



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 3, 2018 – 06:05 PM EST

PDB ID : 6C3O  
EMDB ID: : EMD-7338  
Title : Cryo-EM structure of human KATP bound to ATP and ADP in quatrefoil form  
Authors : Lee, K.P.K.; Chen, J.; MacKinnon, R.  
Deposited on : 2018-01-10  
Resolution : 3.90 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

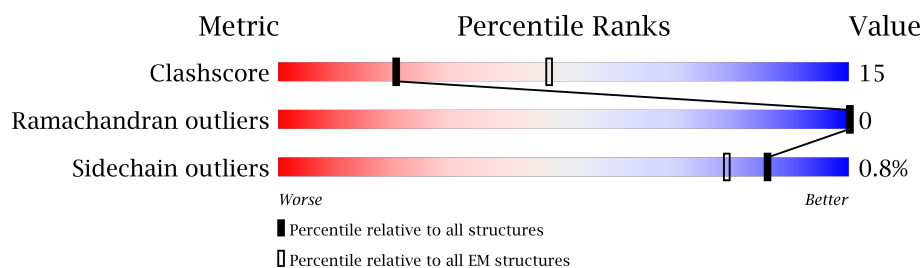
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	406	
1	B	406	
1	C	406	
1	D	406	
2	E	1581	
2	F	1581	
2	G	1581	
2	H	1581	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 49055 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ATP-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	328	Total	C	N	O	S	0	0
			2501	1616	427	441	17		
1	C	328	Total	C	N	O	S	0	0
			2501	1616	427	441	17		
1	B	328	Total	C	N	O	S	0	0
			2501	1616	427	441	17		
1	D	328	Total	C	N	O	S	0	0
			2501	1616	427	441	17		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	SER	-	expression tag	UNP Q14654
A	-4	ALA	-	expression tag	UNP Q14654
A	-3	SER	-	expression tag	UNP Q14654
A	-2	ALA	-	expression tag	UNP Q14654
A	-1	SER	-	expression tag	UNP Q14654
A	0	ALA	-	expression tag	UNP Q14654
A	391	SER	-	expression tag	UNP Q14654
A	392	ASN	-	expression tag	UNP Q14654
A	393	SER	-	expression tag	UNP Q14654
A	394	LEU	-	expression tag	UNP Q14654
A	395	GLU	-	expression tag	UNP Q14654
A	396	VAL	-	expression tag	UNP Q14654
A	397	LEU	-	expression tag	UNP Q14654
A	398	PHE	-	expression tag	UNP Q14654
A	399	GLN	-	expression tag	UNP Q14654
A	400	GLY	-	expression tag	UNP Q14654
C	-5	SER	-	expression tag	UNP Q14654
C	-4	ALA	-	expression tag	UNP Q14654
C	-3	SER	-	expression tag	UNP Q14654
C	-2	ALA	-	expression tag	UNP Q14654
C	-1	SER	-	expression tag	UNP Q14654
C	0	ALA	-	expression tag	UNP Q14654

*Continued on next page...*

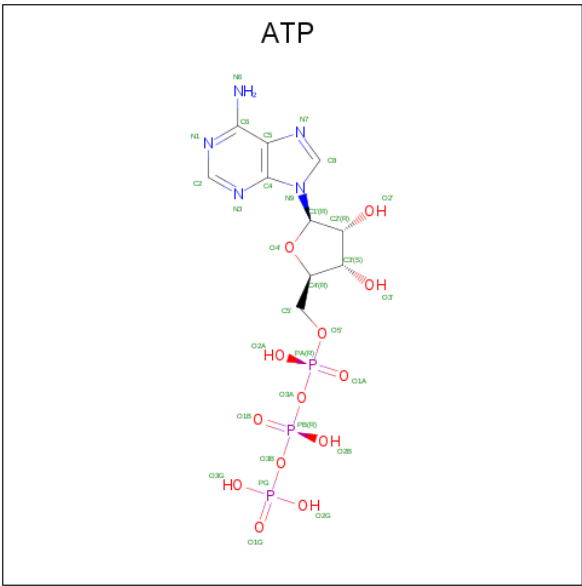
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	391	SER	-	expression tag	UNP Q14654
C	392	ASN	-	expression tag	UNP Q14654
C	393	SER	-	expression tag	UNP Q14654
C	394	LEU	-	expression tag	UNP Q14654
C	395	GLU	-	expression tag	UNP Q14654
C	396	VAL	-	expression tag	UNP Q14654
C	397	LEU	-	expression tag	UNP Q14654
C	398	PHE	-	expression tag	UNP Q14654
C	399	GLN	-	expression tag	UNP Q14654
C	400	GLY	-	expression tag	UNP Q14654
B	-5	SER	-	expression tag	UNP Q14654
B	-4	ALA	-	expression tag	UNP Q14654
B	-3	SER	-	expression tag	UNP Q14654
B	-2	ALA	-	expression tag	UNP Q14654
B	-1	SER	-	expression tag	UNP Q14654
B	0	ALA	-	expression tag	UNP Q14654
B	391	SER	-	expression tag	UNP Q14654
B	392	ASN	-	expression tag	UNP Q14654
B	393	SER	-	expression tag	UNP Q14654
B	394	LEU	-	expression tag	UNP Q14654
B	395	GLU	-	expression tag	UNP Q14654
B	396	VAL	-	expression tag	UNP Q14654
B	397	LEU	-	expression tag	UNP Q14654
B	398	PHE	-	expression tag	UNP Q14654
B	399	GLN	-	expression tag	UNP Q14654
B	400	GLY	-	expression tag	UNP Q14654
D	-5	SER	-	expression tag	UNP Q14654
D	-4	ALA	-	expression tag	UNP Q14654
D	-3	SER	-	expression tag	UNP Q14654
D	-2	ALA	-	expression tag	UNP Q14654
D	-1	SER	-	expression tag	UNP Q14654
D	0	ALA	-	expression tag	UNP Q14654
D	391	SER	-	expression tag	UNP Q14654
D	392	ASN	-	expression tag	UNP Q14654
D	393	SER	-	expression tag	UNP Q14654
D	394	LEU	-	expression tag	UNP Q14654
D	395	GLU	-	expression tag	UNP Q14654
D	396	VAL	-	expression tag	UNP Q14654
D	397	LEU	-	expression tag	UNP Q14654
D	398	PHE	-	expression tag	UNP Q14654
D	399	GLN	-	expression tag	UNP Q14654
D	400	GLY	-	expression tag	UNP Q14654

- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	1290	Total	C	N	O	S	0	0
			9671	6307	1626	1687	51		
2	H	1290	Total	C	N	O	S	0	0
			9671	6307	1626	1687	51		
2	G	1290	Total	C	N	O	S	0	0
			9671	6307	1626	1687	51		
2	F	1290	Total	C	N	O	S	0	0
			9671	6307	1626	1687	51		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



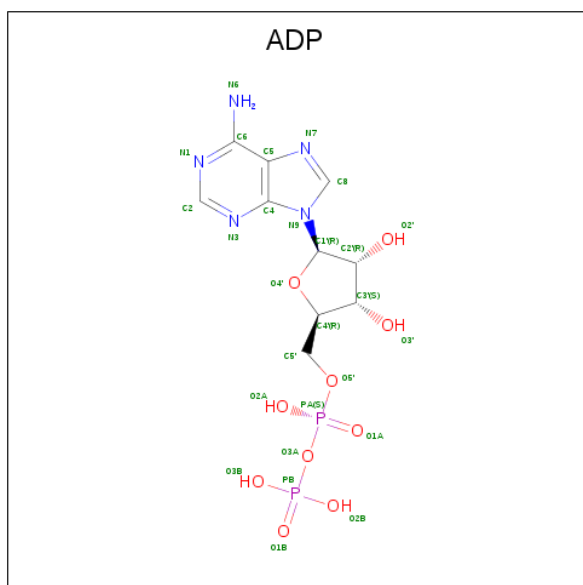
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
4	A	3	Total	K	0
			3	3	

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

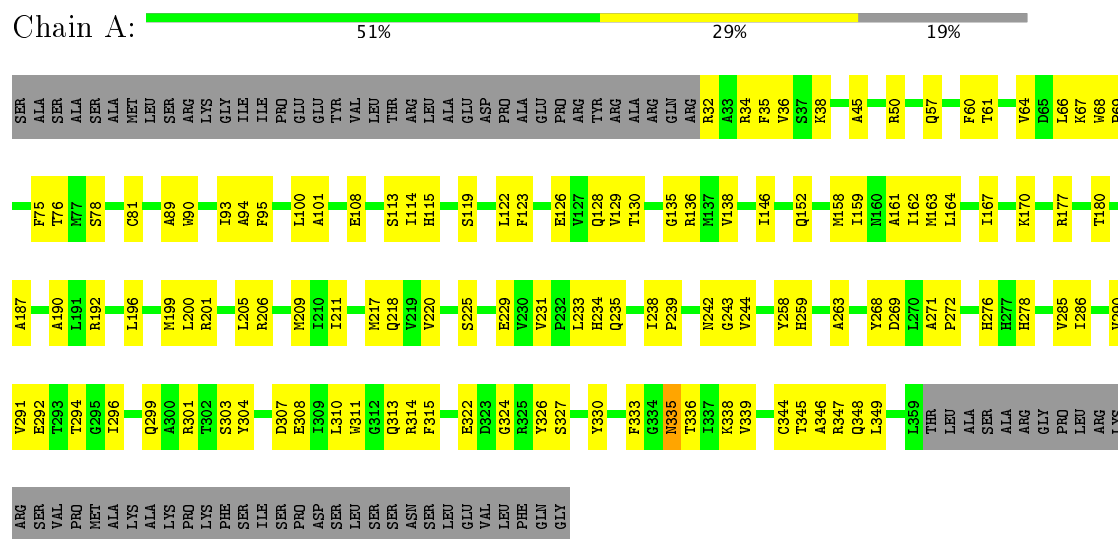


Mol	Chain	Residues	Atoms		AltConf
6	H	2	Total 2	Mg 2	0
6	G	2	Total 2	Mg 2	0
6	F	2	Total 2	Mg 2	0
6	E	2	Total 2	Mg 2	0

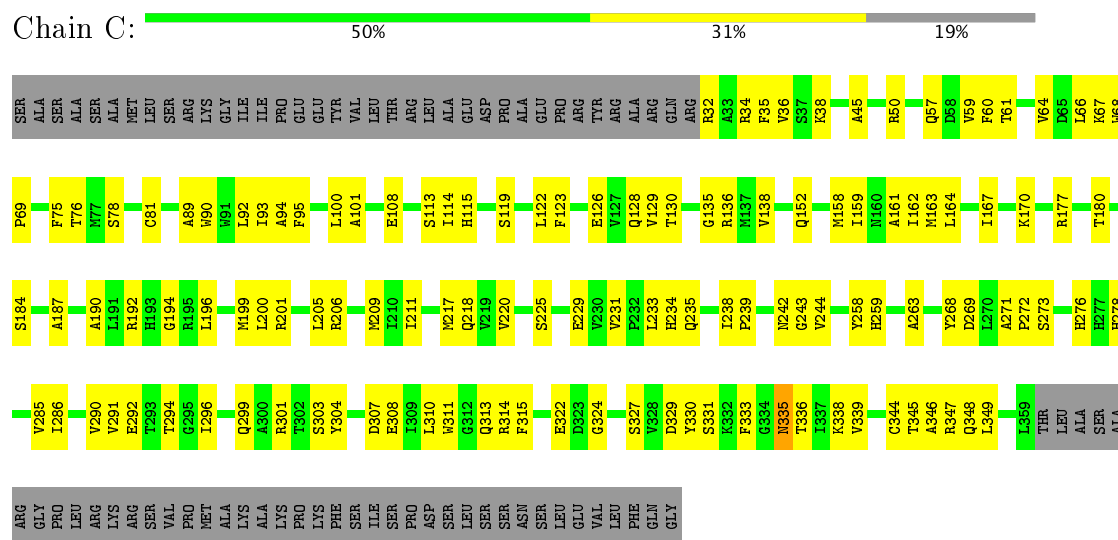
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: ATP-sensitive inward rectifier potassium channel 11



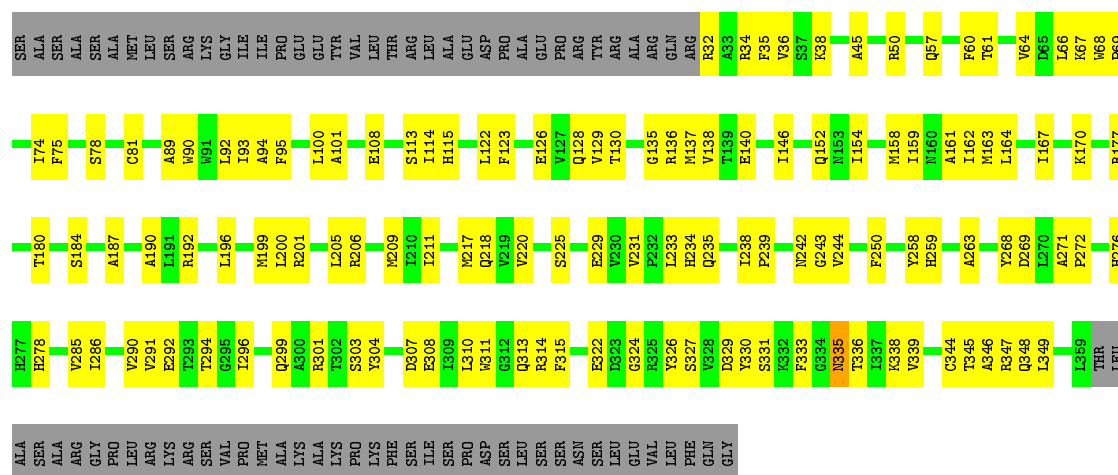
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

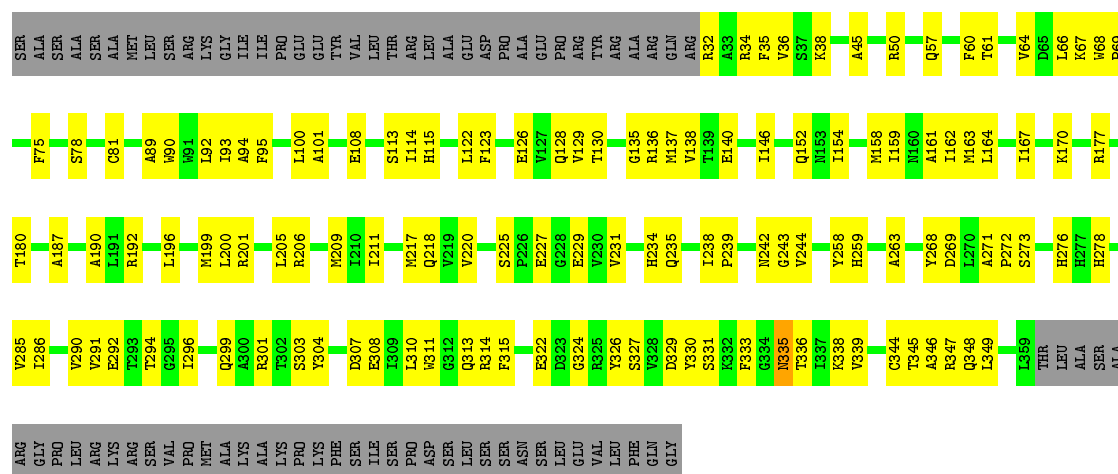






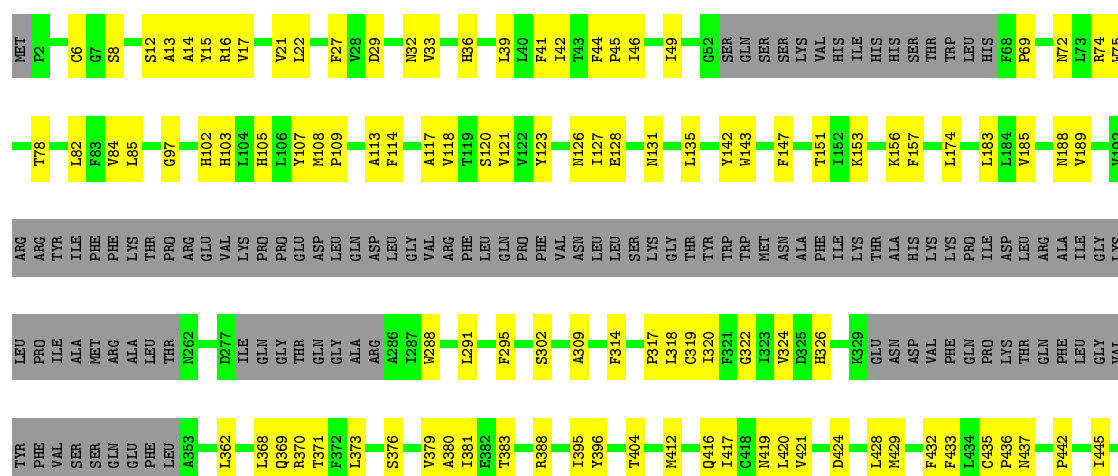
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

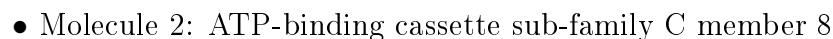
Chain D: 50% 31% 19%



• Molecule 2: ATP-binding cassette sub-family C member 8

Chain E: 56% 25% 18%





Response	Percentage
Yes	56%
No	26%
Don't know	18%



I1549	C1445	A1310	T1194	L1073	HIS	L950	P809	L723	ALA	I557	L451	VAL	ILE
D1560	S1446	R1313	H1202	G1074	GLN	MET	D810	L727	VAL	V563	L452	PRO	GLY
K1561	I1314	I1314	H1202	I1075	ARG	ASN	R811		LEU		Y453	VAL	LEU
P1562	T1449	Y1325	T1212	W1087	E994	GLN	H816	V733	ARG	PHE	Y454	SER	PRO
R1568	E1455		R1213	L1090	Y1003	ASP	T820	V737	VAL	PHE	I455	SER	ILE
K1569	I1346	I1347	R1214	L1091	L1004	GLN	Q821	F738	VAL	LYS	L456	GLN	ALA
D1570	K1460	L1348	F1216	V1092	L1011	LEU	R822	W739	ASN	GLU	G457	GLU	MET
S1571	L1349	L1349	R1217	N1102	L1012	GLU	G823	S740	LYS	ALA	Y458	PHE	ARG
K1581	S1350	S1350	Y1218	N1102	L1012	LYS	L429	SER	ARG	PHE	L461	LEU	ALA
	V1351	V1351		F1124	H1023	THR		PRO	PRO	SER	L465	THR	THR
	D1471		L1226		H1024	VAL	Q833	ASP	ALA	S574		L362	W262
	A1472	S1355	D1231	D1127	V1025	THR	R834	SER	ARG	V575	I468	I368	D277
	I1473	S1356	L1231	C1128	L1026	GLU	Q835	THR	GLU	A576		Q369	ILE
	I1474	S1232	S1232	N1129	V1027	ARG	R836	ILE	CYS	F577	A471	R370	GLN
	L1361	N1233	N1233	T1130	A1028	LYS	R841	GLU	ARG	L582	V472	P372	GLY
	K1362	H1234	H1234	I1131	I1029	ALA		ASP	GLY	F583	V477	L373	THR
	H1363	I1235	I1235	D1132	D1030	THR	H846	LEU	LEU	L592		L373	GLN
	V1364			Q1133	Y1031	GLU	V849	PRO	GLY	V587	K480	V379	GLN
	I1372	N1244	N1244	I1135	W1032	PRO	V850	PRO	PRO	L593	A380	A380	ALA
	G1375	W1246	W1246	P1136	K1035	GLN	P851	GLU	LEU	F591	S487	I381	ARG
	I1376	E1248	E1248	F1138	D1038	LEU	D865	GLU	SER	L592	E490	T383	W288
	L1488			L1139	SER	SER		THR	LEU	F591		R388	L291
	L1491	M1251	M1251	L1142	ALA	ARG	G871	ALA	VAL	L593	E494	R388	L291
	K1384	I1254	I1254	S1143	LEU	ALA		THR	THR	S594	R495	I395	F295
	R1493	G1255	G1255	R1144	THR	MET	L875	ASP	SER	V596	L496	I395	F295
	F1392				LEU	SER		LEU	ALA	W697	Q497	Y396	
	T1397	V1289	V1289	S1151	PRO	SER	D878	ILE	ASP	R598	Q498	T404	A309
	F1398	A1263	A1263	A1152	ALA	ARG	R881	LYS	ASP	S599	T499	T404	F314
	E1399	I1267	I1267	A1154	ARG	LEU	V886		ASN	T600	N500	M412	
	G1400	S1268	S1268	V1155	ASN	LEU	T887	V769	C677	L604	R504	Q416	P317
	H1401	N1269	N1269	I1156	CYS	GLN	R888	A770	C678	V605	K510	L318	L318
	I1402	S1270	S1270	S1157	SER	ASP	R889	Y771	W679	S606	R519	I417	C319
	I1409	L1271	L1271	V1162	LEU	GLU	L890	P776	Q680	V607	R521	I418	I320
	L1417	R1273	R1273	F1163	GLN	GLU	Q891	W777	Q681	GLU	R521	L420	G322
	R1418	H1274	H1274	V1165	CYS	GLU	L933	L778	W685	GLN	A537	V324	V324
	S1422	L1275	L1275	A1166	THR	GLU	P894	L779		CYS	I538	D325	D325
	I1423	S1276	S1276	L1167	LEU	GLU	H895	A781	I701	ALA	T540	L428	L428
	I1424	A1277	A1277	L1168	ASP	ALA	A896		R702	PRO	M429	M429	M429
	V1429	L1284	L1284	P1169	GLN	ALA	D897	I768	I703	HIS	S543	F432	GLU
	L1430	T1285	T1285	L1170	T1061	GLU	T898		L708	GLU	S543	F432	ASN
	F1431	Y1286	Y1286	A1171	V1062	SER	T899	S791	I709	PRO	R547	F433	ASP
	A1287	A1287	A1287	I1172	A1064	GLU	I900	Y798	W710	THR	T548	L434	VAL
	N1292	N1292	N1292	I1177	M1065	ASP	G905	Y798	I711	PRO	T548	L434	PHE
	F1437	N1293	N1293	Y1180	V1066	ASN	T906	I802	W712	GLN	A549	C435	GLN
	N1438	L1294	L1294	F1181	F1067	LEU	I907	I802	V713	PRO	P551	P436	PRO
	L1439	N1295	N1295	R1182	T1068	LEU	R918	C805	G713	ALA	T552	P442	LYS
	D1440			V1183	V1069	SER	D922	S806	Q714	SER	A553	I445	GLN
	E1442			L1191	C1071	SER		Q808	W715	LYS	A554	I445	GLN
					S1072	LEU			C717	THR	V555	I445	PHE
										GLN	L556	G448	GLY

