HD12	1:A:435:VAL:CG1	2.41	0.51
1:B:1202:HIS:CD2	1:B:1204:GLN:CB	2.94	0.51
1:B:1346:LEU:HG	1:B:1347:ILE:N	2.26	0.51
1:B:1429:PRO:HB3	1:B:1488:LEU:CD2	2.41	0.51
1:B:272:ARG:CG	1:B:273:GLU:H	2.24	0.51
1:B:364:LYS:H	1:B:364:LYS:HD3	1.74	0.51
1:A:702:GLY:HA2	1:A:728:PHE:CD1	2.46	0.50
1:B:1432:ILE:O	1:B:1433:SER:O	2.28	0.50
1:B:173:MET:O	1:B:174:VAL:HB	2.11	0.50
1:B:30:ILE:HG22	1:B:31:PHE:O	2.11	0.50
1:B:936:ARG:NH1	1:B:1002:HIS:CE1	2.78	0.50
1:A:78:LYS:NZ	2:X:144:GLY:HA2	2.26	0.50
1:A:150:ASP:N	1:A:150:ASP:OD2	2.44	0.50
1:A:271:ILE:O	1:A:272:ARG:HB2	2.11	0.50
1:A:352:TYR:HD1	1:A:375:VAL:HG11	1.76	0.50
1:B:1431:GLY:C	1:B:1432:ILE:HG12	2.32	0.50
1:B:244:LYS:HE3	1:B:304:GLU:CD	2.31	0.50
1:B:450:GLU:HB3	1:B:452:TYR:CE2	2.47	0.50
1:B:953:ILE:O	1:B:953:ILE:HG13	2.10	0.50
1:A:1111:TYR:CE1	1:A:1121:ASN:HB2	2.47	0.50
1:A:987:ILE:CD1	1:A:1294:ILE:HD12	2.41	0.50
1:A:1343:ASN:N	1:A:1343:ASN:HD22	2.08	0.50
1:A:983:LEU:HD11	1:A:1356:LEU:HD22	1.92	0.50
1:A:242:ASN:HB3	1:A:245:ASN:OD1	2.10	0.50
1:A:412:ARG:HD3	1:A:414:ASP:CG	2.32	0.50
1:A:491:PRO:O	1:A:492:TYR:C	2.48	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ILE:HG22	1:A:55:SER:N	2.27	0.50
1:A:571:LEU:HD21	1:A:600:VAL:HG13	1.93	0.50
1:A:679:LEU:HD22	1:A:738:LEU:HD11	1.94	0.50
1:A:683:ILE:HD13	1:A:735:ALA:HB2	1.93	0.50
1:A:700:TYR:CE1	1:A:758:LEU:HD12	2.46	0.50
1:B:1404:ALA:C	1:B:1474:CYS:SG	2.89	0.50
1:B:234:GLU:C	1:B:235:TYR:HD2	2.15	0.50
1:B:946:PRO:HD2	1:B:947:ARG:H	1.75	0.50
2:Y:193:LEU:HD23	2:Y:221:ILE:HG12	1.93	0.50
1:A:1210:SER:OG	1:A:1211:ALA:N	2.44	0.50
1:A:139:GLN:O	1:A:190:ILE:HG12	2.12	0.50
1:A:42:GLN:HG3	1:A:80:GLN:NE2	2.25	0.50
1:A:485:ILE:CG2	1:A:487:THR:HG23	2.41	0.50
1:A:905:ILE:CD1	1:A:931:PRO:HG3	2.42	0.50
1:A:950:TYR:CE2	1:A:1356:LEU:HD11	2.47	0.50
1:B:59:TYR:CD1	1:B:103:TYR:HE1	2.30	0.50
1:B:1274:LEU:CB	1:B:1297:LEU:HD11	2.38	0.50
1:B:1488:LEU:HD11	1:B:1510:SER:OG	2.12	0.50
1:B:159:THR:HG22	1:B:160:VAL:N	2.25	0.50
1:B:256:TYR:C	1:B:257:ASN:HD22	2.14	0.50
1:B:720:LEU:HD11	1:B:1446:VAL:HG22	1.94	0.50
1:B:599:TRP:HE3	1:B:778:HIS:O	1.94	0.50
1:B:902:PRO:O	1:B:903:LEU:HD13	2.11	0.50
1:A:105:GLU:HA	1:A:114:SER:HB3	1.94	0.50
1:A:161:LEU:CG	1:A:185:PHE:CE1	2.94	0.50
1:A:536:PRO:HG3	1:A:624:PHE:CE2	2.45	0.50
1:A:56:ILE:HD13	1:A:86:THR:H	1.76	0.50
1:B:1093:VAL:HG12	1:B:1095:GLN:NE2	2.27	0.50
1:B:1151:GLY:O	1:B:1152:ILE:C	2.48	0.50
1:B:1323:LEU:CG	1:B:1324:HIS:H	2.24	0.50
1:B:136:THR:HB	1:B:137:PRO:HD2	1.94	0.50
1:B:365:PRO:HD2	1:B:464:TYR:CE2	2.46	0.50
1:B:693:SER:O	1:B:696:LYS:HB3	2.11	0.50
1:B:700:TYR:C	1:B:702:GLY:H	2.14	0.50
1:B:942:VAL:HG22	1:B:957:LYS:HD3	1.94	0.50
2:X:190:THR:HG22	2:X:200:GLU:HG2	1.93	0.50
1:A:1049:LEU:CD2	1:A:1089:VAL:HG13	2.42	0.50
1:A:1082:ALA:O	1:A:1083:LEU:C	2.48	0.50
1:A:1128:LYS:HE2	1:A:1129:LEU:O	2.10	0.50
1:A:1434:ALA:CA	1:A:1479:ILE:HG22	2.34	0.50
1:A:224:LEU:HD13	1:A:225:PRO:HD2	1.93	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1016:VAL:HG12	1:B:1017:PRO:CD	2.41	0.50
1:B:1081:PHE:CE1	1:B:1288:GLN:NE2	2.77	0.50
1:B:1376:SER:O	1:B:1409:LYS:HB2	2.11	0.50
1:B:1429:PRO:HB3	1:B:1488:LEU:HD22	1.94	0.50
1:B:1466:SER:CB	1:B:1468:PRO:HD3	2.42	0.50
1:B:234:GLU:C	1:B:235:TYR:CD2	2.85	0.50
1:B:835:ARG:HH21	1:B:971:THR:HG22	1.76	0.50
1:A:1022:PHE:CE2	1:A:1092:TYR:CG	3.00	0.50
1:A:1299:GLU:O	1:A:1302:LEU:HB2	2.11	0.50
1:A:1466:SER:CB	1:A:1468:PRO:HD3	2.41	0.50
1:B:1069:TRP:HE1	1:B:1463:GLN:HE21	1.58	0.50
1:B:109:LYS:HD2	1:B:110:HIS:HB2	1.93	0.50
1:B:149:ASN:O	1:B:152:LEU:N	2.41	0.50
1:B:816:LYS:O	1:B:817:ALA:HB2	2.12	0.50
1:B:866:CYS:HB2	1:B:901:LEU:O	2.12	0.50
1:B:853:MET:O	1:B:888:VAL:HG22	2.11	0.50
1:A:1240:PRO:O	1:A:1242:THR:HG23	2.11	0.50
1:A:1423:VAL:HG21	1:A:1496:TYR:HE1	1.75	0.50
1:A:128:ILE:CG1	1:A:215:ALA:HB2	2.42	0.50
1:A:227:PHE:CE1	1:A:338:GLU:CB	2.94	0.50
1:A:316:GLU:O	1:A:318:LEU:N	2.45	0.50
1:A:478:VAL:O	1:A:478:VAL:HG13	2.12	0.50
1:A:594:THR:HB	1:A:596:MET:O	2.12	0.50
1:B:1189:ALA:O	1:B:1192:ALA:HB3	2.11	0.50
1:B:1226:ARG:N	1:B:1269:PRO:O	2.31	0.50
1:B:150:ASP:N	1:B:150:ASP:OD2	2.45	0.50
1:B:839:ILE:HG13	1:B:840:GLN:N	2.26	0.50
1:B:927:LEU:HD23	1:B:928:ARG:N	2.27	0.50
1:A:1080:ALA:O	1:A:1083:LEU:HB2	2.12	0.50
1:A:834:VAL:HG11	1:A:1489:SER:CB	2.42	0.50
1:A:260:VAL:HG12	1:A:261:THR:N	2.27	0.50
1:A:395:ILE:O	1:A:429:THR:CG2	2.60	0.50
1:A:485:ILE:HG22	1:A:487:THR:HG23	1.94	0.50
1:A:52:ALA:CB	1:A:73:LEU:HD21	2.41	0.50
1:B:1115:ASN:ND2	1:B:1115:ASN:C	2.65	0.50
1:B:1334:LEU:O	1:B:1335:GLY:O	2.29	0.50
1:B:532:GLN:O	1:B:535:VAL:HG22	2.12	0.50
1:B:592:MET:HE1	1:B:784:LYS:O	2.12	0.50
2:Y:186:TYR:O	2:Y:229:LYS:HB3	2.12	0.50
1:A:349:LEU:HD22	1:A:349:LEU:C	2.32	0.49
1:A:777:VAL:HG12	1:A:778:HIS:N	2.26	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:TYR:C	1:B:466:TYR:CD1	2.85	0.49
1:B:553:GLU:OE1	1:B:555:VAL:CG2	2.60	0.49
1:B:683:ILE:CD1	1:B:735:ALA:HB2	2.41	0.49
1:A:1376:SER:O	1:A:1409:LYS:HB2	2.12	0.49
1:A:149:ASN:N	1:A:155:ALA:HB2	2.27	0.49
1:A:330:ILE:HA	1:A:337:SER:HA	1.95	0.49
1:A:467:ILE:HD12	1:A:484:ILE:HD11	1.94	0.49
1:A:800:GLN:O	1:A:800:GLN:HG2	2.11	0.49
1:A:820:PHE:HE2	1:A:848:TYR:HD2	1.57	0.49
1:A:979:VAL:HB	1:A:1326:TYR:OH	2.12	0.49
1:B:1421:HIS:CE1	1:B:1498:TYR:CG	2.99	0.49
1:B:188:PHE:C	1:B:188:PHE:CD1	2.86	0.49
1:B:412:ARG:HD3	1:B:414:ASP:CG	2.33	0.49
1:A:1229:LYS:CD	1:A:1239:VAL:HG12	2.42	0.49
1:A:1245:ALA:HA	1:A:1285:TYR:HB3	1.93	0.49
1:A:1286:SER:OG	1:A:1287:THR:N	2.41	0.49
1:A:1381:ILE:HD13	1:A:1509:TYR:CE1	2.47	0.49
1:A:571:LEU:CD2	1:A:600:VAL:HG13	2.42	0.49
1:A:727:ALA:O	1:A:731:CYS:SG	2.71	0.49
1:A:85:LEU:H	1:A:85:LEU:CD2	2.20	0.49
1:B:1439:LEU:HD12	1:B:1455:ILE:HD11	1.95	0.49
1:B:493:ILE:CG2	1:B:494:ASP:N	2.75	0.49
1:B:849:ARG:CB	1:B:853:MET:HE1	2.42	0.49
2:Y:136:LEU:N	2:Y:136:LEU:HD23	2.27	0.49
1:A:1183:GLN:O	1:A:1232:LEU:HD22	2.12	0.49
1:A:1332:ASN:O	1:A:1332:ASN:CG	2.51	0.49
1:A:1496:TYR:HB3	1:A:1504:GLN:HG3	1.93	0.49
1:A:128:ILE:HG13	1:A:214:THR:O	2.11	0.49
1:A:440:PRO:HD2	1:A:441:ASP:H	1.77	0.49
1:A:700:TYR:HE1	1:A:758:LEU:CB	2.24	0.49
1:A:825:LEU:HA	1:A:845:VAL:HA	1.94	0.49
1:A:855:PHE:HD1	1:A:856:CYS:N	2.10	0.49
1:B:1024:TYR:HB2	1:B:1298:THR:HG23	1.94	0.49
1:B:1221:ASN:ND2	1:B:1222:PRO:HA	2.27	0.49
1:B:52:ALA:CB	1:B:73:LEU:HD21	2.42	0.49
1:B:534:MET:O	1:B:537:SER:O	2.30	0.49
1:B:634:CYS:SG	1:B:635:GLY:N	2.85	0.49
1:B:96:GLN:O	1:B:98:PRO:CD	2.51	0.49
1:A:558:SER:OG	1:A:638:GLY:N	2.44	0.49
1:A:765:ILE:HD11	1:A:769:PHE:HE2	1.76	0.49
1:A:906:GLY:N	1:A:929:VAL:HB	2.28	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:LEU:HD23	1:A:1309:LEU:CD1	2.42	0.49
1:B:1128:LYS:HE2	1:B:1129:LEU:O	2.12	0.49
1:B:855:PHE:CE2	1:B:888:VAL:HG13	2.47	0.49
1:A:1225:TYR:HD1	1:A:1273:TRP:HB2	1.77	0.49
1:A:1328:MET:O	1:A:1329:THR:HG23	2.11	0.49
1:A:824:PHE:HE1	1:A:846:TYR:HD1	1.59	0.49
1:B:1202:HIS:O	1:B:1204:GLN:N	2.45	0.49
1:B:161:LEU:C	1:B:162:THR:HG22	2.31	0.49
1:B:27:ALA:HB1	1:B:28:PRO:HD2	1.95	0.49
1:B:352:TYR:HD1	1:B:375:VAL:HG13	1.77	0.49
1:B:896:VAL:HG12	1:B:897:THR:N	2.27	0.49
2:X:140:LYS:HE3	2:X:228:LEU:HD12	1.93	0.49
1:A:1268:ASN:N	1:A:1269:PRO:CD	2.75	0.49
1:A:195:ARG:HH11	1:A:195:ARG:HG2	1.77	0.49
1:A:243:PHE:CE2	1:A:316:GLU:CG	2.95	0.49
1:A:394:THR:CG2	1:A:428:VAL:HG23	2.42	0.49
1:A:707:ASN:HB3	1:A:739:ARG:HH12	1.78	0.49
1:A:781:PRO:O	1:A:782:ARG:HB2	2.13	0.49
1:B:1284:PHE:HD2	1:B:1285:TYR:CD1	2.31	0.49
1:B:224:LEU:HD13	1:B:225:PRO:HD2	1.95	0.49
1:A:1308:ARG:HH11	1:A:1308:ARG:HG2	1.78	0.49
1:A:1450:PHE:CZ	1:A:1475:VAL:HB	2.48	0.49
1:A:1439:LEU:CD1	1:A:1455:ILE:HD11	2.42	0.49
1:A:1423:VAL:HG22	1:A:1496:TYR:CD1	2.48	0.49
1:A:281:GLU:O	1:A:282:MET:O	2.29	0.49
1:A:922:ILE:O	1:A:922:ILE:HG22	2.12	0.49
1:B:120:THR:CG2	1:B:121:TYR:N	2.54	0.49
1:B:1435:ASN:O	1:B:1436:GLU:C	2.51	0.49
1:B:191:PRO:CG	1:B:194:PRO:HB3	2.41	0.49
1:B:371:ILE:CD1	1:B:390:LEU:HD21	2.42	0.49
1:B:460:LEU:C	1:B:462:GLN:H	2.16	0.49
1:B:703:ALA:HB1	1:B:735:ALA:HB3	1.95	0.49
1:B:71:VAL:HG11	1:B:82:SER:O	2.12	0.49
1:B:982:LEU:CD2	1:B:1309:LEU:CD1	2.90	0.49
2:Y:166:ASP:OD2	2:Y:201:ILE:HD13	2.12	0.49
1:A:1148:THR:O	1:A:1152:ILE:HD12	2.12	0.49
1:A:1429:PRO:O	1:A:1432:ILE:HG12	2.12	0.49
1:A:123:ASN:C	1:A:211:THR:HG21	2.34	0.49
1:A:386:VAL:N	1:A:411:THR:HG22	2.23	0.49
1:A:540:LEU:O	1:A:558:SER:HB2	2.13	0.49
1:A:606:ASP:O	1:A:608:ALA:N	2.45	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:GLN:O	1:A:626:PHE:C	2.51	0.49
1:B:100:SER:O	1:B:101:TYR:CD2	2.66	0.49
1:B:1432:ILE:O	1:B:1433:SER:C	2.50	0.49
1:B:173:MET:O	1:B:174:VAL:CB	2.61	0.49
1:B:395:ILE:O	1:B:429:THR:CG2	2.60	0.49
1:B:494:ASP:HA	1:B:496:ILE:HD11	1.95	0.49
1:B:51:ASP:OD2	1:B:70:HIS:NE2	2.43	0.49
1:B:58:SER:HB3	1:B:66:TYR:OH	2.12	0.49
1:A:1076:THR:O	1:A:1079:THR:HB	2.13	0.49
1:A:1132:THR:HG22	1:A:1134:PRO:HD2	1.93	0.49
1:A:1342:LEU:N	1:A:1342:LEU:HD23	2.27	0.49
1:A:1401:ARG:HB2	1:A:1478:ARG:CB	2.43	0.49
1:A:839:ILE:HD11	1:A:1483:PHE:CZ	2.48	0.49
1:A:606:ASP:C	1:A:608:ALA:H	2.16	0.49
1:B:1096:ASN:HD22	1:B:1096:ASN:C	2.15	0.49
1:B:685:GLU:HG3	1:B:686:ILE:CD1	2.42	0.49
2:Y:194:LYS:HG3	2:Y:195:ASP:H	1.78	0.49
1:A:1244:THR:HG23	1:A:1502:ASP:OD2	2.12	0.48
1:A:129:HIS:CD2	1:A:129:HIS:O	2.66	0.48
1:A:415:ASP:OD1	1:A:417:VAL:HG23	2.13	0.48
1:A:457:TYR:CD2	1:A:457:TYR:O	2.66	0.48
1:A:855:PHE:C	1:A:855:PHE:CD1	2.86	0.48
1:B:1108:VAL:HG13	1:B:1109:GLU:N	2.28	0.48
1:B:1341:LEU:CB	1:B:1342:LEU:HD23	2.43	0.48
1:B:149:ASN:N	1:B:155:ALA:HB2	2.28	0.48
1:B:438:ASP:C	1:B:439:ALA:O	2.51	0.48
1:B:838:GLN:HA	1:B:901:LEU:HB2	1.95	0.48
1:A:1184:SER:HA	1:A:1232:LEU:CB	2.43	0.48
1:A:124:GLY:O	1:A:125:PHE:CG	2.66	0.48
1:A:1439:LEU:HD12	1:A:1455:ILE:HD11	1.94	0.48
1:A:940:SER:HB2	1:A:959:PHE:CE1	2.48	0.48
1:B:1003:LEU:HD22	1:B:1004:PRO:HD2	1.94	0.48
1:B:1317:TYR:CB	1:B:1320:LYS:HB3	2.43	0.48
1:B:269:PHE:CD1	1:B:286:ALA:HB1	2.48	0.48
1:B:465:LEU:HD13	1:B:544:TYR:CD1	2.48	0.48
1:B:897:THR:C	1:B:898:PHE:CD2	2.87	0.48
1:B:907:LEU:HD12	1:B:908:HIS:H	1.77	0.48
1:A:1008:ALA:CB	1:A:1059:TYR:CD2	2.96	0.48
1:A:1249:GLU:OE2	1:A:1288:GLN:HB3	2.13	0.48
1:A:1381:ILE:CG2	1:A:1509:TYR:CD1	2.97	0.48
1:A:147:SER:O	1:A:148:LEU:HD12	2.14	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ALA:CB	1:A:39:ILE:HD12	2.43	0.48
1:A:735:ALA:HB1	1:A:754:MET:CE	2.40	0.48
1:A:182:ILE:HD12	1:A:777:VAL:HG11	1.96	0.48
1:B:1047:LYS:C	1:B:1049:LEU:N	2.64	0.48
1:B:229:VAL:HG22	1:B:252:ALA:HB2	1.95	0.48
1:B:281:GLU:O	1:B:282:MET:O	2.31	0.48
1:B:727:ALA:O	1:B:731:CYS:SG	2.71	0.48
1:B:733:VAL:HG13	1:B:737:GLN:NE2	2.28	0.48
1:A:1098:ASN:HA	1:A:1101:CYS:HB2	1.95	0.48
1:A:1199:ASP:OD1	1:A:1201:THR:OG1	2.29	0.48
1:A:1427:SER:HB3	1:A:1491:ALA:HB1	1.93	0.48
1:A:165:ASP:C	1:A:165:ASP:OD1	2.51	0.48
1:A:352:TYR:CD1	1:A:375:VAL:HG11	2.48	0.48
1:A:365:PRO:HG2	1:A:464:TYR:CE2	2.49	0.48
1:A:53:THR:HA	1:A:69:GLY:O	2.14	0.48
1:A:686:ILE:C	1:A:688:ALA:N	2.65	0.48
1:A:981:GLY:HA3	1:A:1309:LEU:CD1	2.42	0.48
