



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 10:36 AM UTC

PDB ID : 3HOU / pdb_00003hou
Title : Complete RNA polymerase II elongation complex I with a T-U mismatch
Authors : Sydow, J.F.; Brueckner, F.; Cheung, A.C.M.; Damsma, G.E.; Dengl, S.;
Lehmann, E.; Vassylyev, D.; Cramer, P.
Deposited on : 2009-06-03
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

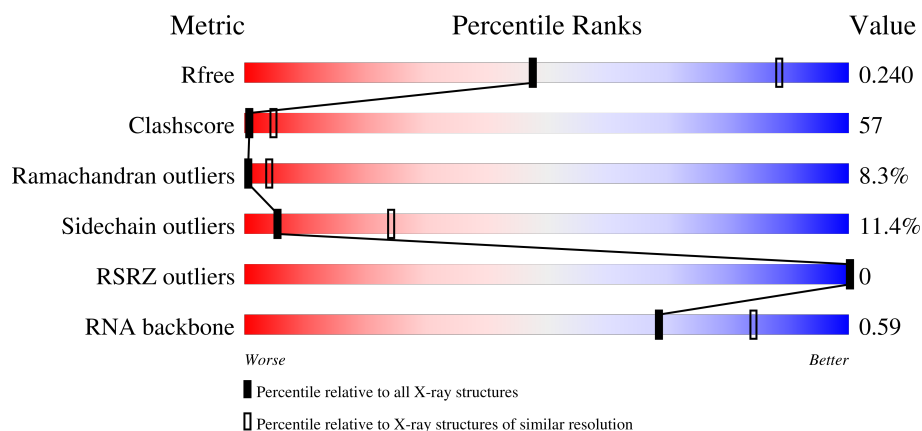
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

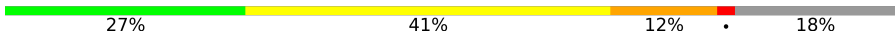
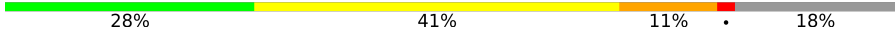
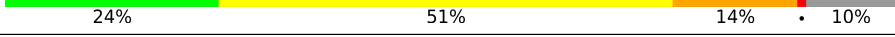
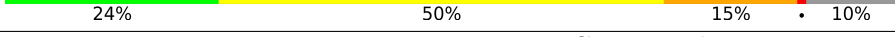
The reported resolution of this entry is 3.20 Å.

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



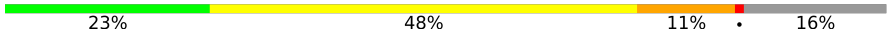
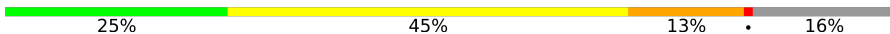
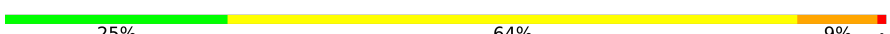
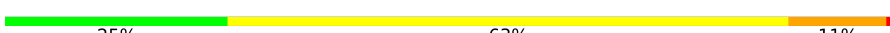
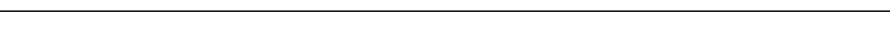
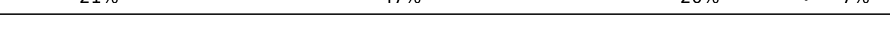
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	1733	
1	M	1733	
2	B	1224	
2	N	1224	

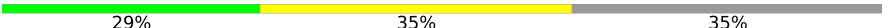
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	318	
3	O	318	
4	D	221	
4	P	221	
5	E	215	
5	Q	215	
6	F	155	
6	R	155	
7	G	171	
7	S	171	
8	H	146	
8	T	146	
9	I	122	
9	U	122	
10	J	70	
10	V	70	
11	K	120	
11	W	120	
12	L	70	
12	X	70	
13	1	26	
13	4	26	
14	2	13	
14	5	13	
15	3	17	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	6	17	 A horizontal bar chart showing the quality of chain 6. The bar is divided into three segments: a green segment on the left labeled '29%', a yellow segment in the middle labeled '35%', and a grey segment on the right labeled '35%'. The total length of the bar represents 100%.

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 63664 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1416	Total	C	N	O	S	0	0	0
			11143	7021	1949	2111	62			
1	M	1416	Total	C	N	O	S	0	0	0
			11143	7021	1949	2111	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1104	Total	C	N	O	S	0	0	0
			8779	5560	1537	1627	55			
2	N	1104	Total	C	N	O	S	0	0	0
			8779	5560	1537	1627	55			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			
4	P	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			
6	R	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			
7	S	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1076	677	182	213	4			
8	T	134	Total	C	N	O	S	0	0	0
			1076	677	182	213	4			

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

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

Continued on next page...

Continued from previous page...

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

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

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			
12	X	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*A*AP*GP*TP*AP*GP*TP*TP*AP*TP*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	1	18	Total 368	Br 1	C 176	N 66	O 108	P 17	0	0	0
13	4	18	Total 368	Br 1	C 176	N 66	O 108	P 17	0	0	0

- Molecule 14 is a DNA chain called 5'-D(*A*AP*CP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	2	6	Total	C	N	O	P	0	0	0
			117	58	20	34	5			
14	5	6	Total	C	N	O	P	0	0	0
			117	58	20	34	5			

- Molecule 15 is a RNA chain called 5'-R(*UP*GP*CP*AP*UP*U*UP*CP*GP*AP*CP*CP*AP*GP*GP*CP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	3	11	Total	C	N	O	P	0	0	0
			230	104	41	75	10			
15	6	11	Total	C	N	O	P	0	0	0
			230	104	41	75	10			

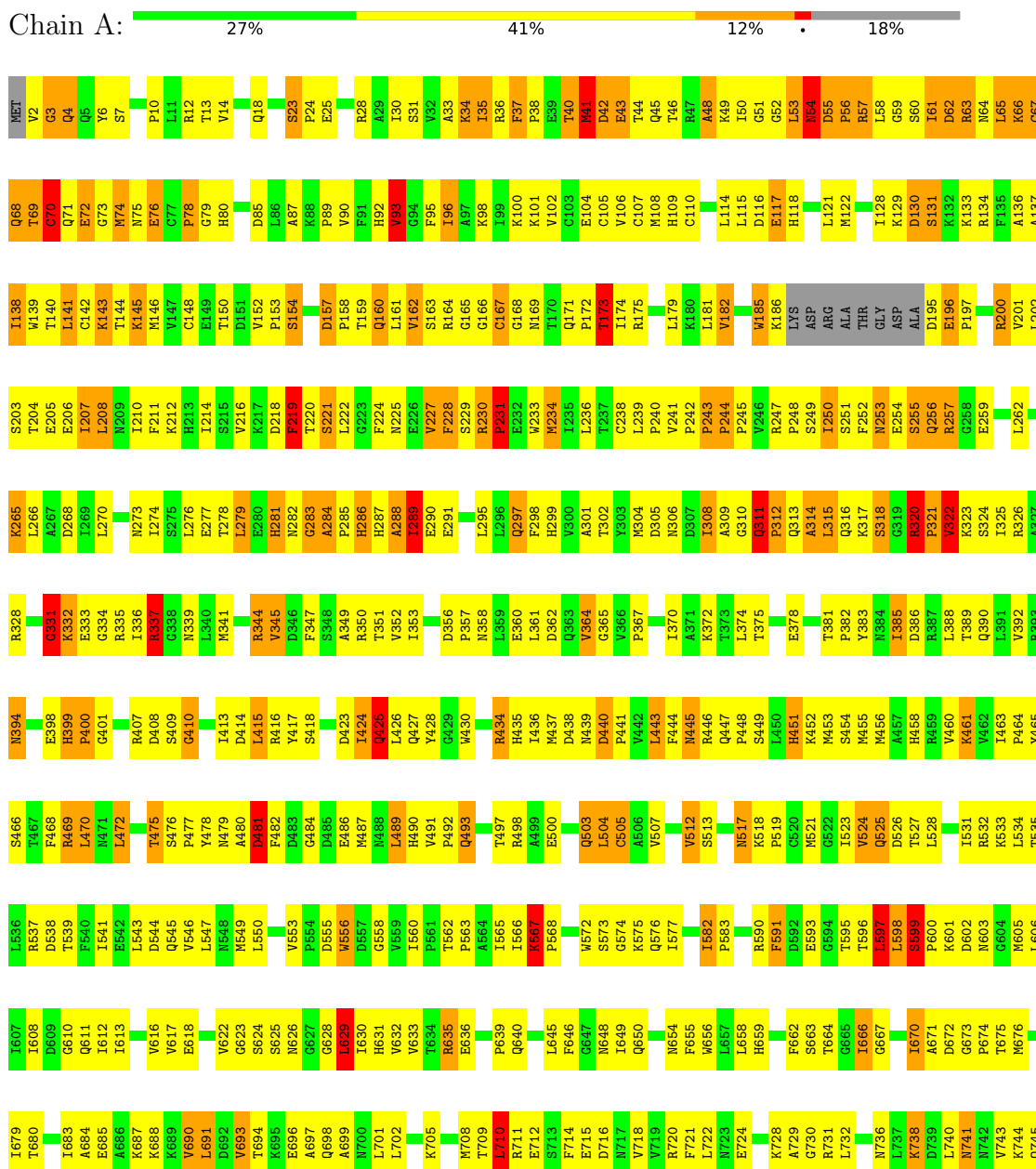
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	2	Total	Zn	0	0
			2	2		
16	B	1	Total	Zn	0	0
			1	1		
16	C	1	Total	Zn	0	0
			1	1		
16	I	2	Total	Zn	0	0
			2	2		
16	J	1	Total	Zn	0	0
			1	1		
16	L	1	Total	Zn	0	0
			1	1		
16	M	2	Total	Zn	0	0
			2	2		
16	N	1	Total	Zn	0	0
			1	1		
16	O	1	Total	Zn	0	0
			1	1		
16	U	2	Total	Zn	0	0
			2	2		
16	V	1	Total	Zn	0	0
			1	1		
16	X	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