- Molecule 2: ATP-binding cassette sub-family C member 8

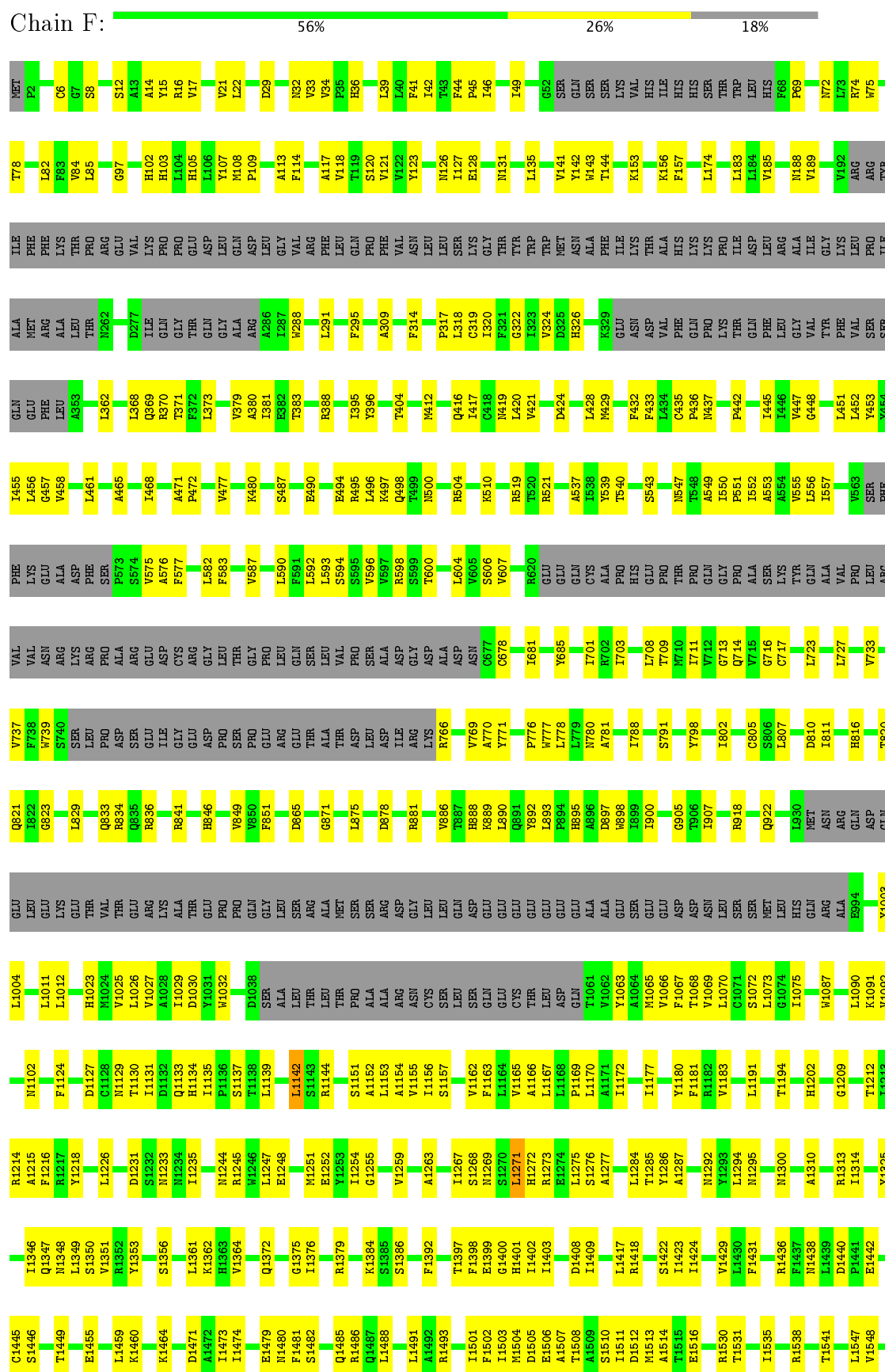
Chain G:  55% 26% 18%

MET	F2	C6	G7	S8	S12	A13	A14	Y15	R16	V17	V21	L22	F27	V28	D29	N32	V33	V34	P35	H36	L39	L40	F41	I42	T43	F44	P45	I46	I49	G52	SER	GLN	SER	SER	LYS	VAL	HIS	ILE	HIS	HIS	HIS	SER	THR	TRP	HIS	F68	P69	T1541	N72	L73	R74
-----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-------	-----	-----	-----

L1541	N1438	R1313	H1202	W1087	ALA	ARG	D810	L727	ALA	I567	L451	TYR	GLY	V192	H75
L1547	L1499	I1314	G1209	L1090	E994	GLN	I811	L727	VAL	V563	L452	PHE	LYS	ARG	T78
V1548	P1441	Y1325	T1212	K1091	Y1003	ASP	H816	V733	PRO	PHE	Y453	SER	LEU	ARG	
I1549	E1442	Y1325	I1213	V1092	L1004	GLU	T820	V737	VAL	PHE	Y454	GLN	ALA	ILE	L82
	G1445	I1346	R1214	N1102	L1011	LEU	Q821	F738	VAL	GLY	L455	GLU	VAL	PHE	F83
D1560	S1446	Q1347	A1215	N1102	L1012	GLY	I822	W739	ASN	LYS	L456	PHE	ASN	PHE	V84
K1561	T1449	N1348	F1216	F1124	M1023	GLU	G823	SER	ARG	ASP	G457	LEU	ARG	PHE	L85
P1562	E1455	S1349	Y1218	N1124	H1024	THR	L829	SER	LYS	PHE	Y458		ALA	LYS	
R1568	R1352	V1351	L1226	D1127	V1025	VAL	L829	PRO	ARG	SER	L461	L362	THR	THR	G97
S1571	L1459	Y1353	L1226	C1128	L1026	GLU	Q833	ASP	PRO	P573	A465	L362	I2262	ARG	H102
K1581	K1460	D1354	D1231	N1129	V1027	ARG	R834	SER	ARG	S574	T468	L368	I2277	GLU	H103
	K1464	S1355	S1232	I1131	A1028	LYS	Q836	ILE	GLU	V575		Q369	ILE	VAL	L104
	K1464	S1356	N1233	D1132	D1030	ALA	Q836	GLY	ASP	A576		R370	GLN	LYS	H105
	D1471	L1361	N1234	Q1133	Y1031	THR	R841	GLU	ARG	F577	A471	F371	THR	PRO	L106
A1472	I1473	K1362	I1235	H1134	W1032	PRO	R846	ASP	GLY	L582	P472	L373	GLN	GLU	M108
I1474	H1363	V1364	N1244	I1135	W1032	PRO	R846	PRO	LEU	F583		Q374	ALA	ASP	P109
E1479	I1473	V1364	W1246	P1136	K1035	GLY	V849	SER	THR	V587	K480	V379	GLY	LEU	A113
F1481	S1482	Q1372	E1248	T1137	D1038	ARG	F851	THR	GLY	L590	S487	A380	ARG	GLN	F114
S1482	Q1485	G1375	M1251	L1142	SER	ALA	D865	THR	LEU	L592		I381	LEU	LEU	A117
Q1485	R1486	I1376	I1254	S1143	LEU	THR	G871	ALA	LEU	L593	E490	F382	VAL	ARG	V118
Q1487	R1486	R1379	G1255	R1144	THR	SER	F871	THR	THR	S594	E494	R388	GLY	PHE	I119
L1488	K1384	I1486	I1259	S1151	PRO	ARG	L875	ASP	PRO	V595	R495	I395	GLN	LEU	V120
L1491	S1385	K1385	V1259	L1152	ALA	ASP	D878	ASP	LEU	V596	L496	Y396	PRO	PRO	V122
A1492	S1386	S1386	A1263	A1154	ALA	GLY	R881	ILE	ASP	V597	Q498	T404	PHE	PHE	Y123
R1493	F1392	I1392	I1267	V1155	ARG	LEU	R881	GLY	ASP	R598	T499	M412	VAL	VAL	H126
I1501	T1397	F1398	S1268	S1157	ASN	LEU	V886	R766	ASP	T600	N500		LEU	ASN	I127
F1502	F1398	E1399	N1269	S1162	LEU	GLU	T887	V769	ASN	L604	R504	Q416	LEU	LEU	E128
I1503	G1400	G1400	L1270	F1163	SER	GLU	R888	A770	GLY	V605	R510	I417	LYS	LYS	M131
M1504	H1401	H1401	L1271	L1164	GLN	GLU	K889	Y771	ASP	S606	R519	C418	GLY	GLY	L135
E1505	I1402	I1402	R1273	V1165	CYS	GLU	Q891	P776	PRO	V607	T520	N420	THR	THR	Y142
A1506	I1403	I1403	E1274	A1166	THR	GLU	Y892	W777	ILE	R620	R521	L420	TRP	TRP	W143
T1508	D1408	D1408	L1275	L1167	LEU	GLU	L893	L778	GLY	GLU	A537	D424	D325	MET	F147
A1509	S1409	I1409	S1276	P1169	ASP	ALA	H895	L779	GLN	CYS	T538		H226	ASN	I148
I1511	I1417	L1417	A1277	L1170	GLN	GLU	A896	N780	ALA	ALA	T539	L428	K329	ALA	T151
M1512	R1418	R1418	T1285	I1172	Y1063	SER	D897	A781	PRO	PRO	T540	M429	GLU	ILE	I152
M1513	S1422	S1422	Y1286	I1177	A1064	GLU	W898	I788	HIS	GLU	S543	F432	ASN	LYS	K153
A1514	I1423	I1423	A1287	I1177	M1065	ASP	I900	S781	PRO	THR	R547	F433	VAL	THR	K156
E1516	I1424	I1424	N1292	Y1180	V1066	ASN	I907	Y798	THR	PRO	T548	L434	PHE	ALA	F157
R1530	I1429	I1429	L1294	F1181	F1067	LEU	R918	I802	PRO	GLN	C435	C435	GLN	LYS	L174
T1531	I1430	I1430	N1295	R1182	V1069	SER	R918	I802	GLY	GLY	A549	N437	PRO	PRO	L174
T1535	F1431	F1431	N1300	V1183	C1071	MET	Q822	C805	GLY	ALA	T552	P442	THR	ILE	L183
R1538	R1436	F1437	A1310	L1191	S1072	LEU	I930	S886	ALA	SER	A553	P442	GLN	ASP	I182
				T1194	G1074	HIS	MET	Q808	LYS	TYR	A554	I445	PHE	LEU	V185
					I1075	ARG	ASN	P809	L723	GLN	L556	G448	VAL	ARG	M188
														ILE	V189

- Molecule 2: ATP-binding cassette sub-family C member 8

## Chain F:



D1560				
K1561				
P1562				
R1568				
S1571				
K1581				



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	47282	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.18	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, K, MG, ADP

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.38	0/2557	0.47	0/3482
1	B	0.38	0/2557	0.47	0/3482
1	C	0.38	0/2557	0.47	0/3482
1	D	0.38	0/2557	0.47	0/3482
2	E	0.33	0/9862	0.48	0/13439
2	F	0.33	0/9862	0.48	0/13439
2	G	0.33	0/9862	0.48	0/13439
2	H	0.33	0/9862	0.48	0/13439
All	All	0.34	0/49676	0.48	0/67684

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2501	0	2491	98	0
1	B	2501	0	2491	102	0
1	C	2501	0	2491	115	0
1	D	2501	0	2491	110	0
2	E	9671	0	9660	277	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	9671	0	9660	283	0
2	G	9671	0	9660	297	0
2	H	9671	0	9660	293	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
3	C	31	0	12	1	0
3	D	31	0	12	1	0
3	E	31	0	12	3	0
3	F	31	0	12	3	0
3	G	31	0	12	3	0
3	H	31	0	12	3	0
4	A	3	0	0	0	0
5	E	27	0	12	0	0
5	F	27	0	12	0	0
5	G	27	0	12	0	0
5	H	27	0	12	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
6	G	2	0	0	0	0
6	H	2	0	0	0	0
All	All	49055	0	48748	1483	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 15.

All (1483) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:888:HIS:ND1	2:G:1512:ASP:OD1	1.66	1.28
2:F:888:HIS:ND1	2:F:1512:ASP:OD1	1.66	1.25
2:H:888:HIS:ND1	2:H:1512:ASP:OD1	1.66	1.24
2:E:888:HIS:ND1	2:E:1512:ASP:OD1	1.66	1.24
1:C:276:HIS:CD2	2:G:1355:SER:HB2	1.89	1.06
1:C:276:HIS:HD2	2:G:1355:SER:HB2	1.20	0.98
1:D:101:ALA:HB2	2:H:16:ARG:HB2	1.51	0.92
2:G:888:HIS:CE1	2:G:1512:ASP:OD1	2.23	0.92
2:F:888:HIS:CE1	2:F:1512:ASP:OD1	2.23	0.91
2:H:888:HIS:CE1	2:H:1512:ASP:OD1	2.23	0.91
2:E:888:HIS:CE1	2:E:1512:ASP:OD1	2.23	0.91
1:D:278:HIS:CG	2:H:1356:SER:OG	2.24	0.91
1:A:81:CYS:HB2	2:E:41:PHE:HB3	1.54	0.89