1:B:1007:SER:OG	1:B:1008:ALA:N	2.47	0.48
1:B:102:VAL:HG13	1:B:119:ILE:HG21	1.95	0.48
1:B:1259:LEU:HD21	1:B:1267:VAL:HG11	1.95	0.48
1:B:304:GLU:O	1:B:305:THR:C	2.52	0.48
1:B:38:ASN:C	1:B:39:ILE:HD13	2.30	0.48
1:B:489:LYS:O	1:B:490:SER:CB	2.62	0.48
1:B:564:GLU:HG3	1:B:564:GLU:O	2.13	0.48
1:B:857:VAL:HG21	1:B:896:VAL:CG1	2.44	0.48
1:B:978:SER:OG	1:B:980:LYS:HD3	2.13	0.48
2:Y:179:LEU:HA	2:Y:184:THR:HB	1.95	0.48
2:Y:217:ASN:HB2	2:Y:220:ASP:CG	2.34	0.48
1:A:1408:TYR:CD1	1:A:1409:LYS:N	2.81	0.48
1:A:837:GLU:OE2	1:A:1488:LEU:CA	2.61	0.48
1:A:1509:TYR:CD2	1:A:1509:TYR:C	2.86	0.48
1:A:208:ASP:O	1:A:209:PHE:CG	2.67	0.48
1:A:357:VAL:O	1:A:359:THR:HG23	2.14	0.48
1:A:373:VAL:CG2	1:A:374:GLN:N	2.75	0.48
1:A:489:LYS:O	1:A:490:SER:CB	2.60	0.48
1:A:589:SER:HB2	1:A:785:GLN:HE21	1.77	0.48
1:B:1019:PHE:CE2	1:B:1088:GLN:HB3	2.49	0.48
1:B:1244:THR:HB	1:B:1247:MET:H	1.79	0.48
1:B:1189:ALA:HB1	1:B:1253:TYR:HB2	1.94	0.48
1:B:377:ASP:O	1:B:379:LEU:N	2.47	0.48
1:B:857:VAL:HG12	1:B:914:LEU:HB3	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:PRO:CB	1:A:1352:PHE:O	2.62	0.48
1:A:146:TYR:HE1	1:A:182:ILE:HG23	1.77	0.48
1:A:352:TYR:O	1:A:448:ALA:CB	2.61	0.48
1:A:90:LYS:O	1:A:92:LEU:HG	2.14	0.48
1:A:969:PRO:O	1:A:971:THR:HG23	2.14	0.48
1:B:1248:VAL:CG2	1:B:1277:GLU:HG2	2.38	0.48
1:B:1452:ASP:O	1:B:1462:LEU:HA	2.14	0.48
1:B:830:PRO:HG3	1:B:1483:PHE:CZ	2.48	0.48
1:B:377:ASP:C	1:B:379:LEU:H	2.17	0.48
1:B:616:ALA:O	1:B:617:LYS:C	2.51	0.48
2:X:153:PHE:CG	2:X:154:SER:N	2.81	0.48
2:Y:146:LEU:HD13	2:Y:146:LEU:C	2.34	0.48
1:A:1262:LYS:O	1:A:1264:ILE:HG13	2.14	0.48
1:A:1226:ARG:CD	1:A:1266:TYR:CE1	2.96	0.48
1:A:1509:TYR:O	1:A:1509:TYR:CD2	2.66	0.48
1:A:29:LYS:HE2	1:A:666:ASP:CB	2.38	0.48
1:A:494:ASP:C	1:A:496:ILE:H	2.17	0.48
1:A:634:CYS:HB3	1:A:648:LEU:HD23	1.95	0.48
1:A:588:VAL:CG1	1:A:790:LEU:HD11	2.44	0.48
1:B:1022:PHE:HE2	1:B:1092:TYR:CG	2.32	0.48
1:B:1205:PHE:O	1:B:1209:VAL:HG23	2.13	0.48
1:B:1215:GLU:OE2	1:B:1233:GLN:HB3	2.14	0.48
1:B:837:GLU:OE2	1:B:1488:LEU:HA	2.13	0.48
1:B:494:ASP:C	1:B:496:ILE:HD12	2.33	0.48
1:B:592:MET:CE	1:B:784:LYS:HB3	2.43	0.48
1:B:710:THR:HG23	1:B:713:GLN:OE1	2.14	0.48
1:B:946:PRO:HB3	1:B:1352:PHE:O	2.13	0.48
2:X:183:THR:HG1	2:X:230:GLN:HB3	1.78	0.48
1:A:1228:TRP:H	1:A:1251:THR:HG22	1.77	0.48
1:A:423:ASN:H	1:A:423:ASN:ND2	2.11	0.48
1:A:505:SER:CB	1:A:510:ILE:HD11	2.43	0.48
1:A:716:ALA:C	1:A:718:ILE:H	2.17	0.48
1:A:77:ASN:HD22	1:A:81:ASN:ND2	2.11	0.48
1:A:837:GLU:C	1:A:901:LEU:HD12	2.34	0.48
1:A:83:ALA:O	1:A:85:LEU:HD22	2.14	0.48
1:B:100:SER:O	1:B:101:TYR:CB	2.61	0.48
1:B:105:GLU:HA	1:B:114:SER:HB3	1.95	0.48
1:B:1189:ALA:HB1	1:B:1253:TYR:CB	2.44	0.48
1:B:1203:PRO:O	1:B:1206:ARG:CB	2.61	0.48
1:B:486:VAL:HG12	1:B:486:VAL:O	2.14	0.48
1:B:66:TYR:HD1	1:B:90:LYS:CE	2.03	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:975:ARG:O	1:B:1339:GLU:HA	2.14	0.48
1:A:1280:TYR:HD1	1:A:1362:THR:CG2	2.25	0.48
1:A:1507:MET:HG2	1:A:1508:PHE:O	2.13	0.48
1:A:159:THR:HG23	1:A:204:LYS:O	2.13	0.48
1:A:162:THR:O	1:A:164:ILE:HG13	2.13	0.48
1:A:317:ASP:C	1:A:319:ASN:N	2.64	0.48
1:A:361:LEU:N	1:A:361:LEU:HD12	2.29	0.48
1:A:409:SER:OG	1:A:410:VAL:N	2.47	0.48
1:A:707:ASN:HB3	1:A:739:ARG:HH22	1.78	0.48
1:B:1240:PRO:O	1:B:1242:THR:HG23	2.13	0.48
1:B:1296:GLY:O	1:B:1299:GLU:N	2.47	0.48
1:B:978:SER:N	1:B:1360:HIS:O	2.43	0.48
1:B:349:LEU:CD2	1:B:446:ASN:HD22	2.27	0.48
1:B:394:THR:CG2	1:B:428:VAL:HG23	2.44	0.48
1:B:825:LEU:HD11	1:B:827:MET:SD	2.54	0.48
1:A:1128:LYS:HZ1	1:A:1415:SER:HB3	1.78	0.48
1:A:393:GLN:O	1:A:431:LEU:HD23	2.13	0.48
1:A:349:LEU:CD2	1:A:446:ASN:HD22	2.27	0.48
1:A:44:TYR:HE1	1:A:497:THR:OG1	1.79	0.48
1:A:602:LEU:HD12	1:A:774:LEU:HD22	1.96	0.48
1:A:88:GLN:HB3	1:A:89:PRO:HD2	1.94	0.48
1:B:1290:THR:HA	1:B:1293:ALA:HB3	1.96	0.48
1:B:1496:TYR:HD1	1:B:1496:TYR:O	1.96	0.48
1:B:304:GLU:O	1:B:305:THR:O	2.32	0.48
1:B:503:ILE:HG12	1:B:540:LEU:CB	2.42	0.48
1:B:505:SER:O	1:B:506:LYS:HB2	2.14	0.48
1:B:593:ALA:HA	1:B:782:ARG:O	2.13	0.48
1:B:833:VAL:O	1:B:929:VAL:HA	2.14	0.48
1:B:938:SER:OG	1:B:1279:ARG:NH1	2.47	0.48
1:A:1056:ILE:O	1:A:1058:SER:N	2.47	0.47
1:A:977:LEU:HD13	1:A:1346:LEU:CD2	2.44	0.47
1:A:395:ILE:HA	1:A:400:GLU:O	2.14	0.47
1:A:637:GLY:O	1:A:638:GLY:O	2.32	0.47
1:B:1217:LEU:O	1:B:1218:VAL:CG1	2.53	0.47
1:B:292:LEU:HD22	1:B:296:ILE:C	2.34	0.47
1:B:792:ASP:O	1:B:793:SER:HB2	2.14	0.47
1:B:88:GLN:HB3	1:B:89:PRO:CD	2.43	0.47
1:A:1049:LEU:HD21	1:A:1089:VAL:HG13	1.96	0.47
1:A:1053:MET:HE1	1:A:1086:LEU:HD13	1.94	0.47
1:A:1203:PRO:O	1:A:1206:ARG:HB2	2.13	0.47
1:A:1227:PHE:HA	1:A:1228:TRP:HE3	1.78	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1196:SER:HB2	1:A:1257:THR:HG23	1.96	0.47
1:A:1284:PHE:HD2	1:A:1285:TYR:CD1	2.32	0.47
1:A:692:HIS:NE2	1:A:694:VAL:HG23	2.28	0.47
1:B:1200:LYS:HE3	1:B:1261:LEU:HD23	1.96	0.47
1:B:515:ARG:HH22	1:B:527:ASN:H	1.60	0.47
1:B:646:PHE:O	1:B:651:LEU:HB2	2.14	0.47
1:B:23:TYR:O	1:B:655:THR:HG23	2.14	0.47
1:B:942:VAL:HG23	1:B:959:PHE:HZ	1.78	0.47
1:A:1056:ILE:HD11	1:A:1066:TYR:CE2	2.49	0.47
1:A:1153:ARG:O	1:A:1154:LYS:C	2.52	0.47
1:A:1204:GLN:O	1:A:1207:SER:N	2.47	0.47
1:A:198:MET:HE1	1:A:218:GLU:HB2	1.96	0.47
1:A:61:ASP:OD1	1:A:63:LYS:HB2	2.14	0.47
1:A:647:HIS:C	1:A:649:ALA:N	2.67	0.47
1:A:41:ILE:HD13	1:A:73:LEU:HD22	1.96	0.47
1:B:1117:SER:HB3	1:B:1174:PHE:CD1	2.49	0.47
1:B:1173:ASN:O	1:B:1174:PHE:C	2.52	0.47
1:B:1244:THR:O	1:B:1285:TYR:CD2	2.67	0.47
1:B:718:ILE:HG12	1:B:1446:VAL:O	2.15	0.47
1:B:466:TYR:CD1	1:B:467:ILE:N	2.82	0.47
1:A:1157:ASP:C	1:A:1160:PRO:HD3	2.34	0.47
1:A:123:ASN:HD22	1:A:124:GLY:N	2.11	0.47
1:A:1379:LEU:HD12	1:A:1507:MET:HE2	1.96	0.47
1:A:351:PRO:O	1:A:377:ASP:HA	2.15	0.47
1:A:96:GLN:O	1:A:98:PRO:CD	2.52	0.47
1:B:1453:TYR:HA	1:B:1462:LEU:HD23	1.96	0.47
1:B:260:VAL:HG12	1:B:261:THR:N	2.29	0.47
1:B:431:LEU:CD2	1:B:431:LEU:C	2.83	0.47
1:B:520:ASP:CG	1:B:521:ALA:N	2.66	0.47
1:B:558:SER:OG	1:B:638:GLY:N	2.46	0.47
1:B:905:ILE:CD1	1:B:931:PRO:HG3	2.44	0.47
1:B:935:LYS:HA	1:B:935:LYS:HD2	1.67	0.47
1:B:938:SER:HB3	1:B:1362:THR:OG1	2.14	0.47
2:X:150:ILE:HG13	2:X:150:ILE:O	2.14	0.47
1:A:1024:TYR:HB2	1:A:1298:THR:CG2	2.44	0.47
1:A:1053:MET:HE1	1:A:1086:LEU:HD22	1.96	0.47
1:A:1090:ASN:HD21	1:A:1158:ILE:CG2	2.18	0.47
1:A:1174:PHE:O	1:A:1178:ASN:HB2	2.14	0.47
1:A:129:HIS:CD2	1:A:129:HIS:C	2.86	0.47
1:A:1346:LEU:HD12	1:A:1347:ILE:H	1.78	0.47
1:A:396:ASP:N	1:A:400:GLU:O	2.39	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:GLU:O	1:A:564:GLU:HG3	2.14	0.47
1:A:592:MET:HE2	1:A:780:VAL:HG21	1.96	0.47
1:A:700:TYR:C	1:A:702:GLY:H	2.17	0.47
1:A:707:ASN:HB3	1:A:739:ARG:NH1	2.30	0.47
1:B:1031:TRP:CE3	1:B:1031:TRP:HA	2.50	0.47
1:B:1050:LYS:O	1:B:1053:MET:CB	2.63	0.47
1:B:1439:LEU:CD1	1:B:1455:ILE:HD11	2.45	0.47
1:B:352:TYR:O	1:B:448:ALA:CB	2.61	0.47
1:B:481:HIS:HE1	1:B:529:PRO:HG3	1.79	0.47
1:B:569:ASN:ND2	1:B:598:SER:HB2	2.29	0.47
1:B:606:ASP:C	1:B:608:ALA:N	2.68	0.47
1:B:680:GLN:O	1:B:680:GLN:HG2	2.14	0.47
1:B:85:LEU:CD2	1:B:85:LEU:H	2.26	0.47
1:B:896:VAL:O	1:B:897:THR:CG2	2.60	0.47
1:A:987:ILE:HD11	1:A:1294:ILE:HD13	1.97	0.47
1:A:1401:ARG:HB2	1:A:1478:ARG:CA	2.44	0.47
1:A:1381:ILE:HG21	1:A:1509:TYR:CD1	2.49	0.47
1:A:157:ARG:NH1	1:A:209:PHE:CD1	2.82	0.47
1:A:183:ILE:CG2	1:A:185:PHE:CE2	2.97	0.47
1:A:867:THR:HG23	1:A:900:VAL:HG12	1.95	0.47
1:A:987:ILE:O	1:A:1021:VAL:HG21	2.13	0.47
1:B:1290:THR:O	1:B:1290:THR:HG22	2.14	0.47
1:B:1325:ASN:ND2	1:B:1325:ASN:O	2.48	0.47
1:B:394:THR:CG2	1:B:395:ILE:N	2.78	0.47
1:B:440:PRO:HD2	1:B:441:ASP:H	1.80	0.47
1:B:531:THR:HG23	1:B:533:ASN:HB2	1.97	0.47
1:B:653:PHE:O	1:B:660:ASP:HB2	2.14	0.47
1:A:1152:ILE:O	1:A:1156:PHE:HB2	2.14	0.47
1:A:390:LEU:O	1:A:390:LEU:HG	2.15	0.47
1:A:394:THR:CG2	1:A:395:ILE:N	2.77	0.47
1:A:430:VAL:HA	1:A:454:ALA:O	2.15	0.47
1:A:430:VAL:HG22	1:A:455:ILE:HG12	1.97	0.47
1:A:523:TYR:O	1:A:524:GLN:HB3	2.15	0.47
1:A:635:GLY:C	1:A:673:LEU:HA	2.35	0.47
1:A:602:LEU:HB2	1:A:774:LEU:O	2.15	0.47
1:B:1080:ALA:HA	1:B:1083:LEU:HD12	1.97	0.47
1:B:1155:ALA:O	1:B:1158:ILE:HG13	2.15	0.47
1:B:1268:ASN:N	1:B:1269:PRO:HD3	2.29	0.47
1:B:1271:ILE:CD1	1:B:1271:ILE:O	2.61	0.47
1:B:1280:TYR:CD2	1:B:1280:TYR:C	2.86	0.47
1:B:30:ILE:HG23	1:B:119:ILE:HA	1.96	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:TYR:HB3	1:B:556:SER:HB3	1.96	0.47
1:B:621:GLU:O	1:B:625:GLN:HG3	2.15	0.47
1:B:659:ALA:C	1:B:661:ASP:H	2.18	0.47
2:Y:159:GLU:HG2	2:Y:159:GLU:O	2.14	0.47
2:Y:179:LEU:HD12	2:Y:180:TYR:N	2.29	0.47
1:A:1019:PHE:HE2	1:A:1020:TYR:CE1	2.26	0.47
1:A:1021:VAL:O	1:A:1025:LEU:HG	2.14	0.47
1:A:177:ILE:HD11	1:A:179:HIS:HB2	1.96	0.47
1:A:488:PRO:HG2	1:A:499:TYR:OH	2.15	0.47
1:A:707:ASN:HB3	1:A:739:ARG:NH2	2.29	0.47
1:A:975:ARG:HB3	1:A:1363:THR:HA	1.96	0.47
1:B:1047:LYS:O	1:B:1048:LYS:C	2.53	0.47
1:B:933:GLY:HA3	1:B:1367:LYS:O	2.14	0.47
1:B:1404:ALA:O	1:B:1474:CYS:SG	2.73	0.47
2:X:158:GLU:HA	2:X:219:LYS:NZ	2.30	0.47
1:A:1084:ARG:O	1:A:1088:GLN:HG3	2.15	0.47
1:A:1136:GLU:O	1:A:1140:ASN:N	2.32	0.47
1:A:1378:TYR:CE1	1:A:1409:LYS:HE3	2.49	0.47
1:A:1379:LEU:HD22	1:A:1493:PHE:HE2	1.79	0.47
1:A:708:ASP:OD2	1:A:1476:ARG:HD2	2.15	0.47
1:A:1507:MET:HB3	1:A:1507:MET:HE3	1.73	0.47
1:A:922:ILE:HG21	4:A:2001:NAG:C7	2.44	0.47
1:A:323:LEU:HB3	1:A:345:ILE:HB	1.97	0.47
1:B:271:ILE:HD11	1:B:283:MET:SD	2.55	0.47
1:B:351:PRO:O	1:B:377:ASP:HA	2.14	0.47
1:B:352:TYR:HE2	1:B:442:LEU:HD11	1.80	0.47
1:B:536:PRO:HG3	1:B:624:PHE:CE2	2.48	0.47
2:X:136:LEU:HD23	2:X:136:LEU:H	1.80	0.47
2:X:226:VAL:HG12	2:X:227:THR:N	2.30	0.47
1:A:1115:ASN:HD22	1:A:1117:SER:H	1.61	0.47
1:A:1076:THR:HG22	1:A:1120:GLU:HA	1.97	0.47
1:A:1251:THR:HG21	1:A:1273:TRP:CH2	2.50	0.47
1:A:1434:ALA:CB	1:A:1477:PHE:CE1	2.98	0.47
1:A:232:GLU:HA	1:A:233:PRO:HD3	1.59	0.47
1:A:382:LEU:HD22	1:A:416:GLY:HA3	1.97	0.47
1:B:1309:LEU:O	1:B:1310:SER:HB2	2.15	0.47
1:B:214:THR:CG2	1:B:215:ALA:N	2.77	0.47
1:B:475:ALA:C	1:B:476:LEU:HD23	2.35	0.47
1:B:547:THR:O	1:B:547:THR:HG22	2.15	0.47
1:A:110:HIS:CD2	1:A:110:HIS:O	2.68	0.47
1:A:1172:ASP:O	1:A:1175:LEU:HB2	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1180:LEU:HA	1:A:1180:LEU:HD23	1.53	0.47
1:A:1423:VAL:HG22	1:A:1496:TYR:CE1	2.49	0.47
1:A:304:GLU:O	1:A:305:THR:C	2.52	0.47
1:A:515:ARG:CZ	1:A:526:ILE:HG23	2.45	0.47
1:A:58:SER:HB3	1:A:66:TYR:OH	2.14	0.47
1:A:857:VAL:HG21	1:A:896:VAL:CG1	2.44	0.47
1:A:86:THR:HG23	1:A:86:THR:O	2.15	0.47
1:B:1153:ARG:O	1:B:1154:LYS:C	2.52	0.47
1:B:1174:PHE:O	1:B:1178:ASN:HB2	2.15	0.47
1:B:1229:LYS:CD	1:B:1239:VAL:HG12	2.41	0.47
1:B:1401:ARG:HA	1:B:1478:ARG:HA	1.96	0.47
1:B:431:LEU:O	1:B:453:ARG:HA	2.15	0.47
2:X:150:ILE:HD12	2:X:151:ASP:N	2.29	0.47
1:A:1153:ARG:CZ	1:A:1168:LEU:HD22	2.45	0.46
1:A:1024:TYR:HB2	1:A:1298:THR:HG23	1.98	0.46
1:A:1432:ILE:O	1:A:1433:SER:O	2.33	0.46
1:A:838:GLN:H	1:A:1486:GLY:HA3	1.80	0.46
1:A:155:ALA:O	1:A:156:LYS:C	2.53	0.46
1:A:539:ARG:NH1	1:A:631:ASP:OD1	2.49	0.46
1:A:835:ARG:HH21	1:A:971:THR:HG22	1.79	0.46