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

• Molecule 1: DNA-directed RNA polymerase II subunit RPB1





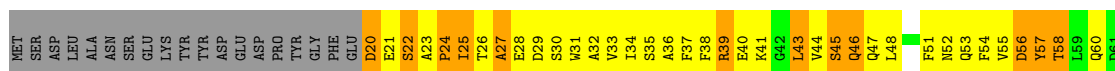
K1039	Q1040	A1041	W1044	V1045	L1046	S1047	I1048	I1049	V1057	V1058	H1059	P1060	M1063	A1069	I1072	G1073	E1074	P1075	A1076	M1079	T1080	L1081	ASN	THR	PHE	HIS	PHE	ALA	GLY	VAL	ALA	SER	K1092	K1093	V1094	T1095	S1096	G1097	V1098	P1099	R1100	L1101	L1102	E1103	L1104	L1105	N1106	V1107	A1108	K1109	R11036	M1110	M1111	T11038					
R962	I963	I964	Q965	Q966	A967	F971	H972	I973	T976	K977	P978	S979	D980	L981	T982	I983	K984	I985	I986	L993	N996	L997	L998	V999	G1002	K1003	N1004	E1005	I1006	N1009	A1010	Q1011	V1015	T1016	K1017	L1018	F1019	C1019	E945	Y946	F947	Y948	D949	G950	E951	R1029	R1030	Q1033	E1034	K1109	R1036	M1110	M1111	T11038					
D926	T927	A928	V929	K930	T931	A932	E933	T934	Y936	R940	L941	R942	K943	A944	L945	E946	D947	R948	M949	R950	H951	Y952	R953	T955	R956	L957	R958	T959	Q965	F966	E967	R968	G969	E970	D971	G972	M973	D974	A975	A976	H977	L978	E979	L983	T986	G987	G988	S989	D990	A991	A992								
F993	R996	Y997	R998	V999	P900	L901	L902	N903	T904	D905	H906	T907	L908	D909	P910	L911	L912	L913	E914	S915	S916	T919	L920	G921	L922	Q926	L929	P930	G931	K934	Q935	Y937	R940	K941	F942	C1019	E945	Y946	F947	Y948	D949	G950	E951	P955	L956	P957	V958	R959	L960	R961									
L756	N757	I758	A759	K760	T761	S762	Q767	Q768	Q769	Q770	E771	R774	F777	F778	F779	F780	D781	R782	T783	L784	P785	H786	F787	S788	K789	P794	S795	S796	K797	F798	F799	V800	E801	R802	S803	Y804	L805	R806	C807	L808	A875	A876	H877	Y878	H879	L883	T886	G887	G888	S889	R890	A891	A892						
K687	K688	K689	Q610	Q611	L612	L613	V616	V617	E618	V622	G623	S624	S625	N626	G627	G628	L629	H630	H631	V632	V633	T634	R635	E636	L645	F646	G647	N648	L649	F655	G656	L657	L658	S663	T664	G665	I666	G667	I670	A671	D672	G673	T674	T675	H676	T679	G681	T682	L683	A684	E685	A686							
L536	R537	L538	T539	F540	L541	Q545	V546	L547	R548	M549	V553	P554	D555	V556	D557	G558	V559	L560	P561	T562	P563	L564	L565	L566	K567	P568	K569	P570	L571	L572	S573	G574	K575	Q576	L577	V580	F581	D582	E583	G584	T585	L586	L587	L588	L589	L590	P600	L603	G604	L605									
S466	T467	F468	R469	L470	R471	L472	S473	V474	T475	L476	L477	L478	L479	L480	L481	F482	D483	G484	M487	N488	L489	H490	V491	P492	Q493	T497	L503	L504	C505	P441	V442	L443	F444	N445	R446	Q447	P448	H451	K452	M453	S454	M455	M456	V524	Q525	R459	L528	R532	A533	L534	T535								
K330	G331	K332	K333	L334	R335	L336	K337	K338	L339	L340	M341	G342	K343	R344	V345	D346	F347	T351	V352	L353	S354	G355	D356	P357	N358	L359	E360	L361	D362	Q363	V364	H365	G366	K367	K368	S369	L370	A371	T373	L374	T375	E378	T381	P382	Y383	K384	L385	D386	Q390	L391	V392	K393	N394						
K285	L286	A287	L288	L289	L290	L291	L292	L293	L294	L295	L296	L297	L298	L299	L300	L301	L302	L303	L304	L305	L306	L307	L308	L309	L310	L311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332												
R200	V201	L202	S203	T204	E205	F206	I207	L208	N209	I210	K143	T144	K145	E146	V147	T148	L149	L150	D151	V152	P153	S154	D157	P158	T159	Q160	V161	V162	S163	R164	G165	C166	C167	G168	N169	T170	Q171	P172	T173	R175	V182	G183	S184	W185	K186	L189	ASP	ASP	ARG	ALA	THR	GLY	ASP	ALA	S255	Q256	R257	E258	E259
K133	R134	F135	A136	E137	G138	V139	T140	L141	C142	K143	T144	K145	E146	V147	T148	L149	L150	D151	V152	P153	S154	D157	P158	T159	Q160	V161	V162	S163	R164	G165	C166	C167	G168	N169	T170	Q171	P172	T173	R175	V182	G183	S184	W185	K186	L189	ASP	ASP	ARG	ALA	THR	GLY	ASP	ALA	S255	Q256	R257	E258	E259	
Q68	T69	C70	Q71	E72	G73	M74	N75	R76	C77	P78	G79	H80	I84	D85	L86	A87	K88	P89	V90	F91	H92	V93	G94	F95	I96	A97	K98	I99	V102	C105	V106	C107	E43	M108	H109	C110	G111	K112	L113	L114	L115	D116	E117	N118	E119	P120	S121	M122	R123	L126	A127	R128	K129	D130	E131	K132			

PRO	SER	SER	ALA	M1454	V1384	S1314	V1243	ASP	T1113
ASN	PRO	PRO	ASP	GLU	T1385	E1315	R1244	GLU	P1114
THR	THR	SER	TYR	GLN	R1386	M1316	PRO	GLU	S1115
PRO	SER	PRO	GLY	LYS	H1387	M1317	LYS	ALA	L1116
THR	SER	PRO	ALA	ILE	F1388		SER	GLU	T1117
TYR	THR	THR	ALA	ILE	F1389	I1322	LEU	GLN	V1118
PRO	THR	THR	THR	THR	M1390	D1323	ASP	SER	Y1119
SER	SER	SER	SER	GLU	R1391	P1324	ALA	PHE	L1120
PRO	PRO	PRO	PRO	ILE	S1392	T1325	GLU	ASP	E1121
THR	THR	THR	PHE	GLU	M1393	R1326	THR	Q1187	P1122
SER	SER	TYR	GLY	ASP	T1394	I1327	GLU	Q1188	G1123
PRO	PRO	SER	ALA	GLY	G1395	V1328		S1189	H1124
THR	THR	PRO	TYR	GLN	A1396	T1329	E1254	P1190	A1125
SER	THR	THR	GLY	ASP	L1397	M1330	E1255		A1126
PRO	SER	GLY	GLU	GLY	M1398	F1331	D1257	L1191	D1127
GLY	PRO	ALA	ALA	GLY	R1399	F1332	H1258	L1193	Q1128
TYR	PRO	THR	PRO	VAL	C1400	T1333	M1259	R1194	E1129
SER	SER	THR	THR	THR	S1401	D1334	L1260	L1195	Q1130
PRO	PRO	SER	SER	PRO	F1402	I1335	K1261		
GLY	SER	PRO	PRO	TYR	E1403	M1336	K1262	D1198	I1134
SER	TYR	THR	GLY	SER	E1404	V1337	I1263		
PRO	SER	PHE	GLY	ASN	T1405	V1338	E1264	M1202	I1138
ALA	PRO	GLY	GLY	GLU	V1406	L1339	T1265	N1203	E1139
THR	THR	VAL	SER	SER	E1407	G1340		D1204	H1140
SER	TYR	TYR	SER	GLY	I1408	I1341	M1267	K1205	T1141
PRO	PRO	SER	SER	LEU	L1409	E1342	L1268	D1206	T1142
LYS	ALA	PRO	PRO	VAL	F1410		E1269	L1207	L1143
GLN	TYR	THR	GLY	ASN	E1411	R1345	N1270	T1208	K1144
ASP	SER	PHE	ASN	ALA	A1412		T1271	M1209	S1145
PRO	PRO	SER	PRO	ASP			T1272		V1146
GLY	THR	THR	PRO	LEU	E1417	L1348	L1273	G1210	T1147
LYS	SER	TYR	THR	ASP	L1418	V1349	R1274	Q1211	I1148
HIS	PRO	SER	SER	VAL	D1419	K1350		V1212	
ASN	SER	PRO	PRO	LYS	E1351	E1352	E1277	G1213	A1149
GLY	TYR	THR	THR	ASP	D1420	V1352		D1214	
SER	SER	THR	THR	GLU	C1421	M1353	N1278	R1215	I1152
ASN	SER	SER	TYR	GLU	R1422	M1354	I1279		Y1153
GLU	PRO	PRO	SER	LEU		V1355	E1280	I1216	Y1154
ASN	THR	SER	PRO	MET	S1425		R1281	K1217	D1155
ASN	SER	TYR	THR	PHE	E1426	Y1362		Q1218	P1156
SER	PRO	SER	SER	SER		V1363	V1291	T1219	D1157
PRO	PRO	PRO	PRO	PRO	Q1432	M1364	P1292	F1220	P1158
THR	TYR	THR	ALA	LEU	M1433	Y1365	S1293	K1221	R1159
SER	SER	SER	TYR	VAL		R1366	P1294	N1222	S1160
PRO	PRO	PRO	SER	ASP	I1436	H1367	T1295	D1223	T1161
THR	THR	SER	PRO	GLY	G1437	M1368	G1296	L1224	V1162
SER	TYR	THR	THR	GLY	T1438	A1369	E1297		I1163
PRO	SER	SER	SER	SER	G1439	L1370	V1298	I1227	P1164
SER	PRO	PRO	PRO	ASN	A1440	V1371	Y1299	W1228	E1165
TYR	TYR	THR	SER	ASP	F1441	V1372	K1300		D1166
SER	SER	TYR	TYR	ALA	D1442	D1373		D1231	E1167
PRO	PRO	SER	SER	MET	V1443	M1374	W1304	N1232	E1168
THR	THR	SER	PRO	ALA	M1444	M1375	V1305	D1233	I1169
SER	THR	THR	THR	GLY	I1445	T1376	L1306		I1170
PRO	SER	SER	SER	GLY		T1377	E1307	L1236	Q1171
PRO	PRO	PRO	PRO	PHE	E1448	Q1378	T1308	L1237	L1172
TYR	TYR	THR	THR	THR	S1449	G1379	D1309	I1238	H1173
SER	SER	TYR	TYR	ALA	L1450	G1380	G1310	R1239	F1174
PRO	PRO	PRO	SER	TYR	V1451	L1381	V1311	C1240	S1175
THR	THR	PRO	PRO	GLY	K1452	T1382	R1241		LEU
SER	SER	TYR	THR	GLY	S1453	S1382	L1312	W1242	