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:309:ALA:O	2:H:369:GLN:NE2	2.08	0.87
1:C:273:SER:OG	2:G:1398:PHE:CD2	2.27	0.87
2:F:309:ALA:O	2:F:369:GLN:NE2	2.08	0.87
1:C:81:CYS:HB2	2:G:41:PHE:HB3	1.56	0.86
1:A:67:LYS:HG2	1:A:69:PRO:HD2	1.58	0.86
1:B:67:LYS:HG2	1:B:69:PRO:HD2	1.58	0.86
2:E:309:ALA:O	2:E:369:GLN:NE2	2.08	0.86
2:G:309:ALA:O	2:G:369:GLN:NE2	2.08	0.86
1:C:67:LYS:HG2	1:C:69:PRO:HD2	1.58	0.85
1:B:101:ALA:HB2	2:F:16:ARG:HB2	1.58	0.85
2:F:723:LEU:HB3	2:F:851:PHE:HZ	1.41	0.85
1:D:67:LYS:HG2	1:D:69:PRO:HD2	1.58	0.84
1:D:278:HIS:CD2	2:H:1356:SER:OG	2.30	0.84
2:H:496:LEU:HD13	2:H:500:ASN:HD21	1.43	0.84
2:H:723:LEU:HB3	2:H:851:PHE:HZ	1.41	0.83
2:E:723:LEU:HB3	2:E:851:PHE:HZ	1.41	0.83
2:F:496:LEU:HD13	2:F:500:ASN:HD21	1.43	0.82
2:E:496:LEU:HD13	2:E:500:ASN:HD21	1.43	0.82
2:G:723:LEU:HB3	2:G:851:PHE:HZ	1.41	0.82
2:G:496:LEU:HD13	2:G:500:ASN:HD21	1.43	0.82
2:G:1510:SER:C	2:G:1511:ILE:HD13	2.03	0.80
1:D:81:CYS:HB2	2:H:41:PHE:HB3	1.62	0.80
2:H:424:ASP:OD1	2:H:606:SER:OG	2.01	0.79
2:E:1510:SER:C	2:E:1511:ILE:HD13	2.03	0.79
2:F:1510:SER:C	2:F:1511:ILE:HD13	2.03	0.79
2:H:1510:SER:C	2:H:1511:ILE:HD13	2.03	0.78
2:E:424:ASP:OD1	2:E:606:SER:OG	2.01	0.78
2:F:1459:LEU:HD21	2:F:1488:LEU:HB3	1.66	0.78
2:H:1025:VAL:HG11	2:H:1073:LEU:HD22	1.66	0.78
2:H:1508:THR:HA	2:H:1511:ILE:HG12	1.65	0.78
2:H:1459:LEU:HD21	2:H:1488:LEU:HB3	1.66	0.78
2:E:1459:LEU:HD21	2:E:1488:LEU:HB3	1.66	0.78
2:E:1025:VAL:HG11	2:E:1073:LEU:HD22	1.66	0.77
2:F:424:ASP:OD1	2:F:606:SER:OG	2.01	0.77
2:G:1459:LEU:HD21	2:G:1488:LEU:HB3	1.66	0.77
2:G:424:ASP:OD1	2:G:606:SER:OG	2.01	0.77
2:F:547:ASN:HD22	2:F:594:SER:HB2	1.50	0.77
2:G:1508:THR:HA	2:G:1511:ILE:HG12	1.66	0.77
2:G:97:GLY:HA2	2:G:1268:SER:HB2	1.67	0.77
1:B:278:HIS:CG	2:F:1356:SER:OG	2.38	0.77
2:H:97:GLY:HA2	2:H:1268:SER:HB2	1.67	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1508:THR:HA	2:F:1511:ILE:HG12	1.65	0.76
2:F:97:GLY:HA2	2:F:1268:SER:HB2	1.67	0.76
1:C:101:ALA:HB2	2:G:16:ARG:HB2	1.67	0.76
2:H:547:ASN:HD22	2:H:594:SER:HB2	1.50	0.76
2:F:1025:VAL:HG11	2:F:1073:LEU:HD22	1.66	0.76
1:B:81:CYS:HB2	2:F:41:PHE:HB3	1.68	0.76
2:E:1508:THR:HA	2:E:1511:ILE:HG12	1.66	0.76
2:G:1025:VAL:HG11	2:G:1073:LEU:HD22	1.65	0.76
2:E:97:GLY:HA2	2:E:1268:SER:HB2	1.67	0.76
2:G:547:ASN:HD22	2:G:594:SER:HB2	1.50	0.76
2:E:1170:LEU:HD21	2:E:1254:ILE:HG23	1.68	0.75
2:H:1216:PHE:HB3	2:H:1218:TYR:HD2	1.51	0.75
2:E:1429:VAL:O	2:E:1493:ARG:NH1	2.18	0.75
2:E:1445:CYS:HG	2:E:1449:THR:HG1	1.30	0.75
2:F:1170:LEU:HD21	2:F:1254:ILE:HG23	1.68	0.74
2:G:598:ARG:NH1	2:G:1137:SER:OG	2.20	0.74
2:E:547:ASN:HD22	2:E:594:SER:HB2	1.50	0.74
2:H:1429:VAL:O	2:H:1493:ARG:NH1	2.17	0.74
2:H:1170:LEU:HD21	2:H:1254:ILE:HG23	1.68	0.74
1:A:136:ARG:NH2	1:B:138:VAL:O	2.18	0.74
2:E:1216:PHE:HB3	2:E:1218:TYR:HD2	1.51	0.74
2:F:29:ASP:OD2	2:F:105:HIS:ND1	2.17	0.74
2:G:1216:PHE:HB3	2:G:1218:TYR:HD2	1.51	0.74
2:F:556:LEU:HD11	2:F:1068:THR:HG22	1.69	0.74
2:H:598:ARG:NH1	2:H:1137:SER:OG	2.20	0.74
2:E:598:ARG:NH1	2:E:1137:SER:OG	2.20	0.74
2:G:1170:LEU:HD21	2:G:1254:ILE:HG23	1.68	0.74
2:G:1429:VAL:O	2:G:1493:ARG:NH1	2.17	0.74
2:F:598:ARG:NH1	2:F:1137:SER:OG	2.20	0.73
2:G:6:CYS:HA	2:G:103:HIS:HB2	1.70	0.73
2:F:1216:PHE:HB3	2:F:1218:TYR:HD2	1.51	0.73
2:G:556:LEU:HD11	2:G:1068:THR:HG22	1.69	0.73
2:H:6:CYS:HA	2:H:103:HIS:HB2	1.70	0.73
2:F:1501:ILE:HG22	2:F:1531:THR:HB	1.70	0.73
2:G:711:ILE:HB	2:G:886:VAL:HG12	1.71	0.73
2:E:6:CYS:HA	2:E:103:HIS:HB2	1.70	0.73
2:H:1501:ILE:HG22	2:H:1531:THR:HB	1.70	0.73
2:H:711:ILE:HB	2:H:886:VAL:HG12	1.71	0.73
2:E:1511:ILE:HD13	2:E:1511:ILE:N	2.04	0.72
2:E:437:ASN:HD22	2:E:592:LEU:HD23	1.54	0.72
2:F:437:ASN:HD22	2:F:592:LEU:HD23	1.54	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:556:LEU:HD11	2:E:1068:THR:HG22	1.69	0.72
2:F:6:CYS:HA	2:F:103:HIS:HB2	1.70	0.72
2:H:437:ASN:HD22	2:H:592:LEU:HD23	1.55	0.72
1:B:34:ARG:HH12	1:B:38:LYS:HG2	1.54	0.72
2:G:29:ASP:OD2	2:G:105:HIS:ND1	2.17	0.72
1:D:92:LEU:HD22	2:H:34:VAL:HG21	1.72	0.72
1:C:34:ARG:HH12	1:C:38:LYS:HG2	1.54	0.72
2:E:1501:ILE:HG22	2:E:1531:THR:HB	1.70	0.72
2:E:711:ILE:HB	2:E:886:VAL:HG12	1.71	0.72
2:H:556:LEU:HD11	2:H:1068:THR:HG22	1.69	0.72
2:F:711:ILE:HB	2:F:886:VAL:HG12	1.71	0.71
2:H:1511:ILE:HD13	2:H:1511:ILE:N	2.04	0.71
1:C:136:ARG:NH2	1:D:138:VAL:O	2.21	0.71
2:F:714:GLN:C	2:F:1512:ASP:OD2	2.29	0.71
2:G:714:GLN:C	2:G:1512:ASP:OD2	2.29	0.71
2:G:1501:ILE:HG22	2:G:1531:THR:HB	1.70	0.71
2:G:437:ASN:HD22	2:G:592:LEU:HD23	1.54	0.71
2:H:714:GLN:C	2:H:1512:ASP:OD2	2.29	0.71
2:E:714:GLN:C	2:E:1512:ASP:OD2	2.29	0.71
2:E:29:ASP:OD2	2:E:105:HIS:ND1	2.17	0.71
2:F:1511:ILE:HD13	2:F:1511:ILE:N	2.04	0.71
1:C:278:HIS:CG	2:G:1356:SER:OG	2.44	0.71
2:G:1511:ILE:HD13	2:G:1511:ILE:N	2.04	0.71
1:B:278:HIS:CD2	2:F:1356:SER:OG	2.43	0.71
2:G:739:TRP:HE3	2:G:766:ARG:HA	1.55	0.71
2:G:587:VAL:HA	2:G:590:LEU:HD12	1.72	0.70
2:H:29:ASP:OD2	2:H:105:HIS:ND1	2.17	0.70
2:F:1429:VAL:O	2:F:1493:ARG:NH1	2.17	0.70
2:H:1029:ILE:HD12	2:H:1070:LEU:HB3	1.74	0.70
2:E:739:TRP:HE3	2:E:766:ARG:HA	1.55	0.70
2:G:1029:ILE:HD12	2:G:1070:LEU:HB3	1.74	0.70
2:E:1029:ILE:HD12	2:E:1070:LEU:HB3	1.74	0.70
2:F:739:TRP:HE3	2:F:766:ARG:HA	1.55	0.70
2:F:587:VAL:HA	2:F:590:LEU:HD12	1.72	0.70
1:A:34:ARG:HH12	1:A:38:LYS:HG2	1.54	0.70
2:E:587:VAL:HA	2:E:590:LEU:HD12	1.72	0.70
2:H:739:TRP:HE3	2:H:766:ARG:HA	1.56	0.69
1:B:66:LEU:O	1:B:170:LYS:NZ	2.26	0.69
1:D:66:LEU:O	1:D:170:LYS:NZ	2.26	0.69
1:D:34:ARG:HH12	1:D:38:LYS:HG2	1.54	0.69
1:A:66:LEU:O	1:A:170:LYS:NZ	2.26	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:865:ASP:OD1	2:E:892:TYR:OH	2.11	0.69
2:F:1029:ILE:HD12	2:F:1070:LEU:HB3	1.74	0.69
2:F:118:VAL:HG11	2:F:1172:ILE:HG21	1.75	0.69
2:H:118:VAL:HG11	2:H:1172:ILE:HG21	1.75	0.69
2:H:587:VAL:HA	2:H:590:LEU:HD12	1.72	0.69
1:B:192:ARG:NH2	1:B:199:MET:SD	2.66	0.69
1:D:192:ARG:NH2	1:D:199:MET:SD	2.66	0.69
2:G:118:VAL:HG11	2:G:1172:ILE:HG21	1.75	0.69
2:G:865:ASP:OD1	2:G:892:TYR:OH	2.11	0.68
1:B:113:SER:OG	1:B:135:GLY:O	2.12	0.68
1:C:66:LEU:O	1:C:170:LYS:NZ	2.26	0.68
1:C:177:ARG:HH12	1:C:206:ARG:HB2	1.59	0.68
1:A:192:ARG:NH2	1:A:199:MET:SD	2.66	0.68
1:C:192:ARG:NH2	1:C:199:MET:SD	2.66	0.68
1:C:273:SER:OG	2:G:1398:PHE:HD2	1.75	0.68
2:E:118:VAL:HG11	2:E:1172:ILE:HG21	1.75	0.68
1:B:177:ARG:HH12	1:B:206:ARG:HB2	1.58	0.68
2:F:865:ASP:OD1	2:F:892:TYR:OH	2.11	0.68
2:H:1479:GLU:HA	2:H:1486:ARG:HH11	1.59	0.68
1:A:113:SER:OG	1:A:135:GLY:O	2.12	0.68
2:F:1479:GLU:HA	2:F:1486:ARG:HH11	1.59	0.68
1:C:278:HIS:CD2	2:G:1356:SER:OG	2.47	0.68
1:C:113:SER:OG	1:C:135:GLY:O	2.12	0.68
2:F:547:ASN:OD1	2:F:590:LEU:HB3	1.94	0.68
1:D:276:HIS:HD2	2:H:1355:SER:HB2	1.59	0.67
2:H:1259:VAL:HA	2:H:1287:ALA:HB1	1.76	0.67
2:H:322:GLY:O	2:H:326:HIS:ND1	2.22	0.67
2:E:1259:VAL:HA	2:E:1287:ALA:HB1	1.76	0.67
2:G:547:ASN:OD1	2:G:590:LEU:HB3	1.94	0.67
2:E:547:ASN:OD1	2:E:590:LEU:HB3	1.94	0.67
1:D:177:ARG:HH12	1:D:206:ARG:HB2	1.59	0.67
2:F:322:GLY:O	2:F:326:HIS:ND1	2.22	0.67
2:H:865:ASP:OD1	2:H:892:TYR:OH	2.11	0.67
2:F:1259:VAL:HA	2:F:1287:ALA:HB1	1.76	0.66
2:G:1259:VAL:HA	2:G:1287:ALA:HB1	1.76	0.66
2:E:1479:GLU:HA	2:E:1486:ARG:HH11	1.59	0.66
2:H:547:ASN:OD1	2:H:590:LEU:HB3	1.94	0.66
1:A:177:ARG:HH12	1:A:206:ARG:HB2	1.59	0.66
1:C:220:VAL:HG22	1:C:235:GLN:HG2	1.77	0.66
2:E:370:ARG:HD3	2:E:373:LEU:HD12	1.77	0.66
2:G:1479:GLU:HA	2:G:1486:ARG:HH11	1.59	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:HIS:CD2	2:H:1355:SER:HB2	2.30	0.66
1:B:272:PRO:HG3	1:B:311:TRP:CE2	2.31	0.66
1:A:272:PRO:HG3	1:A:311:TRP:CE2	2.31	0.66
2:F:370:ARG:HD3	2:F:373:LEU:HD12	1.77	0.66
2:H:889:LYS:HB3	2:H:1538:ARG:HH22	1.61	0.66
1:B:220:VAL:HG22	1:B:235:GLN:HG2	1.77	0.66
1:C:239:PRO:O	1:C:259:HIS:ND1	2.25	0.66
1:D:278:HIS:CD2	2:H:1356:SER:HG	2.12	0.66
1:A:220:VAL:HG22	1:A:235:GLN:HG2	1.77	0.66
2:G:889:LYS:HB3	2:G:1538:ARG:HH22	1.61	0.66
2:E:322:GLY:O	2:E:326:HIS:ND1	2.22	0.65
1:C:272:PRO:HG3	1:C:311:TRP:CE2	2.31	0.65
1:D:272:PRO:HG3	1:D:311:TRP:CE2	2.31	0.65
1:C:273:SER:HG	2:G:1398:PHE:HD2	1.39	0.65
1:D:113:SER:OG	1:D:135:GLY:O	2.12	0.65
2:E:889:LYS:HB3	2:E:1538:ARG:HH22	1.61	0.65
2:F:889:LYS:HB3	2:F:1538:ARG:HH22	1.61	0.65
1:D:220:VAL:HG22	1:D:235:GLN:HG2	1.77	0.65
2:G:370:ARG:HD3	2:G:373:LEU:HD12	1.77	0.65
2:F:1127:ASP:HB3	2:F:1314:ILE:HD11	1.79	0.65
2:G:1127:ASP:HB3	2:G:1314:ILE:HD11	1.79	0.65
2:H:370:ARG:HD3	2:H:373:LEU:HD12	1.77	0.65
1:A:167:ILE:HG21	1:B:161:ALA:HB1	1.78	0.65
1:B:239:PRO:O	1:B:259:HIS:ND1	2.25	0.65
2:G:322:GLY:O	2:G:326:HIS:ND1	2.22	0.65
2:E:1424:ILE:HD12	2:E:1504:MET:HG2	1.79	0.65
1:C:278:HIS:ND1	2:G:1355:SER:OG	2.27	0.64
2:E:1127:ASP:HB3	2:E:1314:ILE:HD11	1.79	0.64
2:G:1011:LEU:HD21	2:G:1087:TRP:CE3	2.33	0.64
2:G:314:PHE:CZ	2:G:448:GLY:HA2	2.33	0.64
2:H:1011:LEU:HD21	2:H:1087:TRP:CE3	2.33	0.64
2:H:314:PHE:CZ	2:H:448:GLY:HA2	2.33	0.64
2:F:1011:LEU:HD21	2:F:1087:TRP:CE3	2.33	0.64
2:E:1011:LEU:HD21	2:E:1087:TRP:CE3	2.33	0.64
2:E:69:PRO:HD2	2:E:189:VAL:HG12	1.80	0.64
2:H:69:PRO:HD2	2:H:189:VAL:HG12	1.80	0.64
2:E:314:PHE:CZ	2:E:448:GLY:HA2	2.33	0.63
2:H:1127:ASP:HB3	2:H:1314:ILE:HD11	1.79	0.63
2:F:314:PHE:CZ	2:F:448:GLY:HA2	2.33	0.63
2:F:1424:ILE:HD12	2:F:1504:MET:HG2	1.79	0.63
1:B:92:LEU:HD22	2:F:34:VAL:HG21	1.80	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1424:ILE:HD12	2:G:1504:MET:HG2	1.79	0.63
1:C:273:SER:HB2	2:G:1399:GLU:OE2	1.99	0.63
2:F:510:LYS:NZ	2:F:1325:TYR:OH	2.31	0.63
2:H:510:LYS:NZ	2:H:1325:TYR:OH	2.31	0.63
2:G:510:LYS:NZ	2:G:1325:TYR:OH	2.31	0.63
2:G:1409:ILE:HG13	2:G:1417:LEU:HD11	1.81	0.62
2:H:1424:ILE:HD12	2:H:1504:MET:HG2	1.79	0.62
2:F:295:PHE:CZ	2:F:383:THR:HB	2.34	0.62
2:G:69:PRO:HD2	2:G:189:VAL:HG12	1.80	0.62
2:E:510:LYS:NZ	2:E:1325:TYR:OH	2.31	0.62
1:A:101:ALA:HB2	2:E:16:ARG:HB2	1.81	0.62
2:E:723:LEU:HB3	2:E:851:PHE:CZ	2.31	0.62
2:G:1424:ILE:HD13	2:G:1491:LEU:HG	1.82	0.62
2:G:295:PHE:CZ	2:G:383:THR:HB	2.34	0.62
2:G:420:LEU:O	2:G:424:ASP:HB3	2.00	0.62
2:H:380:ALA:O	2:H:383:THR:OG1	2.18	0.62
1:B:95:PHE:HD1	1:B:100:LEU:HD12	1.65	0.62
2:F:69:PRO:HD2	2:F:189:VAL:HG12	1.80	0.62
1:D:313:GLN:HG2	1:D:338:LYS:HA	1.82	0.62
2:H:829:LEU:HD13	2:H:833:GLN:HB2	1.82	0.62
2:E:420:LEU:O	2:E:424:ASP:HB3	2.00	0.62
2:H:1424:ILE:HD13	2:H:1491:LEU:HG	1.82	0.61
1:A:313:GLN:HG2	1:A:338:LYS:HA	1.82	0.61
1:C:167:ILE:HG21	1:D:161:ALA:HB1	1.81	0.61
2:E:36:HIS:CE1	2:E:113:ALA:HB2	2.35	0.61
2:G:36:HIS:CE1	2:G:113:ALA:HB2	2.35	0.61
1:A:239:PRO:O	1:A:259:HIS:ND1	2.25	0.61
1:B:313:GLN:HG2	1:B:338:LYS:HA	1.82	0.61
2:E:1409:ILE:HG13	2:E:1417:LEU:HD11	1.81	0.61
2:E:295:PHE:CZ	2:E:383:THR:HB	2.34	0.61
2:F:420:LEU:O	2:F:424:ASP:HB3	2.00	0.61
2:H:295:PHE:CZ	2:H:383:THR:HB	2.34	0.61
2:E:380:ALA:O	2:E:383:THR:OG1	2.18	0.61
2:F:1409:ILE:HG13	2:F:1417:LEU:HD11	1.81	0.61
2:H:1409:ILE:HG13	2:H:1417:LEU:HD11	1.81	0.61
2:F:74:ARG:HH21	2:F:185:VAL:HG12	1.66	0.61
1:C:95:PHE:HD1	1:C:100:LEU:HD12	1.65	0.61
1:C:278:HIS:HB2	2:G:1355:SER:HG	1.66	0.61
2:H:420:LEU:O	2:H:424:ASP:HB3	2.00	0.61
2:H:723:LEU:HB3	2:H:851:PHE:CZ	2.31	0.61
2:E:1560:ASP:OD1	2:E:1561:LYS:N	2.32	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:74:ARG:HH21	2:E:185:VAL:HG12	1.66	0.61
2:E:829:LEU:HD13	2:E:833:GLN:HB2	1.82	0.61
2:F:1482:SER:OG	3:F:2004:ATP:O3A	2.19	0.61
2:G:829:LEU:HD13	2:G:833:GLN:HB2	1.82	0.61
2:E:78:THR:HG21	2:E:121:VAL:HG21	1.82	0.61
2:F:829:LEU:HD13	2:F:833:GLN:HB2	1.82	0.61
1:C:61:THR:HA	1:C:64:VAL:HG12	1.82	0.60
1:D:95:PHE:HD1	1:D:100:LEU:HD12	1.65	0.60
2:F:36:HIS:CE1	2:F:113:ALA:HB2	2.35	0.60
2:F:380:ALA:O	2:F:383:THR:OG1	2.18	0.60
2:G:74:ARG:HH21	2:G:185:VAL:HG12	1.66	0.60
1:C:92:LEU:HD22	2:G:34:VAL:HG21	1.83	0.60
2:H:36:HIS:CE1	2:H:113:ALA:HB2	2.35	0.60
2:E:1482:SER:OG	3:E:2004:ATP:O3A	2.19	0.60
2:G:412:MET:HA	2:G:416:GLN:HE21	1.66	0.60
1:B:61:THR:HA	1:B:64:VAL:HG12	1.82	0.60
2:F:810:ASP:OD2	2:F:836:ARG:NH2	2.35	0.60
2:G:1473:ILE:O	2:G:1480:ASN:ND2	2.34	0.60
1:A:95:PHE:HD1	1:A:100:LEU:HD12	1.65	0.60
1:C:313:GLN:HG2	1:C:338:LYS:HA	1.82	0.60
1:D:239:PRO:O	1:D:259:HIS:ND1	2.25	0.60
2:F:78:THR:HG21	2:F:121:VAL:HG21	1.82	0.60
2:F:1424:ILE:HD13	2:F:1491:LEU:HG	1.82	0.60
2:F:412:MET:HA	2:F:416:GLN:HE21	1.66	0.60
1:A:61:THR:HA	1:A:64:VAL:HG12	1.82	0.60
1:D:314:ARG:HE	1:D:339:VAL:HG21	1.66	0.60
2:E:1424:ILE:HD13	2:E:1491:LEU:HG	1.82	0.60
2:E:8:SER:H	2:E:12:SER:CB	2.14	0.60
2:F:1263:ALA:O	2:F:1267:ILE:HG12	2.02	0.60
2:G:78:THR:HG21	2:G:121:VAL:HG21	1.82	0.60
2:H:1473:ILE:O	2:H:1480:ASN:ND2	2.34	0.60
2:H:412:MET:HA	2:H:416:GLN:HE21	1.66	0.60
2:F:770:ALA:HA	2:F:1216:PHE:HE1	1.67	0.60
2:F:452:LEU:HB3	2:F:461:LEU:HD22	1.84	0.60
2:G:8:SER:H	2:G:12:SER:CB	2.14	0.60
2:H:78:THR:HG21	2:H:121:VAL:HG21	1.82	0.60
2:H:810:ASP:OD2	2:H:836:ARG:NH2	2.35	0.60
1:D:61:THR:HA	1:D:64:VAL:HG12	1.82	0.60
2:F:8:SER:H	2:F:12:SER:CB	2.14	0.60
2:G:1350:SER:HB2	2:G:1399:GLU:HB2	1.84	0.60
2:H:74:ARG:HH21	2:H:185:VAL:HG12	1.66	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:ARG:HE	1:C:339:VAL:HG21	1.66	0.60
2:E:1263:ALA:O	2:E:1267:ILE:HG12	2.02	0.60
2:E:1350:SER:HB2	2:E:1399:GLU:HB2	1.84	0.60
2:G:288:TRP:HE1	2:G:607:VAL:HG21	1.67	0.60