1:B:1105:LEU:O	1:B:1109:GLU:HG3	2.15	0.46
1:B:1113:LEU:N	1:B:1117:SER:O	2.46	0.46
1:B:1278:GLN:O	1:B:1360:HIS:NE2	2.48	0.46
1:B:1370:THR:CG2	1:B:1370:THR:O	2.63	0.46
1:B:175:GLU:O	1:B:176:GLU:HB2	2.15	0.46
1:B:307:VAL:HG12	1:B:313:TYR:O	2.15	0.46
1:B:542:VAL:C	1:B:556:SER:HB2	2.35	0.46
1:B:692:HIS:NE2	1:B:694:VAL:HG23	2.30	0.46
1:B:886:GLN:HG3	1:B:887:LYS:H	1.80	0.46
2:X:208:GLN:O	2:X:212:MET:HG3	2.14	0.46
1:A:1247:MET:HB2	1:A:1247:MET:HE3	1.77	0.46
1:A:1488:LEU:HD12	1:A:1488:LEU:C	2.34	0.46
1:B:1016:VAL:O	1:B:1018:VAL:N	2.48	0.46
1:B:1087:GLY:HA3	1:B:1155:ALA:HA	1.96	0.46
1:B:386:VAL:O	1:B:410:VAL:HG13	2.16	0.46
1:B:488:PRO:HG2	1:B:499:TYR:OH	2.15	0.46
1:B:600:VAL:HG12	1:B:601:ALA:H	1.80	0.46
1:B:968:VAL:HG23	1:B:971:THR:HG21	1.98	0.46
1:B:975:ARG:HB3	1:B:1363:THR:HA	1.96	0.46
1:B:976:ILE:HG22	1:B:977:LEU:H	1.79	0.46
1:A:1202:HIS:CD2	1:A:1204:GLN:HB3	2.50	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1310:SER:O	1:A:1311:MET:O	2.32	0.46
1:A:964:PRO:HG2	1:A:1365:VAL:HG11	1.98	0.46
1:A:461:SER:C	1:A:463:SER:H	2.18	0.46
1:A:520:ASP:CG	1:A:521:ALA:N	2.68	0.46
1:A:477:LEU:HA	1:A:564:GLU:CG	2.45	0.46
1:B:1024:TYR:CE2	1:B:1030:HIS:HD2	2.27	0.46
1:B:1440:LYS:NZ	1:B:1453:TYR:OH	2.45	0.46
1:B:1003:LEU:CD1	1:B:1498:TYR:CE1	2.98	0.46
1:B:24:VAL:HG11	1:B:543:TYR:OH	2.15	0.46
1:B:25:ILE:HD13	1:B:41:ILE:HB	1.98	0.46
1:B:697:LYS:HE3	1:B:701:ASP:OD2	2.15	0.46
2:Y:183:THR:HB	2:Y:230:GLN:HB3	1.97	0.46
1:A:1003:LEU:CD1	1:A:1498:TYR:CE1	2.97	0.46
1:A:1244:THR:O	1:A:1285:TYR:HD2	1.98	0.46
1:A:1129:LEU:HD23	1:A:1246:ARG:HH12	1.79	0.46
1:A:1256:LEU:HD21	1:A:1295:GLU:HG2	1.97	0.46
1:A:1251:THR:OG1	1:A:1273:TRP:HZ3	1.94	0.46
1:A:976:ILE:O	1:A:1361:VAL:HG22	2.16	0.46
1:A:220:LYS:HG2	1:A:763:PRO:HB3	1.97	0.46
1:A:234:GLU:HG3	1:A:247:GLU:HB3	1.98	0.46
1:A:313:TYR:CE2	1:A:321:LYS:HD2	2.50	0.46
1:A:373:VAL:HG23	1:A:374:GLN:H	1.80	0.46
1:A:385:GLY:H	1:A:411:THR:HG23	1.79	0.46
1:A:478:VAL:CG1	1:A:478:VAL:O	2.62	0.46
1:A:544:TYR:HE1	1:A:555:VAL:CG1	2.27	0.46
1:B:1129:LEU:CD1	1:B:1139:GLU:HB3	2.45	0.46
1:B:1162:VAL:CG2	1:B:1163:LYS:H	2.15	0.46
1:B:240:TYR:C	1:B:240:TYR:CD1	2.86	0.46
1:B:544:TYR:CE1	1:B:555:VAL:CG1	2.99	0.46
1:A:1008:ALA:HB3	1:A:1078:LEU:CD1	2.46	0.46
1:A:1008:ALA:O	1:A:1009:GLU:C	2.53	0.46
1:A:123:ASN:C	1:A:123:ASN:ND2	2.66	0.46
1:A:191:PRO:C	1:A:193:ASN:N	2.69	0.46
1:A:365:PRO:HD2	1:A:464:TYR:CE2	2.49	0.46
1:A:73:LEU:HD12	1:A:79:PHE:CD2	2.49	0.46
1:B:1263:ASP:OD1	1:B:1266:TYR:HB2	2.16	0.46
1:B:966:ASP:O	1:B:1368:THR:HG23	2.16	0.46
1:B:189:LYS:HG3	1:B:190:ILE:O	2.15	0.46
1:B:157:ARG:NH1	1:B:209:PHE:CD1	2.84	0.46
1:B:685:GLU:HG3	1:B:686:ILE:HD13	1.96	0.46
1:B:987:ILE:CD1	1:B:1294:ILE:CD1	2.93	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1085:VAL:O	1:A:1089:VAL:HG23	2.15	0.46
1:A:1320:LYS:HG2	1:A:1342:LEU:CD1	2.45	0.46
1:A:933:GLY:HA3	1:A:1367:LYS:O	2.15	0.46
1:A:830:PRO:HG3	1:A:1483:PHE:CZ	2.51	0.46
1:A:23:TYR:HE1	1:A:656:ASN:H	1.63	0.46
1:A:588:VAL:HG11	1:A:790:LEU:HD11	1.97	0.46
1:A:916:THR:HG22	1:A:917:TRP:N	2.31	0.46
1:B:1104:LEU:HD12	1:B:1159:CYS:HB3	1.98	0.46
1:B:1307:LEU:H	1:B:1307:LEU:HD12	1.81	0.46
1:B:1492:THR:HG22	1:B:1508:PHE:CD1	2.50	0.46
1:B:193:ASN:OD1	1:B:1070:LYS:HE2	2.15	0.46
1:B:388:VAL:HG21	1:B:418:ALA:CB	2.46	0.46
1:B:503:ILE:HB	1:B:511:HIS:HB2	1.96	0.46
1:B:608:ALA:O	1:B:609:VAL:O	2.34	0.46
1:B:656:ASN:O	1:B:657:ALA:HB2	2.16	0.46
1:B:711:CYS:HB3	1:B:729:THR:HG22	1.97	0.46
1:B:144:ARG:HG2	1:B:775:TRP:CZ2	2.50	0.46
1:B:799:ILE:CG1	1:B:799:ILE:O	2.64	0.46
1:A:1008:ALA:HB3	1:A:1078:LEU:HD11	1.98	0.46
1:A:1097:GLN:O	1:A:1099:SER:N	2.49	0.46
1:A:1249:GLU:HG2	1:A:1253:TYR:CE2	2.50	0.46
1:A:504:LEU:CD1	1:A:509:ILE:HG12	2.46	0.46
1:A:576:SER:HB3	1:A:577:PRO:HD3	1.96	0.46
1:A:855:PHE:CE1	1:A:886:GLN:CB	2.98	0.46
1:A:978:SER:OG	1:A:980:LYS:HD3	2.15	0.46
1:A:987:ILE:CD1	1:A:1294:ILE:CD1	2.94	0.46
1:B:1317:TYR:HB2	1:B:1320:LYS:HB3	1.97	0.46
1:B:313:TYR:CZ	1:B:321:LYS:HD2	2.51	0.46
1:B:586:GLN:O	1:B:790:LEU:HD12	2.14	0.46
1:B:862:VAL:HG21	1:B:909:ASN:O	2.16	0.46
2:X:134:THR:CG2	2:X:153:PHE:HB3	2.43	0.46
1:A:1028:GLY:O	1:A:1030:HIS:CD2	2.69	0.46
1:A:1205:PHE:CZ	1:A:1209:VAL:HG21	2.51	0.46
1:A:1263:ASP:OD1	1:A:1266:TYR:HB2	2.15	0.46
1:A:161:LEU:HD13	1:A:163:PHE:CE1	2.51	0.46
1:A:234:GLU:HB3	1:A:235:TYR:HD2	1.79	0.46
1:A:265:VAL:HG23	1:A:292:LEU:N	2.29	0.46
1:A:397:VAL:C	1:A:399:GLN:H	2.19	0.46
1:A:478:VAL:HG12	1:A:564:GLU:OE1	2.16	0.46
1:B:102:VAL:O	1:B:116:ARG:HA	2.16	0.46
1:B:1117:SER:HB3	1:B:1174:PHE:CE1	2.51	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:TYR:CZ	1:B:141:VAL:HG22	2.51	0.46
1:B:144:ARG:O	1:B:145:VAL:HG23	2.16	0.46
1:B:272:ARG:O	1:B:273:GLU:OE2	2.34	0.46
1:B:363:LEU:HD21	1:B:431:LEU:HB2	1.97	0.46
1:B:594:THR:HB	1:B:596:MET:O	2.16	0.46
1:A:1280:TYR:HD1	1:A:1362:THR:HG22	1.81	0.46
1:A:137:PRO:HG3	1:A:196:TYR:OH	2.16	0.46
1:A:849:ARG:CG	1:A:853:MET:HE1	2.41	0.46
1:B:1180:LEU:HD23	1:B:1180:LEU:HA	1.63	0.46
1:B:30:ILE:CG2	1:B:119:ILE:HA	2.46	0.46
1:B:31:PHE:HB2	1:B:119:ILE:HB	1.98	0.46
1:B:1244:THR:CG2	1:B:1245:ALA:N	2.78	0.46
1:B:1348:VAL:HG21	1:B:1359:VAL:CG1	2.42	0.46
1:B:324:TYR:CD2	1:B:324:TYR:C	2.88	0.46
1:B:330:ILE:HA	1:B:337:SER:HA	1.98	0.46
1:B:504:LEU:HD12	1:B:509:ILE:HA	1.97	0.46
1:B:857:VAL:HA	1:B:913:SER:O	2.15	0.46
1:B:967:LEU:HD12	1:B:968:VAL:H	1.81	0.46
2:Y:143:GLY:C	2:Y:145:ASN:N	2.68	0.46
2:Y:179:LEU:O	2:Y:180:TYR:HB2	2.16	0.46
2:Y:222:ASN:O	2:Y:223:LYS:HG3	2.16	0.46
1:A:1043:GLN:OE1	1:A:1043:GLN:HA	2.15	0.46
1:A:1273:TRP:CZ3	1:A:1274:LEU:CD2	2.99	0.46
1:A:1318:LYS:HA	1:A:1347:ILE:HD11	1.98	0.46
1:A:486:VAL:HG21	1:A:526:ILE:CD1	2.45	0.46
1:A:694:VAL:O	1:A:698:CYS:SG	2.74	0.46
1:A:834:VAL:O	1:A:835:ARG:C	2.52	0.46
1:B:1049:LEU:HD21	1:B:1089:VAL:HG13	1.97	0.46
1:B:115:LYS:HE2	1:B:117:MET:CE	2.46	0.46
1:B:327:VAL:HG12	1:B:328:THR:N	2.31	0.46
1:B:492:TYR:OH	1:B:548:GLY:HA2	2.16	0.46
1:B:834:VAL:HG12	1:B:835:ARG:O	2.15	0.46
1:A:950:TYR:CE1	1:A:1271:ILE:HD11	2.50	0.45
1:A:1225:TYR:CE1	1:A:1272:LYS:HG3	2.51	0.45
1:A:1283:GLY:CA	1:A:1290:THR:CG2	2.92	0.45
1:A:1439:LEU:HD13	1:A:1453:TYR:HD2	1.81	0.45
1:A:177:ILE:HG13	1:A:177:ILE:O	2.16	0.45
1:A:227:PHE:CE1	1:A:338:GLU:HB2	2.51	0.45
1:A:466:TYR:CD1	1:A:467:ILE:N	2.83	0.45
1:A:540:LEU:CD1	1:A:540:LEU:C	2.84	0.45
1:A:539:ARG:NH2	1:A:634:CYS:C	2.69	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:PHE:CE1	1:A:660:ASP:HB3	2.52	0.45
1:B:157:ARG:O	1:B:178:ASP:CB	2.63	0.45
1:B:271:ILE:HG22	1:B:272:ARG:H	1.81	0.45
1:B:543:TYR:HA	1:B:555:VAL:O	2.16	0.45
1:A:1012:LEU:O	1:A:1015:VAL:HG13	2.16	0.45
1:A:984:VAL:CG1	1:A:1024:TYR:CE1	2.84	0.45
1:A:1169:ILE:C	1:A:1171:ALA:N	2.67	0.45
1:A:1412:ARG:O	1:A:1413:GLU:HB2	2.17	0.45
1:A:1432:ILE:HG21	1:A:1479:ILE:HD12	1.97	0.45
1:A:183:ILE:HG22	1:A:185:PHE:CE2	2.52	0.45
1:A:235:TYR:HD2	1:A:235:TYR:N	2.13	0.45
1:A:387:PRO:HG2	1:A:438:ASP:C	2.37	0.45
1:A:609:VAL:CG2	1:A:610:TYR:N	2.51	0.45
1:A:625:GLN:C	1:A:629:LYS:HE2	2.36	0.45
1:B:1041:GLU:O	1:B:1045:LEU:HG	2.16	0.45
1:B:1503:LYS:CD	1:B:1503:LYS:N	2.78	0.45
1:B:177:ILE:O	1:B:177:ILE:HG13	2.15	0.45
1:B:42:GLN:HB2	1:B:80:GLN:NE2	2.32	0.45
1:B:938:SER:CB	1:B:1362:THR:HA	2.47	0.45
1:B:977:LEU:HD21	1:B:1315:VAL:HG21	1.99	0.45
2:X:217:ASN:ND2	2:X:220:ASP:OD2	2.47	0.45
1:A:1244:THR:N	1:A:1285:TYR:CE2	2.85	0.45
1:A:1313:ILE:HG22	1:A:1314:ASP:H	1.78	0.45
1:A:1317:TYR:CB	1:A:1320:LYS:HB3	2.47	0.45
1:A:1488:LEU:HD11	1:A:1510:SER:OG	2.16	0.45
1:A:316:GLU:HB3	1:A:317:ASP:H	1.54	0.45
1:A:829:ILE:HD11	1:A:925:LYS:HG2	1.98	0.45
1:B:37:GLU:HA	1:B:37:GLU:OE1	2.17	0.45
1:B:57:LYS:HG2	1:B:64:PHE:O	2.16	0.45
1:B:592:MET:HG2	1:B:600:VAL:HG21	1.97	0.45
1:B:654:LEU:HA	1:B:654:LEU:HD12	1.55	0.45
2:X:159:GLU:HG2	2:X:159:GLU:O	2.17	0.45
1:A:1049:LEU:O	1:A:1050:LYS:C	2.54	0.45
1:A:109:LYS:HD2	1:A:110:HIS:HB2	1.98	0.45
1:A:1466:SER:C	1:A:1468:PRO:HD3	2.37	0.45
1:A:160:VAL:O	1:A:160:VAL:HG12	2.13	0.45
1:A:23:TYR:CD1	1:A:23:TYR:N	2.81	0.45
1:A:544:TYR:CE1	1:A:555:VAL:CG1	2.98	0.45
1:A:754:MET:O	1:A:755:LYS:CG	2.65	0.45
1:A:835:ARG:NH1	1:A:835:ARG:CG	2.77	0.45
1:B:57:LYS:HD2	1:B:105:GLU:OE1	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1008:ALA:N	1:B:1068:VAL:O	2.50	0.45
1:B:1023:HIS:CD2	1:B:1092:TYR:OH	2.69	0.45
1:B:1202:HIS:O	1:B:1205:PHE:N	2.49	0.45
1:B:432:GLU:OE2	1:B:453:ARG:NH2	2.50	0.45
1:B:586:GLN:O	1:B:789:ALA:HA	2.16	0.45
1:B:927:LEU:HD22	1:B:929:VAL:HG22	1.97	0.45
1:A:1143:TYR:CE2	1:A:1147:PHE:HD1	2.35	0.45
1:A:1200:LYS:HE3	1:A:1261:LEU:CD2	2.46	0.45
1:A:977:LEU:HD13	1:A:1346:LEU:HD21	1.99	0.45
1:A:161:LEU:H	1:A:161:LEU:HG	1.61	0.45
1:A:319:ASN:OD1	1:A:321:LYS:HG2	2.17	0.45
1:A:412:ARG:HD3	1:A:414:ASP:OD2	2.16	0.45
1:A:685:GLU:HG3	1:A:686:ILE:HD13	1.98	0.45
1:A:729:THR:O	1:A:733:VAL:HG23	2.16	0.45
1:B:1040:ILE:HA	1:B:1040:ILE:HD13	1.78	0.45
1:B:1311:MET:HG2	1:B:1350:THR:OG1	2.17	0.45
1:B:498:HIS:HB3	1:B:514:THR:HG21	1.98	0.45
1:B:599:TRP:CE3	1:B:778:HIS:O	2.70	0.45
1:A:1188:LEU:HA	1:A:1188:LEU:HD12	1.70	0.45
1:A:148:LEU:HD23	1:A:152:LEU:HD12	1.98	0.45
1:A:23:TYR:H	1:A:23:TYR:HD1	1.65	0.45
1:A:27:ALA:O	1:A:28:PRO:O	2.35	0.45
1:A:656:ASN:O	1:A:657:ALA:HB2	2.17	0.45
1:B:1080:ALA:O	1:B:1083:LEU:HB2	2.17	0.45
1:B:1509:TYR:CD2	1:B:1509:TYR:C	2.87	0.45
1:B:240:TYR:O	1:B:240:TYR:CD1	2.70	0.45
1:B:290:THR:O	1:B:290:THR:HG22	2.17	0.45
1:B:397:VAL:C	1:B:399:GLN:H	2.20	0.45
1:B:42:GLN:HB2	1:B:80:GLN:CD	2.37	0.45
1:B:498:HIS:HB3	1:B:514:THR:HG23	1.99	0.45
1:B:590:LEU:HD12	1:B:591:ASN:N	2.31	0.45
1:B:913:SER:HA	1:B:921:GLU:O	2.17	0.45
2:X:184:THR:O	2:X:185:LYS:HB3	2.16	0.45
1:A:1007:SER:OG	1:A:1008:ALA:N	2.50	0.45
1:A:100:SER:O	1:A:101:TYR:HD2	2.00	0.45
1:A:1205:PHE:CE2	1:A:1209:VAL:HG21	2.52	0.45
1:A:1274:LEU:CB	1:A:1297:LEU:HD11	2.44	0.45
1:A:169:SER:O	1:A:171:VAL:HG23	2.17	0.45
1:A:589:SER:HA	1:A:787:GLN:HA	1.98	0.45
1:A:659:ALA:C	1:A:661:ASP:H	2.20	0.45
1:B:194:PRO:HA	1:B:1058:SER:OG	2.16	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLU:HA	1:B:233:PRO:HD3	1.57	0.45
1:B:492:TYR:C	1:B:492:TYR:CD2	2.87	0.45
1:B:820:PHE:CZ	1:B:848:TYR:HD2	2.34	0.45
1:B:820:PHE:HE2	1:B:848:TYR:HD2	1.62	0.45
1:B:976:ILE:HG21	1:B:1280:TYR:CE1	2.50	0.45
2:Y:138:VAL:HG11	2:Y:177:TYR:CD2	2.51	0.45
2:Y:140:LYS:O	2:Y:146:LEU:CD2	2.65	0.45
1:A:1228:TRP:CZ3	1:A:1270:VAL:HG22	2.51	0.45
1:B:122:ASP:OD2	1:B:211:THR:HG22	2.17	0.45
1:B:1217:LEU:CD2	1:B:1235:LYS:HE3	2.46	0.45
1:B:1245:ALA:HA	1:B:1285:TYR:HB3	1.99	0.45
1:B:1307:LEU:HB2	1:B:1355:GLY:HA2	1.97	0.45
1:B:981:GLY:HA3	1:B:1309:LEU:CD1	2.47	0.45
1:B:1460:VAL:O	1:B:1460:VAL:HG12	2.16	0.45
1:B:315:LEU:HB2	1:B:318:LEU:HD12	1.99	0.45
1:B:243:PHE:CZ	1:B:316:GLU:HA	2.51	0.45
1:B:386:VAL:N	1:B:411:THR:HG22	2.25	0.45
1:B:605:VAL:CG1	1:B:606:ASP:N	2.80	0.45
1:B:979:VAL:C	1:B:980:LYS:HD2	2.37	0.45
2:X:194:LYS:HA	2:X:194:LYS:HD2	1.80	0.45
1:A:1050:LYS:O	1:A:1053:MET:CB	2.63	0.45
1:A:1104:LEU:HD13	1:A:1164:ILE:CD1	2.44	0.45