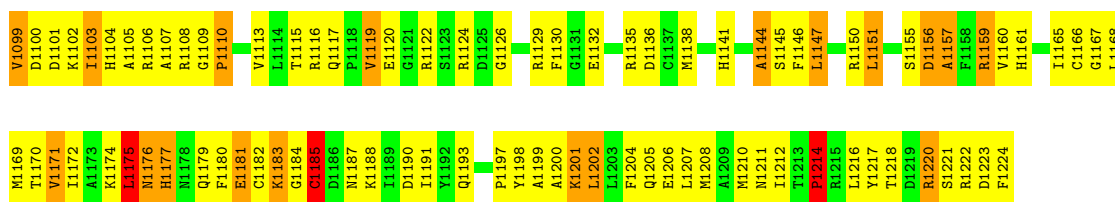
● Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B: 24% 51% 14% 10%

	K257																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
--	------	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--

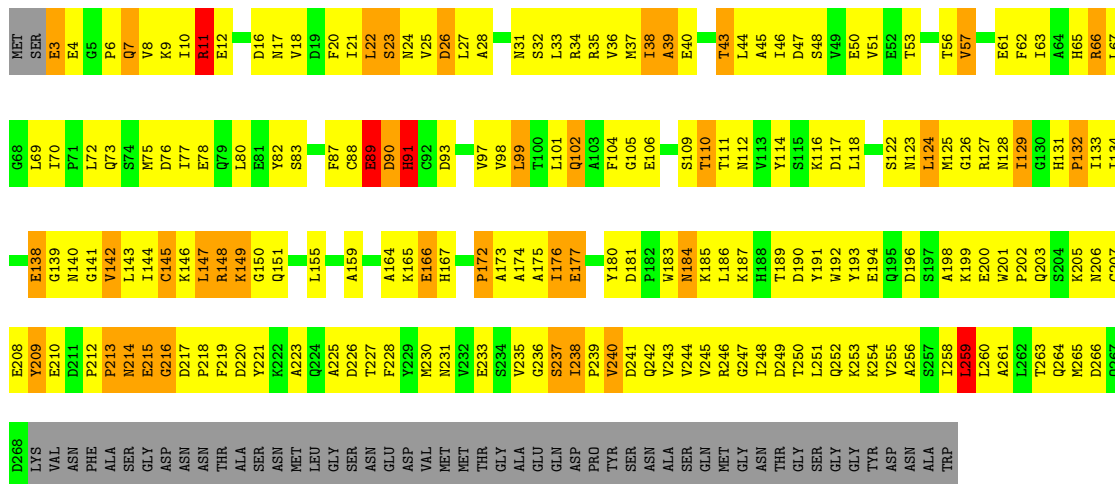


H1025	L1026	I1027	L1028	C1029	L1030	L1031	S1032	K965	V966	R967	V968	R969	T970	T971	P974	Q975	I976	G977	D978	K979	F980	R983	I1050	T1051	V1052	E1053	T989	I990	G991	I992	T993	Y994	Y1064	Q1065	S1066	R1067	G1068	F1069	E1070	V1071	M1072	Y1073	K1079	P1080	D1009	L1010	L1011	L1012	F1086	F1087	N1013	Y1091	R1094	L1095	R1096	L1020	H1097	L1098			
Q957	Q958	D959	G960	L961	K962	F963	V964	K965	R966	R967	V968	R969	T970	T971	P974	Q975	I976	G977	D978	K979	F980	R983	I1050	T1051	V1052	E1053	T989	I990	G991	I992	T993	Y994	Y1064	Q1065	S1066	R1067	G1068	F1069	E1070	V1071	M1072	Y1073	K1079	P1080	D1009	L1010	L1011	L1012	F1086	F1087	N1013	Y1091	R1094	L1095	R1096	L1020	H1097	L1098			
E836	D837	S838	M839	L840	H841	N842	Q843	S844	S845	L846	D847	S848	G849	V850	R851	R852	S853	L854	F855	F856	R857	S858	S859	D860	Q861	Q862	E863	K864	K865	Y866	E867	R868	S869	L870	T871	E872	N873	R874	E875	K876	P877	Q878	R879	ASN	THR	LEU	R884	M885	K886	H887	G888	T889	Y890	D891	K892	L893	D894	D895			
M773	G774	K775	Q776	A777	M778	G779	V780	F781	L782	T783	N784	V785	N786	V787	R788	M789	D790	T791	H792	A793	Y794	Y795	L796	Y797	Y798	Q800	K801	P802	L803	G804	T806	R807	P745	S746	N747	L748	L749	G750	V751	A752	R815	E816	L817	P818	ASN	THR	LEU	R822	A823	R884	M885	K886	H887	G888	T889	Y890	D891	K892	L893	D894	D895
E708	D709	L710	E711	E714	A715	ASN	GLU	GLU	GLU	ASN	ASP	LEU	D722	V723	H724	K727	A728	R729	L730	S731	S732	H733	H734	A735	T736	T737	F738	G741	E742	I743	H744	P745	S746	N747	L748	L749	G750	V751	A752	I756	F757	F758	P759	D760	H761	N762	Q763	S764	F765	R766	L767	Y768	Y769	Q770	S771	A772					
L646	G647	H648	K649	E650	L651	K652	V653	H654	K655	L656	H657	L658	E659	K660	L661	M662	A663	T664	E665	D668	I669	GLU	GLY	GLY	PHE	GLU	ASP	VAL	GLU	E676	H679	T680	H681	S682	S683	L684	L685	N686	E687	G688	L689	V690	E691	Y692	I693	D694	A695	E696	E697	E698	E699	S700	L701	L702	K705	Q706	P707				
V585	W586	V589	H590	H591	S592	F593	A594	R595	L596	M597	L598	E599	T599	L600	R601	N602	L603	R604	R605	K606	D607	D608	L609	M610	P611	S612	S614	M615	L616	R617	D618	L619	F620	L621	K622	E623	L624	K625	L626	F627	D628	D629	A630	G631	R632	V633	Y634	R635	P636	L637	F638	L639	S640	F641	D642	E643	E644	S645			
M516	T517	H518	M519	G520	V521	V522	S523	P524	A525	E526	M527	P528	E529	Q530	Q531	A532	L533	M534	M542	I545	S546	Y547	G548	T549	D550	F557	L558	E559	E560	W561	G562	M563	L566	Y569	P570	H572	G573	Y634	S574	P575	D576	A577	T578	R579	V580	F581	V582	L583	G584	S645											
K451	T452	L453	T454	L457	K458	Y459	A460	L461	G464	M465	D466	E467	E468	Q469	K470	LYS	A472	S474	S475	R476	A477	G478	V479	S480	T487	Y488	S489	S490	T491	L492	L495	R496	R497	T498	T502	GLY	ARG	ALA	ASP	GLY	D576	L508	A509	K510	L578	P511	R512	Q513	L514	H515											
R384	L385	L386	L387	C388	L389	D391	R392	K393	D394	L395	D396	D397	R398	D399	H400	F401	G402	R405	L406	S407	L408	L416	F417	R418	R427	T428	F429	R430	Y431	M432	Q433	R434	T435	V436	E437	GLU	ALA	HIS	ASP	PHE	L508	ASN	MET	LYS	L446	A447	N448	L449	A450												
I323	I324	Q325	L326	R327	A330	L331	D332	F333	L334	G335	R336	ARG	GLY	THR	ALA	LEU	GLY	LYS	E345	E346	K347	R348	I349	Q350	Y351	A352	K353	D354	I355	L356	Q357	E359	F360	L361	P362	H363	T365	Q366	L367	E368	G369	D307	W308	A243	Q309	M310	L311	E312	M313	L314	K315	L378	G379	Y380	N381	L382	N383				
V256	K257	L258	G260	R261	E262	G263	S264	I269	T272	L273	P274	Y275	L276	K277	V211	L212	E216	R217	S218	A219	G220	N221	V222	Q224	V225	F226	K227	K228	L229	P231	G232	P233	I234	S235	H236	V237	A238	E239	I240	R241	S242	A243	L244	E245	K246	G247	L248	S249	F250	K251	S252	T253	L254	Q255							
G127	L128	F129	V130	D131	K134	ARG	THR	GLU	TYR	GLU	GLN	ALA	ASP	VAL	PRO	GLY	ARG	GLU	LEU	LYS	ASP	LYS	TYR	GLU	SER	I90	S91	F92	G93	R94	Y95	Y96	Y97	T98	R99	P100	M101	V102	K164	V165	F166	I167	G168	R169	L170	P171	I172	M173	L174	N178	G179	Y180	L181	T185	R186	S187	D188	L189	Y190	S125	K191
I62	I63	C64	E65	D66	S67	T68	L69	I70	LEU	GLU	GLN	ALA	ASP	GLN	HIS	THR	THR	GLU	SER	ASP	ASN	ILE	GLU	S91	F92	G93	R94	Y95	Y96	Y97	T98	R99	P100	M101	V102	K164	V165	F166	I167	G168	R169	L170	P171	I172	M173	L174	N178	G179	Y180	L181	T185	R186	S187	D188	L189	Y190	S125	K191			



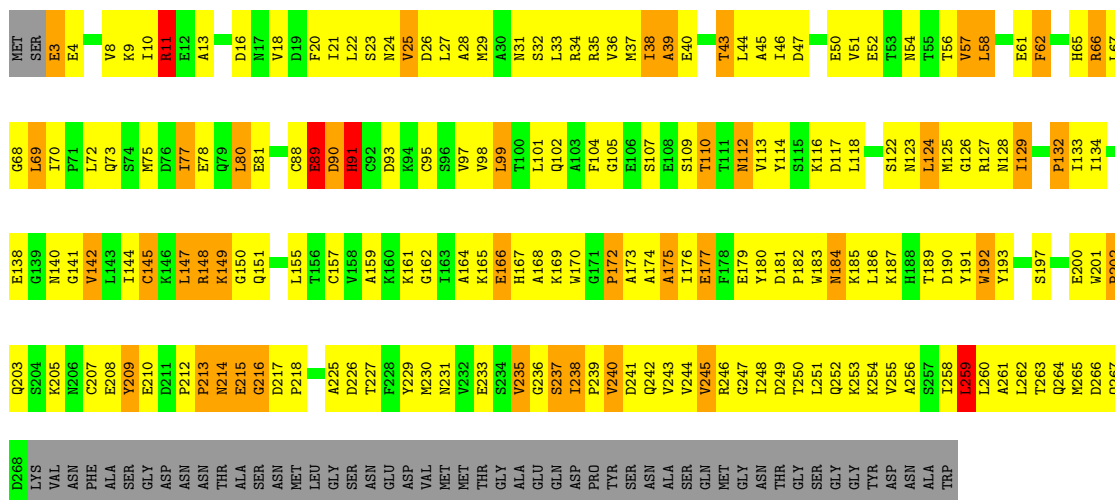
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 23% 48% 11% 16%