2:G:810:ASP:OD2	2:G:836:ARG:NH2	2.35	0.60
1:B:218:GLN:HE21	1:B:235:GLN:HB3	1.67	0.60
2:F:1473:ILE:O	2:F:1480:ASN:ND2	2.34	0.60
1:C:273:SER:OG	2:G:1398:PHE:CE2	2.51	0.60
2:H:770:ALA:HA	2:H:1216:PHE:HE1	1.67	0.60
1:C:218:GLN:HE21	1:C:235:GLN:HB3	1.67	0.60
3:C:501:ATP:N1	1:D:50:ARG:N	2.47	0.60
2:G:452:LEU:HB3	2:G:461:LEU:HD22	1.84	0.60
1:B:238:ILE:HD11	1:B:259:HIS:CD2	2.37	0.59
2:G:778:LEU:HA	2:G:841:ARG:HH12	1.67	0.59
1:D:238:ILE:HD11	1:D:259:HIS:CD2	2.37	0.59
2:H:1263:ALA:O	2:H:1267:ILE:HG12	2.02	0.59
2:H:1350:SER:HB2	2:H:1399:GLU:HB2	1.84	0.59
2:E:1473:ILE:O	2:E:1480:ASN:ND2	2.34	0.59
2:E:288:TRP:HE1	2:E:607:VAL:HG21	1.67	0.59
2:E:412:MET:HA	2:E:416:GLN:HE21	1.66	0.59
2:E:452:LEU:HB3	2:E:461:LEU:HD22	1.84	0.59
2:F:114:PHE:CE2	2:F:1169:PRO:HB3	2.37	0.59
2:F:778:LEU:HA	2:F:841:ARG:HH12	1.67	0.59
2:H:1027:VAL:HG21	2:H:1151:SER:HB2	1.84	0.59
2:H:288:TRP:HE1	2:H:607:VAL:HG21	1.67	0.59
1:A:95:PHE:HE1	2:E:16:ARG:HG2	1.67	0.59
2:F:1027:VAL:HG21	2:F:1151:SER:HB2	1.84	0.59
2:F:319:CYS:SG	2:F:362:LEU:HB2	2.42	0.59
2:G:1263:ALA:O	2:G:1267:ILE:HG12	2.02	0.59
2:G:1482:SER:OG	3:G:2004:ATP:O3A	2.19	0.59
2:H:452:LEU:HB3	2:H:461:LEU:HD22	1.84	0.59
1:A:218:GLN:HE21	1:A:235:GLN:HB3	1.67	0.59
1:D:218:GLN:HE21	1:D:235:GLN:HB3	1.67	0.59
2:E:1216:PHE:HB3	2:E:1218:TYR:CD2	2.37	0.59
2:E:810:ASP:OD2	2:E:836:ARG:NH2	2.35	0.59
2:G:114:PHE:CE2	2:G:1169:PRO:HB3	2.37	0.59
2:G:319:CYS:SG	2:G:362:LEU:HB2	2.42	0.59
2:H:1216:PHE:HB3	2:H:1218:TYR:CD2	2.37	0.59
2:H:8:SER:H	2:H:12:SER:CB	2.14	0.59
2:G:1560:ASP:OD1	2:G:1561:LYS:N	2.32	0.59
1:A:314:ARG:HE	1:A:339:VAL:HG21	1.66	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:ILE:HD11	1:C:259:HIS:CD2	2.37	0.59
2:E:1027:VAL:HG21	2:E:1151:SER:HB2	1.85	0.59
2:H:114:PHE:CE2	2:H:1169:PRO:HB3	2.38	0.59
1:B:314:ARG:HE	1:B:339:VAL:HG21	1.66	0.59
1:D:217:MET:HG2	1:D:285:VAL:HG22	1.84	0.59
2:E:770:ALA:HA	2:E:1216:PHE:HE1	1.67	0.59
2:F:1350:SER:HB2	2:F:1399:GLU:HB2	1.84	0.59
2:F:496:LEU:HD13	2:F:500:ASN:ND2	2.16	0.59
2:G:1027:VAL:HG21	2:G:1151:SER:HB2	1.84	0.59
2:G:496:LEU:HD13	2:G:500:ASN:ND2	2.16	0.59
1:B:217:MET:HG2	1:B:285:VAL:HG22	1.84	0.59
2:E:320:ILE:HG12	2:E:1284:LEU:HD13	1.85	0.59
2:E:778:LEU:HA	2:E:841:ARG:HH12	1.67	0.59
2:G:320:ILE:HG12	2:G:1284:LEU:HD13	1.85	0.59
2:H:1560:ASP:OD1	2:H:1561:LYS:N	2.33	0.59
1:A:238:ILE:HD11	1:A:259:HIS:CD2	2.37	0.59
2:E:319:CYS:SG	2:E:362:LEU:HB2	2.42	0.59
1:C:217:MET:HG2	1:C:285:VAL:HG22	1.84	0.58
2:F:918:ARG:NH2	2:F:922:GLN:OE1	2.36	0.58
2:F:320:ILE:HG12	2:F:1284:LEU:HD13	1.85	0.58
2:G:770:ALA:HA	2:G:1216:PHE:HE1	1.67	0.58
2:H:319:CYS:SG	2:H:362:LEU:HB2	2.42	0.58
1:B:276:HIS:NE2	1:B:278:HIS:O	2.37	0.58
1:A:50:ARG:N	3:D:501:ATP:N1	2.45	0.58
2:E:114:PHE:CE2	2:E:1169:PRO:HB3	2.37	0.58
2:E:477:VAL:HG11	2:E:543:SER:HB2	1.85	0.58
2:F:288:TRP:HE1	2:F:607:VAL:HG21	1.67	0.58
2:G:380:ALA:O	2:G:383:THR:OG1	2.18	0.58
2:F:477:VAL:HG11	2:F:543:SER:HB2	1.85	0.58
2:H:320:ILE:HG12	2:H:1284:LEU:HD13	1.85	0.58
1:D:273:SER:OG	2:H:1398:PHE:CE2	2.56	0.58
2:H:1482:SER:OG	3:H:2004:ATP:O3A	2.19	0.58
1:A:276:HIS:NE2	1:A:278:HIS:O	2.37	0.58
1:C:276:HIS:NE2	1:C:278:HIS:O	2.37	0.58
2:F:723:LEU:HB3	2:F:851:PHE:CZ	2.31	0.58
2:G:309:ALA:C	2:G:369:GLN:HE22	2.04	0.58
2:G:477:VAL:HG11	2:G:543:SER:HB2	1.85	0.58
1:A:239:PRO:HB3	1:D:244:VAL:HG22	1.86	0.58
2:E:918:ARG:NH2	2:E:922:GLN:OE1	2.36	0.58
2:G:918:ARG:NH2	2:G:922:GLN:OE1	2.36	0.58
2:H:318:LEU:HD21	2:H:451:LEU:HD21	1.86	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:477:VAL:HG11	2:H:543:SER:HB2	1.85	0.58
2:H:555:VAL:HG12	2:H:583:PHE:HD2	1.69	0.58
2:H:778:LEU:HA	2:H:841:ARG:HH12	1.67	0.58
1:A:217:MET:HG2	1:A:285:VAL:HG22	1.85	0.57
1:C:75:PHE:O	1:C:78:SER:OG	2.19	0.57
1:D:276:HIS:NE2	1:D:278:HIS:O	2.37	0.57
2:F:776:PRO:O	2:F:834:ARG:NH2	2.37	0.57
2:G:1436:ARG:NH2	2:G:1471:ASP:OD1	2.37	0.57
2:G:318:LEU:HD21	2:G:451:LEU:HD21	1.86	0.57
2:H:1436:ARG:NH2	2:H:1471:ASP:OD1	2.37	0.57
2:H:455:ILE:HG23	2:H:456:LEU:HG	1.86	0.57
2:F:1351:VAL:HG22	2:F:1361:LEU:HB3	1.87	0.57
2:F:318:LEU:HD21	2:F:451:LEU:HD21	1.87	0.57
2:H:496:LEU:HD13	2:H:500:ASN:ND2	2.16	0.57
2:H:918:ARG:NH2	2:H:922:GLN:OE1	2.36	0.57
2:F:1153:LEU:HD11	2:F:1167:LEU:HG	1.87	0.57
2:H:1153:LEU:HD11	2:H:1167:LEU:HG	1.87	0.57
2:F:309:ALA:C	2:F:369:GLN:HE22	2.04	0.57
2:G:723:LEU:HB3	2:G:851:PHE:CZ	2.31	0.57
2:F:456:LEU:HD22	2:F:575:VAL:HA	1.87	0.57
2:E:1351:VAL:HG22	2:E:1361:LEU:HB3	1.87	0.57
2:E:318:LEU:HD21	2:E:451:LEU:HD21	1.86	0.57
2:E:309:ALA:C	2:E:369:GLN:HE22	2.04	0.57
2:E:776:PRO:O	2:E:834:ARG:NH2	2.37	0.57
2:F:1436:ARG:NH2	2:F:1471:ASP:OD1	2.37	0.57
2:G:1153:LEU:HD11	2:G:1167:LEU:HG	1.87	0.57
1:C:239:PRO:HB3	1:B:244:VAL:HG22	1.85	0.57
2:E:1436:ARG:NH2	2:E:1471:ASP:OD1	2.37	0.57
2:E:455:ILE:HG23	2:E:456:LEU:HG	1.86	0.57
2:G:455:ILE:HG23	2:G:456:LEU:HG	1.86	0.57
2:H:776:PRO:O	2:H:834:ARG:NH2	2.38	0.57
2:G:555:VAL:HG12	2:G:583:PHE:HD2	1.69	0.56
2:E:117:ALA:O	2:E:120:SER:OG	2.17	0.56
2:G:1351:VAL:HG22	2:G:1361:LEU:HB3	1.87	0.56
1:C:122:LEU:HD21	1:D:146:ILE:HG12	1.87	0.56
2:E:1153:LEU:HD11	2:E:1167:LEU:HG	1.87	0.56
2:E:555:VAL:HG12	2:E:583:PHE:HD2	1.69	0.56
2:E:456:LEU:HD22	2:E:575:VAL:HA	1.87	0.56
2:G:776:PRO:O	2:G:834:ARG:NH2	2.37	0.56
2:F:1560:ASP:OD1	2:F:1561:LYS:N	2.33	0.56
2:F:455:ILE:HG23	2:F:456:LEU:HG	1.85	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:496:LEU:HD13	2:E:500:ASN:ND2	2.16	0.56
2:E:711:ILE:HG13	2:E:900:ILE:HB	1.87	0.56
1:B:211:ILE:HB	1:B:290:VAL:HB	1.88	0.56
1:C:211:ILE:HB	1:C:290:VAL:HB	1.87	0.56
2:G:498:GLN:HE22	2:G:521:ARG:NH1	2.04	0.56
2:H:498:GLN:HE22	2:H:521:ARG:NH1	2.04	0.56
2:F:498:GLN:HE22	2:F:521:ARG:NH1	2.04	0.56
2:G:1191:LEU:HA	2:G:1194:THR:HG22	1.88	0.56
2:H:1191:LEU:HA	2:H:1194:THR:HG22	1.88	0.56
2:F:555:VAL:HG12	2:F:583:PHE:HD2	1.69	0.56
2:G:711:ILE:HG13	2:G:900:ILE:HB	1.87	0.55
2:F:1191:LEU:HA	2:F:1194:THR:HG22	1.88	0.55
2:H:1351:VAL:HG22	2:H:1361:LEU:HB3	1.87	0.55
2:E:498:GLN:HE22	2:E:521:ARG:NH1	2.04	0.55
1:A:161:ALA:HB1	1:D:167:ILE:HG21	1.87	0.55
2:E:1191:LEU:HA	2:E:1194:THR:HG22	1.88	0.55
2:H:117:ALA:O	2:H:120:SER:OG	2.17	0.55
2:H:309:ALA:C	2:H:369:GLN:HE22	2.04	0.55
2:H:711:ILE:HG13	2:H:900:ILE:HB	1.87	0.55
2:H:456:LEU:HD22	2:H:575:VAL:HA	1.87	0.55
2:F:14:ALA:HA	2:F:17:VAL:HG13	1.89	0.55
2:F:381:ILE:HG13	2:F:433:PHE:CE1	2.42	0.55
2:F:455:ILE:O	2:F:457:GLY:N	2.40	0.55
2:F:711:ILE:HG13	2:F:900:ILE:HB	1.87	0.55
1:D:269:ASP:OD1	1:D:347:ARG:NE	2.33	0.55
1:A:211:ILE:HB	1:A:290:VAL:HB	1.88	0.55
1:D:75:PHE:O	1:D:78:SER:OG	2.19	0.55
2:E:1506:GLU:H	2:E:1535:ILE:HB	1.72	0.55
2:E:295:PHE:HZ	2:E:383:THR:HB	1.72	0.55
2:G:14:ALA:HA	2:G:17:VAL:HG13	1.89	0.55
1:A:138:VAL:O	1:D:136:ARG:NH2	2.32	0.54
2:E:388:ARG:NH1	2:E:429:MET:SD	2.80	0.54
2:E:455:ILE:O	2:E:457:GLY:N	2.40	0.54
2:G:388:ARG:NH1	2:G:429:MET:SD	2.81	0.54
2:G:455:ILE:O	2:G:457:GLY:N	2.40	0.54
2:H:388:ARG:NH1	2:H:429:MET:SD	2.80	0.54
2:E:14:ALA:HA	2:E:17:VAL:HG13	1.89	0.54
2:F:1506:GLU:H	2:F:1535:ILE:HB	1.72	0.54
2:F:404:THR:OG1	2:F:1214:ARG:NH2	2.41	0.54
2:G:456:LEU:HD22	2:G:575:VAL:HA	1.87	0.54
2:F:388:ARG:NH1	2:F:429:MET:SD	2.80	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:455:ILE:O	2:H:457:GLY:N	2.40	0.54
2:E:708:LEU:O	2:E:897:ASP:N	2.40	0.54
2:G:1506:GLU:H	2:G:1535:ILE:HB	1.72	0.54
2:H:14:ALA:HA	2:H:17:VAL:HG13	1.89	0.54
2:H:1506:GLU:H	2:H:1535:ILE:HB	1.72	0.54
2:E:381:ILE:HG13	2:E:433:PHE:CE1	2.42	0.54
2:G:381:ILE:HG13	2:G:433:PHE:CE1	2.42	0.54
2:H:33:VAL:HG22	2:H:109:PRO:HB3	1.89	0.54
1:C:129:VAL:O	1:C:130:THR:OG1	2.23	0.54
1:D:211:ILE:HB	1:D:290:VAL:HB	1.88	0.54
2:E:102:HIS:HD2	2:E:1273:ARG:HH11	1.56	0.54
2:G:480:LYS:HG3	2:G:539:TYR:CE2	2.43	0.54
2:H:1177:ILE:HD11	2:H:1251:MET:SD	2.48	0.54
2:H:295:PHE:HZ	2:H:383:THR:HB	1.73	0.54
2:F:708:LEU:O	2:F:897:ASP:N	2.41	0.54
2:G:404:THR:OG1	2:G:1214:ARG:NH2	2.41	0.54
2:H:102:HIS:HD2	2:H:1273:ARG:HH11	1.56	0.54
1:A:129:VAL:O	1:A:130:THR:OG1	2.23	0.54
2:F:1216:PHE:HB3	2:F:1218:TYR:CD2	2.37	0.54
2:H:381:ILE:HG13	2:H:433:PHE:CE1	2.42	0.54
2:F:1177:ILE:HD11	2:F:1251:MET:SD	2.48	0.54
2:G:1177:ILE:HD11	2:G:1251:MET:SD	2.48	0.54
2:G:6:CYS:H	2:G:16:ARG:NH1	2.06	0.54
2:G:708:LEU:O	2:G:897:ASP:N	2.41	0.54
2:E:1177:ILE:HD11	2:E:1251:MET:SD	2.48	0.53
2:E:33:VAL:HG22	2:E:109:PRO:HB3	1.89	0.53
2:H:404:THR:OG1	2:H:1214:ARG:NH2	2.40	0.53
2:G:495:ARG:NH1	2:G:1124:PHE:O	2.38	0.53
2:G:102:HIS:HD2	2:G:1273:ARG:HH11	1.56	0.53
2:G:727:LEU:HD21	2:G:1215:ALA:HB2	1.90	0.53
2:E:1066:VAL:HA	2:E:1069:VAL:HG12	1.90	0.53
2:E:404:THR:OG1	2:E:1214:ARG:NH2	2.41	0.53
2:E:575:VAL:HG23	2:E:576:ALA:H	1.74	0.53
2:E:6:CYS:H	2:E:16:ARG:NH1	2.06	0.53
2:F:1066:VAL:HA	2:F:1069:VAL:HG12	1.90	0.53
2:G:33:VAL:HG22	2:G:109:PRO:HB3	1.89	0.53
1:D:95:PHE:CD2	2:H:27:PHE:HD1	2.26	0.53
2:H:480:LYS:HG3	2:H:539:TYR:CE2	2.43	0.53
1:C:269:ASP:OD1	1:C:347:ARG:NE	2.33	0.53
2:F:33:VAL:HG22	2:F:109:PRO:HB3	1.89	0.53
2:H:6:CYS:H	2:H:16:ARG:NH1	2.06	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:802:ILE:HG23	2:H:807:LEU:HB3	1.91	0.53
2:G:1216:PHE:HB3	2:G:1218:TYR:CD2	2.37	0.53
1:C:95:PHE:HE2	2:G:27:PHE:HB2	1.72	0.53
2:E:727:LEU:HD21	2:E:1215:ALA:HB2	1.90	0.53
2:G:74:ARG:HH22	2:G:189:VAL:HG21	1.74	0.53
2:E:495:ARG:NH1	2:E:1124:PHE:O	2.38	0.53
2:E:74:ARG:HH22	2:E:189:VAL:HG21	1.74	0.53
1:A:34:ARG:NH1	1:A:38:LYS:HG2	2.24	0.53
1:C:34:ARG:NH1	1:C:38:LYS:HG2	2.24	0.53
2:F:295:PHE:HZ	2:F:383:THR:HB	1.73	0.53
1:A:95:PHE:HE2	2:E:27:PHE:HB2	1.73	0.53
1:C:161:ALA:HB1	1:B:167:ILE:HG21	1.90	0.53
2:F:1032:TRP:HZ2	2:F:1063:TYR:HD1	1.57	0.53
2:G:1032:TRP:HZ2	2:G:1063:TYR:HD1	1.57	0.53
2:G:1353:TYR:OH	2:G:1386:SER:OG	2.21	0.53
1:A:122:LEU:HD21	1:B:146:ILE:HG12	1.90	0.52
2:E:480:LYS:HG3	2:E:539:TYR:CE2	2.43	0.52
2:F:102:HIS:HD2	2:F:1273:ARG:HH11	1.56	0.52
2:F:74:ARG:HH22	2:F:189:VAL:HG21	1.74	0.52
2:F:480:LYS:HG3	2:F:539:TYR:CE2	2.43	0.52
2:F:727:LEU:HD21	2:F:1215:ALA:HB2	1.90	0.52
2:H:727:LEU:HD21	2:H:1215:ALA:HB2	1.90	0.52
1:A:34:ARG:NH2	1:A:303:SER:OG	2.35	0.52
1:C:327:SER:HA	1:D:45:ALA:HB3	1.90	0.52
1:D:32:ARG:CZ	1:D:278:HIS:HA	2.39	0.52
2:E:802:ILE:HG23	2:E:807:LEU:HB3	1.91	0.52
2:F:1129:ASN:OD1	2:F:1133:GLN:NE2	2.43	0.52
2:F:6:CYS:H	2:F:16:ARG:NH1	2.06	0.52
2:H:575:VAL:HG23	2:H:576:ALA:H	1.74	0.52
1:C:276:HIS:HD2	2:G:1355:SER:CB	2.06	0.52
1:D:273:SER:OG	2:H:1398:PHE:CD2	2.59	0.52
2:H:74:ARG:HH22	2:H:189:VAL:HG21	1.74	0.52
1:C:45:ALA:HB3	1:B:327:SER:HA	1.92	0.52
1:C:138:VAL:O	1:B:136:ARG:NH2	2.34	0.52
2:F:575:VAL:HG23	2:F:576:ALA:H	1.74	0.52
2:G:1066:VAL:HA	2:G:1069:VAL:HG12	1.90	0.52
2:G:802:ILE:HG23	2:G:807:LEU:HB3	1.91	0.52
1:A:187:ALA:O	1:A:310:LEU:N	2.43	0.52
1:A:32:ARG:CZ	1:A:278:HIS:HA	2.40	0.52
1:C:50:ARG:N	3:B:501:ATP:N1	2.51	0.52
2:H:1066:VAL:HA	2:H:1069:VAL:HG12	1.90	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1129:ASN:OD1	2:H:1133:GLN:NE2	2.43	0.52
2:H:593:LEU:HA	2:H:596:VAL:HB	1.92	0.52
1:A:75:PHE:O	1:A:78:SER:OG	2.19	0.52
2:G:1129:ASN:OD1	2:G:1133:GLN:NE2	2.43	0.52
2:H:1032:TRP:HZ3	2:H:1067:PHE:HB2	1.74	0.52
2:H:708:LEU:O	2:H:897:ASP:N	2.40	0.52
1:D:129:VAL:O	1:D:130:THR:OG1	2.23	0.52
1:D:187:ALA:O	1:D:310:LEU:N	2.43	0.52
2:F:802:ILE:HG23	2:F:807:LEU:HB3	1.91	0.52
2:F:495:ARG:NH1	2:F:1124:PHE:O	2.38	0.52
2:G:295:PHE:HZ	2:G:383:THR:HB	1.73	0.52
2:G:593:LEU:HA	2:G:596:VAL:HB	1.92	0.52
2:E:1129:ASN:OD1	2:E:1133:GLN:NE2	2.43	0.51
2:G:487:SER:HA	2:G:490:GLU:HG2	1.92	0.51
2:G:575:VAL:HG23	2:G:576:ALA:H	1.74	0.51
1:C:32:ARG:CZ	1:C:278:HIS:HA	2.39	0.51
2:F:1353:TYR:OH	2:F:1386:SER:OG	2.22	0.51
2:G:412:MET:HA	2:G:416:GLN:NE2	2.26	0.51
2:G:465:ALA:HA	2:G:468:ILE:HD12	1.93	0.51
1:A:327:SER:HA	1:B:45:ALA:HB3	1.92	0.51
1:B:187:ALA:O	1:B:310:LEU:N	2.43	0.51
2:E:1032:TRP:HZ3	2:E:1067:PHE:HB2	1.75	0.51
2:E:465:ALA:HA	2:E:468:ILE:HD12	1.93	0.51
2:F:487:SER:HA	2:F:490:GLU:HG2	1.92	0.51
2:F:739:TRP:CE3	2:F:766:ARG:HA	2.42	0.51
2:G:1269:ASN:O	2:G:1273:ARG:N	2.29	0.51
2:H:846:HIS:ND1	2:H:846:HIS:O	2.44	0.51
1:C:187:ALA:O	1:C:310:LEU:N	2.43	0.51
2:E:846:HIS:ND1	2:E:846:HIS:O	2.44	0.51
1:A:271:ALA:HB2	1:A:345:THR:HG22	1.93	0.51
1:C:34:ARG:NH2	1:C:303:SER:OG	2.35	0.51
2:E:451:LEU:O	2:E:455:ILE:HG22	2.11	0.51
2:F:1032:TRP:HZ3	2:F:1067:PHE:HB2	1.75	0.51
2:H:1032:TRP:HZ2	2:H:1063:TYR:HD1	1.57	0.51
1:A:177:ARG:HG2	1:A:291:VAL:HG22	1.93	0.51
1:B:32:ARG:CZ	1:B:278:HIS:HA	2.39	0.51
2:E:1032:TRP:HZ2	2:E:1063:TYR:HD1	1.57	0.51
2:E:678:CYS:HB2	2:E:703:ILE:O	2.11	0.51
2:F:593:LEU:HA	2:F:596:VAL:HB	1.92	0.51
2:G:500:ASN:O	2:G:504:ARG:HG2	2.11	0.51
2:H:549:ALA:HB1	2:H:1075:ILE:HG13	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:ARG:NH1	1:D:38:LYS:HG2	2.24	0.51
2:E:487:SER:HA	2:E:490:GLU:HG2	1.92	0.51
2:F:537:ALA:HA	2:F:540:THR:HG22	1.93	0.51
2:G:1011:LEU:HD11	2:G:1091:LYS:HD3	1.93	0.51
2:G:678:CYS:HB2	2:G:703:ILE:O	2.11	0.51
2:H:465:ALA:HA	2:H:468:ILE:HD12	1.93	0.51
2:H:487:SER:HA	2:H:490:GLU:HG2	1.92	0.51
2:E:14:ALA:O	2:E:17:VAL:HG22	2.11	0.51
2:E:412:MET:HA	2:E:416:GLN:NE2	2.26	0.51
2:F:1011:LEU:HD11	2:F:1091:LYS:HD3	1.93	0.51
2:F:871:GLY:O	2:F:875:LEU:HG	2.11	0.51
2:G:451:LEU:O	2:G:455:ILE:HG22	2.11	0.51