1:A:983:LEU:HD23	1:A:1271:ILE:HD13	1.98	0.45
1:A:441:ASP:OD2	1:A:441:ASP:N	2.37	0.45
1:A:498:HIS:HB3	1:A:514:THR:HG23	1.99	0.45
1:A:519:SER:O	1:A:520:ASP:C	2.55	0.45
1:A:623:VAL:HG11	1:A:809:ILE:HD13	1.97	0.45
1:A:646:PHE:O	1:A:649:ALA:HB3	2.16	0.45
1:A:50:PHE:CE2	1:A:79:PHE:CE2	3.05	0.45
1:B:31:PHE:CZ	1:B:104:LEU:HD22	2.40	0.45
1:B:104:LEU:O	1:B:114:SER:CB	2.65	0.45
1:B:1056:ILE:HD11	1:B:1066:TYR:CE2	2.52	0.45
1:B:1180:LEU:CD1	1:B:1207:SER:HB3	2.47	0.45
1:B:1204:GLN:O	1:B:1207:SER:N	2.50	0.45
1:B:1280:TYR:HD1	1:B:1362:THR:CG2	2.30	0.45
1:B:1249:GLU:OE2	1:B:1288:GLN:HB3	2.17	0.45
1:B:162:THR:O	1:B:164:ILE:HG13	2.17	0.45
1:B:435:VAL:CG1	1:B:436:LYS:N	2.80	0.45
1:B:469:TRP:HB2	1:B:483:ASN:O	2.17	0.45
1:B:531:THR:HG23	1:B:533:ASN:N	2.32	0.45
1:A:100:SER:O	1:A:101:TYR:CB	2.63	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:LEU:O	1:A:1107:LEU:HD12	2.17	0.45
1:A:1150:ILE:HD11	1:A:1190:ILE:CG2	2.42	0.45
1:A:1185:THR:HG21	1:A:1228:TRP:HB3	1.99	0.45
1:A:1467:ILE:N	1:A:1468:PRO:CD	2.80	0.45
1:A:1423:VAL:CG2	1:A:1496:TYR:HE1	2.29	0.45
1:A:227:PHE:CD1	1:A:227:PHE:O	2.70	0.45
1:A:240:TYR:CZ	1:A:443:PRO:HD2	2.51	0.45
1:A:259:VAL:HG23	1:A:260:VAL:O	2.16	0.45
1:A:590:LEU:HD12	1:A:591:ASN:H	1.81	0.45
1:A:599:TRP:CZ3	1:A:779:LEU:HB2	2.52	0.45
1:A:644:ASN:HD21	1:A:648:LEU:CD1	2.20	0.45
1:A:837:GLU:OE2	1:A:1488:LEU:CB	2.63	0.45
1:A:956:ARG:HG3	1:A:1349:SER:CB	2.37	0.45
1:A:977:LEU:HD12	1:A:1361:VAL:HG23	1.96	0.45
1:B:1200:LYS:HG2	1:B:1200:LYS:H	1.39	0.45
1:B:1332:ASN:O	1:B:1332:ASN:CG	2.53	0.45
1:B:138:ASP:N	1:B:190:ILE:HB	2.32	0.45
1:B:25:ILE:O	1:B:654:LEU:N	2.43	0.45
1:B:54:ILE:HG22	1:B:55:SER:N	2.31	0.45
1:B:41:ILE:CG2	1:B:81:ASN:O	2.64	0.45
1:B:888:VAL:HG12	1:B:894:HIS:HB2	1.97	0.45
1:B:901:LEU:HA	1:B:902:PRO:HD3	1.81	0.45
1:A:31:PHE:CZ	1:A:104:LEU:HD13	2.51	0.44
1:A:101:TYR:CE1	1:A:116:ARG:NE	2.85	0.44
1:A:159:THR:O	1:A:175:GLU:HA	2.17	0.44
1:A:243:PHE:CZ	1:A:316:GLU:CG	2.92	0.44
1:A:315:LEU:HB2	1:A:318:LEU:HD12	1.98	0.44
1:A:469:TRP:HB2	1:A:483:ASN:O	2.17	0.44
1:A:575:LEU:HD23	1:A:575:LEU:HA	1.74	0.44
1:A:758:LEU:O	1:A:760:VAL:N	2.50	0.44
1:A:587:THR:HG22	1:A:789:ALA:HB2	1.99	0.44
1:A:936:ARG:CZ	1:A:1002:HIS:HE1	2.30	0.44
1:B:323:LEU:HG	1:B:347:TYR:HE2	1.82	0.44
1:B:424:LEU:HA	1:B:425:PRO:HD3	1.79	0.44
1:B:396:ASP:O	1:B:429:THR:HG21	2.17	0.44
1:B:431:LEU:C	1:B:431:LEU:HD22	2.37	0.44
1:B:350:SER:OG	1:B:446:ASN:O	2.27	0.44
1:B:363:LEU:CD2	1:B:454:ALA:HB3	2.46	0.44
1:B:608:ALA:HB1	1:B:769:PHE:HE1	1.82	0.44
1:B:849:ARG:HB3	1:B:853:MET:CE	2.46	0.44
2:X:190:THR:HA	2:X:199:GLN:O	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:153:PHE:CG	2:Y:154:SER:N	2.85	0.44
1:A:1056:ILE:HD11	1:A:1066:TYR:HE2	1.82	0.44
1:A:1225:TYR:CD1	1:A:1273:TRP:HB2	2.53	0.44
1:A:1300:TYR:CD2	1:A:1300:TYR:C	2.90	0.44
1:A:1439:LEU:CD1	1:A:1453:TYR:HD2	2.29	0.44
1:A:25:ILE:HD13	1:A:41:ILE:HA	1.99	0.44
1:A:412:ARG:HG2	1:A:413:VAL:H	1.82	0.44
1:A:492:TYR:C	1:A:492:TYR:CD2	2.90	0.44
1:A:57:LYS:HG2	1:A:64:PHE:O	2.17	0.44
1:A:88:GLN:HB3	1:A:89:PRO:CD	2.47	0.44
1:B:1053:MET:HE3	1:B:1086:LEU:HD13	1.99	0.44
1:B:1210:SER:O	1:B:1214:ARG:N	2.45	0.44
1:B:1265:ASN:HA	1:B:1268:ASN:ND2	2.32	0.44
1:B:540:LEU:C	1:B:540:LEU:CD1	2.85	0.44
1:B:583:SER:HA	1:B:584:PRO:HD3	1.87	0.44
1:B:699:CYS:O	1:B:702:GLY:HA3	2.18	0.44
1:B:980:LYS:HB3	1:B:980:LYS:HE3	1.70	0.44
1:A:1244:THR:HG22	1:A:1245:ALA:N	2.32	0.44
1:A:1438:ASP:O	1:A:1441:ALA:HB3	2.17	0.44
1:A:227:PHE:CE1	1:A:338:GLU:HB3	2.53	0.44
1:B:1378:TYR:CE2	1:B:1409:LYS:HG2	2.53	0.44
1:B:183:ILE:HG22	1:B:185:PHE:CE2	2.52	0.44
1:B:515:ARG:HH22	1:B:527:ASN:CA	2.30	0.44
1:B:590:LEU:HD12	1:B:591:ASN:H	1.82	0.44
1:B:944:LEU:HD23	1:B:944:LEU:HA	1.61	0.44
1:B:991:VAL:HG21	1:B:1017:PRO:O	2.17	0.44
2:Y:226:VAL:HG12	2:Y:227:THR:N	2.32	0.44
1:A:1226:ARG:CZ	1:A:1266:TYR:HE1	2.30	0.44
1:A:1339:GLU:O	1:A:1341:LEU:HD22	2.18	0.44
1:A:961:TYR:CE2	1:A:1343:ASN:HA	2.53	0.44
1:A:165:ASP:HA	1:A:166:PRO:HD3	1.78	0.44
1:A:494:ASP:C	1:A:496:ILE:HD12	2.38	0.44
1:A:847:ASN:O	1:A:848:TYR:CD1	2.71	0.44
1:A:820:PHE:CZ	1:A:848:TYR:HB2	2.42	0.44
1:B:1012:LEU:O	1:B:1015:VAL:CG1	2.65	0.44
1:B:1255:LEU:HD11	1:B:1259:LEU:HD11	1.99	0.44
1:B:1323:LEU:CG	1:B:1324:HIS:N	2.80	0.44
1:B:1432:ILE:HD13	1:B:1481:GLU:HG2	2.00	0.44
1:B:173:MET:C	1:B:174:VAL:HG12	2.38	0.44
1:B:183:ILE:CG2	1:B:185:PHE:CE2	3.01	0.44
1:B:361:LEU:HD12	1:B:361:LEU:N	2.32	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:PHE:CE2	1:B:79:PHE:CD2	3.06	0.44
1:B:544:TYR:CE1	1:B:555:VAL:HG12	2.52	0.44
1:B:754:MET:O	1:B:755:LYS:CG	2.65	0.44
2:X:211:ARG:O	2:X:214:ASP:HB2	2.17	0.44
1:A:1041:GLU:O	1:A:1045:LEU:HG	2.18	0.44
1:A:1047:LYS:C	1:A:1049:LEU:N	2.68	0.44
1:A:1105:LEU:HA	1:A:1108:VAL:HG11	2.00	0.44
1:A:1175:LEU:HA	1:A:1175:LEU:HD23	1.79	0.44
1:A:325:ILE:O	1:A:342:ILE:N	2.30	0.44
1:A:773:TRP:HZ3	1:A:788:PHE:CE1	2.34	0.44
1:B:1127:ILE:HD12	1:B:1127:ILE:O	2.16	0.44
1:B:1228:TRP:N	1:B:1228:TRP:CE3	2.86	0.44
1:B:1229:LYS:HD2	1:B:1239:VAL:CG1	2.42	0.44
1:B:1279:ARG:CD	1:B:1284:PHE:CG	2.98	0.44
1:B:1259:LEU:HD11	1:B:1300:TYR:HB2	1.99	0.44
1:B:33:VAL:HB	1:B:209:PHE:CE2	2.51	0.44
1:B:500:ASN:O	1:B:542:VAL:HA	2.18	0.44
1:B:61:ASP:CG	1:B:61:ASP:O	2.56	0.44
1:B:735:ALA:HB1	1:B:754:MET:CE	2.45	0.44
1:B:777:VAL:HG12	1:B:778:HIS:N	2.32	0.44
2:Y:140:LYS:O	2:Y:146:LEU:HA	2.17	0.44
1:A:1047:LYS:O	1:A:1048:LYS:C	2.56	0.44
1:A:1225:TYR:OH	1:A:1272:LYS:HE3	2.18	0.44
1:A:600:VAL:HG12	1:A:601:ALA:H	1.82	0.44
1:B:1018:VAL:O	1:B:1019:PHE:C	2.56	0.44
1:B:1037:ASP:OD1	1:B:1038:PRO:N	2.51	0.44
1:B:1136:GLU:OE1	1:B:1415:SER:HB3	2.17	0.44
1:B:1497:GLU:O	1:B:1498:TYR:C	2.55	0.44
1:B:415:ASP:OD1	1:B:417:VAL:HG23	2.18	0.44
1:B:834:VAL:HG11	1:B:1489:SER:HB3	2.00	0.44
2:X:166:ASP:OD2	2:X:201:ILE:HD13	2.17	0.44
2:X:192:ASN:HB2	2:X:223:LYS:O	2.18	0.44
2:Y:150:ILE:HD12	2:Y:151:ASP:N	2.32	0.44
1:A:1104:LEU:HD12	1:A:1159:CYS:HB3	1.98	0.44
1:A:1243:GLY:HA3	1:A:1285:TYR:CE2	2.53	0.44
1:A:271:ILE:HG22	1:A:272:ARG:H	1.82	0.44
1:A:290:THR:O	1:A:291:MET:O	2.35	0.44
1:A:450:GLU:HB3	1:A:452:TYR:HE2	1.81	0.44
1:A:912:PHE:O	1:A:922:ILE:HA	2.18	0.44
1:B:227:PHE:CZ	1:B:338:GLU:HB2	2.53	0.44
1:B:867:THR:HG23	1:B:900:VAL:CG1	2.47	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:981:GLY:C	1:B:982:LEU:HD23	2.38	0.44
1:A:1037:ASP:HA	1:A:1038:PRO:HD3	1.76	0.44
1:A:1061:ASN:HB2	1:A:1065:SER:O	2.18	0.44
1:A:1135:VAL:HG12	1:A:1136:GLU:N	2.33	0.44
1:A:1323:LEU:CG	1:A:1324:HIS:H	2.31	0.44
1:A:153:LYS:O	1:A:155:ALA:N	2.51	0.44
1:A:159:THR:CG2	1:A:160:VAL:N	2.81	0.44
1:A:367:ILE:HG23	1:A:368:PRO:CD	2.47	0.44
1:A:412:ARG:HG2	1:A:413:VAL:N	2.32	0.44
1:A:478:VAL:CG1	1:A:566:LYS:HD3	2.47	0.44
1:A:489:LYS:O	1:A:491:PRO:HD2	2.17	0.44
1:A:609:VAL:HG23	1:A:610:TYR:CD2	2.53	0.44
1:B:1016:VAL:O	1:B:1017:PRO:C	2.56	0.44
1:B:1161:LEU:HG	1:B:1164:ILE:HG23	1.99	0.44
1:B:1379:LEU:HD22	1:B:1493:PHE:HE2	1.77	0.44
1:B:1496:TYR:HD2	1:B:1504:GLN:OE1	2.01	0.44
1:B:284:GLN:O	1:B:310:LEU:HD13	2.18	0.44
1:B:367:ILE:CD1	1:B:466:TYR:HB3	2.48	0.44
1:B:544:TYR:CD1	1:B:544:TYR:N	2.84	0.44
2:Y:183:THR:CB	2:Y:230:GLN:HB3	2.48	0.44
1:A:968:VAL:HG22	1:A:1366:HIS:O	2.18	0.44
1:A:494:ASP:O	1:A:496:ILE:N	2.46	0.44
1:A:56:ILE:O	1:A:66:TYR:CD2	2.70	0.44
1:A:576:SER:CB	1:A:577:PRO:CD	2.95	0.44
1:A:609:VAL:CG2	1:A:610:TYR:CD2	3.01	0.44
1:A:859:MET:HE2	1:A:912:PHE:CZ	2.52	0.44
1:A:930:VAL:HG12	1:A:931:PRO:N	2.33	0.44
1:A:938:SER:OG	1:A:1279:ARG:NE	2.50	0.44
1:B:1083:LEU:HD11	1:B:1107:LEU:HD11	1.99	0.44
1:B:1084:ARG:O	1:B:1088:GLN:HG3	2.17	0.44
1:B:107:VAL:HG12	1:B:108:SER:N	2.33	0.44
1:B:1125:GLN:O	1:B:1421:HIS:N	2.49	0.44
1:B:1133:LEU:N	1:B:1134:PRO:CD	2.81	0.44
1:B:1190:ILE:HG12	1:B:1253:TYR:CD1	2.53	0.44
1:B:1401:ARG:HB2	1:B:1478:ARG:CA	2.48	0.44
1:B:1423:VAL:HG22	1:B:1496:TYR:CE1	2.51	0.44
1:B:1069:TRP:NE1	1:B:1463:GLN:NE2	2.60	0.44
1:B:272:ARG:CG	1:B:273:GLU:N	2.81	0.44
1:B:388:VAL:O	1:B:420:PHE:HZ	2.00	0.44
1:B:423:ASN:ND2	1:B:423:ASN:H	2.15	0.44
1:B:61:ASP:OD1	1:B:63:LYS:HB2	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:621:GLU:O	1:B:622:ARG:C	2.56	0.44
1:B:667:GLU:N	1:B:667:GLU:OE1	2.51	0.44
1:B:220:LYS:HG2	1:B:763:PRO:HB3	2.00	0.44
1:A:1057:MET:O	1:A:1060:ARG:HB3	2.18	0.43
1:A:1019:PHE:HE2	1:A:1088:GLN:HE21	1.64	0.43
1:A:1226:ARG:HB3	1:A:1270:VAL:HG23	2.01	0.43
1:A:1243:GLY:HA3	1:A:1285:TYR:HE2	1.82	0.43
1:A:1300:TYR:CE1	1:A:1304:VAL:HG21	2.53	0.43
1:A:1429:PRO:O	1:A:1432:ILE:CG1	2.66	0.43
1:A:144:ARG:O	1:A:145:VAL:HG23	2.18	0.43
1:A:1435:ASN:ND2	1:A:1478:ARG:HB2	2.27	0.43
1:A:303:SER:HB3	1:A:347:TYR:OH	2.18	0.43
1:A:442:LEU:O	1:A:443:PRO:C	2.52	0.43
1:A:439:ALA:O	1:A:447:GLN:NE2	2.50	0.43
1:A:606:ASP:C	1:A:608:ALA:N	2.71	0.43
1:A:724:CYS:O	1:A:727:ALA:N	2.51	0.43
1:A:768:TYR:HE2	1:A:770:PRO:HA	1.83	0.43
1:A:88:GLN:HE21	1:A:88:GLN:HB3	1.63	0.43
1:B:1081:PHE:O	1:B:1081:PHE:CD2	2.71	0.43
1:B:1188:LEU:HA	1:B:1188:LEU:HD12	1.73	0.43
1:B:1228:TRP:N	1:B:1228:TRP:HE3	2.16	0.43
1:B:1305:LYS:HE3	1:B:1305:LYS:HB2	1.68	0.43
1:B:158:GLU:CB	1:B:206:LYS:HE2	2.48	0.43
1:B:465:LEU:HD22	1:B:542:VAL:O	2.18	0.43
1:B:701:ASP:OD1	1:B:702:GLY:N	2.51	0.43
2:X:172:HIS:O	2:X:176:ASN:N	2.49	0.43
1:A:1031:TRP:CE3	1:A:1031:TRP:HA	2.53	0.43
1:A:1052:GLY:O	1:A:1055:SER:HB3	2.17	0.43
1:A:1370:THR:HG21	1:A:1506:THR:O	2.18	0.43
1:A:190:ILE:HG22	1:A:194:PRO:CG	2.47	0.43
1:A:319:ASN:OD1	1:A:321:LYS:CG	2.66	0.43
1:A:777:VAL:CG1	1:A:778:HIS:N	2.81	0.43
1:A:994:GLN:NE2	1:A:998:ASN:HD22	2.16	0.43
1:B:113:LYS:HZ3	1:B:656:ASN:HD21	1.65	0.43
1:B:1247:MET:O	1:B:1251:THR:HG23	2.18	0.43
1:B:259:VAL:HG23	1:B:260:VAL:O	2.17	0.43
1:B:271:ILE:HD11	1:B:307:VAL:CG2	2.48	0.43
1:B:356:LEU:CD1	1:B:452:TYR:CD1	3.00	0.43
1:B:454:ALA:C	1:B:455:ILE:HG13	2.38	0.43
1:B:531:THR:O	1:B:534:MET:HG3	2.18	0.43
1:B:53:THR:HA	1:B:69:GLY:O	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:ASN:O	1:B:666:ASP:HB3	2.18	0.43
1:B:582:TYR:HB2	1:B:819:VAL:HG12	2.00	0.43
1:B:840:GLN:O	1:B:1483:PHE:CD2	2.70	0.43
1:B:257:ASN:ND2	1:B:893:SER:O	2.51	0.43
1:B:896:VAL:C	1:B:897:THR:CG2	2.86	0.43
2:X:193:LEU:HD23	2:X:221:ILE:HG12	1.99	0.43
1:A:1169:ILE:O	1:A:1170:LYS:C	2.57	0.43
1:A:1176:LEU:H	1:A:1176:LEU:HG	1.51	0.43
1:A:1206:ARG:CG	1:A:1206:ARG:NH1	2.73	0.43
1:A:968:VAL:CG1	1:A:1368:THR:CG2	2.86	0.43
1:A:838:GLN:HB3	1:A:1486:GLY:CA	2.48	0.43
1:A:1126:PRO:C	1:A:1499:HIS:HD1	2.21	0.43
1:A:23:TYR:HA	1:A:43:VAL:HG23	2.00	0.43
1:A:469:TRP:CD1	1:A:482:LEU:HD21	2.53	0.43
1:A:541:LEU:HD23	1:A:541:LEU:C	2.38	0.43
1:A:758:LEU:HD22	1:A:760:VAL:H	1.84	0.43
1:B:1024:TYR:CD2	1:B:1025:LEU:N	2.83	0.43
1:B:511:HIS:NE2	1:B:531:THR:HG21	2.31	0.43
2:Y:224:ILE:C	2:Y:225:GLU:HG3	2.39	0.43
1:A:1087:GLY:HA3	1:A:1155:ALA:HA	2.01	0.43
1:A:975:ARG:O	1:A:1339:GLU:HA	2.19	0.43
1:A:1352:PHE:CG	1:A:1353:GLY:N	2.83	0.43
1:A:59:TYR:CD2	1:A:60:PRO:CD	2.97	0.43
1:A:59:TYR:CG	1:A:60:PRO:CD	2.97	0.43
1:A:647:HIS:C	1:A:649:ALA:H	2.22	0.43