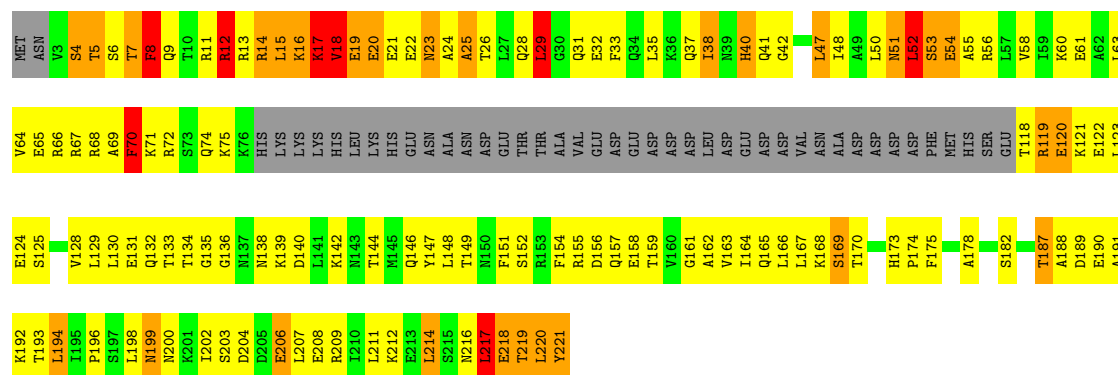
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain O: 25% 45% 13% 16%

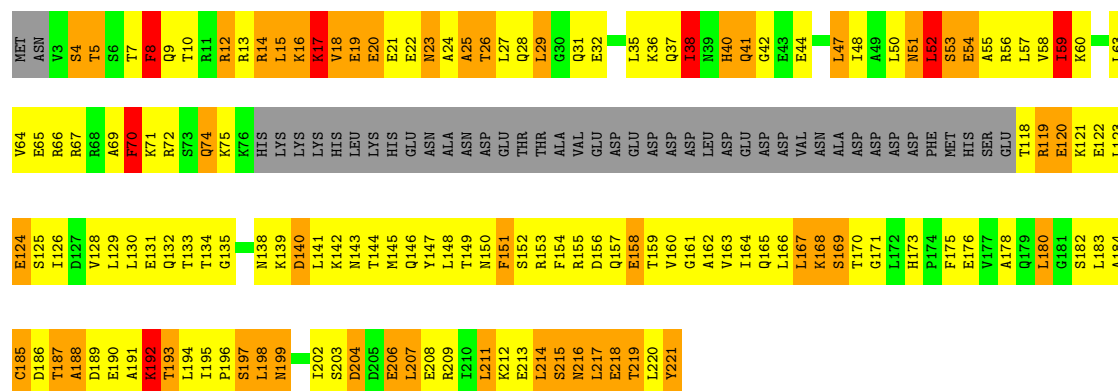


• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

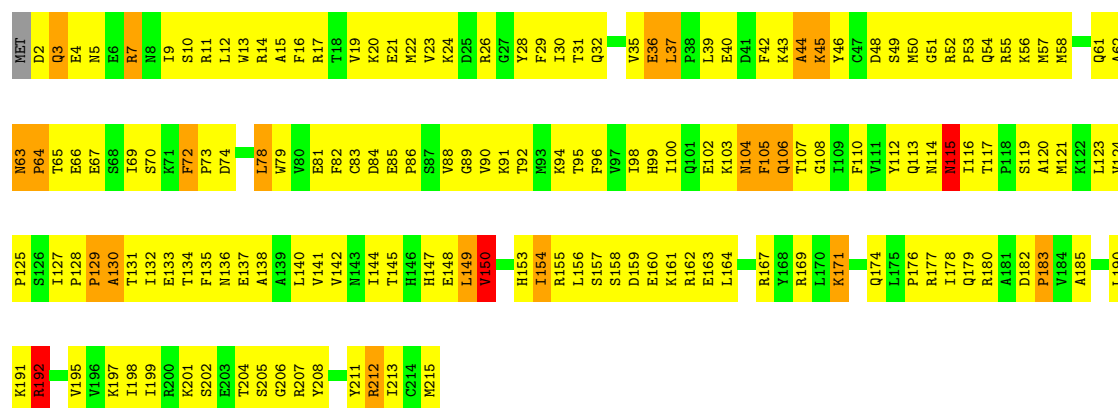
Chain D: 20% 44% 13% 19%



• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



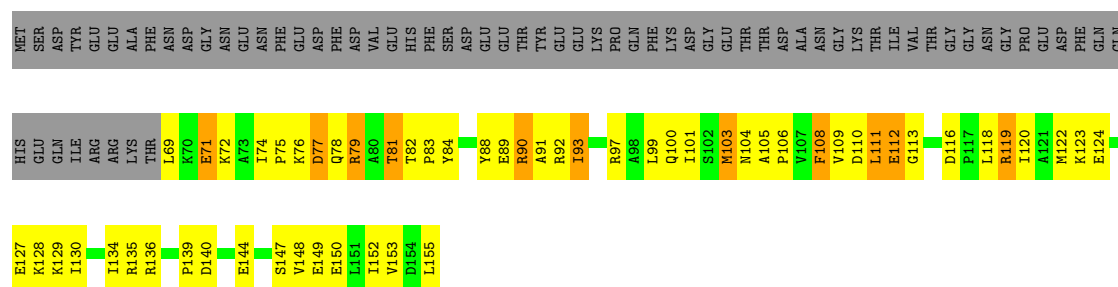
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1





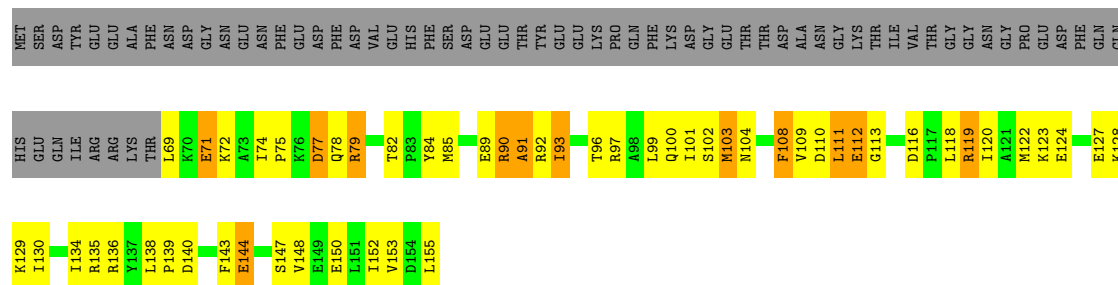
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 19% 30% 7% 44%



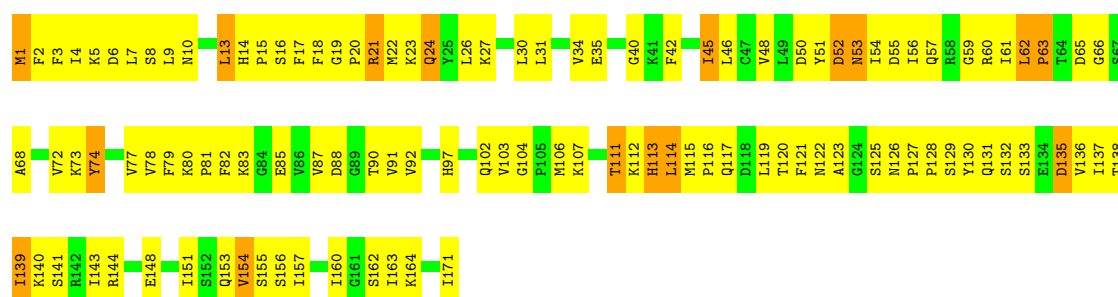
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain R: 21% 28% 8% 44%

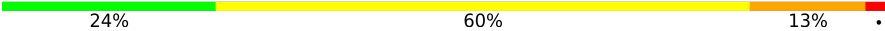


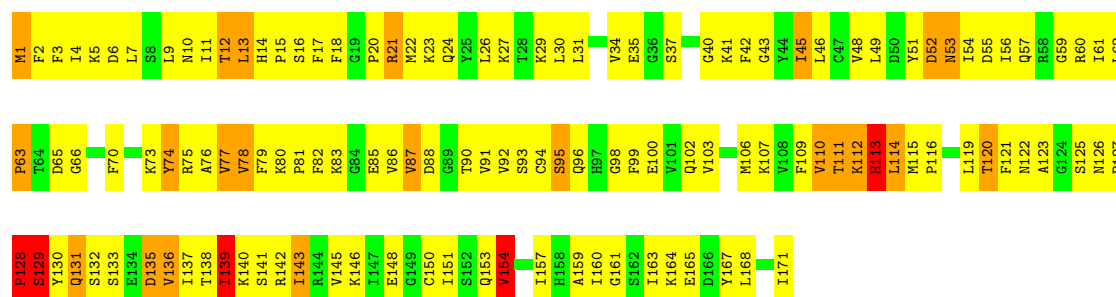
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G: 34% 57% 9%



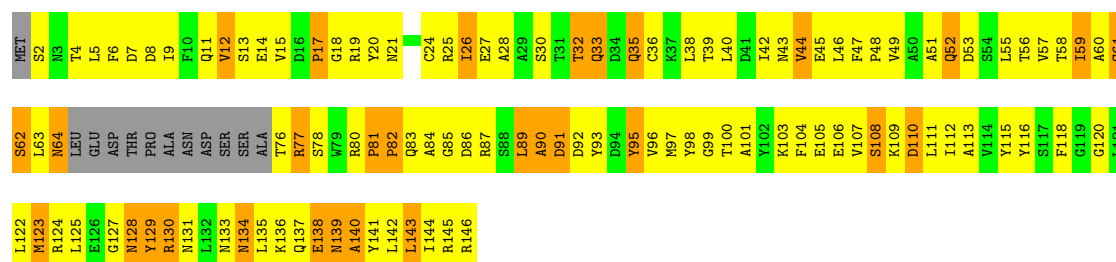
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain S: 



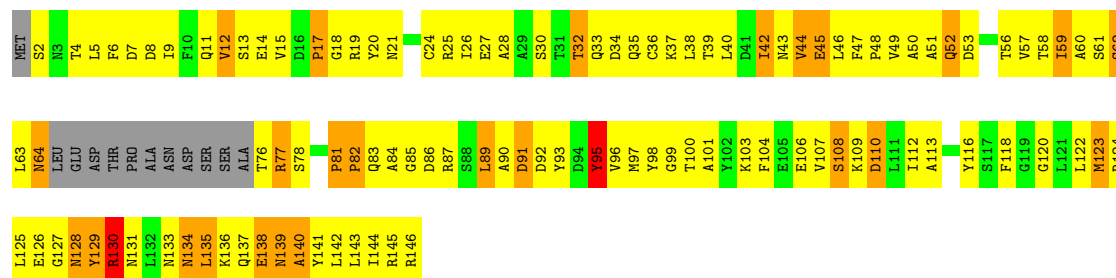
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 