2:H:1011:LEU:HD11	2:H:1091:LYS:HD3	1.93	0.51
2:H:1445:CYS:SG	2:H:1449:THR:OG1	2.54	0.51
2:H:14:ALA:O	2:H:17:VAL:HG22	2.11	0.51
2:H:412:MET:HA	2:H:416:GLN:NE2	2.26	0.51
1:B:271:ALA:HB2	1:B:345:THR:HG22	1.93	0.51
2:E:500:ASN:O	2:E:504:ARG:HG2	2.11	0.51
2:G:1032:TRP:HZ3	2:G:1067:PHE:HB2	1.75	0.51
2:G:871:GLY:O	2:G:875:LEU:HG	2.11	0.51
2:H:451:LEU:O	2:H:455:ILE:HG22	2.11	0.51
1:B:177:ARG:HG2	1:B:291:VAL:HG22	1.93	0.51
1:D:314:ARG:NE	1:D:339:VAL:HG21	2.26	0.51
2:E:442:PRO:HA	2:E:445:ILE:HG22	1.93	0.51
2:F:451:LEU:O	2:F:455:ILE:HG22	2.11	0.51
2:G:537:ALA:HA	2:G:540:THR:HG22	1.93	0.51
2:H:678:CYS:HB2	2:H:703:ILE:O	2.11	0.51
2:H:871:GLY:O	2:H:875:LEU:HG	2.11	0.51
1:B:209:MET:O	1:B:292:GLU:HB2	2.11	0.50
1:C:231:VAL:HB	1:C:234:HIS:HB2	1.94	0.50
1:D:177:ARG:HG2	1:D:291:VAL:HG22	1.93	0.50
2:E:1011:LEU:HD11	2:E:1091:LYS:HD3	1.93	0.50
2:E:600:THR:O	2:E:604:LEU:HD23	2.12	0.50
2:E:871:GLY:O	2:E:875:LEU:HG	2.11	0.50
2:F:465:ALA:HA	2:F:468:ILE:HD12	1.93	0.50
2:F:500:ASN:O	2:F:504:ARG:HG2	2.11	0.50
1:C:209:MET:O	1:C:292:GLU:HB2	2.11	0.50
2:E:593:LEU:HA	2:E:596:VAL:HB	1.92	0.50
2:F:1445:CYS:SG	2:F:1449:THR:OG1	2.54	0.50
2:F:678:CYS:HB2	2:F:703:ILE:O	2.11	0.50
2:G:14:ALA:O	2:G:17:VAL:HG22	2.11	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:442:PRO:HA	2:G:445:ILE:HG22	1.94	0.50
2:G:519:ARG:HD2	2:G:1102:ASN:OD1	2.12	0.50
2:H:21:VAL:HG23	2:H:22:LEU:HD12	1.93	0.50
1:B:231:VAL:HB	1:B:234:HIS:HB2	1.94	0.50
1:D:271:ALA:HB2	1:D:345:THR:HG22	1.93	0.50
2:F:442:PRO:HA	2:F:445:ILE:HG22	1.94	0.50
2:F:497:LYS:HA	2:F:500:ASN:HD22	1.76	0.50
2:G:846:HIS:O	2:G:846:HIS:ND1	2.44	0.50
2:H:547:ASN:ND2	2:H:590:LEU:O	2.29	0.50
2:H:600:THR:O	2:H:604:LEU:HD23	2.12	0.50
1:A:209:MET:O	1:A:292:GLU:HB2	2.11	0.50
1:A:314:ARG:NE	1:A:339:VAL:HG21	2.26	0.50
1:C:322:GLU:O	1:C:324:GLY:N	2.44	0.50
2:E:1131:ILE:HA	2:E:1135:ILE:HD12	1.93	0.50
2:F:1202:HIS:HD2	2:F:1226:LEU:HD12	1.77	0.50
2:F:1422:SER:HB2	2:F:1502:PHE:CB	2.42	0.50
2:F:600:THR:O	2:F:604:LEU:HD23	2.12	0.50
2:G:600:THR:O	2:G:604:LEU:HD23	2.12	0.50
2:H:1375:GLY:N	2:H:1547:LEU:O	2.45	0.50
2:E:549:ALA:HB1	2:E:1075:ILE:HG13	1.93	0.50
2:E:739:TRP:CE3	2:E:766:ARG:HA	2.42	0.50
2:F:412:MET:HA	2:F:416:GLN:NE2	2.26	0.50
2:F:846:HIS:O	2:F:846:HIS:ND1	2.44	0.50
2:G:497:LYS:HA	2:G:500:ASN:HD22	1.76	0.50
1:C:177:ARG:HG2	1:C:291:VAL:HG22	1.93	0.50
1:D:209:MET:O	1:D:292:GLU:HB2	2.11	0.50
1:D:335:ASN:HD22	1:D:336:THR:N	2.10	0.50
2:F:6:CYS:HB3	2:F:105:HIS:CD2	2.47	0.50
2:F:1482:SER:HG	3:F:2004:ATP:PB	2.34	0.50
2:H:442:PRO:HA	2:H:445:ILE:HG22	1.94	0.50
2:H:500:ASN:O	2:H:504:ARG:HG2	2.11	0.50
2:H:537:ALA:HA	2:H:540:THR:HG22	1.93	0.50
2:H:739:TRP:CE3	2:H:766:ARG:HA	2.43	0.50
1:B:335:ASN:HD22	1:B:336:THR:N	2.10	0.50
1:C:314:ARG:NE	1:C:339:VAL:HG21	2.26	0.50
1:D:95:PHE:HE2	2:H:27:PHE:HB2	1.76	0.50
2:E:1026:LEU:O	2:E:1029:ILE:HG22	2.12	0.50
2:E:1422:SER:HB2	2:E:1502:PHE:CB	2.42	0.50
2:F:549:ALA:HB1	2:F:1075:ILE:HG13	1.93	0.50
2:G:1422:SER:HB2	2:G:1502:PHE:CB	2.42	0.50
2:H:780:ASN:HA	2:H:823:GLY:HA3	1.94	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:VAL:HB	2:G:49:ILE:HD12	1.93	0.50
1:D:113:SER:HA	1:D:115:HIS:CE1	2.47	0.50
2:G:549:ALA:HB1	2:G:1075:ILE:HG13	1.93	0.50
2:G:1375:GLY:N	2:G:1547:LEU:O	2.45	0.50
2:H:495:ARG:NH1	2:H:1124:PHE:O	2.38	0.50
2:H:1202:HIS:HD2	2:H:1226:LEU:HD12	1.77	0.50
1:C:225:SER:OG	1:C:229:GLU:N	2.45	0.50
2:E:781:ALA:HA	2:E:821:GLN:HE22	1.77	0.50
2:G:117:ALA:O	2:G:120:SER:OG	2.17	0.50
2:H:1131:ILE:HA	2:H:1135:ILE:HD12	1.93	0.50
2:H:1392:PHE:HD1	2:H:1418:ARG:HG2	1.77	0.50
1:A:101:ALA:HB1	2:E:13:ALA:O	2.12	0.49
1:A:231:VAL:HB	1:A:234:HIS:HB2	1.94	0.49
1:C:335:ASN:HD22	1:C:336:THR:N	2.10	0.49
2:E:1202:HIS:HD2	2:E:1226:LEU:HD12	1.77	0.49
2:E:537:ALA:HA	2:E:540:THR:HG22	1.93	0.49
2:F:1026:LEU:O	2:F:1029:ILE:HG22	2.12	0.49
2:F:14:ALA:O	2:F:17:VAL:HG22	2.11	0.49
2:F:519:ARG:HD2	2:F:1102:ASN:OD1	2.12	0.49
2:H:519:ARG:HD2	2:H:1102:ASN:OD1	2.12	0.49
1:C:271:ALA:HB2	1:C:345:THR:HG22	1.93	0.49
1:D:225:SER:OG	1:D:229:GLU:N	2.45	0.49
1:D:322:GLU:O	1:D:324:GLY:N	2.44	0.49
2:E:452:LEU:HD21	2:E:582:LEU:HD22	1.95	0.49
1:A:225:SER:OG	1:A:229:GLU:N	2.45	0.49
2:E:497:LYS:HA	2:E:500:ASN:HD22	1.76	0.49
2:F:1131:ILE:HA	2:F:1135:ILE:HD12	1.93	0.49
2:G:1131:ILE:HA	2:G:1135:ILE:HD12	1.93	0.49
2:G:396:TYR:CD1	2:G:1226:LEU:HD13	2.48	0.49
2:G:781:ALA:HA	2:G:821:GLN:HE22	1.77	0.49
1:A:322:GLU:O	1:A:324:GLY:N	2.45	0.49
1:D:177:ARG:NH1	1:D:206:ARG:HB2	2.26	0.49
2:F:781:ALA:HA	2:F:821:GLN:HE22	1.77	0.49
2:F:780:ASN:HA	2:F:823:GLY:HA3	1.94	0.49
2:H:1026:LEU:O	2:H:1029:ILE:HG22	2.12	0.49
2:H:396:TYR:CD1	2:H:1226:LEU:HD13	2.48	0.49
2:H:781:ALA:HA	2:H:821:GLN:HE22	1.77	0.49
1:B:322:GLU:O	1:B:324:GLY:N	2.45	0.49
1:B:75:PHE:O	1:B:78:SER:OG	2.19	0.49
1:C:113:SER:HA	1:C:115:HIS:CE1	2.47	0.49
1:D:231:VAL:HB	1:D:234:HIS:HB2	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1392:PHE:HD1	2:E:1418:ARG:HG2	1.77	0.49
2:E:21:VAL:HG23	2:E:22:LEU:HD12	1.93	0.49
2:G:1026:LEU:O	2:G:1029:ILE:HG22	2.12	0.49
2:G:1202:HIS:HD2	2:G:1226:LEU:HD12	1.77	0.49
1:B:314:ARG:NE	1:B:339:VAL:HG21	2.26	0.49
1:D:273:SER:HG	2:H:1398:PHE:HD2	1.51	0.49
2:E:519:ARG:HD2	2:E:1102:ASN:OD1	2.12	0.49
2:F:396:TYR:CD1	2:F:1226:LEU:HD13	2.48	0.49
2:F:1375:GLY:N	2:F:1547:LEU:O	2.45	0.49
2:F:21:VAL:HG23	2:F:22:LEU:HD12	1.93	0.49
2:F:452:LEU:HD21	2:F:582:LEU:HD22	1.94	0.49
2:H:452:LEU:HD21	2:H:582:LEU:HD22	1.94	0.49
1:A:113:SER:HA	1:A:115:HIS:CE1	2.47	0.49
1:A:335:ASN:HD22	1:A:336:THR:N	2.10	0.49
1:B:113:SER:HA	1:B:115:HIS:CE1	2.47	0.49
1:B:34:ARG:NH2	1:B:303:SER:OG	2.35	0.49
2:E:780:ASN:HA	2:E:823:GLY:HA3	1.94	0.49
2:G:1392:PHE:HD1	2:G:1418:ARG:HG2	1.77	0.49
2:G:428:LEU:O	2:G:432:PHE:HD2	1.96	0.49
2:G:780:ASN:HA	2:G:823:GLY:HA3	1.94	0.49
2:H:1422:SER:HB2	2:H:1502:PHE:CB	2.42	0.49
1:A:177:ARG:NH1	1:A:206:ARG:HB2	2.26	0.49
1:A:45:ALA:HB3	1:D:327:SER:HA	1.94	0.49
2:E:396:TYR:CD1	2:E:1226:LEU:HD13	2.48	0.49
2:G:6:CYS:HB3	2:G:105:HIS:CD2	2.47	0.49
2:G:21:VAL:HG23	2:G:22:LEU:HD12	1.93	0.49
2:H:428:LEU:O	2:H:432:PHE:HD2	1.96	0.49
1:B:225:SER:OG	1:B:229:GLU:N	2.45	0.49
2:E:6:CYS:HB3	2:E:105:HIS:CD2	2.47	0.49
1:B:278:HIS:CD2	2:F:1356:SER:HG	2.29	0.49
2:F:713:GLY:O	2:F:1512:ASP:OD2	2.31	0.49
2:E:428:LEU:O	2:E:432:PHE:HD2	1.96	0.49
2:F:547:ASN:ND2	2:F:590:LEU:O	2.29	0.49
2:H:6:CYS:HB3	2:H:105:HIS:CD2	2.47	0.49
2:E:1423:ILE:HG13	2:E:1503:ILE:HG23	1.94	0.48
2:G:739:TRP:CE3	2:G:766:ARG:HA	2.43	0.48
2:H:1516:GLU:OE2	2:H:1541:THR:OG1	2.21	0.48
2:E:547:ASN:ND2	2:E:594:SER:HB2	2.26	0.48
2:F:1269:ASN:O	2:F:1273:ARG:N	2.29	0.48
1:A:344:CYS:SG	1:A:349:LEU:HD22	2.53	0.48
2:E:1032:TRP:HH2	2:E:1063:TYR:O	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:547:ASN:ND2	2:F:594:SER:HB2	2.25	0.48
2:H:1153:LEU:HD12	2:H:1156:ILE:HD11	1.96	0.48
1:B:344:CYS:SG	1:B:349:LEU:HD22	2.53	0.48
1:A:95:PHE:CE1	2:E:16:ARG:HG2	2.49	0.48
2:F:1032:TRP:HH2	2:F:1063:TYR:O	1.96	0.48
2:H:1423:ILE:HG13	2:H:1503:ILE:HG23	1.94	0.48
1:C:344:CYS:SG	1:C:349:LEU:HD22	2.53	0.48
2:E:713:GLY:O	2:E:1512:ASP:OD2	2.31	0.48
2:F:1423:ILE:HG13	2:F:1503:ILE:HG23	1.94	0.48
2:F:428:LEU:O	2:F:432:PHE:HD2	1.96	0.48
2:G:452:LEU:HD21	2:G:582:LEU:HD22	1.94	0.48
2:H:1275:LEU:HD12	2:H:1276:SER:N	2.29	0.48
2:H:497:LYS:HA	2:H:500:ASN:HD22	1.76	0.48
1:D:66:LEU:HD23	1:D:67:LYS:N	2.29	0.48
2:E:143:TRP:HB2	2:E:183:LEU:HD23	1.96	0.48
2:H:713:GLY:O	2:H:1512:ASP:OD2	2.31	0.48
1:B:129:VAL:O	1:B:130:THR:OG1	2.23	0.48
1:A:244:VAL:HG22	1:B:239:PRO:HB3	1.95	0.48
1:D:344:CYS:SG	1:D:349:LEU:HD22	2.53	0.48
2:E:453:TYR:O	2:E:458:VAL:HA	2.14	0.48
2:F:1392:PHE:HD1	2:F:1418:ARG:HG2	1.77	0.48
2:G:1032:TRP:HH2	2:G:1063:TYR:O	1.96	0.48
2:H:1375:GLY:O	2:H:1549:ILE:N	2.40	0.48
2:H:143:TRP:HB2	2:H:183:LEU:HD23	1.96	0.48
1:D:34:ARG:NH2	1:D:303:SER:OG	2.35	0.48
2:E:135:LEU:O	2:E:135:LEU:HD13	2.14	0.48
2:F:1275:LEU:HD12	2:F:1276:SER:N	2.29	0.48
2:G:1153:LEU:HD12	2:G:1156:ILE:HD11	1.96	0.48
2:G:453:TYR:O	2:G:458:VAL:HA	2.14	0.48
1:A:307:ASP:OD1	1:A:308:GLU:N	2.47	0.48
1:C:159:ILE:O	1:C:163:MET:HG2	2.14	0.48
2:F:816:HIS:HB2	2:F:820:THR:HA	1.96	0.48
2:G:429:MET:HG2	2:G:433:PHE:CZ	2.49	0.48
2:H:135:LEU:O	2:H:135:LEU:HD13	2.14	0.48
2:H:453:TYR:O	2:H:458:VAL:HA	2.14	0.48
1:C:263:ALA:HA	1:C:268:TYR:CG	2.49	0.48
1:D:263:ALA:HA	1:D:268:TYR:CG	2.49	0.48
1:D:307:ASP:OD1	1:D:308:GLU:N	2.47	0.48
2:G:713:GLY:O	2:G:1512:ASP:OD2	2.31	0.48
2:G:547:ASN:ND2	2:G:590:LEU:O	2.30	0.48
1:B:307:ASP:OD1	1:B:308:GLU:N	2.47	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1139:LEU:O	2:F:1142:LEU:HD23	2.14	0.47
2:F:143:TRP:HB2	2:F:183:LEU:HD23	1.96	0.47
2:F:453:TYR:O	2:F:458:VAL:HA	2.14	0.47
2:G:1275:LEU:HD12	2:G:1276:SER:N	2.29	0.47
2:G:1445:CYS:SG	2:G:1449:THR:OG1	2.54	0.47
2:H:1032:TRP:HH2	2:H:1063:TYR:O	1.96	0.47
2:H:429:MET:HG2	2:H:433:PHE:CZ	2.49	0.47
1:B:94:ALA:HB2	1:B:114:ILE:HD11	1.96	0.47
1:B:330:TYR:O	1:B:333:PHE:HB2	2.14	0.47
2:E:1087:TRP:HA	2:E:1090:LEU:HD12	1.96	0.47
2:G:1154:ALA:O	2:G:1157:SER:OG	2.26	0.47
2:G:135:LEU:O	2:G:135:LEU:HD13	2.14	0.47
2:G:816:HIS:HB2	2:G:820:THR:HA	1.96	0.47
1:B:66:LEU:HD23	1:B:67:LYS:N	2.29	0.47
1:C:57:GLN:O	1:C:60:PHE:HB3	2.15	0.47
1:D:94:ALA:HB2	1:D:114:ILE:HD11	1.96	0.47
2:E:1275:LEU:HD12	2:E:1276:SER:N	2.29	0.47
2:G:1423:ILE:HG13	2:G:1503:ILE:HG23	1.94	0.47
2:G:143:TRP:HB2	2:G:183:LEU:HD23	1.96	0.47
2:H:1032:TRP:CZ3	2:H:1067:PHE:HB2	2.49	0.47
1:A:263:ALA:HA	1:A:268:TYR:CG	2.49	0.47
3:A:501:ATP:N1	1:B:50:ARG:N	2.57	0.47
1:A:76:THR:HG22	1:B:154:ILE:HG21	1.97	0.47
1:B:159:ILE:O	1:B:163:MET:HG2	2.14	0.47
1:B:57:GLN:O	1:B:60:PHE:HB3	2.14	0.47
1:C:330:TYR:O	1:C:333:PHE:HB2	2.14	0.47
2:E:429:MET:HG2	2:E:433:PHE:CZ	2.49	0.47
2:F:1153:LEU:HD12	2:F:1156:ILE:HD11	1.96	0.47
2:G:1032:TRP:CZ3	2:G:1067:PHE:HB2	2.49	0.47
2:H:816:HIS:HB2	2:H:820:THR:HA	1.96	0.47
1:A:330:TYR:O	1:A:333:PHE:HB2	2.14	0.47
1:B:35:PHE:CD2	1:B:36:VAL:HG23	2.50	0.47
1:B:34:ARG:NH1	1:B:38:LYS:HG2	2.24	0.47
1:C:307:ASP:OD1	1:C:308:GLU:N	2.47	0.47
1:C:35:PHE:CD2	1:C:36:VAL:HG23	2.50	0.47
1:C:94:ALA:HB2	1:C:114:ILE:HD11	1.97	0.47
2:E:547:ASN:ND2	2:E:590:LEU:O	2.29	0.47
2:E:816:HIS:HB2	2:E:820:THR:HA	1.96	0.47
2:G:1548:VAL:HG23	2:G:1562:PRO:HG3	1.97	0.47
2:H:1139:LEU:O	2:H:1142:LEU:HD23	2.14	0.47
2:H:1245:ARG:NH2	2:H:1248:GLU:OE1	2.42	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ALA:O	1:A:93:ILE:HG12	2.15	0.47
1:C:66:LEU:HD23	1:C:67:LYS:N	2.29	0.47
1:D:330:TYR:O	1:D:333:PHE:HB2	2.14	0.47
2:E:1375:GLY:O	2:E:1549:ILE:N	2.40	0.47
2:E:550:ILE:HD11	2:E:590:LEU:HD13	1.97	0.47
2:F:1032:TRP:CZ3	2:F:1067:PHE:HB2	2.49	0.47
2:F:1087:TRP:HA	2:F:1090:LEU:HD12	1.97	0.47
1:C:177:ARG:NH1	1:C:206:ARG:HB2	2.26	0.47
2:E:1139:LEU:O	2:E:1142:LEU:HD23	2.14	0.47
2:F:82:LEU:HG	2:F:114:PHE:CE1	2.50	0.47
2:G:577:PHE:HE2	2:G:1285:THR:HG1	1.63	0.47
2:H:550:ILE:HD11	2:H:590:LEU:HD13	1.97	0.47
1:A:94:ALA:HB2	1:A:114:ILE:HD11	1.97	0.47
1:A:159:ILE:O	1:A:163:MET:HG2	2.14	0.47
2:E:1032:TRP:CZ3	2:E:1067:PHE:HB2	2.49	0.47
2:E:798:TYR:CZ	2:E:802:ILE:HD11	2.50	0.47
2:F:1481:PHE:HB3	2:F:1485:GLN:HB2	1.97	0.47
2:F:429:MET:HG2	2:F:433:PHE:CZ	2.49	0.47
1:C:95:PHE:CD2	2:G:27:PHE:HD1	2.32	0.47
2:H:1269:ASN:O	2:H:1273:ARG:N	2.29	0.47
2:H:1284:LEU:HD12	2:H:1285:THR:N	2.30	0.47
2:H:798:TYR:CZ	2:H:802:ILE:HD11	2.50	0.47
1:A:66:LEU:HD23	1:A:67:LYS:N	2.29	0.47
1:D:201:ARG:HD2	1:D:315:PHE:HB3	1.97	0.47
2:E:324:VAL:HG13	2:E:1277:ALA:HB1	1.97	0.47
2:F:1422:SER:HB2	2:F:1502:PHE:HB3	1.96	0.47
1:D:278:HIS:ND1	2:H:1355:SER:OG	2.34	0.47
2:H:701:ILE:HD11	2:H:907:ILE:HG21	1.97	0.47
2:H:82:LEU:HG	2:H:114:PHE:CE1	2.50	0.47
1:B:263:ALA:HA	1:B:268:TYR:CG	2.49	0.47
2:E:1153:LEU:HD12	2:E:1156:ILE:HD11	1.96	0.47
2:E:1398:PHE:CD2	2:E:1399:GLU:HG2	2.50	0.47
2:E:1481:PHE:HB3	2:E:1485:GLN:HB2	1.97	0.47
2:F:135:LEU:HD13	2:F:135:LEU:O	2.14	0.47
2:H:85:LEU:HD11	2:H:113:ALA:HB3	1.97	0.47
1:C:89:ALA:O	1:C:93:ILE:HG12	2.15	0.47
1:D:57:GLN:O	1:D:60:PHE:HB3	2.14	0.47
2:E:1422:SER:HB2	2:E:1502:PHE:HB3	1.96	0.47
2:F:1398:PHE:CD2	2:F:1399:GLU:HG2	2.50	0.47
2:F:798:TYR:CZ	2:F:802:ILE:HD11	2.50	0.47
2:G:547:ASN:ND2	2:G:594:SER:HB2	2.25	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1422:SER:HB2	2:H:1502:PHE:HB3	1.96	0.47
1:A:201:ARG:HD2	1:A:315:PHE:HB3	1.97	0.46
1:A:95:PHE:HE1	2:E:16:ARG:CG	2.27	0.46
1:A:136:ARG:HH12	1:B:137:MET:CG	2.28	0.46
1:B:177:ARG:NH1	1:B:206:ARG:HB2	2.26	0.46
1:B:201:ARG:HD2	1:B:315:PHE:HB3	1.97	0.46
2:E:82:LEU:HG	2:E:114:PHE:CE1	2.50	0.46
2:E:1181:PHE:CG	2:E:1247:LEU:HD22	2.51	0.46
2:E:1284:LEU:HD12	2:E:1285:THR:N	2.30	0.46
2:E:1446:SER:O	2:E:1449:THR:OG1	2.34	0.46
2:E:701:ILE:HD11	2:E:907:ILE:HG21	1.97	0.46
2:F:324:VAL:HG13	2:F:1277:ALA:HB1	1.97	0.46
2:F:1516:GLU:OE2	2:F:1541:THR:OG1	2.21	0.46
2:G:1181:PHE:CG	2:G:1247:LEU:HD22	2.51	0.46
2:G:1284:LEU:HD12	2:G:1285:THR:N	2.30	0.46
2:G:1516:GLU:OE2	2:G:1541:THR:OG1	2.21	0.46
2:G:701:ILE:HD11	2:G:907:ILE:HG21	1.97	0.46
2:E:1349:LEU:HB3	2:E:1364:VAL:HG13	1.97	0.46
2:F:1446:SER:O	2:F:1449:THR:OG1	2.33	0.46
2:F:701:ILE:HD11	2:F:907:ILE:HG21	1.97	0.46
2:G:1481:PHE:HB3	2:G:1485:GLN:HB2	1.97	0.46