1:B:1422:ALA:HA	1:B:1498:TYR:H	1.83	0.43
1:B:1480:PHE:O	1:B:1481:GLU:C	2.56	0.43
1:B:166:PRO:HD3	1:B:199:TRP:CE2	2.53	0.43
1:B:216:TYR:CD2	1:B:216:TYR:N	2.86	0.43
1:B:515:ARG:CZ	1:B:526:ILE:HG23	2.49	0.43
1:B:554:LEU:O	1:B:555:VAL:HG23	2.18	0.43
1:B:571:LEU:HD12	1:B:571:LEU:C	2.29	0.43
1:B:758:LEU:O	1:B:760:VAL:N	2.50	0.43
1:B:50:PHE:HE2	1:B:79:PHE:CE2	2.35	0.43
2:X:140:LYS:O	2:X:146:LEU:HA	2.17	0.43
2:Y:136:LEU:HD23	2:Y:136:LEU:H	1.83	0.43
2:Y:153:PHE:HZ	2:Y:168:LYS:HD2	1.84	0.43
1:A:115:LYS:HG3	1:A:116:ARG:H	1.77	0.43
1:A:1203:PRO:O	1:A:1206:ARG:N	2.52	0.43
1:A:1435:ASN:HB3	1:A:1438:ASP:CG	2.38	0.43
1:A:496:ILE:CD1	1:A:517:LYS:NZ	2.82	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:TYR:N	1:A:544:TYR:CD1	2.81	0.43
1:A:605:VAL:O	1:A:797:TRP:HE3	2.01	0.43
1:A:61:ASP:C	1:A:63:LYS:H	2.20	0.43
1:A:641:ASN:O	1:A:642:ASN:C	2.57	0.43
1:A:820:PHE:HZ	1:A:848:TYR:CB	2.27	0.43
1:B:625:GLN:O	1:B:626:PHE:C	2.56	0.43
1:B:699:CYS:SG	1:B:727:ALA:O	2.76	0.43
2:Y:217:ASN:ND2	2:Y:220:ASP:OD2	2.47	0.43
1:A:106:VAL:CG1	1:A:107:VAL:N	2.81	0.43
1:A:494:ASP:HA	1:A:496:ILE:HD11	2.00	0.43
1:A:560:TRP:CH2	1:A:562:ASN:CB	2.99	0.43
1:A:609:VAL:HG23	1:A:610:TYR:CG	2.53	0.43
1:A:832:SER:O	1:A:1430:THR:HG23	2.19	0.43
1:B:1128:LYS:NZ	1:B:1415:SER:HB3	2.34	0.43
1:B:128:ILE:HA	1:B:145:VAL:HG22	2.00	0.43
1:B:1352:PHE:CG	1:B:1353:GLY:N	2.84	0.43
1:B:488:PRO:CG	1:B:499:TYR:OH	2.66	0.43
2:X:158:GLU:HA	2:X:219:LYS:HZ1	1.83	0.43
1:A:1120:GLU:OE2	1:A:1121:ASN:N	2.51	0.43
1:A:1158:ILE:HG13	1:A:1158:ILE:H	1.63	0.43
1:A:1206:ARG:O	1:A:1210:SER:HB3	2.19	0.43
1:A:974:LYS:HE3	1:A:1339:GLU:OE1	2.17	0.43
1:A:223:VAL:HG12	1:A:224:LEU:N	2.33	0.43
1:A:231:ILE:HD12	1:A:327:VAL:HG23	2.01	0.43
1:A:560:TRP:HZ3	1:A:562:ASN:HB2	1.74	0.43
1:A:743:SER:OG	1:A:752:LEU:HD22	2.19	0.43
1:A:995:GLU:O	1:A:996:GLY:O	2.36	0.43
1:B:1068:VAL:HA	1:B:1078:LEU:HD13	2.01	0.43
1:B:1082:ALA:O	1:B:1086:LEU:N	2.49	0.43
1:B:1286:SER:OG	1:B:1287:THR:N	2.50	0.43
1:B:1342:LEU:C	1:B:1343:ASN:HD22	2.22	0.43
1:B:1429:PRO:O	1:B:1432:ILE:HG12	2.19	0.43
1:B:342:ILE:HG22	1:B:343:PRO:HD2	2.01	0.43
1:B:323:LEU:O	1:B:345:ILE:HB	2.17	0.43
1:B:472:ASN:OD1	1:B:473:HIS:CE1	2.72	0.43
1:B:820:PHE:CZ	1:B:821:LYS:O	2.72	0.43
1:B:982:LEU:N	1:B:982:LEU:CD2	2.81	0.43
1:A:1016:VAL:O	1:A:1017:PRO:C	2.55	0.43
1:A:1054:LEU:C	1:A:1056:ILE:H	2.23	0.43
1:A:1096:ASN:ND2	1:A:1096:ASN:C	2.71	0.43
1:A:1318:LYS:HE2	1:A:1345:ASP:HB2	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:VAL:HG11	1:A:1489:SER:HB3	2.00	0.43
1:A:327:VAL:HG12	1:A:328:THR:N	2.33	0.43
1:A:387:PRO:HA	1:A:410:VAL:HG22	1.99	0.43
1:A:557:ASP:CG	1:A:558:SER:H	2.22	0.43
1:A:599:TRP:HE3	1:A:778:HIS:O	2.01	0.43
1:A:78:LYS:HE3	2:X:143:GLY:O	2.18	0.43
1:A:859:MET:CE	1:A:912:PHE:CZ	3.02	0.43
1:A:90:LYS:HB2	1:A:91:GLN:H	1.58	0.43
1:A:968:VAL:O	1:A:969:PRO:O	2.37	0.43
1:B:988:LEU:CD2	1:B:1021:VAL:HG13	2.49	0.43
1:B:1091:LYS:HE2	1:B:1091:LYS:HB3	1.73	0.43
1:B:1133:LEU:H	1:B:1133:LEU:CD1	2.32	0.43
1:B:1132:THR:CG2	1:B:1134:PRO:HD2	2.49	0.43
1:B:101:TYR:HD1	1:B:116:ARG:CG	2.31	0.43
1:B:1372:GLU:HG3	1:B:1373:GLU:HG3	2.01	0.43
1:B:292:LEU:C	1:B:292:LEU:HD13	2.38	0.43
1:B:504:LEU:HD21	1:B:651:LEU:CG	2.46	0.43
1:B:609:VAL:HG23	1:B:610:TYR:CG	2.52	0.43
1:B:647:HIS:C	1:B:649:ALA:N	2.71	0.43
1:B:951:GLY:O	1:B:952:THR:HG22	2.19	0.43
1:A:127:PHE:HE1	1:A:626:PHE:CE2	2.36	0.43
1:A:1307:LEU:HD12	1:A:1307:LEU:H	1.84	0.43
1:A:1438:ASP:OD2	1:A:1478:ARG:N	2.49	0.43
1:B:979:VAL:HB	1:B:1326:TYR:OH	2.19	0.43
1:B:208:ASP:O	1:B:209:PHE:CG	2.72	0.43
1:B:51:ASP:OD1	1:B:72:HIS:ND1	2.49	0.43
1:B:644:ASN:HD22	1:B:644:ASN:C	2.22	0.43
1:B:707:ASN:HB3	1:B:739:ARG:CZ	2.49	0.43
1:B:773:TRP:HZ3	1:B:788:PHE:CE1	2.37	0.43
1:B:50:PHE:HE2	1:B:79:PHE:CD2	2.37	0.43
2:X:192:ASN:HB2	2:X:223:LYS:H	1.83	0.43
2:X:227:THR:C	2:X:228:LEU:HD23	2.39	0.43
1:A:1042:LYS:HG2	1:A:1046:LYS:HE3	2.01	0.43
1:A:1259:LEU:HD21	1:A:1300:TYR:HD1	1.84	0.43
1:A:133:PRO:O	1:A:134:VAL:CG2	2.53	0.43
1:A:1383:THR:HG22	1:A:1402:ILE:HG12	2.00	0.43
1:A:198:MET:CE	1:A:218:GLU:HB2	2.49	0.43
1:A:269:PHE:CB	1:A:283:MET:HE3	2.48	0.43
1:A:356:LEU:HG	1:A:452:TYR:CZ	2.53	0.43
1:A:465:LEU:CD2	1:A:542:VAL:O	2.66	0.43
1:A:685:GLU:HG3	1:A:686:ILE:CD1	2.48	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:PHE:CZ	1:A:821:LYS:O	2.72	0.43
1:A:971:THR:OG1	1:A:971:THR:O	2.36	0.43
1:B:1068:VAL:HG22	1:B:1069:TRP:N	2.34	0.43
1:B:1283:GLY:O	1:B:1290:THR:OG1	2.36	0.43
1:B:1328:MET:O	1:B:1329:THR:CG2	2.66	0.43
1:B:641:ASN:C	1:B:643:ALA:N	2.67	0.43
1:B:634:CYS:SG	1:B:672:ILE:HG22	2.59	0.43
2:X:146:LEU:C	2:X:146:LEU:HD13	2.39	0.43
1:A:1082:ALA:O	1:A:1086:LEU:HD23	2.19	0.42
1:A:1149:VAL:HA	1:A:1152:ILE:HD12	2.01	0.42
1:A:162:THR:HG21	1:A:204:LYS:HE2	2.00	0.42
1:A:386:VAL:HA	1:A:387:PRO:HD3	1.71	0.42
1:A:760:VAL:O	1:A:761:SER:HB3	2.18	0.42
1:A:947:ARG:NH1	1:A:1354:SER:HB3	2.33	0.42
1:B:1053:MET:HE1	1:B:1086:LEU:CD2	2.46	0.42
1:B:1068:VAL:HG22	1:B:1069:TRP:CD2	2.54	0.42
1:B:121:TYR:O	1:B:210:SER:N	2.43	0.42
1:B:1440:LYS:O	1:B:1444:GLU:CB	2.67	0.42
1:B:170:GLU:O	1:B:171:VAL:HG23	2.19	0.42
4:B:2001:NAG:HO3	4:B:2002:NAG:C1	2.32	0.42
1:B:270:GLY:N	1:B:324:TYR:O	2.52	0.42
1:B:330:ILE:HB	1:B:336:PHE:O	2.19	0.42
1:B:386:VAL:CG1	1:B:387:PRO:HD2	2.39	0.42
1:B:392:ALA:HB3	1:B:404:LEU:CD1	2.45	0.42
1:B:562:ASN:OD1	1:B:563:ILE:N	2.52	0.42
1:B:561:LEU:O	1:B:563:ILE:HG23	2.19	0.42
2:X:138:VAL:HG11	2:X:177:TYR:CD2	2.54	0.42
1:A:1050:LYS:O	1:A:1053:MET:N	2.52	0.42
1:A:1129:LEU:CD1	1:A:1139:GLU:HB3	2.49	0.42
1:A:1225:TYR:HE1	1:A:1272:LYS:HG3	1.84	0.42
1:A:350:SER:HB2	1:A:446:ASN:C	2.39	0.42
1:A:367:ILE:HD12	1:A:466:TYR:HB2	2.00	0.42
1:A:472:ASN:OD1	1:A:473:HIS:CE1	2.72	0.42
1:A:700:TYR:CE1	1:A:758:LEU:CB	2.99	0.42
1:A:735:ALA:O	1:A:754:MET:SD	2.77	0.42
1:A:834:VAL:HG12	1:A:835:ARG:O	2.18	0.42
1:A:988:LEU:HA	1:A:988:LEU:HD23	1.89	0.42
1:B:1023:HIS:HD2	1:B:1092:TYR:OH	2.03	0.42
1:B:1438:ASP:OD2	1:B:1478:ARG:N	2.50	0.42
1:B:1467:ILE:N	1:B:1468:PRO:CD	2.82	0.42
1:B:1381:ILE:HG21	1:B:1509:TYR:CD1	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:VAL:HG12	1:B:224:LEU:N	2.34	0.42
1:B:232:GLU:OE2	1:B:251:LYS:CE	2.60	0.42
1:B:297:ALA:O	1:B:298:GLN:CG	2.65	0.42
1:B:505:SER:HB3	1:B:510:ILE:CD1	2.49	0.42
1:B:691:LYS:O	1:B:692:HIS:HB2	2.20	0.42
1:B:722:PRO:HA	1:B:725:ILE:HG13	2.01	0.42
1:B:88:GLN:HE21	1:B:88:GLN:HB3	1.64	0.42
1:B:909:ASN:N	1:B:926:THR:HG22	2.33	0.42
2:Y:134:THR:CG2	2:Y:153:PHE:HB3	2.47	0.42
1:A:142:LYS:HD3	1:A:775:TRP:CD1	2.54	0.42
1:A:502:LEU:HD12	1:A:502:LEU:HA	1.81	0.42
1:A:592:MET:HB3	1:A:780:VAL:HG11	2.01	0.42
1:A:61:ASP:O	1:A:61:ASP:CG	2.57	0.42
1:A:762:LYS:HA	1:A:763:PRO:HD3	1.91	0.42
1:A:829:ILE:HG22	1:A:830:PRO:CD	2.49	0.42
1:A:968:VAL:HG23	1:A:971:THR:CG2	2.49	0.42
1:B:1008:ALA:HB2	1:B:1068:VAL:O	2.20	0.42
1:B:1093:VAL:O	1:B:1094:GLU:C	2.58	0.42
1:B:1206:ARG:O	1:B:1210:SER:HB3	2.19	0.42
1:B:128:ILE:HB	1:B:215:ALA:HB2	2.00	0.42
1:B:1376:SER:OG	1:B:1503:LYS:HA	2.20	0.42
1:B:161:LEU:HD13	1:B:163:PHE:CE1	2.54	0.42
1:B:354:LEU:HD12	1:B:435:VAL:HG12	2.00	0.42
1:B:501:TYR:OH	2:Y:147:ASP:HB3	2.19	0.42
1:B:561:LEU:O	1:B:563:ILE:HG22	2.18	0.42
1:B:56:ILE:HD13	1:B:86:THR:H	1.84	0.42
1:B:576:SER:HB3	1:B:577:PRO:HD3	2.01	0.42
1:B:61:ASP:OD1	1:B:61:ASP:O	2.38	0.42
1:B:847:ASN:HD22	1:B:888:VAL:CG2	2.32	0.42
1:B:859:MET:HE2	1:B:912:PHE:CZ	2.54	0.42
1:B:922:ILE:O	1:B:922:ILE:HG22	2.18	0.42
2:X:146:LEU:HD11	2:X:148:ALA:CB	2.45	0.42
1:A:1028:GLY:O	1:A:1029:ASN:O	2.38	0.42
1:A:111:PHE:CD2	1:A:112:SER:N	2.86	0.42
1:A:1203:PRO:O	1:A:1206:ARG:CB	2.68	0.42
1:A:132:LYS:NZ	1:A:139:GLN:NE2	2.67	0.42
1:A:214:THR:HG22	1:A:215:ALA:H	1.84	0.42
1:A:961:TYR:OH	1:A:1343:ASN:CG	2.58	0.42
1:B:1244:THR:HB	1:B:1247:MET:HB3	2.01	0.42
1:B:1428:LEU:HA	1:B:1429:PRO:HD3	1.87	0.42
1:B:191:PRO:HD2	1:B:194:PRO:HG3	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:SER:HB2	1:B:446:ASN:C	2.40	0.42
1:B:352:TYR:CD1	1:B:375:VAL:CG1	3.01	0.42
1:B:540:LEU:O	1:B:540:LEU:HD12	2.20	0.42
1:B:735:ALA:O	1:B:754:MET:SD	2.77	0.42
1:B:844:THR:HG22	1:B:895:LEU:HG	2.00	0.42
1:B:88:GLN:HB3	1:B:89:PRO:HD2	2.02	0.42
2:X:194:LYS:HG3	2:X:195:ASP:N	2.35	0.42
2:X:189:ILE:CD1	2:X:203:LEU:HD21	2.48	0.42
2:Y:190:THR:HA	2:Y:199:GLN:O	2.19	0.42
2:Y:211:ARG:O	2:Y:214:ASP:HB2	2.19	0.42
1:A:1011:GLU:HG3	1:A:1055:SER:OG	2.20	0.42
1:A:1283:GLY:H	1:A:1290:THR:HG21	1.84	0.42
1:A:1427:SER:CB	1:A:1491:ALA:HB1	2.50	0.42
1:A:205:TYR:HD1	1:A:211:THR:OG1	2.03	0.42
1:A:461:SER:C	1:A:463:SER:N	2.72	0.42
1:A:55:SER:CB	1:A:67:SER:O	2.68	0.42
1:A:685:GLU:C	1:A:687:ALA:H	2.22	0.42
1:A:55:SER:HB3	1:A:68:SER:CB	2.50	0.42
1:A:796:THR:HG23	1:A:818:LYS:HB3	2.02	0.42
1:A:981:GLY:O	1:A:982:LEU:CB	2.68	0.42
1:B:1185:THR:HG21	1:B:1228:TRP:HB3	2.01	0.42
1:B:1129:LEU:HD23	1:B:1246:ARG:HH12	1.84	0.42
1:B:272:ARG:HG2	1:B:273:GLU:H	1.84	0.42
1:B:350:SER:OG	1:B:448:ALA:N	2.52	0.42
1:B:504:LEU:CD1	1:B:509:ILE:HG12	2.49	0.42
1:B:829:ILE:CG2	1:B:830:PRO:HD2	2.48	0.42
1:B:830:PRO:HG3	1:B:1483:PHE:HZ	1.85	0.42
1:A:1019:PHE:CE2	1:A:1020:TYR:CD1	3.08	0.42
1:A:284:GLN:O	1:A:310:LEU:CD1	2.68	0.42
1:A:349:LEU:HD22	1:A:446:ASN:HD22	1.84	0.42
1:A:489:LYS:C	1:A:491:PRO:HD2	2.40	0.42
1:A:502:LEU:HD12	1:A:512:PHE:HB3	2.01	0.42
1:B:1175:LEU:O	1:B:1179:THR:OG1	2.36	0.42
1:B:1199:ASP:C	1:B:1199:ASP:OD1	2.58	0.42
1:B:159:THR:O	1:B:175:GLU:HA	2.19	0.42
1:B:31:PHE:HZ	1:B:104:LEU:CD2	2.25	0.42
1:B:518:PHE:O	1:B:519:SER:C	2.58	0.42
1:B:589:SER:HA	1:B:787:GLN:HA	2.00	0.42
1:B:738:LEU:O	1:B:742:ILE:HG13	2.19	0.42
1:B:834:VAL:HG11	1:B:1489:SER:CB	2.50	0.42
1:B:84:ILE:HD13	2:Y:135:HIS:CD2	2.55	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ILE:HG13	1:B:84:ILE:O	2.19	0.42
1:B:855:PHE:HD1	1:B:856:CYS:N	2.18	0.42
1:B:862:VAL:O	1:B:863:GLU:C	2.58	0.42
1:B:950:TYR:HE1	1:B:1271:ILE:HD11	1.83	0.42
2:Y:227:THR:C	2:Y:228:LEU:HD23	2.40	0.42
1:A:1003:LEU:HA	1:A:1004:PRO:HD2	1.49	0.42
1:A:1108:VAL:HG22	1:A:1109:GLU:N	2.35	0.42
1:A:935:LYS:O	1:A:1365:VAL:O	2.36	0.42
1:A:1434:ALA:CB	1:A:1477:PHE:HE1	2.32	0.42
1:A:38:ASN:C	1:A:39:ILE:HD13	2.38	0.42
1:A:503:ILE:HG12	1:A:540:LEU:CB	2.48	0.42
1:A:577:PRO:HD2	1:A:588:VAL:CG2	2.37	0.42
1:A:610:TYR:HB2	1:A:611:GLY:H	1.68	0.42
1:A:626:PHE:O	1:A:628:GLU:N	2.53	0.42
1:B:1083:LEU:O	1:B:1086:LEU:HB2	2.19	0.42
1:B:1159:CYS:N	1:B:1160:PRO:CD	2.82	0.42
1:B:1278:GLN:NE2	1:B:1278:GLN:CA	2.83	0.42
1:B:1429:PRO:O	1:B:1430:THR:C	2.58	0.42
1:B:166:PRO:HG3	1:B:199:TRP:CD1	2.54	0.42
1:B:137:PRO:HD3	1:B:220:LYS:O	2.19	0.42
1:B:254:TYR:CE2	1:B:260:VAL:HG22	2.53	0.42
1:B:438:ASP:O	1:B:439:ALA:O	2.38	0.42
1:B:617:LYS:O	1:B:618:LYS:CG	2.49	0.42
1:B:840:GLN:HB2	1:B:1484:GLU:HB2	2.02	0.42
1:B:982:LEU:C	1:B:984:VAL:H	2.22	0.42
2:X:192:ASN:HD22	2:X:223:LYS:HB2	1.85	0.42
1:A:100:SER:O	1:A:101:TYR:CD2	2.72	0.42
1:A:1024:TYR:HD2	1:A:1025:LEU:N	2.17	0.42
1:A:1022:PHE:O	1:A:1026:GLU:HB3	2.20	0.42
1:A:1161:LEU:CD1	1:A:1162:VAL:HG22	2.46	0.42