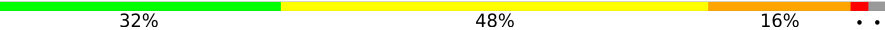


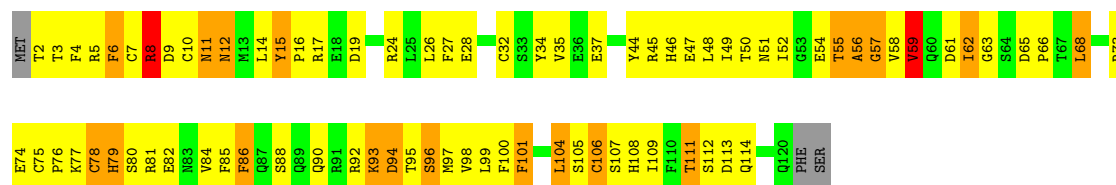
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain T: 

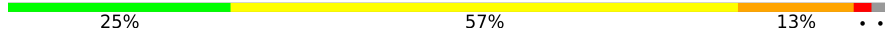


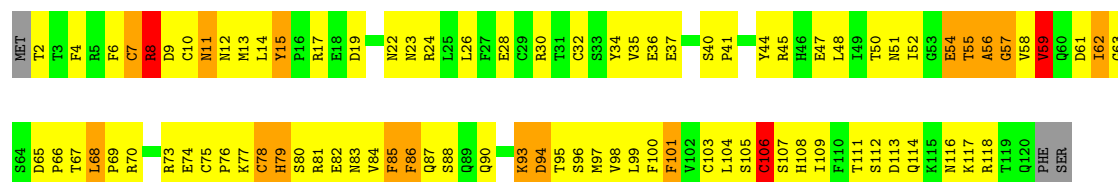
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 

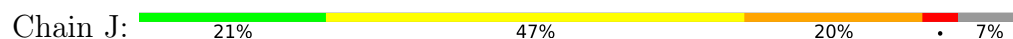


- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

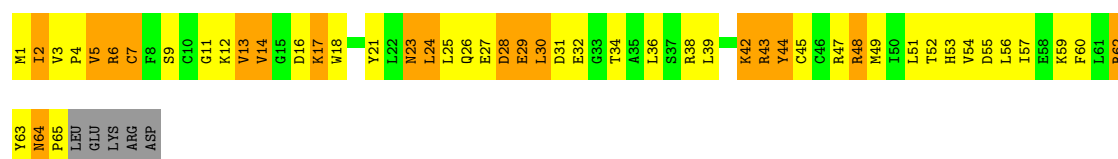
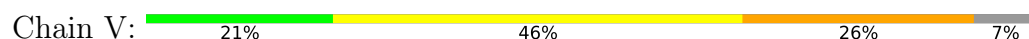
Chain U: 



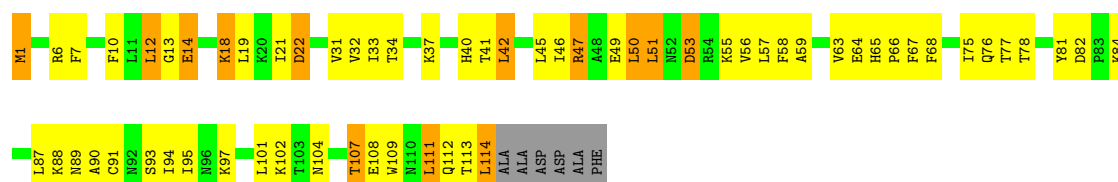
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



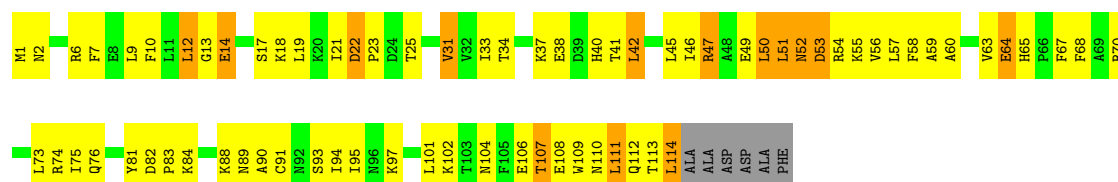
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



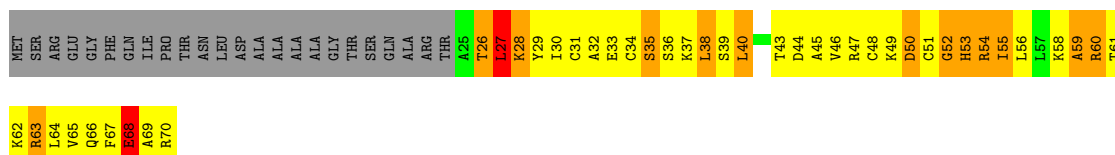
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4





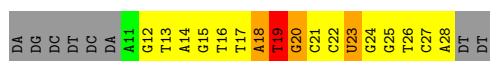
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain X: 6% 39% 19% 34%



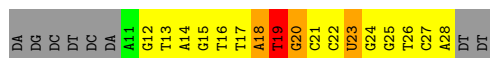
- Molecule 13: 5'-D(*AP*GP*CP*TP*CP*A*AP*GP*TP*AP*GP*TP*TP*AP*TP*GP*CP*C P*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3'

Chain 1: 50% 12% 31%



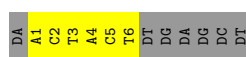
- Molecule 13: 5'-D(*AP*GP*CP*TP*CP*A*AP*GP*TP*AP*GP*TP*TP*AP*TP*GP*CP*C P*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3'

Chain 4: 50% 12% 31%



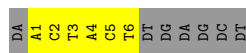
- Molecule 14: 5'-D(*A*AP*CP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'

Chain 2: 46% 54%



- Molecule 14: 5'-D(*A*AP*CP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'

Chain 5: 46% 54%



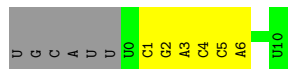
- Molecule 15: 5'-R(*UP*GP*CP*AP*UP*U*UP*CP*GP*AP*CP*CP*AP*GP*GP*CP*U)-3',

Chain 3: 29% 35% 35%



- Molecule 15: 5'-R(*UP*GP*CP*AP*UP*U*UP*CP*GP*AP*CP*CP*AP*GP*GP*CP*U)-3',

Chain 6:  29% 35% 35%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	394.26Å 221.61Å 283.45Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 40.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.6 (40.00-3.20) 90.8 (40.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.233 , 0.252 0.234 , 0.240	Depositor DCC
R_{free} test set	20910 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.017 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.018 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.017 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.017 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.257 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	63664	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.63	3/11342 (0.0%)	1.15	99/15337 (0.6%)
1	M	0.62	1/11342 (0.0%)	1.15	96/15337 (0.6%)
2	B	0.59	0/8948	1.08	55/12062 (0.5%)
2	N	0.58	0/8948	1.09	53/12062 (0.4%)
3	C	0.59	0/2133	1.11	15/2891 (0.5%)
3	O	0.59	0/2133	1.10	13/2891 (0.4%)
4	D	0.51	0/1444	1.15	19/1935 (1.0%)
4	P	0.64	0/1444	1.24	18/1935 (0.9%)
5	E	0.53	0/1788	1.12	12/2406 (0.5%)
5	Q	0.54	0/1788	1.13	11/2406 (0.5%)
6	F	0.70	0/717	1.26	4/967 (0.4%)
6	R	0.68	0/717	1.25	5/967 (0.5%)
7	G	0.54	0/1368	1.15	12/1844 (0.7%)
7	S	0.69	0/1368	1.27	11/1844 (0.6%)
8	H	0.47	0/1094	1.04	4/1481 (0.3%)
8	T	0.47	0/1094	1.04	7/1481 (0.5%)
9	I	0.50	0/989	1.10	6/1331 (0.5%)
9	U	0.50	0/989	1.06	5/1331 (0.4%)
10	J	0.60	0/541	1.09	2/727 (0.3%)
10	V	0.58	0/541	1.04	1/727 (0.1%)
11	K	0.55	0/937	1.00	4/1265 (0.3%)
11	W	0.56	0/937	0.99	5/1265 (0.4%)
12	L	0.64	0/365	1.16	2/485 (0.4%)
12	X	0.63	0/365	1.16	2/485 (0.4%)
13	1	0.40	0/389	1.01	1/597 (0.2%)
13	4	0.39	0/389	1.01	1/597 (0.2%)
14	2	0.36	0/130	0.75	0/198
14	5	0.35	0/130	0.73	0/198
15	3	0.45	0/256	0.79	0/397
15	6	0.45	0/256	0.78	0/397
All	All	0.59	4/64882 (0.0%)	1.12	463/87846 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	N	0	2
13	1	0	4
13	4	0	4
All	All	0	11

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	437	MET	SD-CE	6.51	1.95	1.79
1	M	437	MET	SD-CE	5.76	1.94	1.79
1	A	1398	MET	SD-CE	5.56	1.93	1.79
1	A	55	ASP	CA-C	-5.38	1.46	1.52