2:H:1181:PHE:CG	2:H:1247:LEU:HD22	2.51	0.46
2:H:46:ILE:HD12	2:H:123:TYR:OH	2.16	0.46
1:A:344:CYS:HB2	1:A:348:GLN:OE1	2.16	0.46
1:A:57:GLN:O	1:A:60:PHE:HB3	2.15	0.46
1:D:159:ILE:O	1:D:163:MET:HG2	2.14	0.46
1:D:89:ALA:O	1:D:93:ILE:HG12	2.15	0.46
2:E:1269:ASN:O	2:E:1273:ARG:N	2.29	0.46
2:G:1139:LEU:O	2:G:1142:LEU:HD23	2.14	0.46
2:G:85:LEU:HD11	2:G:113:ALA:HB3	1.97	0.46
2:G:550:ILE:HD11	2:G:590:LEU:HD13	1.97	0.46
2:G:798:TYR:CZ	2:G:802:ILE:HD11	2.50	0.46
2:H:1087:TRP:HA	2:H:1090:LEU:HD12	1.97	0.46
2:H:770:ALA:HA	2:H:1216:PHE:CE1	2.50	0.46
1:B:344:CYS:HB2	1:B:348:GLN:OE1	2.16	0.46
1:D:344:CYS:HB2	1:D:348:GLN:OE1	2.16	0.46
2:E:1548:VAL:HG23	2:E:1562:PRO:HG3	1.97	0.46
2:F:1548:VAL:HG23	2:F:1562:PRO:HG3	1.97	0.46
2:G:770:ALA:HA	2:G:1216:PHE:CE1	2.49	0.46
2:G:82:LEU:HG	2:G:114:PHE:CE1	2.50	0.46
2:H:1481:PHE:HB3	2:H:1485:GLN:HB2	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:VAL:HG22	1:D:239:PRO:HB3	1.98	0.46
1:D:35:PHE:CD2	1:D:36:VAL:HG23	2.50	0.46
2:F:379:VAL:O	2:F:383:THR:HG23	2.16	0.46
2:F:550:ILE:HD11	2:F:590:LEU:HD13	1.97	0.46
2:G:1349:LEU:HB3	2:G:1364:VAL:HG13	1.97	0.46
2:G:1375:GLY:O	2:G:1549:ILE:N	2.40	0.46
2:H:1398:PHE:CD2	2:H:1399:GLU:HG2	2.50	0.46
1:C:201:ARG:HD2	1:C:315:PHE:HB3	1.97	0.46
2:F:1003:TYR:CE1	2:F:1092:VAL:HG11	2.51	0.46
2:F:577:PHE:HE2	2:F:1285:THR:HG1	1.61	0.46
2:G:1087:TRP:HA	2:G:1090:LEU:HD12	1.96	0.46
2:G:324:VAL:HG13	2:G:1277:ALA:HB1	1.97	0.46
2:G:153:LYS:O	2:G:157:PHE:HB2	2.16	0.46
2:H:1548:VAL:HG23	2:H:1562:PRO:HG3	1.97	0.46
1:A:35:PHE:CD2	1:A:36:VAL:HG23	2.50	0.46
1:C:329:ASP:OD1	1:C:331:SER:OG	2.31	0.46
1:A:233:LEU:HD21	1:D:326:TYR:CZ	2.51	0.46
2:E:577:PHE:HE2	2:E:1285:THR:HG1	1.63	0.46
2:F:1284:LEU:HD12	2:F:1285:THR:N	2.30	0.46
2:G:1003:TYR:CE1	2:G:1092:VAL:HG11	2.51	0.46
2:G:1152:ALA:O	2:G:1156:ILE:HG12	2.16	0.46
2:G:1398:PHE:CD2	2:G:1399:GLU:HG2	2.50	0.46
1:B:89:ALA:O	1:B:93:ILE:HG12	2.15	0.46
1:C:218:GLN:NE2	1:C:235:GLN:OE1	2.49	0.46
2:E:1030:ASP:OD2	2:E:1286:TYR:OH	2.32	0.46
2:E:1375:GLY:N	2:E:1547:LEU:O	2.45	0.46
2:E:379:VAL:O	2:E:383:THR:HG23	2.16	0.46
2:E:46:ILE:HD12	2:E:123:TYR:OH	2.16	0.46
2:F:108:MET:N	2:F:109:PRO:HD2	2.31	0.46
2:F:1181:PHE:CG	2:F:1247:LEU:HD22	2.50	0.46
2:F:494:GLU:O	2:F:498:GLN:HG2	2.16	0.46
2:G:127:ILE:O	2:G:131:ASN:N	2.45	0.46
2:G:1379:ARG:O	2:G:1384:LYS:NZ	2.49	0.46
2:H:1349:LEU:HB3	2:H:1364:VAL:HG13	1.97	0.46
2:H:1446:SER:O	2:H:1449:THR:OG1	2.34	0.46
2:H:379:VAL:O	2:H:383:THR:HG23	2.16	0.46
1:A:218:GLN:NE2	1:A:235:GLN:OE1	2.49	0.46
2:E:1231:ASP:O	2:E:1235:ILE:HG12	2.16	0.46
2:F:45:PRO:O	2:F:49:ILE:HG23	2.16	0.46
2:G:1231:ASP:O	2:G:1235:ILE:HG12	2.16	0.46
2:G:379:VAL:O	2:G:383:THR:HG23	2.16	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:324:VAL:HG13	2:H:1277:ALA:HB1	1.97	0.46
2:H:461:LEU:O	2:H:461:LEU:HD12	2.16	0.46
2:H:494:GLU:O	2:H:498:GLN:HG2	2.16	0.46
2:H:547:ASN:ND2	2:H:594:SER:HB2	2.26	0.46
1:C:344:CYS:HB2	1:C:348:GLN:OE1	2.16	0.46
2:E:85:LEU:HD11	2:E:113:ALA:HB3	1.97	0.46
2:G:108:MET:N	2:G:109:PRO:HD2	2.31	0.46
2:H:1152:ALA:O	2:H:1156:ILE:HG12	2.16	0.46
2:H:45:PRO:O	2:H:49:ILE:HG23	2.16	0.46
1:B:218:GLN:NE2	1:B:235:GLN:OE1	2.49	0.45
1:C:200:LEU:HD21	1:C:285:VAL:HG21	1.98	0.45
1:C:194:GLY:N	1:D:227:GLU:OE2	2.24	0.45
2:E:45:PRO:O	2:E:49:ILE:HG23	2.16	0.45
2:F:681:ILE:HG12	2:F:737:VAL:HG22	1.98	0.45
2:G:1422:SER:HB2	2:G:1502:PHE:HB3	1.96	0.45
2:G:1431:PHE:HB2	2:G:1438:ASN:ND2	2.31	0.45
2:H:681:ILE:HG12	2:H:737:VAL:HG22	1.98	0.45
2:E:108:MET:N	2:E:109:PRO:HD2	2.31	0.45
2:F:85:LEU:HD11	2:F:113:ALA:HB3	1.97	0.45
2:F:1231:ASP:O	2:F:1235:ILE:HG12	2.16	0.45
2:F:46:ILE:HD12	2:F:123:TYR:OH	2.16	0.45
2:F:1379:ARG:O	2:F:1384:LYS:NZ	2.49	0.45
2:F:153:LYS:O	2:F:157:PHE:HB2	2.16	0.45
2:G:45:PRO:O	2:G:49:ILE:HG23	2.16	0.45
2:H:108:MET:N	2:H:109:PRO:HD2	2.31	0.45
2:H:1431:PHE:HB2	2:H:1438:ASN:ND2	2.31	0.45
2:H:1372:GLN:HA	2:H:1530:ARG:O	2.17	0.45
1:B:200:LEU:HD21	1:B:285:VAL:HG21	1.98	0.45
2:E:1152:ALA:O	2:E:1156:ILE:HG12	2.16	0.45
2:E:153:LYS:O	2:E:157:PHE:HB2	2.16	0.45
2:G:1482:SER:HG	3:G:2004:ATP:PB	2.40	0.45
1:D:218:GLN:NE2	1:D:235:GLN:OE1	2.49	0.45
2:E:1003:TYR:CE1	2:E:1092:VAL:HG11	2.51	0.45
2:F:1152:ALA:O	2:F:1156:ILE:HG12	2.16	0.45
2:F:1431:PHE:HB2	2:F:1438:ASN:ND2	2.31	0.45
2:G:1446:SER:O	2:G:1449:THR:OG1	2.34	0.45
2:G:461:LEU:O	2:G:461:LEU:HD12	2.16	0.45
2:H:1231:ASP:O	2:H:1235:ILE:HG12	2.16	0.45
1:C:233:LEU:HD21	1:B:326:TYR:CZ	2.51	0.45
1:C:199:MET:HG2	1:C:258:TYR:HB3	1.99	0.45
1:C:299:GLN:NE2	1:C:301:ARG:HD2	2.32	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1431:PHE:HB2	2:E:1438:ASN:ND2	2.31	0.45
2:H:455:ILE:C	2:H:457:GLY:H	2.20	0.45
2:E:1151:SER:O	2:E:1155:VAL:HG23	2.17	0.45
2:E:32:ASN:ND2	2:E:153:LYS:HD2	2.32	0.45
2:F:1072:SER:O	2:F:1075:ILE:HG22	2.17	0.45
2:F:117:ALA:O	2:F:120:SER:OG	2.17	0.45
2:F:1181:PHE:CD2	2:F:1247:LEU:HD22	2.52	0.45
2:F:455:ILE:C	2:F:457:GLY:H	2.20	0.45
2:F:788:ILE:HG22	2:F:791:SER:H	1.82	0.45
2:G:32:ASN:ND2	2:G:153:LYS:HD2	2.32	0.45
2:G:46:ILE:HD12	2:G:123:TYR:OH	2.16	0.45
2:G:681:ILE:HG12	2:G:737:VAL:HG22	1.98	0.45
2:H:1003:TYR:CE1	2:H:1092:VAL:HG11	2.51	0.45
2:H:1023:HIS:HE1	2:H:1144:ARG:HA	1.82	0.45
2:H:153:LYS:O	2:H:157:PHE:HB2	2.16	0.45
1:A:299:GLN:NE2	1:A:301:ARG:HD2	2.32	0.45
1:B:346:ALA:HA	1:B:349:LEU:HB2	1.99	0.45
1:D:199:MET:HG2	1:D:258:TYR:HB3	1.99	0.45
2:E:455:ILE:C	2:E:457:GLY:H	2.20	0.45
2:E:788:ILE:HG22	2:E:791:SER:H	1.82	0.45
2:G:716:GLY:N	3:G:2004:ATP:O2G	2.34	0.45
1:B:299:GLN:NE2	1:B:301:ARG:HD2	2.32	0.45
1:C:346:ALA:HA	1:C:349:LEU:HB2	1.99	0.45
1:D:128:GLN:HB2	1:D:152:GLN:HE21	1.82	0.45
1:D:68:TRP:CD2	1:D:170:LYS:HE3	2.52	0.45
2:F:291:LEU:O	2:F:295:PHE:HB3	2.16	0.45
2:G:1023:HIS:HE1	2:G:1144:ARG:HA	1.82	0.45
2:H:1030:ASP:OD2	2:H:1286:TYR:OH	2.32	0.45
2:H:1151:SER:O	2:H:1155:VAL:HG23	2.17	0.45
2:H:893:LEU:C	2:H:895:HIS:H	2.20	0.45
2:E:461:LEU:O	2:E:461:LEU:HD12	2.16	0.45
2:E:494:GLU:O	2:E:498:GLN:HG2	2.16	0.45
2:F:1349:LEU:HB3	2:F:1364:VAL:HG13	1.97	0.45
2:G:1245:ARG:NH2	2:G:1248:GLU:OE1	2.42	0.45
2:G:807:LEU:HG	2:G:811:ILE:HG13	1.99	0.45
2:H:1310:ALA:HA	2:H:1313:ARG:NH2	2.32	0.45
1:A:269:ASP:OD1	1:A:347:ARG:NE	2.33	0.45
1:A:90:TRP:CE2	1:A:123:PHE:HE2	2.35	0.45
1:C:268:TYR:CZ	1:C:347:ARG:HA	2.52	0.45
1:D:200:LEU:HD21	1:D:285:VAL:HG21	1.98	0.45
1:D:294:THR:OG1	1:D:296:ILE:HG12	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1023:HIS:HE1	2:E:1144:ARG:HA	1.82	0.45
2:E:1372:GLN:HA	2:E:1530:ARG:O	2.17	0.45
2:F:1151:SER:O	2:F:1155:VAL:HG23	2.17	0.45
2:G:1181:PHE:CD2	2:G:1247:LEU:HD22	2.52	0.45
2:H:1181:PHE:CD2	2:H:1247:LEU:HD22	2.52	0.45
2:H:1379:ARG:O	2:H:1384:LYS:NZ	2.49	0.45
1:A:68:TRP:CD2	1:A:170:LYS:HE3	2.52	0.44
1:B:294:THR:OG1	1:B:296:ILE:HG12	2.17	0.44
1:B:268:TYR:CZ	1:B:347:ARG:HA	2.52	0.44
1:D:90:TRP:CE2	1:D:123:PHE:HE2	2.36	0.44
2:E:1072:SER:O	2:E:1075:ILE:HG22	2.17	0.44
2:F:1271:LEU:HG	2:F:1272:HIS:CD2	2.52	0.44
2:G:1351:VAL:HG12	2:G:1397:THR:HA	1.99	0.44
2:G:1372:GLN:HA	2:G:1530:ARG:O	2.17	0.44
2:G:771:TYR:HD2	2:G:1212:THR:HG22	1.82	0.44
2:H:1072:SER:O	2:H:1075:ILE:HG22	2.17	0.44
2:H:1154:ALA:O	2:H:1157:SER:OG	2.26	0.44
1:A:200:LEU:HD21	1:A:285:VAL:HG21	1.98	0.44
1:D:268:TYR:CZ	1:D:347:ARG:HA	2.52	0.44
2:E:1271:LEU:HG	2:E:1272:HIS:CD2	2.52	0.44
2:E:1516:GLU:OE2	2:E:1541:THR:OG1	2.21	0.44
2:E:291:LEU:O	2:E:295:PHE:HB3	2.17	0.44
2:F:1310:ALA:HA	2:F:1313:ARG:NH2	2.32	0.44
2:F:417:ILE:O	2:F:420:LEU:HG	2.18	0.44
2:F:381:ILE:HG13	2:F:433:PHE:CZ	2.53	0.44
2:F:461:LEU:HD12	2:F:461:LEU:O	2.16	0.44
2:G:291:LEU:O	2:G:295:PHE:HB3	2.16	0.44
2:G:36:HIS:HD2	2:G:142:TYR:HE1	1.66	0.44
2:G:455:ILE:C	2:G:457:GLY:H	2.20	0.44
2:G:494:GLU:O	2:G:498:GLN:HG2	2.16	0.44
2:G:788:ILE:HG22	2:G:791:SER:H	1.82	0.44
2:H:1351:VAL:HG12	2:H:1397:THR:HA	2.00	0.44
1:D:95:PHE:HD2	2:H:27:PHE:HD1	1.65	0.44
1:A:268:TYR:CZ	1:A:347:ARG:HA	2.52	0.44
1:B:286:ILE:HG23	1:B:299:GLN:HE21	1.83	0.44
1:D:299:GLN:NE2	1:D:301:ARG:HD2	2.32	0.44
2:E:1181:PHE:CD2	2:E:1247:LEU:HD22	2.52	0.44
2:E:893:LEU:C	2:E:895:HIS:H	2.20	0.44
2:F:1023:HIS:HE1	2:F:1144:ARG:HA	1.82	0.44
2:F:771:TYR:HD2	2:F:1212:THR:HG22	1.82	0.44
2:G:1151:SER:O	2:G:1155:VAL:HG23	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:32:ASN:HD21	2:G:153:LYS:HD2	1.83	0.44
1:B:128:GLN:HB2	1:B:152:GLN:HE21	1.82	0.44
1:B:68:TRP:CD2	1:B:170:LYS:HE3	2.52	0.44
1:C:294:THR:OG1	1:C:296:ILE:HG12	2.17	0.44
1:C:76:THR:HG22	1:D:154:ILE:HG21	1.99	0.44
1:A:278:HIS:ND1	2:E:1355:SER:OG	2.47	0.44
2:E:417:ILE:O	2:E:420:LEU:HG	2.18	0.44
2:E:807:LEU:HG	2:E:811:ILE:HG13	1.99	0.44
2:F:1245:ARG:NH2	2:F:1248:GLU:OE1	2.42	0.44
2:F:1348:ASN:O	2:F:1350:SER:N	2.49	0.44
2:F:1372:GLN:HA	2:F:1530:ARG:O	2.17	0.44
2:F:36:HIS:HD2	2:F:142:TYR:HE1	1.66	0.44
2:F:889:LYS:NZ	2:F:892:TYR:HE2	2.16	0.44
2:G:1310:ALA:HA	2:G:1313:ARG:NH2	2.32	0.44
2:G:381:ILE:HG13	2:G:433:PHE:CZ	2.53	0.44
2:G:889:LYS:NZ	2:G:892:TYR:HE2	2.16	0.44
2:H:291:LEU:O	2:H:295:PHE:HB3	2.17	0.44
1:A:199:MET:HG2	1:A:258:TYR:HB3	1.99	0.44
1:A:164:LEU:HD11	1:B:164:LEU:HD13	1.99	0.44
1:C:68:TRP:CD2	1:C:170:LYS:HE3	2.52	0.44
1:D:286:ILE:HG23	1:D:299:GLN:HE21	1.82	0.44
2:E:1348:ASN:O	2:E:1350:SER:N	2.49	0.44
2:E:36:HIS:HD2	2:E:142:TYR:HE1	1.66	0.44
2:E:471:ALA:HB3	2:E:472:PRO:HD3	2.00	0.44
2:E:889:LYS:NZ	2:E:892:TYR:HE2	2.16	0.44
2:F:32:ASN:ND2	2:F:153:LYS:HD2	2.32	0.44
2:F:770:ALA:HA	2:F:1216:PHE:CE1	2.50	0.44
2:G:1455:GLU:OE1	2:G:1460:LYS:HB3	2.18	0.44
2:G:417:ILE:O	2:G:420:LEU:HG	2.18	0.44
2:G:893:LEU:C	2:G:895:HIS:H	2.20	0.44
2:H:771:TYR:HD2	2:H:1212:THR:HG22	1.82	0.44
1:A:294:THR:OG1	1:A:296:ILE:HG12	2.17	0.44
1:B:329:ASP:OD1	1:B:331:SER:OG	2.31	0.44
2:E:1066:VAL:O	2:E:1069:VAL:HG12	2.18	0.44
2:E:32:ASN:HD21	2:E:153:LYS:HD2	1.83	0.44
2:E:681:ILE:HG12	2:E:737:VAL:HG22	1.98	0.44
2:F:1455:GLU:OE1	2:F:1460:LYS:HB3	2.18	0.44
2:G:1348:ASN:O	2:G:1350:SER:N	2.49	0.44
2:H:1376:ILE:HB	2:H:1535:ILE:HD13	2.00	0.44
2:H:36:HIS:HD2	2:H:142:TYR:HE1	1.66	0.44
2:H:471:ALA:HB3	2:H:472:PRO:HD3	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:788:ILE:HG22	2:H:791:SER:H	1.82	0.44
1:A:128:GLN:HB2	1:A:152:GLN:HE21	1.82	0.44
2:E:1455:GLU:OE1	2:E:1460:LYS:HB3	2.18	0.44
2:F:32:ASN:HD21	2:F:153:LYS:HD2	1.83	0.44
2:F:893:LEU:C	2:F:895:HIS:H	2.20	0.44
2:H:1066:VAL:O	2:H:1069:VAL:HG12	2.18	0.44
1:A:346:ALA:HA	1:A:349:LEU:HB2	1.99	0.44
1:B:199:MET:HG2	1:B:258:TYR:HB3	1.99	0.44
1:C:90:TRP:CE2	1:C:123:PHE:HE2	2.36	0.44
1:C:286:ILE:HG23	1:C:299:GLN:HE21	1.82	0.44
1:D:199:MET:HG2	1:D:258:TYR:CB	2.48	0.44
2:G:437:ASN:ND2	2:G:592:LEU:HD23	2.29	0.44
2:H:32:ASN:ND2	2:H:153:LYS:HD2	2.32	0.44
2:H:435:CYS:N	2:H:436:PRO:HD2	2.33	0.44
2:H:807:LEU:HG	2:H:811:ILE:HG13	1.99	0.44
1:A:286:ILE:HG23	1:A:299:GLN:HE21	1.82	0.44
1:C:126:GLU:OE2	1:C:136:ARG:NH1	2.51	0.44
1:C:229:GLU:HB3	1:B:314:ARG:CZ	2.48	0.44
2:E:127:ILE:O	2:E:131:ASN:N	2.45	0.44
2:E:381:ILE:HG13	2:E:433:PHE:CZ	2.53	0.44
2:F:1460:LYS:O	2:F:1464:LYS:HG2	2.18	0.44
2:G:1066:VAL:O	2:G:1069:VAL:HG12	2.18	0.44
2:G:127:ILE:HG23	2:G:128:GLU:N	2.33	0.44
2:H:32:ASN:HD21	2:H:153:LYS:HD2	1.83	0.44
1:D:126:GLU:OE2	1:D:136:ARG:NH1	2.51	0.43
2:E:1379:ARG:O	2:E:1384:LYS:NZ	2.49	0.43
2:F:807:LEU:HG	2:F:811:ILE:HG13	1.99	0.43
2:G:1271:LEU:HG	2:G:1272:HIS:CD2	2.52	0.43
2:G:1251:MET:HE3	2:G:1294:LEU:HD11	1.99	0.43
2:H:127:ILE:O	2:H:131:ASN:N	2.45	0.43
2:H:127:ILE:HG23	2:H:128:GLU:N	2.33	0.43
2:H:141:VAL:O	2:H:144:THR:OG1	2.32	0.43
1:A:119:SER:OG	1:B:140:GLU:OE2	2.17	0.43
1:B:269:ASP:OD1	1:B:347:ARG:NE	2.33	0.43
1:C:190:ALA:O	1:C:196:LEU:HD12	2.18	0.43
1:C:199:MET:HG2	1:C:258:TYR:CB	2.48	0.43
1:D:346:ALA:HA	1:D:349:LEU:HB2	1.99	0.43
2:F:1030:ASP:OD2	2:F:1286:TYR:OH	2.32	0.43
2:G:1460:LYS:O	2:G:1464:LYS:HG2	2.19	0.43
2:G:1376:ILE:HB	2:G:1535:ILE:HD13	2.00	0.43
2:H:1251:MET:HE3	2:H:1294:LEU:HD11	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ALA:O	1:B:196:LEU:HD12	2.18	0.43
1:B:199:MET:HG2	1:B:258:TYR:CB	2.48	0.43
2:E:1310:ALA:HA	2:E:1313:ARG:NH2	2.32	0.43
2:F:1251:MET:HE3	2:F:1294:LEU:HD11	1.99	0.43
2:F:1351:VAL:HG12	2:F:1397:THR:HA	1.99	0.43
2:G:1180:TYR:O	2:G:1183:VAL:HG12	2.19	0.43
2:H:1180:TYR:O	2:H:1183:VAL:HG12	2.19	0.43
2:H:417:ILE:O	2:H:420:LEU:HG	2.18	0.43
1:A:199:MET:HG2	1:A:258:TYR:CB	2.48	0.43
1:D:122:LEU:O	1:D:126:GLU:HG3	2.19	0.43
1:D:190:ALA:O	1:D:196:LEU:HD12	2.18	0.43
2:E:1376:ILE:HB	2:E:1535:ILE:HD13	2.00	0.43
2:E:1351:VAL:HG12	2:E:1397:THR:HA	1.99	0.43
2:F:1130:THR:O	2:F:1134:HIS:HB2	2.19	0.43
2:G:1072:SER:O	2:G:1075:ILE:HG22	2.17	0.43
2:G:1491:LEU:HD11	2:G:1507:ALA:HB1	2.00	0.43
2:G:471:ALA:HB3	2:G:472:PRO:HD3	2.00	0.43
2:H:1271:LEU:HG	2:H:1272:HIS:CD2	2.52	0.43
2:H:1460:LYS:O	2:H:1464:LYS:HG2	2.18	0.43
2:H:309:ALA:HB1	2:H:369:GLN:OE1	2.19	0.43
1:B:90:TRP:CE2	1:B:123:PHE:HE2	2.36	0.43
1:B:184:SER:O	1:B:304:TYR:OH	2.32	0.43
1:D:200:LEU:HD22	1:D:304:TYR:CE2	2.54	0.43
2:F:1154:ALA:O	2:F:1157:SER:OG	2.26	0.43
2:F:309:ALA:HB1	2:F:369:GLN:OE1	2.19	0.43
2:F:314:PHE:HZ	2:F:448:GLY:HA2	1.83	0.43
2:G:39:LEU:HA	2:G:42:ILE:HG22	2.01	0.43
2:H:381:ILE:HG13	2:H:433:PHE:CZ	2.53	0.43
1:A:126:GLU:OE2	1:A:136:ARG:NH1	2.51	0.43