1:A:982:LEU:HD11	1:A:1306:GLN:OE1	2.20	0.42
1:A:1317:TYR:HB2	1:A:1320:LYS:HB3	2.02	0.42
1:A:1496:TYR:CD1	1:A:1496:TYR:C	2.93	0.42
1:A:136:THR:HA	1:A:220:LYS:O	2.20	0.42
1:A:253:ARG:HG3	1:A:253:ARG:O	2.19	0.42
1:A:292:LEU:HD13	1:A:292:LEU:C	2.39	0.42
1:A:359:THR:HG21	1:A:372:LYS:N	2.23	0.42
1:A:41:ILE:O	1:A:81:ASN:N	2.49	0.42
1:A:497:THR:HG23	1:A:498:HIS:N	2.29	0.42
1:A:515:ARG:HH22	1:A:527:ASN:H	1.68	0.42
1:A:500:ASN:O	1:A:542:VAL:HA	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1012:LEU:C	1:B:1014:SER:H	2.23	0.42
1:B:1379:LEU:HD21	1:B:1495:VAL:CG1	2.48	0.42
1:B:1379:LEU:HD12	1:B:1507:MET:HE2	2.01	0.42
1:B:396:ASP:N	1:B:400:GLU:O	2.50	0.42
1:B:240:TYR:CZ	1:B:443:PRO:HD3	2.53	0.42
1:B:831:TYR:O	1:B:928:ARG:HB2	2.19	0.42
2:Y:192:ASN:HB2	2:Y:223:LYS:O	2.20	0.42
2:Y:217:ASN:HB2	2:Y:220:ASP:OD2	2.19	0.42
1:A:1069:TRP:NE1	1:A:1463:GLN:NE2	2.68	0.42
1:A:159:THR:HG22	1:A:160:VAL:H	1.84	0.42
1:A:284:GLN:HG2	1:A:310:LEU:HD13	2.02	0.42
1:A:350:SER:HA	1:A:351:PRO:HD3	1.74	0.42
1:A:497:THR:OG1	1:A:498:HIS:ND1	2.52	0.42
1:A:592:MET:HG2	1:A:600:VAL:HG21	2.01	0.42
1:A:855:PHE:CD1	1:A:856:CYS:N	2.87	0.42
1:A:902:PRO:O	1:A:903:LEU:HD13	2.20	0.42
1:A:907:LEU:HD12	1:A:908:HIS:N	2.34	0.42
1:B:1148:THR:OG1	1:B:1152:ILE:HD11	2.19	0.42
1:B:125:PHE:N	1:B:125:PHE:CD1	2.87	0.42
1:B:1307:LEU:HD13	1:B:1356:LEU:HD12	2.02	0.42
1:B:1408:TYR:O	1:B:1410:PRO:HD3	2.20	0.42
1:B:23:TYR:OH	1:B:656:ASN:HB2	2.20	0.42
1:B:415:ASP:OD1	1:B:417:VAL:CG2	2.67	0.42
1:B:369:TYR:HE2	1:B:433:PHE:HE1	1.66	0.42
1:B:531:THR:CG2	1:B:533:ASN:HB2	2.49	0.42
1:B:61:ASP:C	1:B:63:LYS:H	2.21	0.42
1:A:1054:LEU:C	1:A:1056:ILE:N	2.71	0.42
1:A:1227:PHE:HB2	1:A:1251:THR:HG21	2.02	0.42
1:A:337:SER:HB3	1:A:1437:GLU:CD	2.40	0.42
1:A:191:PRO:O	1:A:194:PRO:HD3	2.20	0.42
1:A:216:TYR:O	1:A:217:PHE:HB3	2.19	0.42
1:A:616:ALA:O	1:A:617:LYS:C	2.57	0.42
1:B:1307:LEU:CD1	1:B:1356:LEU:HD12	2.49	0.42
1:B:157:ARG:CZ	1:B:209:PHE:CE1	3.03	0.42
1:B:331:GLU:OE1	1:B:336:PHE:HD1	2.02	0.42
1:B:42:GLN:CG	1:B:80:GLN:NE2	2.81	0.42
1:B:504:LEU:HD12	1:B:509:ILE:HG23	2.02	0.42
1:B:576:SER:CB	1:B:577:PRO:CD	2.97	0.42
1:A:1113:LEU:C	1:A:1115:ASN:H	2.23	0.41
1:A:140:SER:OG	1:A:187:ASP:HB3	2.20	0.41
1:A:1435:ASN:O	1:A:1436:GLU:C	2.59	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLY:N	1:A:283:MET:CE	2.83	0.41
1:A:356:LEU:CD1	1:A:452:TYR:CD1	3.03	0.41
1:A:665:ASN:CG	1:A:666:ASP:H	2.23	0.41
1:A:667:GLU:N	1:A:667:GLU:OE1	2.53	0.41
1:A:839:ILE:HG13	1:A:840:GLN:N	2.35	0.41
1:A:967:LEU:HD12	1:A:968:VAL:N	2.34	0.41
1:A:976:ILE:O	1:A:1361:VAL:HA	2.20	0.41
1:B:110:HIS:O	1:B:110:HIS:CD2	2.73	0.41
1:B:1117:SER:HA	1:B:1145:THR:CG2	2.48	0.41
1:B:1176:LEU:H	1:B:1176:LEU:HG	1.39	0.41
1:B:1180:LEU:HD11	1:B:1207:SER:HB3	2.02	0.41
1:B:123:ASN:ND2	1:B:123:ASN:C	2.70	0.41
1:B:123:ASN:C	1:B:211:THR:HG21	2.40	0.41
1:B:396:ASP:HB3	1:B:398:ASN:N	2.35	0.41
1:B:440:PRO:CD	1:B:441:ASP:H	2.33	0.41
1:B:972:GLU:HG2	1:B:972:GLU:H	1.51	0.41
2:X:164:GLU:O	2:X:168:LYS:HG3	2.20	0.41
2:X:179:LEU:HD11	2:X:185:LYS:HA	2.03	0.41
1:A:1019:PHE:CD2	1:A:1020:TYR:CE1	3.08	0.41
1:A:1096:ASN:ND2	1:A:1099:SER:H	2.19	0.41
1:A:1112:GLN:HG3	1:A:1118:PHE:CE1	2.55	0.41
1:A:719:SER:CB	1:A:1123:GLN:HE21	2.33	0.41
1:A:1227:PHE:CA	1:A:1228:TRP:CE3	3.03	0.41
1:A:173:MET:C	1:A:174:VAL:HG12	2.41	0.41
1:A:415:ASP:OD1	1:A:417:VAL:CG2	2.68	0.41
1:A:617:LYS:O	1:A:618:LYS:CG	2.46	0.41
1:A:824:PHE:CE1	1:A:846:TYR:CD1	2.93	0.41
1:A:862:VAL:O	1:A:863:GLU:C	2.57	0.41
1:A:980:LYS:HB3	1:A:980:LYS:HE3	1.78	0.41
1:B:1037:ASP:HA	1:B:1038:PRO:HD3	1.74	0.41
1:B:1162:VAL:O	1:B:1165:ASP:N	2.52	0.41
1:B:1324:HIS:CE1	1:B:1326:TYR:CE2	3.07	0.41
1:B:1435:ASN:HB2	1:B:1478:ARG:O	2.20	0.41
1:B:357:VAL:O	1:B:359:THR:HG23	2.19	0.41
1:B:405:ASP:HA	1:B:406:PRO:HD3	1.60	0.41
1:B:468:ASP:O	1:B:484:ILE:HG13	2.19	0.41
1:B:610:TYR:HB2	1:B:611:GLY:H	1.67	0.41
1:B:695:VAL:HA	1:B:698:CYS:HB2	2.02	0.41
1:B:604:ALA:O	1:B:772:SER:HB3	2.21	0.41
1:B:889:GLU:H	1:B:889:GLU:CD	2.24	0.41
1:B:930:VAL:HG12	1:B:931:PRO:N	2.35	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:947:ARG:C	1:B:949:ILE:N	2.70	0.41
2:Y:179:LEU:HD11	2:Y:185:LYS:HA	2.02	0.41
1:A:1180:LEU:HD11	1:A:1208:ILE:N	2.35	0.41
1:A:33:VAL:HG23	1:A:120:THR:O	2.20	0.41
1:A:1440:LYS:HD3	1:A:1453:TYR:CZ	2.56	0.41
1:A:185:PHE:HB3	1:A:186:PRO:HD3	2.00	0.41
1:A:295:GLY:C	1:A:296:ILE:CG1	2.88	0.41
1:A:504:LEU:HD12	1:A:509:ILE:HA	2.01	0.41
1:A:66:TYR:CE1	1:A:90:LYS:CG	2.97	0.41
1:B:984:VAL:CG1	1:B:1024:TYR:CE1	2.92	0.41
1:B:1081:PHE:CD2	1:B:1081:PHE:C	2.93	0.41
1:B:1175:LEU:HA	1:B:1175:LEU:HD23	1.69	0.41
1:B:369:TYR:HA	1:B:370:PRO:HD3	1.66	0.41
1:B:387:PRO:C	1:B:388:VAL:HG23	2.41	0.41
1:B:743:SER:OG	1:B:752:LEU:HD22	2.20	0.41
2:X:224:ILE:C	2:X:225:GLU:HG3	2.41	0.41
1:A:120:THR:CG2	1:A:121:TYR:N	2.59	0.41
1:A:292:LEU:HD22	1:A:296:ILE:O	2.21	0.41
1:A:420:PHE:O	1:A:421:VAL:HG23	2.20	0.41
1:A:653:PHE:CZ	1:A:660:ASP:CA	2.92	0.41
1:B:1030:HIS:O	1:B:1033:ILE:CG1	2.64	0.41
1:B:1132:THR:N	1:B:1135:VAL:HB	2.35	0.41
1:B:1152:ILE:O	1:B:1153:ARG:C	2.58	0.41
1:B:1401:ARG:HB2	1:B:1478:ARG:CB	2.50	0.41
1:B:1378:TYR:CE1	1:B:1409:LYS:HE3	2.55	0.41
1:B:1429:PRO:HG2	1:B:1511:THR:CB	2.44	0.41
1:B:171:VAL:O	1:B:171:VAL:HG12	2.19	0.41
1:B:244:LYS:HA	1:B:302:ASP:OD2	2.20	0.41
1:B:262:GLU:HG2	1:B:332:SER:HB2	2.03	0.41
1:B:700:TYR:CE1	1:B:758:LEU:CB	3.02	0.41
1:B:841:LEU:HD12	1:B:859:MET:CE	2.42	0.41
1:B:93:PRO:HG2	1:B:96:GLN:OE1	2.21	0.41
2:Y:194:LYS:HA	2:Y:194:LYS:HD2	1.84	0.41
1:A:1401:ARG:HB2	1:A:1478:ARG:CG	2.48	0.41
1:A:262:GLU:HG2	1:A:332:SER:HB2	2.02	0.41
1:A:44:TYR:OH	1:A:497:THR:HB	2.21	0.41
1:A:935:LYS:HD2	1:A:935:LYS:HA	1.83	0.41
1:B:936:ARG:CZ	1:B:1002:HIS:HE1	2.34	0.41
1:B:1191:SER:O	1:B:1195:LEU:HG	2.20	0.41
1:B:244:LYS:HE3	1:B:304:GLU:OE2	2.21	0.41
1:B:461:SER:C	1:B:463:SER:H	2.22	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:PHE:HE1	1:B:638:GLY:O	2.04	0.41
1:B:903:LEU:N	1:B:903:LEU:HD13	2.35	0.41
2:X:199:GLN:C	2:X:200:GLU:HG3	2.40	0.41
1:A:1076:THR:HG22	1:A:1120:GLU:CD	2.41	0.41
1:A:1148:THR:O	1:A:1152:ILE:CD1	2.69	0.41
1:A:1244:THR:O	1:A:1285:TYR:CD2	2.73	0.41
1:A:1279:ARG:HE	1:A:1279:ARG:HB3	1.65	0.41
1:A:256:TYR:HB2	1:A:895:LEU:HD12	2.02	0.41
1:A:30:ILE:HG22	1:A:31:PHE:O	2.20	0.41
1:A:337:SER:HB3	1:A:1437:GLU:OE2	2.21	0.41
1:A:700:TYR:O	1:A:702:GLY:N	2.53	0.41
1:B:1000:LEU:HD23	1:B:1000:LEU:HA	1.87	0.41
1:B:1227:PHE:HA	1:B:1228:TRP:CE3	2.55	0.41
1:B:1278:GLN:CA	1:B:1278:GLN:HE21	2.33	0.41
1:B:938:SER:HB3	1:B:1362:THR:HA	2.03	0.41
1:B:185:PHE:HB3	1:B:186:PRO:HD3	2.02	0.41
1:B:388:VAL:HG12	1:B:420:PHE:HZ	1.85	0.41
1:B:436:LYS:HD2	1:B:437:THR:O	2.20	0.41
1:B:752:LEU:C	1:B:753:HIS:CG	2.93	0.41
2:Y:184:THR:O	2:Y:185:LYS:HB3	2.20	0.41
2:Y:186:TYR:HD2	2:Y:229:LYS:HD3	1.80	0.41
1:A:1144:LEU:O	1:A:1148:THR:CG2	2.67	0.41
1:A:1153:ARG:O	1:A:1155:ALA:N	2.53	0.41
1:A:1427:SER:HB3	1:A:1492:THR:N	2.29	0.41
1:A:1440:LYS:O	1:A:1444:GLU:CB	2.68	0.41
1:A:1456:LYS:O	1:A:1459:HIS:N	2.46	0.41
1:A:150:ASP:O	1:A:152:LEU:HD22	2.20	0.41
1:A:166:PRO:HG3	1:A:199:TRP:CD1	2.56	0.41
1:A:545:ILE:HG12	1:A:554:LEU:HD21	2.03	0.41
1:A:644:ASN:C	1:A:644:ASN:ND2	2.74	0.41
1:A:798:GLU:O	1:A:798:GLU:HG2	2.19	0.41
1:B:1005:LYS:HE3	1:B:1005:LYS:HB3	1.86	0.41
1:B:1100:ILE:HG13	1:B:1158:ILE:HD12	2.03	0.41
1:B:1148:THR:O	1:B:1152:ILE:CG1	2.67	0.41
1:B:1162:VAL:O	1:B:1164:ILE:N	2.53	0.41
1:B:1342:LEU:HD23	1:B:1342:LEU:H	1.85	0.41
1:B:1364:VAL:HG12	1:B:1365:VAL:N	2.35	0.41
1:B:1488:LEU:HD12	1:B:1488:LEU:C	2.40	0.41
1:B:165:ASP:HA	1:B:166:PRO:HD3	1.82	0.41
1:B:169:SER:C	1:B:170:GLU:O	2.57	0.41
1:B:35:ALA:O	1:B:37:GLU:N	2.53	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:VAL:HG12	1:B:420:PHE:CZ	2.56	0.41
1:B:431:LEU:HD13	1:B:433:PHE:CD1	2.56	0.41
1:B:477:LEU:HA	1:B:564:GLU:CG	2.51	0.41
1:B:502:LEU:HA	1:B:502:LEU:HD12	1.77	0.41
1:B:560:TRP:CH2	1:B:562:ASN:CB	2.97	0.41
1:B:719:SER:HB2	1:B:1123:GLN:HE21	1.85	0.41
1:B:729:THR:O	1:B:733:VAL:HG23	2.20	0.41
1:A:107:VAL:HG12	1:A:108:SER:N	2.36	0.41
1:A:1096:ASN:HD22	1:A:1099:SER:H	1.69	0.41
1:A:102:VAL:HG13	1:A:119:ILE:HG21	2.03	0.41
1:A:149:ASN:HB2	1:A:150:ASP:OD2	2.21	0.41
1:A:35:ALA:HA	1:A:150:ASP:OD1	2.21	0.41
1:A:237:PHE:O	1:A:238:ILE:CG1	2.69	0.41
1:A:43:VAL:HG22	1:A:44:TYR:N	2.36	0.41
1:A:553:GLU:OE1	1:A:555:VAL:HG23	2.21	0.41
1:A:56:ILE:CD1	1:A:66:TYR:HB2	2.51	0.41
1:A:703:ALA:CB	1:A:732:CYS:HA	2.51	0.41
1:A:840:GLN:HB3	1:A:840:GLN:HE21	1.75	0.41
1:A:897:THR:C	1:A:898:PHE:CD2	2.94	0.41
1:B:1076:THR:HG22	1:B:1120:GLU:CD	2.41	0.41
1:B:1176:LEU:O	1:B:1178:ASN:N	2.54	0.41
1:B:1324:HIS:HE1	1:B:1326:TYR:CE2	2.39	0.41
1:B:1405:CYS:N	1:B:1474:CYS:SG	2.87	0.41
1:B:162:THR:OG1	1:B:162:THR:O	2.32	0.41
1:B:56:ILE:O	1:B:66:TYR:CD2	2.74	0.41
1:A:1117:SER:HA	1:A:1145:THR:HG21	2.02	0.41
1:A:1173:ASN:O	1:A:1174:PHE:C	2.59	0.41
1:A:1212:LEU:O	1:A:1215:GLU:N	2.53	0.41
1:A:987:ILE:CG1	1:A:1294:ILE:HD12	2.51	0.41
1:A:1497:GLU:O	1:A:1498:TYR:C	2.58	0.41
1:A:324:TYR:OH	1:A:326:ALA:HB2	2.20	0.41
1:A:438:ASP:C	1:A:439:ALA:O	2.58	0.41
1:A:54:ILE:O	1:A:55:SER:HB3	2.21	0.41
1:A:654:LEU:HD12	1:A:654:LEU:HA	1.57	0.41
1:A:944:LEU:HD23	1:A:944:LEU:HA	1.77	0.41
1:A:946:PRO:CD	1:A:947:ARG:H	2.30	0.41
1:B:193:ASN:OD1	1:B:1070:LYS:CE	2.69	0.41
1:B:1284:PHE:CD2	1:B:1285:TYR:CD1	3.08	0.41
1:B:1443:VAL:CG2	1:B:1444:GLU:N	2.84	0.41
1:B:1489:SER:HA	1:B:1490:PRO:HD3	1.95	0.41
1:B:257:ASN:O	1:B:257:ASN:CG	2.59	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:GLN:CD	1:B:310:LEU:HD22	2.41	0.41
1:B:760:VAL:O	1:B:761:SER:HB3	2.21	0.41
1:B:589:SER:CB	1:B:785:GLN:HE21	2.33	0.41
1:B:80:GLN:HB3	1:B:512:PHE:HE1	1.84	0.41
1:B:909:ASN:H	1:B:926:THR:HA	1.86	0.41
2:X:217:ASN:HB2	2:X:220:ASP:CG	2.41	0.41
1:A:1040:ILE:HD13	1:A:1040:ILE:HA	1.86	0.41
1:A:50:PHE:CB	1:A:109:LYS:HE2	2.51	0.41
1:A:1127:ILE:HD12	1:A:1127:ILE:O	2.21	0.41
1:A:1166:THR:HG22	1:A:1167:ALA:N	2.35	0.41
1:A:1290:THR:O	1:A:1294:ILE:CG1	2.67	0.41
1:A:144:ARG:HG2	1:A:775:TRP:HZ2	1.84	0.41
1:A:149:ASN:O	1:A:150:ASP:C	2.58	0.41
1:A:33:VAL:HB	1:A:209:PHE:HE2	1.86	0.41
1:A:431:LEU:O	1:A:453:ARG:HA	2.21	0.41
1:A:614:ARG:O	1:A:615:GLY:C	2.59	0.41
1:B:1023:HIS:HA	1:B:1092:TYR:OH	2.21	0.41
1:B:1193:TYR:CZ	1:B:1256:LEU:HD13	2.55	0.41
1:B:313:TYR:CE2	1:B:321:LYS:HD2	2.56	0.41
1:B:350:SER:HA	1:B:351:PRO:HD3	1.74	0.41
1:B:504:LEU:HA	1:B:509:ILE:HA	2.03	0.41
1:B:515:ARG:NH1	1:B:526:ILE:HA	2.36	0.41
1:B:599:TRP:CZ3	1:B:779:LEU:HB2	2.56	0.41
1:B:587:THR:HA	1:B:789:ALA:HA	2.03	0.41
1:B:838:GLN:HB3	1:B:1486:GLY:CA	2.50	0.41
1:B:855:PHE:CD2	1:B:888:VAL:HG13	2.56	0.41
1:B:897:THR:O	1:B:898:PHE:CD2	2.74	0.41
2:Y:158:GLU:HA	2:Y:219:LYS:HZ1	1.85	0.41
2:Y:162:LEU:HA	2:Y:165:LEU:CB	2.50	0.41
1:A:1069:TRP:HE1	1:A:1463:GLN:HE21	1.67	0.41
1:A:1500:ARG:HA	1:A:1501:PRO:HD2	1.95	0.41
1:A:27:ALA:HB1	1:A:28:PRO:HD2	2.03	0.41
1:A:308:LYS:HB2	1:A:308:LYS:HE3	1.83	0.41
1:A:355:ASN:O	1:A:356:LEU:C	2.58	0.41