All (463) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	71	GLU	N-CA-C	-13.70	95.91	113.17
6	R	71	GLU	N-CA-C	-13.55	96.10	113.17
5	E	5	ASN	N-CA-C	-12.47	97.50	113.72
5	Q	5	ASN	N-CA-C	-12.36	97.65	113.72
1	M	3	GLY	N-CA-C	-11.12	98.93	115.72
1	A	3	GLY	N-CA-C	-11.10	98.89	115.32
2	N	1185	CYS	N-CA-C	-10.97	98.49	114.39
2	B	1185	CYS	N-CA-C	-10.91	98.57	114.39
4	P	26	THR	N-CA-C	-10.48	99.36	112.88
3	C	39	ALA	N-CA-C	10.46	127.11	112.04
7	S	65	ASP	N-CA-C	-10.12	95.48	110.46
4	P	31	GLN	N-CA-C	-10.12	100.20	112.54
5	Q	171	LYS	N-CA-C	-10.03	96.05	110.59
7	G	65	ASP	N-CA-C	-10.01	95.64	110.46
5	E	171	LYS	N-CA-C	-9.99	96.11	110.59
3	O	39	ALA	N-CA-C	9.88	126.27	112.04
2	N	363	HIS	N-CA-C	-9.72	98.13	110.19
4	D	26	THR	N-CA-C	-9.59	99.95	112.41
2	B	363	HIS	N-CA-C	-9.44	98.49	110.19
7	S	62	LEU	CA-C-N	-9.31	108.20	119.84
7	S	62	LEU	C-N-CA	-9.31	108.20	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ALA	N-CA-C	-9.25	100.58	114.64
1	M	288	ALA	N-CA-C	-9.24	100.60	114.64
2	B	473	MET	N-CA-C	-9.21	101.75	113.16
2	N	473	MET	N-CA-C	-9.05	101.94	113.16
2	N	851	PHE	N-CA-C	8.99	123.90	113.38
4	D	31	GLN	N-CA-C	-8.93	101.65	112.54
2	B	296	GLU	N-CA-C	-8.92	101.97	113.12
5	Q	149	LEU	CA-C-N	-8.84	116.59	122.60
5	Q	149	LEU	C-N-CA	-8.84	116.59	122.60
7	G	62	LEU	CA-C-N	-8.79	108.85	119.84
7	G	62	LEU	C-N-CA	-8.79	108.85	119.84
1	A	1256	GLU	N-CA-C	8.78	120.78	111.03
2	B	851	PHE	N-CA-C	8.77	123.56	112.86
2	N	428	ILE	N-CA-C	-8.68	101.77	110.62
2	N	296	GLU	N-CA-C	-8.57	102.41	113.12
2	B	976	ILE	N-CA-C	8.54	119.12	110.23
4	D	38	ILE	N-CA-C	8.52	120.13	108.89
2	B	428	ILE	N-CA-C	-8.49	101.95	110.62
5	E	149	LEU	CA-C-N	-8.46	116.84	122.60
5	E	149	LEU	C-N-CA	-8.46	116.84	122.60
1	M	1311	VAL	N-CA-C	8.42	120.23	107.77
4	D	41	GLN	N-CA-C	-8.38	104.08	112.97
1	M	646	PHE	N-CA-C	-8.38	102.14	111.28
1	M	117	GLU	N-CA-C	-8.38	102.32	112.54
1	A	117	GLU	N-CA-C	-8.32	102.39	112.54
1	A	1311	VAL	N-CA-C	8.25	119.98	107.77
1	A	56	PRO	N-CA-C	-8.21	95.55	112.47
1	M	56	PRO	N-CA-C	-8.19	95.59	112.47
1	A	646	PHE	N-CA-C	-8.16	102.34	111.07
4	P	188	ALA	N-CA-C	-8.04	102.57	112.38
7	S	151	ILE	CB-CA-C	-8.04	103.11	111.23
4	P	72	ARG	N-CA-C	-8.03	102.12	112.23
1	M	1005	GLU	N-CA-C	7.93	119.55	111.07
2	B	901	PRO	N-CA-C	7.92	124.20	113.98
1	A	289	ILE	N-CA-C	-7.91	103.54	110.74
1	A	629	LEU	N-CA-C	-7.88	102.65	111.71
7	G	40	GLY	N-CA-C	-7.88	104.89	114.66
2	N	976	ILE	N-CA-C	7.82	118.36	110.23
4	P	38	ILE	N-CA-C	7.81	119.20	108.89
2	N	628	THR	N-CA-C	-7.75	102.92	113.30
1	A	466	SER	N-CA-C	7.74	121.32	112.57
4	D	72	ARG	N-CA-C	-7.73	102.49	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	466	SER	N-CA-C	7.70	121.27	112.57
10	V	5	VAL	N-CA-C	-7.64	98.80	108.89
10	J	5	VAL	N-CA-C	-7.62	98.83	108.89
3	C	40	GLU	N-CA-C	7.59	122.67	112.88
1	M	629	LEU	N-CA-C	-7.58	102.99	111.71
1	A	1005	GLU	N-CA-C	7.55	119.15	111.07
1	M	242	PRO	CA-C-N	7.52	128.13	120.38
1	M	242	PRO	C-N-CA	7.52	128.13	120.38
1	A	481	ASP	N-CA-C	-7.48	98.55	109.18
4	P	41	GLN	N-CA-C	-7.46	105.06	112.97
1	M	481	ASP	N-CA-C	-7.45	98.60	109.18
1	M	311	GLN	N-CA-C	7.44	126.25	109.81
1	M	289	ILE	N-CA-C	-7.39	104.01	110.74
3	O	40	GLU	N-CA-C	7.36	122.38	112.88
1	A	311	GLN	N-CA-C	7.36	126.07	109.81
1	A	266	LEU	N-CA-C	-7.33	102.68	111.69
2	N	1177	HIS	N-CA-C	-7.30	103.46	112.88
1	M	1104	ILE	N-CA-C	7.29	117.37	110.30
2	B	934	LYS	N-CA-C	7.28	121.30	107.75
1	A	454	SER	N-CA-C	-7.28	104.42	113.38
5	Q	63	ASN	N-CA-C	7.27	119.89	108.55
1	A	875	ALA	N-CA-C	7.23	120.03	111.71
4	P	54	GLU	N-CA-C	-7.21	103.59	112.38
5	E	63	ASN	CA-C-N	7.19	128.83	119.84
5	E	63	ASN	C-N-CA	7.19	128.83	119.84
12	X	68	GLU	N-CA-C	-7.18	99.19	109.96
2	N	41	LYS	N-CA-C	7.17	118.89	111.14
3	C	200	GLU	N-CA-C	7.16	119.17	111.36
7	S	52	ASP	N-CA-C	7.14	119.06	111.28
2	B	628	THR	N-CA-C	-7.12	103.75	113.30
4	D	188	ALA	N-CA-C	-7.12	103.70	112.38
1	A	1258	HIS	N-CA-C	-7.10	103.58	111.82
2	B	41	LYS	N-CA-C	7.09	119.09	111.36
1	M	710	LEU	N-CA-C	-7.09	103.63	111.36
2	N	934	LYS	N-CA-C	7.09	120.93	107.75
1	M	4	GLN	N-CA-C	7.08	125.89	110.80
1	M	829	VAL	N-CA-C	-7.08	105.72	111.81
1	M	266	LEU	N-CA-C	-7.06	102.78	111.40
2	B	1177	HIS	N-CA-C	-7.06	103.78	112.88
5	E	63	ASN	N-CA-C	7.04	119.54	108.55
2	B	555	ILE	N-CA-C	-7.00	103.84	110.42
1	A	281	HIS	N-CA-C	-6.99	103.86	112.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	63	ASN	CA-C-N	6.99	128.57	119.84
5	Q	63	ASN	C-N-CA	6.99	128.57	119.84
2	B	1201	LYS	N-CA-C	-6.93	102.57	111.02
4	P	8	PHE	N-CA-C	6.92	125.55	110.80
12	L	52	GLY	N-CA-C	-6.90	104.50	112.50
11	K	22	ASP	CA-C-N	6.88	128.44	119.84
11	K	22	ASP	C-N-CA	6.88	128.44	119.84
1	A	40	THR	N-CA-C	-6.85	103.43	111.03
2	N	1066	SER	N-CA-C	6.84	119.58	111.71
1	M	281	HIS	N-CA-C	-6.84	104.14	113.30
2	N	1201	LYS	N-CA-C	-6.84	102.91	111.11
2	N	1184	GLY	N-CA-C	-6.83	105.37	114.25
1	M	886	ILE	N-CA-C	6.82	116.83	110.42
1	M	40	THR	N-CA-C	-6.82	103.46	111.03
1	A	1162	VAL	N-CA-C	-6.81	103.81	113.07
1	A	4	GLN	N-CA-C	6.77	125.22	110.80
4	D	8	PHE	N-CA-C	6.76	125.20	110.80
6	F	108	PHE	N-CA-C	6.76	120.42	112.72
1	M	1258	HIS	N-CA-C	-6.75	103.73	112.23
1	M	1389	PHE	N-CA-C	6.74	119.48	111.33
4	P	70	PHE	N-CA-C	-6.73	105.14	113.15
2	B	1066	SER	N-CA-C	6.73	119.45	111.71
1	M	454	SER	N-CA-C	-6.73	104.69	113.17
1	M	227	VAL	CB-CA-C	-6.68	103.86	111.55
12	X	52	GLY	N-CA-C	-6.67	104.77	112.50
1	A	242	PRO	CA-C-N	6.66	127.24	120.38
1	A	242	PRO	C-N-CA	6.66	127.24	120.38
1	A	553	VAL	CA-C-N	6.65	126.35	119.56
1	A	553	VAL	C-N-CA	6.65	126.35	119.56
2	N	801	LYS	N-CA-C	-6.65	101.44	110.36
1	A	320	ARG	CA-C-N	6.65	128.15	119.84
1	A	320	ARG	C-N-CA	6.65	128.15	119.84
2	N	805	THR	N-CA-C	6.64	118.62	109.18
1	M	1162	VAL	N-CA-C	-6.63	104.05	113.07
2	B	829	CYS	N-CA-C	-6.63	99.21	109.76
1	M	553	VAL	CA-C-N	6.63	126.32	119.56
1	M	553	VAL	C-N-CA	6.63	126.32	119.56
12	L	68	GLU	N-CA-C	-6.63	99.22	109.76
2	N	66	ASP	N-CA-C	-6.59	103.73	113.61
4	D	24	ALA	N-CA-C	6.57	117.29	108.23
3	O	112	ASN	N-CA-C	6.56	119.42	108.73
1	M	513	SER	N-CA-C	6.55	117.90	109.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1009	ASP	N-CA-C	-6.54	105.43	113.41
2	B	66	ASP	N-CA-C	-6.54	103.72	112.94
2	N	829	CYS	N-CA-C	-6.54	99.37	109.76
2	N	555	ILE	N-CA-C	-6.53	104.28	110.42
1	A	1403	GLU	N-CA-C	6.53	124.71	110.80
1	M	1403	GLU	N-CA-C	6.52	124.69	110.80
2	N	43	LEU	N-CA-C	6.51	120.81	112.34
1	M	320	ARG	CA-C-N	6.48	127.94	119.84
1	M	320	ARG	C-N-CA	6.48	127.94	119.84
3	O	200	GLU	N-CA-C	6.47	118.42	111.36
1	M	505	CYS	N-CA-C	6.47	120.55	111.30