1:B:126:GLU:OE2	1:B:136:ARG:NH1	2.51	0.43
1:C:128:GLN:HB2	1:C:152:GLN:HE21	1.82	0.43
2:E:552:ILE:HA	2:E:555:VAL:HG22	2.01	0.43
2:F:1066:VAL:O	2:F:1069:VAL:HG12	2.18	0.43
2:F:127:ILE:O	2:F:131:ASN:N	2.45	0.43
2:F:1491:LEU:HD11	2:F:1507:ALA:HB1	1.99	0.43
2:F:435:CYS:N	2:F:436:PRO:HD2	2.33	0.43
2:G:771:TYR:HD1	2:G:851:PHE:HD2	1.66	0.43
2:H:1482:SER:HG	3:H:2004:ATP:PB	2.41	0.43
1:A:122:LEU:O	1:A:126:GLU:HG3	2.19	0.43
2:E:1130:THR:O	2:E:1134:HIS:HB2	2.19	0.43
2:E:127:ILE:HG23	2:E:128:GLU:N	2.33	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1491:LEU:HD11	2:E:1507:ALA:HB1	1.99	0.43
2:F:471:ALA:HB3	2:F:472:PRO:HD3	2.00	0.43
2:H:1130:THR:O	2:H:1134:HIS:HB2	2.19	0.43
2:H:1491:LEU:HD11	2:H:1507:ALA:HB1	1.99	0.43
2:H:889:LYS:NZ	2:H:892:TYR:HE2	2.16	0.43
1:A:108:GLU:N	1:A:108:GLU:OE1	2.52	0.43
1:A:190:ALA:O	1:A:196:LEU:HD12	2.18	0.43
1:C:108:GLU:OE1	1:C:108:GLU:N	2.52	0.43
1:C:200:LEU:HD22	1:C:304:TYR:CE2	2.54	0.43
2:E:39:LEU:HA	2:E:42:ILE:HG22	2.01	0.43
2:E:771:TYR:HD1	2:E:851:PHE:HD2	1.66	0.43
2:H:395:ILE:HG21	2:H:421:VAL:HG12	2.01	0.43
2:H:39:LEU:HA	2:H:42:ILE:HG22	2.01	0.43
2:H:890:LEU:O	2:H:893:LEU:HG	2.19	0.43
1:B:242:ASN:OD1	1:B:243:GLY:N	2.52	0.43
1:C:286:ILE:HD13	1:B:250:PHE:CD1	2.54	0.43
1:B:34:ARG:HH21	1:B:303:SER:HG	1.61	0.43
2:E:771:TYR:HD2	2:E:1212:THR:HG22	1.82	0.43
2:E:1251:MET:HE3	2:E:1294:LEU:HD11	2.00	0.43
2:E:309:ALA:HB1	2:E:369:GLN:OE1	2.19	0.43
2:F:1180:TYR:O	2:F:1183:VAL:HG12	2.19	0.43
2:H:552:ILE:HA	2:H:555:VAL:HG22	2.01	0.43
2:E:1460:LYS:O	2:E:1464:LYS:HG2	2.19	0.43
2:F:685:TYR:O	2:F:733:VAL:N	2.52	0.43
2:H:368:LEU:O	2:H:371:THR:HG22	2.19	0.43
2:H:771:TYR:HD1	2:H:851:PHE:HD2	1.66	0.43
1:C:158:MET:O	1:C:162:ILE:HG12	2.19	0.42
1:D:108:GLU:OE1	1:D:108:GLU:N	2.52	0.42
2:E:1180:TYR:O	2:E:1183:VAL:HG12	2.19	0.42
2:E:435:CYS:N	2:E:436:PRO:HD2	2.33	0.42
2:F:1065:MET:O	2:F:1068:THR:OG1	2.33	0.42
2:F:141:VAL:O	2:F:144:THR:OG1	2.32	0.42
2:F:395:ILE:HG21	2:F:421:VAL:HG12	2.00	0.42
2:G:1440:ASP:HB3	2:G:1442:GLU:O	2.19	0.42
2:G:714:GLN:HE22	2:G:1514:ALA:HB3	1.84	0.42
2:G:890:LEU:O	2:G:893:LEU:HG	2.19	0.42
2:H:1455:GLU:OE1	2:H:1460:LYS:HB3	2.18	0.42
1:A:200:LEU:HD22	1:A:304:TYR:CE2	2.54	0.42
1:A:242:ASN:OD1	1:A:243:GLY:N	2.52	0.42
1:B:200:LEU:HD22	1:B:304:TYR:CE2	2.54	0.42
1:C:122:LEU:O	1:C:126:GLU:HG3	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:127:ILE:HG23	2:F:128:GLU:N	2.33	0.42
2:F:1440:ASP:HB3	2:F:1442:GLU:O	2.19	0.42
2:G:309:ALA:HB1	2:G:369:GLN:OE1	2.19	0.42
1:B:122:LEU:O	1:B:126:GLU:HG3	2.19	0.42
2:E:395:ILE:HG21	2:E:421:VAL:HG12	2.01	0.42
2:F:1438:ASN:OD1	2:F:1474:ILE:HD12	2.19	0.42
2:F:368:LEU:O	2:F:371:THR:HG22	2.19	0.42
2:F:714:GLN:HE22	2:F:1514:ALA:HB3	1.84	0.42
2:G:368:LEU:O	2:G:371:THR:HG22	2.19	0.42
2:G:552:ILE:HA	2:G:555:VAL:HG22	2.01	0.42
1:A:158:MET:O	1:A:162:ILE:HG12	2.19	0.42
2:F:1376:ILE:HB	2:F:1535:ILE:HD13	2.00	0.42
2:F:552:ILE:HA	2:F:555:VAL:HG22	2.01	0.42
2:G:435:CYS:N	2:G:436:PRO:HD2	2.33	0.42
2:G:685:TYR:O	2:G:733:VAL:N	2.52	0.42
2:H:107:TYR:CD2	2:H:1165:VAL:HG21	2.55	0.42
2:H:1348:ASN:O	2:H:1350:SER:N	2.49	0.42
2:H:685:TYR:O	2:H:733:VAL:N	2.52	0.42
1:C:36:VAL:HB	1:C:303:SER:HB3	2.01	0.42
2:E:1245:ARG:NH2	2:E:1248:GLU:OE1	2.42	0.42
2:E:1438:ASN:OD1	2:E:1474:ILE:HD12	2.19	0.42
2:E:685:TYR:O	2:E:733:VAL:N	2.52	0.42
2:G:1438:ASN:OD1	2:G:1474:ILE:HD12	2.19	0.42
2:G:395:ILE:HG21	2:G:421:VAL:HG12	2.01	0.42
2:H:1162:VAL:O	2:H:1165:VAL:HG22	2.20	0.42
2:H:1142:LEU:HB3	2:H:1300:ASN:HB3	2.01	0.42
2:H:1440:ASP:HB3	2:H:1442:GLU:O	2.19	0.42
1:B:158:MET:O	1:B:162:ILE:HG12	2.19	0.42
1:C:233:LEU:HD21	1:B:326:TYR:CE1	2.54	0.42
2:E:1350:SER:HA	2:E:1362:LYS:HA	2.02	0.42
2:E:890:LEU:O	2:E:893:LEU:HG	2.19	0.42
2:G:1130:THR:O	2:G:1134:HIS:HB2	2.19	0.42
2:H:1350:SER:HA	2:H:1362:LYS:HA	2.02	0.42
1:C:34:ARG:HH21	1:C:303:SER:HG	1.62	0.42
2:E:1440:ASP:HB3	2:E:1442:GLU:O	2.19	0.42
2:F:44:PHE:HB2	2:F:45:PRO:HD3	2.02	0.42
2:G:1162:VAL:O	2:G:1165:VAL:HG22	2.20	0.42
2:G:12:SER:C	2:G:15:TYR:H	2.22	0.42
2:G:314:PHE:HZ	2:G:448:GLY:HA2	1.83	0.42
1:A:180:THR:OG1	1:A:205:LEU:HB2	2.20	0.42
1:A:263:ALA:HA	1:A:268:TYR:CD1	2.55	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:VAL:HB	1:B:303:SER:HB3	2.01	0.42
2:E:317:PRO:HA	2:E:320:ILE:HD12	2.02	0.42
2:E:770:ALA:HA	2:E:1216:PHE:CE1	2.50	0.42
2:F:890:LEU:O	2:F:893:LEU:HG	2.19	0.42
2:G:1166:ALA:C	2:G:1169:PRO:HD2	2.40	0.42
2:G:1350:SER:HA	2:G:1362:LYS:HA	2.02	0.42
2:G:317:PRO:HA	2:G:320:ILE:HD12	2.02	0.42
2:H:716:GLY:N	3:H:2004:ATP:O2G	2.34	0.42
2:H:44:PHE:HB2	2:H:45:PRO:HD3	2.02	0.42
1:C:233:LEU:HD11	1:B:326:TYR:CG	2.55	0.42
1:D:95:PHE:HE2	2:H:27:PHE:CB	2.32	0.42
2:E:368:LEU:O	2:E:371:THR:HG22	2.19	0.42
2:E:44:PHE:HB2	2:E:45:PRO:HD3	2.02	0.42
2:F:39:LEU:HA	2:F:42:ILE:HG22	2.01	0.42
2:G:1251:MET:HB2	2:G:1295:ASN:HD21	1.84	0.42
2:G:878:ASP:OD2	2:G:881:ARG:HB2	2.20	0.42
1:B:108:GLU:N	1:B:108:GLU:OE1	2.52	0.42
1:C:180:THR:OG1	1:C:205:LEU:HB2	2.20	0.42
2:E:1166:ALA:C	2:E:1169:PRO:HD2	2.40	0.42
2:E:714:GLN:HE22	2:E:1514:ALA:HB3	1.84	0.42
2:F:12:SER:C	2:F:15:TYR:H	2.22	0.42
2:F:553:ALA:O	2:F:557:ILE:HG12	2.20	0.42
2:G:107:TYR:CD2	2:G:1165:VAL:HG21	2.55	0.42
2:G:1142:LEU:HB3	2:G:1300:ASN:HB3	2.01	0.42
2:G:553:ALA:O	2:G:557:ILE:HG12	2.20	0.42
2:H:1348:ASN:O	2:H:1400:GLY:HA3	2.20	0.42
2:H:1488:LEU:HD13	2:H:1488:LEU:HA	1.89	0.42
2:H:22:LEU:HB3	2:H:156:LYS:HE3	2.02	0.42
1:A:229:GLU:HB3	1:D:314:ARG:CZ	2.50	0.41
1:A:136:ARG:NH1	1:B:137:MET:SD	2.93	0.41
1:B:180:THR:OG1	1:B:205:LEU:HB2	2.20	0.41
2:E:1163:PHE:CE2	2:E:1167:LEU:HB2	2.55	0.41
2:E:716:GLY:N	3:E:2004:ATP:O2G	2.34	0.41
2:E:769:VAL:HG13	2:E:849:VAL:O	2.20	0.41
2:F:1162:VAL:O	2:F:1165:VAL:HG22	2.20	0.41
2:F:1347:GLN:HE21	2:F:1401:HIS:CE1	2.38	0.41
2:F:317:PRO:HA	2:F:320:ILE:HD12	2.02	0.41
2:F:771:TYR:HD1	2:F:851:PHE:HD2	1.66	0.41
2:G:44:PHE:HB2	2:G:45:PRO:HD3	2.02	0.41
2:H:714:GLN:HE22	2:H:1514:ALA:HB3	1.84	0.41
2:H:317:PRO:HA	2:H:320:ILE:HD12	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ALA:HA	1:B:268:TYR:CD1	2.55	0.41
1:D:263:ALA:HA	1:D:268:TYR:CD1	2.55	0.41
1:D:36:VAL:HB	1:D:303:SER:HB3	2.01	0.41
2:E:1004:LEU:HB2	2:E:1012:LEU:HD21	2.03	0.41
2:H:1438:ASN:OD1	2:H:1474:ILE:HD12	2.19	0.41
2:H:396:TYR:CG	2:H:1226:LEU:HD13	2.55	0.41
2:H:547:ASN:HD21	2:H:590:LEU:C	2.19	0.41
1:D:180:THR:OG1	1:D:205:LEU:HB2	2.20	0.41
2:E:107:TYR:CD2	2:E:1165:VAL:HG21	2.55	0.41
2:E:1142:LEU:HB3	2:E:1300:ASN:HB3	2.02	0.41
2:E:1348:ASN:O	2:E:1400:GLY:HA3	2.20	0.41
2:E:1482:SER:HG	3:E:2004:ATP:PB	2.43	0.41
2:E:22:LEU:HB3	2:E:156:LYS:HE3	2.02	0.41
2:F:107:TYR:CD2	2:F:1165:VAL:HG21	2.55	0.41
2:F:1403:ILE:HD13	2:F:1408:ASP:HA	2.02	0.41
2:F:22:LEU:HB3	2:F:156:LYS:HE3	2.02	0.41
2:F:878:ASP:OD2	2:F:881:ARG:HB2	2.20	0.41
2:G:1403:ILE:HD13	2:G:1408:ASP:HA	2.02	0.41
2:H:1166:ALA:C	2:H:1169:PRO:HD2	2.40	0.41
2:H:1568:ARG:HH21	2:H:1571:SER:HA	1.85	0.41
2:H:314:PHE:HZ	2:H:448:GLY:HA2	1.83	0.41
1:C:263:ALA:HA	1:C:268:TYR:CD1	2.55	0.41
1:D:158:MET:O	1:D:162:ILE:HG12	2.19	0.41
1:C:164:LEU:HD11	1:D:164:LEU:HD13	2.02	0.41
1:D:273:SER:HG	2:H:1398:PHE:HE2	1.58	0.41
1:A:233:LEU:HD11	1:D:326:TYR:CG	2.56	0.41
2:F:1251:MET:HB2	2:F:1295:ASN:HD21	1.84	0.41
2:F:1142:LEU:HB3	2:F:1300:ASN:HB3	2.02	0.41
2:F:1350:SER:HA	2:F:1362:LYS:HA	2.02	0.41
2:G:22:LEU:HB3	2:G:156:LYS:HE3	2.02	0.41
2:H:1251:MET:HB2	2:H:1295:ASN:HD21	1.84	0.41
2:H:769:VAL:HG13	2:H:849:VAL:O	2.20	0.41
2:H:878:ASP:OD2	2:H:881:ARG:HB2	2.20	0.41
2:E:1023:HIS:CE1	2:E:1144:ARG:HA	2.56	0.41
2:E:553:ALA:O	2:E:557:ILE:HG12	2.20	0.41
2:E:437:ASN:ND2	2:E:592:LEU:HD23	2.29	0.41
2:E:878:ASP:OD2	2:E:881:ARG:HB2	2.20	0.41
2:F:1163:PHE:CE2	2:F:1167:LEU:HB2	2.56	0.41
2:F:1568:ARG:HH21	2:F:1571:SER:HA	1.85	0.41
2:F:84:VAL:HG11	2:F:174:LEU:HD12	2.03	0.41
2:F:6:CYS:H	2:F:16:ARG:HH11	1.69	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:805:CYS:O	2:F:836:ARG:HD2	2.20	0.41
2:G:1347:GLN:HE21	2:G:1401:HIS:CE1	2.38	0.41
2:H:1004:LEU:HB2	2:H:1012:LEU:HD21	2.03	0.41
2:H:12:SER:C	2:H:15:TYR:H	2.22	0.41
2:H:1346:ILE:HG22	2:H:1402:ILE:HG13	2.02	0.41
2:H:550:ILE:N	2:H:551:PRO:HD2	2.36	0.41
2:H:72:ASN:HA	2:H:75:TRP:HD1	1.85	0.41
1:C:218:GLN:NE2	1:C:235:GLN:HB3	2.35	0.41
2:E:1162:VAL:O	2:E:1165:VAL:HG22	2.20	0.41
2:E:1251:MET:HB2	2:E:1295:ASN:HD21	1.84	0.41
2:E:1346:ILE:HG22	2:E:1402:ILE:HG13	2.02	0.41
2:F:1346:ILE:HG22	2:F:1402:ILE:HG13	2.02	0.41
2:F:716:GLY:N	3:F:2004:ATP:O2G	2.34	0.41
2:H:1163:PHE:CE2	2:H:1167:LEU:HB2	2.56	0.41
1:C:119:SER:OG	1:D:140:GLU:OE2	2.23	0.41
1:C:314:ARG:CZ	1:D:229:GLU:HB3	2.51	0.41
2:E:6:CYS:H	2:E:16:ARG:HH11	1.68	0.41
2:F:1255:GLY:O	2:F:1259:VAL:HG23	2.21	0.41
2:G:1023:HIS:CE1	2:G:1144:ARG:HA	2.56	0.41
2:G:396:TYR:CG	2:G:1226:LEU:HD13	2.55	0.41
2:G:1348:ASN:O	2:G:1400:GLY:HA3	2.20	0.41
2:H:320:ILE:HG23	2:H:1284:LEU:HD11	2.03	0.41
2:H:428:LEU:HA	2:H:428:LEU:HD23	1.91	0.41
2:H:553:ALA:O	2:H:557:ILE:HG12	2.20	0.41
2:H:84:VAL:HG11	2:H:174:LEU:HD12	2.03	0.41
1:A:38:LYS:NZ	1:A:308:GLU:OE1	2.53	0.41
1:A:36:VAL:HB	1:A:303:SER:HB3	2.01	0.41
2:E:12:SER:C	2:E:15:TYR:H	2.22	0.41
2:E:709:THR:HA	2:E:898:TRP:O	2.21	0.41
2:E:72:ASN:HA	2:E:75:TRP:HD1	1.85	0.41
2:F:1023:HIS:CE1	2:F:1144:ARG:HA	2.56	0.41
2:F:547:ASN:HD21	2:F:590:LEU:C	2.19	0.41
2:G:1568:ARG:HH21	2:G:1571:SER:HA	1.85	0.41
2:G:769:VAL:HG13	2:G:849:VAL:O	2.21	0.41
2:G:84:VAL:HG11	2:G:174:LEU:HD12	2.03	0.41
2:H:1255:GLY:O	2:H:1259:VAL:HG23	2.21	0.41
2:H:147:PHE:O	2:H:151:THR:HG23	2.21	0.41
1:B:335:ASN:HD22	1:B:336:THR:H	1.69	0.41
1:C:242:ASN:OD1	1:C:243:GLY:N	2.52	0.41
2:E:550:ILE:N	2:E:551:PRO:HD2	2.36	0.41
2:E:709:THR:HB	2:E:898:TRP:HB3	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:314:PHE:CE2	2:F:447:VAL:HG12	2.56	0.41
2:F:396:TYR:CG	2:F:1226:LEU:HD13	2.55	0.41
2:F:550:ILE:N	2:F:551:PRO:HD2	2.35	0.41
2:F:72:ASN:HA	2:F:75:TRP:HD1	1.85	0.41
2:G:1255:GLY:O	2:G:1259:VAL:HG23	2.21	0.41
2:G:147:PHE:O	2:G:151:THR:HG23	2.21	0.41
2:G:72:ASN:HA	2:G:75:TRP:HD1	1.85	0.41
1:B:74:ILE:HD13	2:F:49:ILE:HG22	2.03	0.41
1:C:184:SER:O	1:C:304:TYR:OH	2.32	0.41
1:C:95:PHE:HE2	2:G:27:PHE:CB	2.34	0.41
1:C:314:ARG:HD2	1:D:229:GLU:OE1	2.21	0.41
2:E:396:TYR:CG	2:E:1226:LEU:HD13	2.56	0.41
2:E:1255:GLY:O	2:E:1259:VAL:HG23	2.21	0.41
2:E:302:SER:OG	2:E:376:SER:O	2.31	0.41
2:F:320:ILE:HG23	2:F:1284:LEU:HD11	2.03	0.41
2:F:322:GLY:C	2:F:326:HIS:HD1	2.18	0.41
2:G:455:ILE:C	2:G:456:LEU:HG	2.41	0.41
2:G:777:TRP:CZ3	2:G:1209:GLY:HA3	2.56	0.41
2:H:455:ILE:C	2:H:456:LEU:HG	2.41	0.41
1:D:242:ASN:OD1	1:D:243:GLY:N	2.52	0.41
2:E:1347:GLN:HE21	2:E:1401:HIS:CE1	2.38	0.41
2:E:1568:ARG:HH21	2:E:1571:SER:HA	1.85	0.41
2:E:889:LYS:HZ2	2:E:892:TYR:HE2	1.67	0.41
2:F:1166:ALA:C	2:F:1169:PRO:HD2	2.40	0.41
2:G:1131:ILE:HA	2:G:1135:ILE:CD1	2.51	0.41
2:G:547:ASN:HD21	2:G:590:LEU:C	2.19	0.41
2:G:679:VAL:HA	2:G:738:PHE:O	2.21	0.41
2:G:709:THR:HA	2:G:898:TRP:O	2.21	0.41
2:H:1568:ARG:C	2:H:1570:ASP:H	2.24	0.41
1:D:329:ASP:OD1	1:D:331:SER:OG	2.31	0.40
2:E:84:VAL:HG11	2:E:174:LEU:HD12	2.03	0.40
2:E:455:ILE:C	2:E:456:LEU:HG	2.41	0.40
2:E:805:CYS:O	2:E:836:ARG:HD2	2.20	0.40
2:F:1004:LEU:HB2	2:F:1012:LEU:HD21	2.03	0.40
2:F:709:THR:HA	2:F:898:TRP:O	2.21	0.40
2:G:1346:ILE:HG22	2:G:1402:ILE:HG13	2.02	0.40
2:G:805:CYS:O	2:G:836:ARG:HD2	2.20	0.40
2:F:777:TRP:CZ3	2:F:1209:GLY:HA3	2.56	0.40
2:F:1348:ASN:O	2:F:1400:GLY:HA3	2.20	0.40
2:G:36:HIS:HD2	2:G:142:TYR:CE1	2.40	0.40
2:G:374:GLN:NE2	2:G:1245:ARG:HE	2.20	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:808:GLN:HB2	2:G:809:PRO:HD3	2.03	0.40
2:H:1065:MET:O	2:H:1068:THR:OG1	2.33	0.40
2:H:709:THR:HA	2:H:898:TRP:O	2.21	0.40
2:H:679:VAL:HA	2:H:738:PHE:O	2.21	0.40
1:A:146:ILE:HG12	1:D:122:LEU:HD21	2.02	0.40
1:D:218:GLN:NE2	1:D:235:GLN:HB3	2.35	0.40
1:D:335:ASN:HD22	1:D:336:THR:H	1.69	0.40
2:E:147:PHE:O	2:E:151:THR:HG23	2.21	0.40
2:F:370:ARG:HB3	2:F:1252:GLU:HG2	2.04	0.40
2:F:1505:ASP:HA	2:F:1535:ILE:HB	2.03	0.40
2:G:1004:LEU:HB2	2:G:1012:LEU:HD21	2.03	0.40
2:G:1065:MET:O	2:G:1068:THR:OG1	2.33	0.40
2:G:320:ILE:HG23	2:G:1284:LEU:HD11	2.03	0.40
2:H:1131:ILE:HA	2:H:1135:ILE:CD1	2.51	0.40
2:H:1347:GLN:HE21	2:H:1401:HIS:CE1	2.38	0.40
2:H:805:CYS:O	2:H:836:ARG:HD2	2.20	0.40
2:E:370:ARG:HB3	2:E:1252:GLU:HG2	2.04	0.40
2:F:717:CYS:O	2:F:905:GLY:N	2.54	0.40
2:G:1163:PHE:CE2	2:G:1167:LEU:HB2	2.55	0.40
2:H:1031:TYR:CE2	2:H:1035:LYS:HD2	2.57	0.40
2:H:577:PHE:HE2	2:H:1285:THR:HG1	1.63	0.40
2:H:717:CYS:O	2:H:905:GLY:N	2.54	0.40
1:A:326:TYR:CZ	1:B:233:LEU:HD21	2.57	0.40
1:C:229:GLU:OE1	1:B:314:ARG:HD2	2.22	0.40
1:C:136:ARG:HH12	1:D:137:MET:CG	2.34	0.40
2:E:808:GLN:HB2	2:E:809:PRO:HD3	2.03	0.40
2:F:455:ILE:C	2:F:456:LEU:HG	2.41	0.40
2:F:769:VAL:HG13	2:F:849:VAL:O	2.21	0.40
2:F:709:THR:HB	2:F:898:TRP:HB3	2.03	0.40
2:G:1031:TYR:CE2	2:G:1035:LYS:HD2	2.57	0.40
2:G:148:ILE:O	2:G:151:THR:OG1	2.34	0.40
2:G:1505:ASP:HA	2:G:1535:ILE:HB	2.03	0.40
2:G:550:ILE:N	2:G:551:PRO:HD2	2.35	0.40
2:H:808:GLN:HB2	2:H:809:PRO:HD3	2.03	0.40
2:H:709:THR:HB	2:H:898:TRP:HB3	2.03	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 PDB entries followed by that with respect to all EM entries.