1:A:387:PRO:C	1:A:388:VAL:HG23	2.41	0.41
1:A:440:PRO:CD	1:A:441:ASP:H	2.33	0.41
1:A:709:GLU:CA	1:A:713:GLN:OE1	2.69	0.41
1:A:620:LEU:CD1	1:A:811:VAL:H	2.31	0.41
1:A:886:GLN:HG3	1:A:887:LYS:H	1.86	0.41
1:B:1020:TYR:CZ	1:B:1295:GLU:HB2	2.56	0.41
1:B:935:LYS:O	1:B:1365:VAL:O	2.39	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1475:VAL:CG2	1:B:1476:ARG:N	2.84	0.41
1:B:837:GLU:CG	1:B:1488:LEU:HA	2.46	0.41
1:B:23:TYR:HA	1:B:43:VAL:HG23	2.01	0.41
1:B:240:TYR:CE1	1:B:443:PRO:CG	3.04	0.41
1:B:325:ILE:HD13	1:B:325:ILE:HG21	1.81	0.41
1:B:409:SER:OG	1:B:410:VAL:N	2.53	0.41
1:B:412:ARG:HD3	1:B:414:ASP:OD2	2.20	0.41
1:B:356:LEU:HD12	1:B:452:TYR:CD1	2.55	0.41
1:B:614:ARG:O	1:B:615:GLY:C	2.59	0.41
1:B:639:GLY:N	1:B:645:VAL:HA	2.36	0.41
1:B:765:ILE:HD11	1:B:769:PHE:HE2	1.84	0.41
1:B:978:SER:HB2	1:B:1280:TYR:CD2	2.56	0.41
2:X:143:GLY:C	2:X:145:ASN:N	2.66	0.41
2:X:186:TYR:HD2	2:X:229:LYS:HB3	1.86	0.41
1:A:1008:ALA:O	1:A:1011:GLU:N	2.54	0.40
1:A:1202:HIS:HD2	1:A:1204:GLN:N	2.12	0.40
1:A:1443:VAL:CG2	1:A:1444:GLU:N	2.82	0.40
1:A:157:ARG:O	1:A:178:ASP:CB	2.66	0.40
1:A:141:VAL:CG2	1:A:190:ILE:HD11	2.51	0.40
1:A:394:THR:HG21	1:A:428:VAL:HG23	2.02	0.40
1:A:465:LEU:HD13	1:A:544:TYR:CD1	2.57	0.40
1:A:518:PHE:O	1:A:519:SER:C	2.60	0.40
1:A:689:LYS:HB3	1:A:689:LYS:HE2	1.81	0.40
1:A:722:PRO:HA	1:A:725:ILE:HG13	2.03	0.40
1:A:903:LEU:HD13	1:A:903:LEU:N	2.34	0.40
1:B:1061:ASN:HB3	1:B:1062:ALA:H	1.62	0.40
1:B:1077:TRP:HB2	1:B:1120:GLU:OE1	2.21	0.40
1:B:1084:ARG:HB2	1:B:1151:GLY:HA2	2.02	0.40
1:B:1232:LEU:HG	1:B:1232:LEU:O	2.21	0.40
1:B:1278:GLN:N	1:B:1278:GLN:HE21	2.19	0.40
1:B:1259:LEU:HD13	1:B:1300:TYR:HB2	2.02	0.40
1:B:1280:TYR:OH	1:B:1337:PRO:CG	2.69	0.40
1:B:136:THR:HA	1:B:220:LYS:O	2.22	0.40
1:B:305:THR:HB	1:B:306:ALA:H	1.73	0.40
1:B:308:LYS:HA	1:B:313:TYR:O	2.20	0.40
1:B:254:TYR:OH	1:B:331:GLU:HG3	2.22	0.40
1:B:348:VAL:HG12	1:B:350:SER:N	2.36	0.40
1:B:478:VAL:HG12	1:B:564:GLU:OE1	2.20	0.40
1:B:768:TYR:HE2	1:B:770:PRO:HA	1.83	0.40
1:B:912:PHE:O	1:B:922:ILE:HA	2.21	0.40
2:X:179:LEU:HA	2:X:184:THR:HB	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:186:TYR:O	2:X:229:LYS:HB3	2.21	0.40
1:B:512:PHE:CE2	2:Y:148:ALA:HB3	2.56	0.40
1:A:1022:PHE:HE2	1:A:1092:TYR:CD1	2.39	0.40
1:A:1193:TYR:CE2	1:A:1197:LEU:HD11	2.56	0.40
1:A:1464:LEU:HD12	1:A:1464:LEU:N	2.36	0.40
1:A:227:PHE:CZ	1:A:338:GLU:HB2	2.57	0.40
1:A:424:LEU:HA	1:A:424:LEU:HD23	1.73	0.40
1:A:495:LYS:HA	1:A:495:LYS:CE	2.51	0.40
1:A:541:LEU:HG	1:A:556:SER:OG	2.21	0.40
1:A:914:LEU:HD12	1:A:914:LEU:O	2.22	0.40
1:B:1255:LEU:HB2	1:B:1270:VAL:CG1	2.44	0.40
1:B:170:GLU:O	1:B:171:VAL:CG2	2.68	0.40
1:B:189:LYS:HG3	1:B:190:ILE:N	2.33	0.40
1:B:576:SER:OG	1:B:589:SER:CB	2.58	0.40
1:B:144:ARG:NH2	1:B:602:LEU:O	2.50	0.40
1:B:942:VAL:HG22	1:B:957:LYS:CD	2.50	0.40
1:A:1153:ARG:O	1:A:1156:PHE:N	2.46	0.40
1:A:1143:TYR:CE1	1:A:1186:PHE:CZ	3.07	0.40
1:A:1186:PHE:HD1	1:A:1250:THR:CG2	2.28	0.40
1:A:1200:LYS:H	1:A:1200:LYS:HG2	1.39	0.40
1:A:1303:LEU:C	1:A:1303:LEU:HD13	2.41	0.40
1:A:960:PRO:HB3	1:A:1345:ASP:OD1	2.22	0.40
1:A:1446:VAL:O	1:A:1446:VAL:HG12	2.20	0.40
1:A:816:LYS:O	1:A:817:ALA:HB2	2.22	0.40
1:A:832:SER:HB2	1:A:930:VAL:CG2	2.50	0.40
1:A:963:ILE:HA	1:A:964:PRO:HD3	1.94	0.40
1:A:991:VAL:CG1	1:A:991:VAL:O	2.69	0.40
1:B:1042:LYS:HG2	1:B:1046:LYS:HE3	2.03	0.40
1:B:115:LYS:HG3	1:B:116:ARG:H	1.79	0.40
1:B:1180:LEU:HD11	1:B:1208:ILE:N	2.36	0.40
1:B:1295:GLU:O	1:B:1296:GLY:O	2.40	0.40
1:B:936:ARG:HB3	1:B:1364:VAL:HG22	2.01	0.40
1:B:23:TYR:N	1:B:23:TYR:CD1	2.88	0.40
1:B:457:TYR:HD2	1:B:458:SER:O	2.05	0.40
1:B:486:VAL:HG21	1:B:526:ILE:CD1	2.52	0.40
1:B:360:PRO:CA	1:B:636:ALA:HB3	2.45	0.40
1:B:896:VAL:HG12	1:B:897:THR:H	1.86	0.40
1:B:907:LEU:HD12	1:B:908:HIS:N	2.37	0.40
1:B:940:SER:HB2	1:B:959:PHE:CE1	2.49	0.40
2:Y:193:LEU:CD2	2:Y:221:ILE:HG12	2.51	0.40
1:A:1204:GLN:O	1:A:1208:ILE:HG13	2.22	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1280:TYR:CD2	1:A:1281:GLY:N	2.89	0.40
1:A:1295:GLU:O	1:A:1299:GLU:HB2	2.20	0.40
1:A:1323:LEU:CG	1:A:1324:HIS:N	2.84	0.40
1:A:1368:THR:O	1:A:1508:PHE:CE2	2.71	0.40
1:A:1401:ARG:HG3	1:A:1478:ARG:HG2	2.03	0.40
1:A:224:LEU:HD13	1:A:225:PRO:CD	2.52	0.40
1:A:254:TYR:CE2	1:A:260:VAL:HG22	2.57	0.40
1:A:310:LEU:HD23	1:A:310:LEU:N	2.37	0.40
1:A:357:VAL:O	1:A:358:ALA:C	2.59	0.40
1:A:404:LEU:HB3	1:A:405:ASP:H	1.76	0.40
1:A:610:TYR:HB3	1:A:614:ARG:HD2	2.00	0.40
1:A:77:ASN:HD21	1:A:81:ASN:ND2	2.19	0.40
1:A:987:ILE:HG22	1:A:1021:VAL:CG2	2.52	0.40
1:B:1019:PHE:CE2	1:B:1020:TYR:CD1	3.08	0.40
1:B:1062:ALA:C	1:B:1064:TYR:H	2.23	0.40
1:B:1104:LEU:O	1:B:1108:VAL:HG12	2.21	0.40
1:B:1280:TYR:HD1	1:B:1362:THR:HG22	1.86	0.40
1:B:1446:VAL:HG12	1:B:1446:VAL:O	2.22	0.40
1:B:545:ILE:HG12	1:B:554:LEU:HD21	2.02	0.40
1:B:132:LYS:HB2	1:B:609:VAL:HG11	2.02	0.40
1:B:721:GLY:HA2	1:B:722:PRO:HD3	1.97	0.40
1:B:946:PRO:CD	1:B:947:ARG:H	2.35	0.40
1:A:1037:ASP:OD1	1:A:1038:PRO:N	2.54	0.40
1:A:981:GLY:CA	1:A:1309:LEU:HD11	2.47	0.40
1:A:1454:GLN:HG3	1:A:1454:GLN:O	2.22	0.40
1:A:1461:ILE:HG22	1:A:1461:ILE:O	2.22	0.40
1:A:342:ILE:O	1:A:343:PRO:C	2.60	0.40
1:A:357:VAL:CG2	1:A:374:GLN:HB3	2.52	0.40
1:A:758:LEU:C	1:A:760:VAL:N	2.73	0.40
1:B:1161:LEU:HD12	1:B:1162:VAL:CG2	2.52	0.40
1:B:1271:ILE:CD1	1:B:1271:ILE:C	2.86	0.40
1:B:1364:VAL:CG1	1:B:1365:VAL:N	2.84	0.40
1:B:148:LEU:HD12	1:B:148:LEU:HA	1.77	0.40
1:B:309:GLU:HG3	1:B:309:GLU:O	2.22	0.40
1:B:424:LEU:HA	1:B:424:LEU:HD23	1.88	0.40
1:B:576:SER:HB2	1:B:577:PRO:HD3	2.03	0.40
1:B:682:LYS:HD2	1:B:682:LYS:O	2.22	0.40
1:B:987:ILE:O	1:B:1021:VAL:HG21	2.21	0.40
2:Y:219:LYS:CD	2:Y:219:LYS:N	2.73	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1449/1676 (86%)	1039 (72%)	255 (18%)	155 (11%)	0	9
1	B	1449/1676 (86%)	1026 (71%)	274 (19%)	149 (10%)	0	10
2	X	100/103 (97%)	86 (86%)	9 (9%)	5 (5%)	2	26
2	Y	100/103 (97%)	84 (84%)	11 (11%)	5 (5%)	2	26
All	All	3098/3558 (87%)	2235 (72%)	549 (18%)	314 (10%)	0	11

All (314) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	TYR
1	A	86	THR
1	A	97	ASN
1	A	99	VAL
1	A	170	GLU
1	A	174	VAL
1	A	207	GLU
1	A	209	PHE
1	A	282	MET
1	A	289	ASN
1	A	291	MET
1	A	305	THR
1	A	316	GLU
1	A	317	ASP
1	A	318	LEU
1	A	426	SER
1	A	457	TYR
1	A	477	LEU
1	A	480	GLU
1	A	489	LYS
1	A	490	SER
1	A	519	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	520	ASP
1	A	522	SER
1	A	609	VAL
1	A	610	TYR
1	A	638	GLY
1	A	657	ALA
1	A	662	SER
1	A	700	TYR
1	A	704	CYS
1	A	720	LEU
1	A	863	GLU
1	A	1231	ASN
1	A	1264	ILE
1	A	1275	SER
1	A	1284	PHE
1	A	1286	SER
1	A	1297	LEU
1	A	1304	VAL
1	A	1311	MET
1	A	1335	GLY
1	A	1342	LEU
1	A	1373	GLU
1	A	1433	SER
2	X	185	LYS
1	B	59	TYR
1	B	97	ASN
1	B	99	VAL
1	B	133	PRO
1	B	174	VAL
1	B	207	GLU
1	B	209	PHE
1	B	282	MET
1	B	289	ASN
1	B	305	THR
1	B	426	SER
1	B	457	TYR
1	B	490	SER
1	B	520	ASP
1	B	522	SER
1	B	609	VAL
1	B	610	TYR
1	B	638	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	657	ALA
1	B	661	ASP
1	B	700	TYR
1	B	704	CYS
1	B	720	LEU
1	B	863	GLU
1	B	949	ILE
1	B	1068	VAL
1	B	1097	GLN
1	B	1231	ASN
1	B	1264	ILE
1	B	1284	PHE
1	B	1311	MET
1	B	1335	GLY
1	B	1342	LEU
1	B	1373	GLU
1	B	1433	SER
2	Y	185	LYS
1	A	90	LYS
1	A	101	TYR
1	A	150	ASP
1	A	302	ASP
1	A	304	GLU
1	A	306	ALA
1	A	307	VAL
1	A	308	LYS
1	A	523	TYR
1	A	615	GLY
1	A	619	PRO
1	A	661	ASP
1	A	669	CYS
1	A	705	VAL
1	A	814	THR
1	A	817	ALA
1	A	909	ASN
1	A	931	PRO
1	A	996	GLY
1	A	1007	SER
1	A	1029	ASN
1	A	1055	SER
1	A	1097	GLN
1	A	1166	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1216	ALA
1	A	1296	GLY
1	A	1312	ASP
1	A	1321	GLY
1	A	1352	PHE
1	A	1457	ASP
1	A	1486	GLY
2	X	144	GLY
1	B	28	PRO
1	B	86	THR
1	B	90	LYS
1	B	101	TYR
1	B	170	GLU
1	B	291	MET
1	B	302	ASP
1	B	304	GLU
1	B	307	VAL
1	B	308	LYS
1	B	378	SER
1	B	388	VAL
1	B	480	GLU
1	B	489	LYS
1	B	495	LYS
1	B	607	SER
1	B	612	VAL
1	B	619	PRO
1	B	662	SER
1	B	669	CYS
1	B	710	THR
1	B	814	THR
1	B	817	ALA
1	B	909	ASN
1	B	931	PRO
1	B	948	GLY
1	B	996	GLY
1	B	1029	ASN
1	B	1098	ASN
1	B	1162	VAL
1	B	1177	GLU
1	B	1216	ALA
1	B	1286	SER
1	B	1296	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1297	LEU
1	B	1304	VAL
1	B	1310	SER
2	Y	144	GLY
2	Y	195	ASP
1	A	85	LEU
1	A	133	PRO
1	A	173	MET
1	A	231	ILE
1	A	272	ARG
1	A	356	LEU
1	A	388	VAL
1	A	491	PRO
1	A	612	VAL
1	A	625	GLN
1	A	648	LEU
1	A	660	ASP
1	A	663	GLN
1	A	691	LYS
1	A	793	SER
1	A	1240	PRO
1	A	1247	MET
1	A	1263	ASP
1	A	1308	ARG
1	A	1310	SER
2	X	195	ASP
1	B	36	SER
1	B	150	ASP
1	B	186	PRO
1	B	240	TYR
1	B	306	ALA
1	B	356	LEU
1	B	445	GLU
1	B	491	PRO
1	B	519	SER
1	B	617	LYS
1	B	627	LEU
1	B	660	ASP
1	B	663	GLN
1	B	666	ASP
1	B	691	LYS
1	B	793	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	856	CYS
1	B	1105	LEU
1	B	1240	PRO
1	B	1269	PRO
1	B	1280	TYR
1	B	1308	ARG
1	B	1312	ASP
1	B	1341	LEU
1	B	1352	PHE
1	B	1457	ASP
1	A	62	LYS
1	A	129	HIS
1	A	141	VAL
1	A	166	PRO
1	A	186	PRO
1	A	425	PRO
1	A	492	TYR
1	A	495	LYS
1	A	607	SER
1	A	627	LEU
1	A	717	ARG
1	A	815	VAL
1	A	856	CYS
1	A	993	SER
1	A	1016	VAL
1	A	1101	CYS
1	A	1113	LEU
1	A	1114	ASP
1	A	1153	ARG
1	A	1177	GLU
1	A	1280	TYR
1	A	1341	LEU
1	A	1349	SER
1	A	1444	GLU
1	A	1468	PRO
1	B	62	LYS
1	B	166	PRO
1	B	173	MET
1	B	398	ASN
1	B	425	PRO
1	B	492	TYR
1	B	625	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	759	PRO
1	B	952	THR
1	B	982	LEU
1	B	1007	SER
1	B	1055	SER
1	B	1057	MET
1	B	1084	ARG
1	B	1153	ARG
1	B	1444	GLU
1	A	497	THR
1	A	536	PRO
1	A	666	ASP
1	A	710	THR
1	A	759	PRO
1	A	892	SER
1	A	969	PRO
1	A	1122	SER
1	A	1481	GLU
1	A	1501	PRO
1	B	78	LYS
1	B	85	LEU
1	B	312	TYR
1	B	320	ASN
1	B	536	PRO
1	B	664	GLU
1	B	667	GLU
1	B	892	SER
1	B	993	SER
1	B	1126	PRO
1	B	1218	VAL
1	B	1239	VAL
1	B	1468	PRO
1	B	1501	PRO
1	A	299	VAL
1	A	617	LYS
1	A	667	GLU
1	A	760	VAL
1	A	1036	SER
1	A	1126	PRO
1	A	1181	PRO
1	A	1432	ILE
1	B	111	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	343	PRO
1	B	565	GLU
1	B	760	VAL
1	B	815	VAL
1	B	1009	GLU
1	B	1263	ASP
1	B	1486	GLY
1	A	686	ILE
1	A	1269	PRO
2	X	178	GLY
1	A	1108	VAL
2	X	196	GLY
1	B	705	VAL
1	B	1016	VAL
1	B	1268	ASN
1	B	1347	ILE
2	Y	196	GLY
1	A	92	LEU
1	A	765	ILE
1	A	1135	VAL
1	A	1218	VAL
1	A	1239	VAL
1	B	92	LEU
1	B	231	ILE
1	B	615	GLY
1	B	1038	PRO
1	B	1432	ILE
1	A	28	PRO
1	A	296	ILE
1	A	510	ILE
1	A	1162	VAL
1	B	171	VAL
1	B	345	ILE
1	B	686	ILE
2	Y	178	GLY
1	A	238	ILE
1	A	668	PRO
1	A	1038	PRO
1	A	1068	VAL
1	B	668	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1296/1484 (87%)	1061 (82%)	235 (18%)	2	13
1	B	1296/1484 (87%)	1051 (81%)	245 (19%)	1	11
2	X	93/94 (99%)	87 (94%)	6 (6%)	19	51
2	Y	93/94 (99%)	86 (92%)	7 (8%)	15	47
All	All	2778/3156 (88%)	2285 (82%)	493 (18%)	2	14

All (493) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	23	TYR
1	A	41	ILE
1	A	42	GLN
1	A	51	ASP
1	A	56	ILE
1	A	64	PHE
1	A	73	LEU
1	A	81	ASN
1	A	88	GLN
1	A	100	SER
1	A	109	LYS
1	A	112	SER
1	A	114	SER
1	A	116	ARG
1	A	119	ILE
1	A	123	ASN
1	A	125	PHE
1	A	126	LEU
1	A	128	ILE
1	A	130	THR
1	A	131	ASP