3	O	91	HIS	N-CA-C	6.47	118.38	108.42
1	M	398	GLU	N-CA-C	-6.46	102.01	110.53
8	H	35	GLN	N-CA-C	-6.46	106.04	114.04
1	A	710	LEU	N-CA-C	-6.43	104.36	111.36
2	N	903	VAL	N-CA-C	6.41	118.02	109.37
2	B	43	LEU	N-CA-C	6.40	120.67	112.34
7	G	52	ASP	N-CA-C	6.40	118.25	111.28
1	A	829	VAL	N-CA-C	-6.38	105.61	111.67
1	M	173	THR	N-CA-C	-6.38	99.49	109.25
11	W	18	LYS	N-CA-C	-6.38	104.25	111.07
1	M	1405	THR	N-CA-C	6.37	124.37	110.80
1	A	966	ASN	N-CA-C	-6.35	104.28	111.14
1	A	513	SER	N-CA-C	6.32	117.62	109.65
11	K	18	LYS	N-CA-C	-6.32	104.31	111.07
2	B	1009	ASP	N-CA-C	-6.32	105.70	113.41
9	I	68	LEU	CA-C-N	6.31	126.22	119.85
9	I	68	LEU	C-N-CA	6.31	126.22	119.85
6	R	108	PHE	N-CA-C	6.30	119.90	112.72
7	G	135	ASP	N-CA-C	6.28	119.02	110.55
5	E	150	VAL	N-CA-C	6.26	113.26	107.56
2	B	1184	GLY	N-CA-C	-6.25	106.12	114.25
3	O	259	LEU	N-CA-C	-6.25	104.16	110.97
2	B	805	THR	N-CA-C	6.22	118.02	109.18
1	A	1405	THR	N-CA-C	6.22	124.05	110.80
2	B	903	VAL	N-CA-C	6.22	117.77	109.37
1	M	243	PRO	CA-C-N	6.22	126.78	120.38
1	M	243	PRO	C-N-CA	6.22	126.78	120.38
1	M	143	LYS	N-CA-C	-6.21	104.06	111.69
3	O	89	GLU	N-CA-C	-6.20	99.06	108.67
3	C	259	LEU	N-CA-C	-6.19	104.22	110.97
2	B	1084	GLN	N-CA-C	-6.18	100.11	109.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	85	PHE	N-CA-C	6.18	119.56	110.59
8	H	21	ASN	N-CA-C	6.16	120.35	112.34
3	C	91	HIS	N-CA-C	6.16	117.90	108.42
4	P	51	ASN	N-CA-C	-6.14	102.42	110.53
2	B	292	ILE	N-CA-C	6.12	122.11	108.88
11	W	22	ASP	CA-C-N	6.11	127.48	119.84
11	W	22	ASP	C-N-CA	6.11	127.48	119.84
1	A	1104	ILE	N-CA-C	6.11	116.22	110.30
1	M	1421	CYS	N-CA-C	-6.10	103.74	111.92
4	P	169	SER	N-CA-C	-6.10	106.82	114.56
7	S	40	GLY	N-CA-C	-6.10	105.20	113.37
3	C	89	GLU	N-CA-C	-6.09	99.23	108.67
2	B	801	LYS	N-CA-C	-6.08	101.90	110.29
4	D	54	GLU	N-CA-C	-6.06	104.74	111.71
1	A	398	GLU	N-CA-C	-6.05	102.54	110.53
7	S	133	SER	N-CA-C	-6.05	103.85	111.11
1	M	598	LEU	N-CA-C	-6.04	103.26	112.99
4	P	12	ARG	N-CA-C	6.04	119.12	110.24
2	N	606	LYS	N-CA-C	-6.04	106.45	113.88
1	A	505	CYS	N-CA-C	6.03	119.92	111.30
1	A	1389	PHE	N-CA-C	6.03	118.62	111.33
3	C	38	ILE	CB-CA-C	-6.02	104.15	112.04
1	A	243	PRO	CA-C-N	6.02	126.58	120.38
1	A	243	PRO	C-N-CA	6.02	126.58	120.38
2	B	603	LEU	N-CA-C	-6.02	105.02	112.90
2	N	681	TRP	N-CA-C	-6.01	103.38	112.04
5	Q	150	VAL	N-CA-C	6.00	113.02	107.56
2	N	603	LEU	N-CA-C	-6.00	105.04	112.90
1	A	598	LEU	N-CA-C	-6.00	103.34	112.99
1	A	23	SER	N-CA-C	-5.99	102.51	109.93
6	R	103	MET	N-CA-C	-5.96	106.06	113.15
1	A	1163	ILE	CA-C-N	5.96	125.16	118.97
1	A	1163	ILE	C-N-CA	5.96	125.16	118.97
1	A	362	ASP	N-CA-C	5.93	120.13	113.02
8	T	35	GLN	N-CA-C	-5.92	106.69	114.04
1	M	875	ALA	N-CA-C	5.91	119.59	112.38
3	O	38	ILE	CB-CA-C	-5.90	104.31	112.04
6	R	77	ASP	N-CA-C	-5.90	100.94	110.32
4	D	7	THR	N-CA-C	5.89	117.22	107.20
2	N	978	ASP	N-CA-C	5.89	118.77	110.23
4	D	169	SER	N-CA-C	-5.87	107.11	114.56
1	A	1444	MET	N-CA-C	5.87	118.77	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1144	ALA	N-CA-C	5.86	117.36	110.97
2	N	1101	ASP	N-CA-C	-5.86	105.45	113.30
9	U	8	ARG	N-CA-C	-5.86	98.33	110.80
9	U	85	PHE	N-CA-C	5.85	119.08	110.59
1	A	998	LEU	N-CA-C	5.85	118.94	110.28
1	M	539	THR	N-CA-C	5.85	117.57	109.15
2	N	1084	GLN	N-CA-C	-5.83	100.67	109.95
2	N	1130	PHE	N-CA-C	-5.83	96.91	107.75
2	N	292	ILE	N-CA-C	5.82	121.45	108.88
1	M	279	LEU	N-CA-C	-5.80	106.06	114.12
2	B	1130	PHE	N-CA-C	-5.79	96.98	107.75
2	B	825	VAL	N-CA-C	5.78	116.27	108.17
4	P	217	LEU	N-CA-C	-5.78	104.83	112.34
8	H	45	GLU	N-CA-C	-5.78	106.27	113.55
3	C	112	ASN	N-CA-C	5.78	118.14	108.73
1	A	173	THR	N-CA-C	-5.77	100.42	109.25
2	B	707	PRO	N-CA-C	-5.77	105.22	113.47
2	B	681	TRP	N-CA-C	-5.77	103.73	112.04
2	N	1013	ASN	N-CA-C	5.76	117.95	109.42
7	G	104	GLY	CA-C-N	5.76	125.38	119.56
7	G	104	GLY	C-N-CA	5.76	125.38	119.56
1	A	1421	CYS	N-CA-C	-5.74	104.23	111.92
9	I	8	ARG	N-CA-C	-5.74	98.58	110.80
2	N	526	GLU	N-CA-C	5.73	118.08	108.23
8	T	34	ASP	N-CA-C	-5.72	106.90	112.97
1	A	337	ARG	N-CA-C	5.72	118.29	111.71
1	A	886	ILE	N-CA-C	5.71	115.90	110.53
1	M	31	SER	N-CA-C	5.71	118.75	110.42
1	M	78	PRO	N-CA-C	-5.71	100.72	112.47
9	U	68	LEU	N-CA-C	5.70	117.00	109.93
1	A	1269	GLU	N-CA-C	5.70	117.14	110.41
1	M	931	GLU	N-CA-C	-5.69	105.15	111.36
1	M	1169	ILE	N-CA-C	5.68	121.16	109.34
1	M	1163	ILE	CA-C-N	5.67	124.87	118.97
1	M	1163	ILE	C-N-CA	5.67	124.87	118.97
1	A	567	LYS	CA-C-N	-5.67	112.75	119.84
1	A	567	LYS	C-N-CA	-5.67	112.75	119.84
1	M	1269	GLU	N-CA-C	5.67	117.10	110.41
1	A	1169	ILE	N-CA-C	5.67	121.13	109.34
7	G	63	PRO	N-CA-C	5.67	124.14	112.47
2	B	606	LYS	N-CA-C	-5.66	106.92	113.88
2	N	513	GLN	N-CA-C	5.65	118.18	110.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	526	GLU	N-CA-C	5.65	117.94	108.23
9	U	68	LEU	CA-C-N	5.64	125.55	119.85
9	U	68	LEU	C-N-CA	5.64	125.55	119.85
2	N	423	LYS	N-CA-C	-5.64	105.13	112.23
8	H	110	ASP	N-CA-C	-5.63	104.65	112.03
11	K	68	PHE	N-CA-C	5.62	117.58	108.41
1	A	78	PRO	N-CA-C	-5.62	100.90	112.47
1	A	440	ASP	N-CA-C	-5.60	102.99	109.93
7	S	135	ASP	N-CA-C	5.60	117.75	110.53
1	M	582	ILE	CA-C-N	5.59	126.38	120.11
1	M	582	ILE	C-N-CA	5.59	126.38	120.11
1	M	567	LYS	CA-C-N	-5.59	112.85	119.84
1	M	567	LYS	C-N-CA	-5.59	112.85	119.84
11	W	68	PHE	N-CA-C	5.59	117.52	108.41
2	B	127	GLY	N-CA-C	5.58	119.14	111.54
7	G	133	SER	N-CA-C	-5.58	104.41	111.11
3	O	80	LEU	N-CA-C	-5.58	100.79	109.72
1	A	143	LYS	N-CA-C	-5.58	104.83	111.69
1	M	1445	ILE	CB-CA-C	-5.57	103.91	111.15
1	M	234	MET	N-CA-C	-5.57	106.33	113.01
1	M	865	GLN	N-CA-C	-5.56	98.85	108.69
1	A	31	SER	N-CA-C	5.56	118.53	110.42
1	A	227	VAL	N-CA-C	5.56	116.59	111.81
1	A	30	ILE	CB-CA-C	-5.55	104.86	111.97
2	B	891	ASP	N-CA-C	5.55	117.77	111.11
2	N	330	ALA	N-CA-C	-5.54	105.14	111.07
2	N	112	LEU	N-CA-C	5.54	117.45	110.24
1	M	1444	MET	N-CA-C	5.54	118.25	109.50
7	S	63	PRO	N-CA-C	5.53	123.87	112.47
2	N	127	GLY	N-CA-C	5.53	119.06	111.54
2	N	901	PRO	N-CA-C	5.52	123.84	112.47
4	D	70	PHE	N-CA-C	-5.52	106.58	113.15
2	B	330	ALA	N-CA-C	-5.52	105.17	111.07
1	A	55	ASP	N-CA-C	5.50	121.97	109.81
2	B	1101	ASP	N-CA-C	-5.50	105.93	113.30
2	N	498	THR	N-CA-C	5.50	118.52	109.72
4	P	180	LEU	CA-CB-CG	-5.50	97.05	116.30
1	A	1294	PRO	N-CA-C	-5.49	106.37	113.57
1	M	847	ASP	N-CA-C	5.48	120.93	113.37
1	A	539	THR	N-CA-C	5.48	117.04	109.15
2	N	39	ARG	N-CA-C	-5.48	104.54	111.11
8	T	110	ASP	N-CA-C	-5.47	104.86	112.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	GLY	N-CA-C	5.46	126.13	113.18