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	326/406 (80%)	301 (92%)	25 (8%)	0	100	100
1	B	326/406 (80%)	302 (93%)	24 (7%)	0	100	100
1	C	326/406 (80%)	303 (93%)	23 (7%)	0	100	100
1	D	326/406 (80%)	303 (93%)	23 (7%)	0	100	100
2	E	1270/1581 (80%)	1175 (92%)	95 (8%)	0	100	100
2	F	1270/1581 (80%)	1175 (92%)	95 (8%)	0	100	100
2	G	1270/1581 (80%)	1175 (92%)	95 (8%)	0	100	100
2	H	1270/1581 (80%)	1175 (92%)	95 (8%)	0	100	100
All	All	6384/7948 (80%)	5909 (93%)	475 (7%)	0	100	100

There are no Ramachandran outliers to report.

### 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 PDB entries followed by that with respect to all EM entries.

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	264/348 (76%)	263 (100%)	1 (0%)	93	96
1	B	264/348 (76%)	263 (100%)	1 (0%)	93	96
1	C	264/348 (76%)	263 (100%)	1 (0%)	93	96
1	D	264/348 (76%)	263 (100%)	1 (0%)	93	96
2	E	987/1368 (72%)	978 (99%)	9 (1%)	82	92
2	F	987/1368 (72%)	978 (99%)	9 (1%)	82	92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	987/1368 (72%)	978 (99%)	9 (1%)	82	92
2	H	987/1368 (72%)	978 (99%)	9 (1%)	82	92
All	All	5004/6864 (73%)	4964 (99%)	40 (1%)	86	93

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	335	ASN
1	C	335	ASN
1	B	335	ASN
1	D	335	ASN
2	E	126	ASN
2	E	188	ASN
2	E	419	ASN
2	E	1142	LEU
2	E	1233	ASN
2	E	1244	ASN
2	E	1271	LEU
2	E	1292	ASN
2	E	1513	MET
2	H	126	ASN
2	H	188	ASN
2	H	419	ASN
2	H	1142	LEU
2	H	1233	ASN
2	H	1244	ASN
2	H	1271	LEU
2	H	1292	ASN
2	H	1513	MET
2	G	126	ASN
2	G	188	ASN
2	G	419	ASN
2	G	1142	LEU
2	G	1233	ASN
2	G	1244	ASN
2	G	1271	LEU
2	G	1292	ASN
2	G	1513	MET
2	F	126	ASN
2	F	188	ASN
2	F	419	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	F	1142	LEU
2	F	1233	ASN
2	F	1244	ASN
2	F	1271	LEU
2	F	1292	ASN
2	F	1513	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	HIS
1	A	193	HIS
1	A	218	GLN
1	A	235	GLN
1	A	277	HIS
1	A	335	ASN
1	C	115	HIS
1	C	193	HIS
1	C	218	GLN
1	C	235	GLN
1	C	277	HIS
1	C	335	ASN
1	B	115	HIS
1	B	193	HIS
1	B	218	GLN
1	B	235	GLN
1	B	277	HIS
1	B	335	ASN
1	D	115	HIS
1	D	193	HIS
1	D	218	GLN
1	D	235	GLN
1	D	277	HIS
1	D	335	ASN
2	E	36	HIS
2	E	102	HIS
2	E	126	ASN
2	E	188	ASN
2	E	416	GLN
2	E	419	ASN
2	E	437	ASN
2	E	498	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	E	500	ASN
2	E	707	GLN
2	E	714	GLN
2	E	821	GLN
2	E	1129	ASN
2	E	1133	GLN
2	E	1202	HIS
2	E	1244	ASN
2	E	1272	HIS
2	H	36	HIS
2	H	102	HIS
2	H	126	ASN
2	H	188	ASN
2	H	416	GLN
2	H	419	ASN
2	H	437	ASN
2	H	498	GLN
2	H	500	ASN
2	H	707	GLN
2	H	714	GLN
2	H	821	GLN
2	H	1129	ASN
2	H	1133	GLN
2	H	1202	HIS
2	H	1244	ASN
2	H	1272	HIS
2	G	36	HIS
2	G	102	HIS
2	G	126	ASN
2	G	188	ASN
2	G	416	GLN
2	G	419	ASN
2	G	437	ASN
2	G	498	GLN
2	G	500	ASN
2	G	707	GLN
2	G	714	GLN
2	G	821	GLN
2	G	1129	ASN
2	G	1133	GLN
2	G	1202	HIS
2	G	1244	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	G	1272	HIS
2	F	36	HIS
2	F	102	HIS
2	F	126	ASN
2	F	188	ASN
2	F	416	GLN
2	F	419	ASN
2	F	437	ASN
2	F	498	GLN
2	F	500	ASN
2	F	707	GLN
2	F	714	GLN
2	F	821	GLN
2	F	1129	ASN
2	F	1133	GLN
2	F	1202	HIS
2	F	1244	ASN
2	F	1272	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 11 are monoatomic - leaving 12 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	$\# Z  > 2$
3	ATP	A	501	-	27,33,33	0.90	1 (3%)	25,52,52	1.65	2 (8%)
3	ATP	B	501	-	27,33,33	0.91	1 (3%)	25,52,52	1.64	2 (8%)
3	ATP	C	501	-	27,33,33	0.89	1 (3%)	25,52,52	1.65	2 (8%)
3	ATP	D	501	-	27,33,33	0.89	1 (3%)	25,52,52	1.69	2 (8%)
5	ADP	E	2001	6	25,29,29	0.95	1 (4%)	24,45,45	1.62	2 (8%)
3	ATP	E	2004	6	27,33,33	0.91	1 (3%)	25,52,52	1.65	2 (8%)
5	ADP	F	2001	6	25,29,29	0.94	1 (4%)	24,45,45	1.62	2 (8%)
3	ATP	F	2004	6	27,33,33	0.91	1 (3%)	25,52,52	1.65	2 (8%)
5	ADP	G	2001	6	25,29,29	0.94	1 (4%)	24,45,45	1.63	2 (8%)
3	ATP	G	2004	6	27,33,33	0.90	1 (3%)	25,52,52	1.65	3 (12%)
5	ADP	H	2001	6	25,29,29	0.94	1 (4%)	24,45,45	1.62	2 (8%)
3	ATP	H	2004	6	27,33,33	0.91	1 (3%)	25,52,52	1.66	2 (8%)

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
3	ATP	A	501	-	-	0/18/38/38	0/3/3/3
3	ATP	B	501	-	-	0/18/38/38	0/3/3/3
3	ATP	C	501	-	-	0/18/38/38	0/3/3/3
3	ATP	D	501	-	-	0/18/38/38	0/3/3/3
5	ADP	E	2001	6	-	0/12/32/32	0/3/3/3
3	ATP	E	2004	6	-	0/18/38/38	0/3/3/3
5	ADP	F	2001	6	-	0/12/32/32	0/3/3/3
3	ATP	F	2004	6	-	0/18/38/38	0/3/3/3
5	ADP	G	2001	6	-	0/12/32/32	0/3/3/3
3	ATP	G	2004	6	-	0/18/38/38	0/3/3/3
5	ADP	H	2001	6	-	0/12/32/32	0/3/3/3
3	ATP	H	2004	6	-	0/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	ATP	C5-C4	2.78	1.46	1.40
3	G	2004	ATP	C5-C4	2.82	1.46	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2004	ATP	C5-C4	2.82	1.46	1.40
3	A	501	ATP	C5-C4	2.85	1.46	1.40
5	H	2001	ADP	C5-C4	2.86	1.47	1.40
3	C	501	ATP	C5-C4	2.87	1.47	1.40
3	E	2004	ATP	C5-C4	2.89	1.47	1.40
3	B	501	ATP	C5-C4	2.90	1.47	1.40
5	E	2001	ADP	C5-C4	2.91	1.47	1.40
3	F	2004	ATP	C5-C4	2.91	1.47	1.40
5	G	2001	ADP	C5-C4	2.91	1.47	1.40
5	F	2001	ADP	C5-C4	2.92	1.47	1.40

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	ATP	N3-C2-N1	-5.92	123.70	128.86
5	G	2001	ADP	N3-C2-N1	-5.84	123.77	128.86
3	A	501	ATP	N3-C2-N1	-5.84	123.78	128.86
3	B	501	ATP	N3-C2-N1	-5.82	123.79	128.86
3	C	501	ATP	N3-C2-N1	-5.81	123.80	128.86
5	E	2001	ADP	N3-C2-N1	-5.78	123.82	128.86
5	F	2001	ADP	N3-C2-N1	-5.78	123.82	128.86
5	H	2001	ADP	N3-C2-N1	-5.77	123.84	128.86
3	F	2004	ATP	N3-C2-N1	-5.53	124.04	128.86
3	E	2004	ATP	N3-C2-N1	-5.51	124.06	128.86
3	H	2004	ATP	N3-C2-N1	-5.49	124.08	128.86
3	G	2004	ATP	N3-C2-N1	-5.47	124.09	128.86
3	F	2004	ATP	C4-C5-N7	-2.88	106.63	109.41
3	H	2004	ATP	C4-C5-N7	-2.88	106.63	109.41
3	E	2004	ATP	C4-C5-N7	-2.83	106.68	109.41
3	G	2004	ATP	C4-C5-N7	-2.79	106.71	109.41
3	B	501	ATP	C4-C5-N7	-2.78	106.72	109.41
3	C	501	ATP	C4-C5-N7	-2.75	106.75	109.41
3	D	501	ATP	C4-C5-N7	-2.74	106.76	109.41
5	H	2001	ADP	C4-C5-N7	-2.73	106.77	109.41
3	A	501	ATP	C4-C5-N7	-2.72	106.79	109.41
5	E	2001	ADP	C4-C5-N7	-2.70	106.81	109.41
5	G	2001	ADP	C4-C5-N7	-2.69	106.81	109.41
5	F	2001	ADP	C4-C5-N7	-2.68	106.82	109.41
3	G	2004	ATP	C2'-C3'-C4'	2.00	106.52	102.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	ATP	1	0
3	B	501	ATP	1	0
3	C	501	ATP	1	0
3	D	501	ATP	1	0
3	E	2004	ATP	3	0
3	F	2004	ATP	3	0
3	G	2004	ATP	3	0
3	H	2004	ATP	3	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.