1	A	140	SER
1	A	143	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	144	ARG
1	A	151	ASP
1	A	161	LEU
1	A	162	THR
1	A	163	PHE
1	A	169	SER
1	A	175	GLU
1	A	176	GLU
1	A	177	ILE
1	A	180	ILE
1	A	184	SER
1	A	192	SER
1	A	195	ARG
1	A	224	LEU
1	A	231	ILE
1	A	232	GLU
1	A	235	TYR
1	A	242	ASN
1	A	249	THR
1	A	264	ASP
1	A	273	GLU
1	A	280	LYS
1	A	296	ILE
1	A	299	VAL
1	A	312	TYR
1	A	313	TYR
1	A	324	TYR
1	A	333	THR
1	A	349	LEU
1	A	354	LEU
1	A	363	LEU
1	A	364	LYS
1	A	373	VAL
1	A	378	SER
1	A	381	GLN
1	A	383	VAL
1	A	386	VAL
1	A	389	THR
1	A	393	GLN
1	A	394	THR
1	A	403	ASP
1	A	411	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	419	SER
1	A	421	VAL
1	A	422	LEU
1	A	423	ASN
1	A	431	LEU
1	A	433	PHE
1	A	436	LYS
1	A	441	ASP
1	A	457	TYR
1	A	461	SER
1	A	466	TYR
1	A	469	TRP
1	A	473	HIS
1	A	476	LEU
1	A	482	LEU
1	A	484	ILE
1	A	492	TYR
1	A	493	ILE
1	A	495	LYS
1	A	497	THR
1	A	504	LEU
1	A	518	PHE
1	A	528	ILE
1	A	535	VAL
1	A	539	ARG
1	A	540	LEU
1	A	541	LEU
1	A	544	TYR
1	A	556	SER
1	A	563	ILE
1	A	570	GLN
1	A	573	VAL
1	A	588	VAL
1	A	589	SER
1	A	594	THR
1	A	624	PHE
1	A	631	ASP
1	A	640	LEU
1	A	641	ASN
1	A	644	ASN
1	A	648	LEU
1	A	652	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	653	PHE
1	A	667	GLU
1	A	673	LEU
1	A	680	GLN
1	A	705	VAL
1	A	710	THR
1	A	711	CYS
1	A	712	GLU
1	A	724	CYS
1	A	729	THR
1	A	753	HIS
1	A	758	LEU
1	A	767	SER
1	A	786	LEU
1	A	790	LEU
1	A	799	ILE
1	A	800	GLN
1	A	802	ILE
1	A	804	ILE
1	A	809	ILE
1	A	814	THR
1	A	840	GLN
1	A	866	CYS
1	A	867	THR
1	A	886	GLN
1	A	887	LYS
1	A	891	SER
1	A	894	HIS
1	A	895	LEU
1	A	897	THR
1	A	900	VAL
1	A	901	LEU
1	A	903	LEU
1	A	908	HIS
1	A	921	GLU
1	A	924	VAL
1	A	926	THR
1	A	927	LEU
1	A	935	LYS
1	A	936	ARG
1	A	942	VAL
1	A	949	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	952	THR
1	A	957	LYS
1	A	961	TYR
1	A	962	ARG
1	A	973	ILE
1	A	979	VAL
1	A	980	LYS
1	A	982	LEU
1	A	983	LEU
1	A	986	GLU
1	A	995	GLU
1	A	998	ASN
1	A	1001	THR
1	A	1003	LEU
1	A	1015	VAL
1	A	1024	TYR
1	A	1027	THR
1	A	1029	ASN
1	A	1033	ILE
1	A	1039	LEU
1	A	1040	ILE
1	A	1053	MET
1	A	1056	ILE
1	A	1076	THR
1	A	1084	ARG
1	A	1096	ASN
1	A	1101	CYS
1	A	1115	ASN
1	A	1127	ILE
1	A	1128	LYS
1	A	1132	THR
1	A	1140	ASN
1	A	1147	PHE
1	A	1148	THR
1	A	1158	ILE
1	A	1161	LEU
1	A	1164	ILE
1	A	1168	LEU
1	A	1200	LYS
1	A	1208	ILE
1	A	1210	SER
1	A	1217	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1218	VAL
1	A	1228	TRP
1	A	1229	LYS
1	A	1232	LEU
1	A	1251	THR
1	A	1257	THR
1	A	1274	LEU
1	A	1278	GLN
1	A	1291	ILE
1	A	1297	LEU
1	A	1301	SER
1	A	1307	LEU
1	A	1311	MET
1	A	1313	ILE
1	A	1316	SER
1	A	1318	LYS
1	A	1325	ASN
1	A	1332	ASN
1	A	1334	LEU
1	A	1336	ARG
1	A	1342	LEU
1	A	1343	ASN
1	A	1345	ASP
1	A	1347	ILE
1	A	1365	VAL
1	A	1376	SER
1	A	1383	THR
1	A	1401	ARG
1	A	1437	GLU
1	A	1443	VAL
1	A	1464	LEU
1	A	1465	ASN
1	A	1476	ARG
1	A	1480	PHE
1	A	1483	PHE
1	A	1487	PHE
1	A	1488	LEU
1	A	1496	TYR
1	A	1500	ARG
1	A	1503	LYS
1	A	1507	MET
1	A	1509	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1511	THR
2	X	134	THR
2	X	136	LEU
2	X	146	LEU
2	X	150	ILE
2	X	166	ASP
2	X	184	THR
1	B	23	TYR
1	B	24	VAL
1	B	26	SER
1	B	41	ILE
1	B	42	GLN
1	B	51	ASP
1	B	56	ILE
1	B	59	TYR
1	B	64	PHE
1	B	73	LEU
1	B	81	ASN
1	B	88	GLN
1	B	100	SER
1	B	109	LYS
1	B	112	SER
1	B	114	SER
1	B	116	ARG
1	B	119	ILE
1	B	123	ASN
1	B	125	PHE
1	B	126	LEU
1	B	128	ILE
1	B	130	THR
1	B	131	ASP
1	B	148	LEU
1	B	151	ASP
1	B	160	VAL
1	B	161	LEU
1	B	162	THR
1	B	163	PHE
1	B	175	GLU
1	B	176	GLU
1	B	177	ILE
1	B	180	ILE
1	B	184	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	188	PHE
1	B	189	LYS
1	B	194	PRO
1	B	195	ARG
1	B	212	THR
1	B	224	LEU
1	B	231	ILE
1	B	232	GLU
1	B	235	TYR
1	B	242	ASN
1	B	249	THR
1	B	253	ARG
1	B	257	ASN
1	B	264	ASP
1	B	273	GLU
1	B	280	LYS
1	B	290	THR
1	B	296	ILE
1	B	299	VAL
1	B	312	TYR
1	B	317	ASP
1	B	318	LEU
1	B	324	TYR
1	B	333	THR
1	B	349	LEU
1	B	354	LEU
1	B	363	LEU
1	B	364	LYS
1	B	373	VAL
1	B	378	SER
1	B	379	LEU
1	B	383	VAL
1	B	386	VAL
1	B	389	THR
1	B	393	GLN
1	B	394	THR
1	B	403	ASP
1	B	411	THR
1	B	421	VAL
1	B	422	LEU
1	B	423	ASN
1	B	431	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	433	PHE
1	B	436	LYS
1	B	441	ASP
1	B	457	TYR
1	B	461	SER
1	B	463	SER
1	B	466	TYR
1	B	469	TRP
1	B	473	HIS
1	B	476	LEU
1	B	484	ILE
1	B	492	TYR
1	B	493	ILE
1	B	495	LYS
1	B	497	THR
1	B	500	ASN
1	B	502	LEU
1	B	509	ILE
1	B	517	LYS
1	B	528	ILE
1	B	535	VAL
1	B	539	ARG
1	B	540	LEU
1	B	541	LEU
1	B	544	TYR
1	B	553	GLU
1	B	556	SER
1	B	563	ILE
1	B	570	GLN
1	B	573	VAL
1	B	588	VAL
1	B	589	SER
1	B	594	THR
1	B	624	PHE
1	B	640	LEU
1	B	641	ASN
1	B	644	ASN
1	B	648	LEU
1	B	652	THR
1	B	653	PHE
1	B	667	GLU
1	B	669	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	673	LEU
1	B	680	GLN
1	B	699	CYS
1	B	704	CYS
1	B	705	VAL
1	B	707	ASN
1	B	711	CYS
1	B	729	THR
1	B	753	HIS
1	B	758	LEU
1	B	767	SER
1	B	786	LEU
1	B	790	LEU
1	B	795	THR
1	B	799	ILE
1	B	802	ILE
1	B	804	ILE
1	B	809	ILE
1	B	814	THR
1	B	840	GLN
1	B	866	CYS
1	B	867	THR
1	B	886	GLN
1	B	887	LYS
1	B	891	SER
1	B	894	HIS
1	B	895	LEU
1	B	897	THR
1	B	900	VAL
1	B	901	LEU
1	B	903	LEU
1	B	908	HIS
1	B	924	VAL
1	B	926	THR
1	B	927	LEU
1	B	932	GLU
1	B	935	LYS
1	B	936	ARG
1	B	952	THR
1	B	961	TYR
1	B	962	ARG
1	B	972	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	973	ILE
1	B	975	ARG
1	B	976	ILE
1	B	980	LYS
1	B	982	LEU
1	B	983	LEU
1	B	986	GLU
1	B	995	GLU
1	B	998	ASN
1	B	1001	THR
1	B	1003	LEU
1	B	1015	VAL
1	B	1024	TYR
1	B	1027	THR
1	B	1029	ASN
1	B	1040	ILE
1	B	1053	MET
1	B	1056	ILE
1	B	1069	TRP
1	B	1096	ASN
1	B	1108	VAL
1	B	1115	ASN
1	B	1127	ILE
1	B	1128	LYS
1	B	1132	THR
1	B	1140	ASN
1	B	1147	PHE
1	B	1148	THR
1	B	1158	ILE
1	B	1161	LEU
1	B	1164	ILE
1	B	1168	LEU
1	B	1200	LYS
1	B	1206	ARG
1	B	1208	ILE
1	B	1210	SER
1	B	1213	LYS
1	B	1217	LEU
1	B	1218	VAL
1	B	1226	ARG
1	B	1228	TRP
1	B	1232	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1251	THR
1	B	1257	THR
1	B	1269	PRO
1	B	1271	ILE
1	B	1278	GLN
1	B	1279	ARG
1	B	1280	TYR
1	B	1297	LEU
1	B	1301	SER
1	B	1307	LEU
1	B	1311	MET
1	B	1313	ILE
1	B	1316	SER
1	B	1318	LYS
1	B	1325	ASN
1	B	1332	ASN
1	B	1334	LEU
1	B	1336	ARG
1	B	1342	LEU
1	B	1343	ASN
1	B	1344	ASP
1	B	1345	ASP
1	B	1347	ILE
1	B	1358	THR
1	B	1376	SER
1	B	1383	THR
1	B	1401	ARG
1	B	1443	VAL
1	B	1464	LEU
1	B	1465	ASN
1	B	1474	CYS
1	B	1476	ARG
1	B	1480	PHE
1	B	1483	PHE
1	B	1487	PHE
1	B	1488	LEU
1	B	1496	TYR
1	B	1500	ARG
1	B	1502	ASP
1	B	1503	LYS
1	B	1507	MET
1	B	1509	TYR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	Y	134	THR
2	Y	136	LEU
2	Y	138	VAL
2	Y	146	LEU
2	Y	150	ILE
2	Y	184	THR
2	Y	210	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	81	ASN
1	A	88	GLN
1	A	110	HIS
1	A	123	ASN
1	A	139	GLN
1	A	226	HIS
1	A	242	ASN
1	A	279	GLN
1	A	298	GLN
1	A	320	ASN
1	A	393	GLN
1	A	423	ASN
1	A	481	HIS
1	A	625	GLN
1	A	656	ASN
1	A	737	GLN
1	A	785	GLN
1	A	787	GLN
1	A	840	GLN
1	A	886	GLN
1	A	894	HIS
1	A	994	GLN
1	A	1002	HIS
1	A	1023	HIS
1	A	1029	ASN
1	A	1030	HIS
1	A	1090	ASN
1	A	1095	GLN
1	A	1096	ASN
1	A	1115	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1123	GLN
1	A	1140	ASN
1	A	1173	ASN
1	A	1202	HIS
1	A	1221	ASN
1	A	1260	ASN
1	A	1278	GLN
1	A	1306	GLN
1	A	1325	ASN
1	A	1343	ASN
1	A	1366	HIS
1	A	1435	ASN
1	A	1459	HIS
1	A	1463	GLN
1	A	1465	ASN
1	A	1504	GLN
2	X	135	HIS
2	X	192	ASN
1	B	77	ASN
1	B	80	GLN
1	B	88	GLN
1	B	110	HIS
1	B	123	ASN
1	B	139	GLN
1	B	226	HIS
1	B	242	ASN
1	B	257	ASN
1	B	298	GLN
1	B	320	ASN
1	B	381	GLN
1	B	393	GLN
1	B	423	ASN
1	B	481	HIS
1	B	625	GLN
1	B	656	ASN
1	B	737	GLN
1	B	785	GLN
1	B	787	GLN
1	B	840	GLN
1	B	886	GLN
1	B	894	HIS
1	B	994	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1002	HIS
1	B	1023	HIS
1	B	1029	ASN
1	B	1030	HIS
1	B	1090	ASN
1	B	1096	ASN
1	B	1115	ASN
1	B	1123	GLN
1	B	1140	ASN
1	B	1173	ASN
1	B	1202	HIS
1	B	1221	ASN
1	B	1268	ASN
1	B	1278	GLN
1	B	1306	GLN
1	B	1325	ASN
1	B	1343	ASN
1	B	1366	HIS
1	B	1435	ASN
1	B	1463	GLN
1	B	1465	ASN
1	B	1504	GLN
2	Y	135	HIS
2	Y	176	ASN
2	Y	230	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

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	1680	1	14,14,15	0.66	0	17,19,21	1.00	1 (5%)
4	NAG	A	2001	1,4	14,14,15	0.52	0	17,19,21	1.06	1 (5%)
4	NAG	A	2002	4	14,14,15	0.47	0	17,19,21	1.06	2 (11%)
4	NAG	B	1679	1	14,14,15	0.71	1 (7%)	17,19,21	1.11	2 (11%)
4	NAG	B	2001	1,4	14,14,15	0.55	0	17,19,21	0.97	0
4	NAG	B	2002	4	14,14,15	0.47	0	17,19,21	1.02	2 (11%)

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	1680	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2002	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1679	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2002	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1679	NAG	C1-C2	2.04	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1679	NAG	O5-C1-C2	2.01	114.30	111.52
4	A	2002	NAG	O5-C5-C6	2.09	110.45	107.15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2002	NAG	O5-C5-C6	2.21	110.65	107.15
4	B	1679	NAG	O5-C5-C6	2.57	111.21	107.15
4	B	2002	NAG	C1-O5-C5	2.59	115.75	112.19
4	A	1680	NAG	O5-C5-C6	2.90	111.73	107.15
4	A	2001	NAG	C1-O5-C5	2.94	116.23	112.19
4	A	2002	NAG	C1-O5-C5	2.94	116.23	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	NAG	2	0
4	B	2001	NAG	3	0
4	B	2002	NAG	1	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	1459/1676 (87%)	-0.62	11 (0%) 86 79	81, 190, 311, 455	0
1	B	1459/1676 (87%)	-0.63	10 (0%) 87 81	85, 190, 308, 475	0
2	X	102/103 (99%)	0.04	9 (8%) 10 7	157, 292, 386, 530	0
2	Y	102/103 (99%)	0.02	5 (4%) 29 22	156, 292, 377, 494	0
All	All	3122/3558 (87%)	-0.58	35 (1%) 80 72	81, 194, 328, 530	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	671	GLU	4.8
2	Y	193	LEU	4.4
2	X	193	LEU	4.4
1	B	671	GLU	4.0
1	A	670	LYS	3.6
1	B	668	PRO	3.4
2	Y	159	GLU	3.4
1	B	615	GLY	3.4
1	A	672	ILE	3.3
2	X	159	GLU	2.9
1	A	668	PRO	2.8
1	B	670	LYS	2.8
1	A	759	PRO	2.8
2	X	158	GLU	2.7
2	Y	192	ASN	2.7
1	A	883	CYS	2.6
1	A	309	GLU	2.6
2	X	197	GLU	2.5
2	Y	157	LYS	2.5
1	B	309	GLU	2.5
1	A	258	LYS	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	X	129	SER	2.3
1	A	613	GLN	2.3
2	X	192	ASN	2.3
1	B	47	THR	2.2
1	B	613	GLN	2.2
1	B	672	ILE	2.2
2	X	228	LEU	2.2
2	X	227	THR	2.1
2	Y	158	GLU	2.1
1	A	47	THR	2.1
1	A	615	GLY	2.1
2	X	157	LYS	2.1
1	B	258	LYS	2.1
1	B	759	PRO	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CD	A	1679	1/1	0.22	0.12	402,402,402,402	0
3	CD	B	1678	1/1	0.39	0.11	397,397,397,397	0
4	NAG	A	1680	14/15	0.51	0.36	301,301,301,301	0
4	NAG	B	1679	14/15	0.59	0.35	290,290,290,290	0
4	NAG	A	2002	14/15	0.66	0.46	343,343,343,343	0
4	NAG	B	2002	14/15	0.73	0.50	363,363,363,363	0
4	NAG	B	2001	14/15	0.79	0.30	280,280,280,280	0
4	NAG	A	2001	14/15	0.85	0.28	293,293,293,293	0
3	CD	A	1678	1/1	0.87	0.44	481,481,481,481	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CD	A	1677	1/1	0.89	0.09	229,229,229,229	1
3	CD	B	1677	1/1	0.90	0.38	466,466,466,466	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.