1	A	847	ASP	N-CA-C	5.45	120.90	113.37
1	M	966	ASN	N-CA-C	-5.45	105.25	111.14
1	A	227	VAL	CB-CA-C	-5.45	105.28	111.55
1	M	23	SER	N-CA-C	-5.45	103.20	110.07
2	B	978	ASP	N-CA-C	5.45	118.13	110.23
1	M	239	LEU	N-CA-C	5.43	116.80	109.24
3	O	247	GLY	N-CA-C	-5.43	106.20	112.50
1	A	228	PHE	N-CA-C	5.42	120.17	113.50
1	M	321	PRO	N-CA-C	5.42	123.64	112.47
4	D	12	ARG	N-CA-C	5.42	118.21	110.24
1	M	599	SER	CA-C-N	5.42	124.76	118.85
1	M	599	SER	C-N-CA	5.42	124.76	118.85
2	N	707	PRO	N-CA-C	-5.42	105.72	113.47
1	A	74	MET	N-CA-C	5.42	122.34	110.80
4	P	25	ALA	N-CA-C	-5.42	107.23	112.97
1	M	999	VAL	N-CA-C	-5.41	107.58	112.12
1	M	55	ASP	N-CA-C	5.41	121.76	109.81
1	M	226	GLU	N-CA-C	5.40	118.66	111.75
1	A	1424	VAL	CB-CA-C	-5.40	104.97	111.88
2	B	580	VAL	N-CA-C	5.40	116.35	108.58
8	T	13	SER	N-CA-C	-5.40	105.29	111.07
1	M	1294	PRO	N-CA-C	-5.39	106.51	113.57
1	M	1341	ILE	N-CA-C	5.39	116.77	110.62
2	B	498	THR	N-CA-C	5.38	118.33	109.72
3	C	192	TRP	N-CA-C	-5.38	102.56	110.52
1	M	472	LEU	N-CA-C	5.38	117.84	111.33
2	B	693	ILE	CB-CA-C	-5.37	104.43	111.25
5	Q	105	PHE	CA-C-O	5.37	121.06	117.94
2	N	807	ARG	N-CA-C	-5.37	104.88	111.75
7	G	129	SER	N-CA-C	5.36	116.42	108.86
1	A	513	SER	CA-C-N	5.36	125.83	120.04
1	A	513	SER	C-N-CA	5.36	125.83	120.04
2	N	736	THR	N-CA-C	-5.36	106.50	114.64
4	D	51	ASN	N-CA-C	-5.36	103.46	110.53
13	4	19	DT	N1-C1'-C2'	-5.35	105.47	113.50
6	F	77	ASP	N-CA-C	-5.34	101.83	110.32
1	M	636	GLU	N-CA-C	5.34	117.18	111.36
3	O	191	TYR	N-CA-C	5.34	117.77	110.24
9	I	68	LEU	N-CA-C	5.33	116.54	109.93
1	M	362	ASP	N-CA-C	5.32	119.41	113.02
1	A	1339	LEU	N-CA-C	5.32	119.76	113.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1013	ASN	N-CA-C	5.32	117.30	109.42
1	M	535	THR	N-CA-C	5.32	119.84	112.45
3	C	7	GLN	N-CA-C	5.32	118.39	110.52
1	A	279	LEU	N-CA-C	-5.30	106.75	114.12
2	B	896	ASP	N-CA-C	-5.30	106.58	113.16
1	M	74	MET	N-CA-C	5.30	122.10	110.80
1	A	1102	LYS	N-CA-C	-5.30	105.40	111.07
2	B	423	LYS	N-CA-C	-5.30	105.55	112.23
2	B	1034	VAL	N-CA-C	-5.30	105.44	110.42
2	B	736	THR	N-CA-C	-5.30	106.59	114.64
5	Q	177	ARG	N-CA-C	5.30	117.70	110.55
1	M	174	ILE	N-CA-C	5.29	116.60	108.71
2	N	693	ILE	CB-CA-C	-5.29	104.53	111.25
1	A	85	ASP	N-CA-C	-5.29	101.82	109.59
7	S	139	ILE	N-CA-C	5.29	120.33	109.34
3	C	191	TYR	N-CA-C	5.28	117.69	110.24
3	O	173	ALA	N-CA-C	5.28	119.22	111.04
1	A	54	ASN	CA-C-N	5.28	134.67	121.80
1	A	54	ASN	C-N-CA	5.28	134.67	121.80
1	A	582	ILE	CA-C-N	5.27	126.02	120.11
1	A	582	ILE	C-N-CA	5.27	126.02	120.11
3	C	87	PHE	N-CA-C	5.27	119.58	113.20
2	N	858	SER	N-CA-C	5.27	117.25	108.02
5	Q	55	ARG	N-CA-C	5.27	117.02	111.28
1	M	331	GLY	N-CA-C	5.26	125.65	113.18
4	D	25	ALA	N-CA-C	-5.26	106.63	112.57
3	O	192	TRP	N-CA-C	-5.26	102.74	110.52
5	E	105	PHE	CA-C-O	5.26	120.99	117.94
1	A	55	ASP	N-CA-CB	5.25	119.72	110.37
1	M	998	LEU	N-CA-C	5.25	118.05	110.28
1	A	158	PRO	N-CA-C	-5.24	107.91	114.20
6	R	91	ALA	N-CA-C	-5.24	105.46	111.07
4	P	18	VAL	N-CA-C	5.24	115.40	107.75
1	A	321	PRO	N-CA-C	5.24	123.25	112.47
1	A	599	SER	CA-C-N	5.23	124.55	118.85
1	A	599	SER	C-N-CA	5.23	124.55	118.85
2	B	650	GLU	N-CA-C	5.23	117.02	108.76
1	M	3	GLY	CA-C-N	5.23	131.52	121.54
1	M	3	GLY	C-N-CA	5.23	131.52	121.54
1	A	916	GLY	N-CA-C	5.22	119.45	112.77
13	1	19	DT	N1-C1'-C2'	-5.22	105.67	113.50
4	P	171	GLY	N-CA-C	-5.22	108.04	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	29	LEU	N-CA-C	-5.22	103.02	110.59
2	N	1099	VAL	N-CA-C	5.22	115.84	110.36
4	P	59	ILE	CB-CA-C	-5.21	105.29	111.81
2	N	366	GLN	N-CA-C	-5.21	106.31	113.30
1	M	1339	LEU	N-CA-C	5.21	119.62	113.16
2	B	492	LEU	N-CA-C	-5.21	105.29	110.97
1	M	227	VAL	N-CA-C	5.20	116.28	111.81
5	E	105	PHE	CB-CA-C	-5.20	109.59	117.07
1	M	683	ILE	N-CA-C	-5.19	105.78	110.82
4	D	217	LEU	N-CA-C	-5.18	105.60	112.34
1	M	54	ASN	CA-C-N	5.18	134.44	121.80
1	M	54	ASN	C-N-CA	5.18	134.44	121.80
2	N	1034	VAL	N-CA-C	-5.18	105.55	110.42
1	M	834	THR	N-CA-C	-5.17	104.90	111.11
8	T	45	GLU	N-CA-C	-5.17	107.03	113.55
1	M	337	ARG	N-CA-C	5.17	117.65	111.71
2	B	112	LEU	N-CA-C	5.16	116.95	110.24
1	A	636	GLU	N-CA-C	5.16	116.71	111.14
6	F	103	MET	N-CA-C	-5.15	107.02	113.15
8	T	130	ARG	N-CA-C	-5.14	105.73	112.72
1	A	472	LEU	N-CA-C	5.14	118.33	111.75
4	D	194	LEU	N-CA-C	-5.14	107.01	113.28
2	N	990	ILE	N-CA-C	-5.14	104.40	110.21
1	A	1155	ASP	CA-C-N	5.14	125.59	120.04
1	A	1155	ASP	C-N-CA	5.14	125.59	120.04
1	M	142	CYS	N-CA-C	5.12	118.36	112.57
2	B	427	ASP	N-CA-C	-5.11	99.92	110.80
2	N	896	ASP	N-CA-C	-5.11	106.83	113.16
9	I	104	LEU	N-CA-C	-5.11	107.05	113.28
3	C	80	LEU	N-CA-C	-5.10	101.56	109.72
2	N	348	ARG	N-CA-C	5.10	116.52	111.07
1	A	1113	THR	CA-C-N	-5.09	113.47	119.84
1	A	1113	THR	C-N-CA	-5.09	113.47	119.84
2	B	348	ARG	N-CA-C	5.09	116.52	111.07
1	M	1403	GLU	CA-C-N	-5.08	115.59	123.17
1	M	1403	GLU	C-N-CA	-5.08	115.59	123.17
11	W	52	ASN	N-CA-C	-5.08	107.03	113.43
1	A	865	GLN	N-CA-C	-5.08	99.70	108.69
4	D	18	VAL	N-CA-C	5.08	115.28	107.77
1	M	916	GLY	N-CA-C	5.07	119.27	112.77
10	J	3	VAL	CB-CA-C	-5.07	105.91	110.88
2	B	1135	ARG	N-CA-C	-5.07	105.65	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	129	SER	N-CA-C	5.07	116.00	108.86
1	A	174	ILE	N-CA-C	5.06	116.25	108.71
3	C	247	GLY	N-CA-C	-5.06	106.64	112.50
2	B	935	ARG	N-CA-C	-5.05	100.93	109.07
8	T	21	ASN	N-CA-C	5.05	118.90	112.34
1	A	3	GLY	CA-C-N	5.04	131.17	121.54
1	A	3	GLY	C-N-CA	5.04	131.17	121.54
2	B	807	ARG	N-CA-C	-5.04	105.30	111.75
1	A	425	GLN	N-CA-C	-5.04	100.08	108.34
1	M	1170	ILE	N-CA-C	5.04	115.16	110.42
2	N	427	ASP	N-CA-C	-5.04	100.07	110.80
5	E	95	THR	CA-C-N	5.03	127.34	120.54
5	E	95	THR	C-N-CA	5.03	127.34	120.54
2	B	1015	HIS	N-CA-C	5.03	118.51	112.38
1	A	234	MET	N-CA-C	-5.03	106.41	112.54
1	A	1403	GLU	CA-C-N	-5.03	115.68	123.17
1	A	1403	GLU	C-N-CA	-5.03	115.68	123.17
1	M	158	PRO	N-CA-C	-5.02	108.17	114.20
3	C	173	ALA	N-CA-C	5.02	118.83	111.04
1	M	1016	THR	N-CA-C	5.02	117.15	111.02
2	B	1099	VAL	N-CA-C	5.02	115.63	110.36
7	G	114	LEU	N-CA-C	-5.01	105.88	112.94

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	1	18	DA	Sidechain
13	1	19	DT	Sidechain
13	1	20	DG	Sidechain
13	1	21	DC	Sidechain
13	4	18	DA	Sidechain
13	4	19	DT	Sidechain
13	4	20	DG	Sidechain
13	4	21	DC	Sidechain
2	B	833	TYR	Sidechain
2	N	431	TYR	Sidechain
2	N	797	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11143	0	11217	1232	0
1	M	11143	0	11217	1236	0
2	B	8779	0	8808	1124	0
2	N	8779	0	8808	1136	0
3	C	2095	0	2051	244	0
3	O	2095	0	2051	246	0
4	D	1434	0	1460	165	0
4	P	1434	0	1460	288	0
5	E	1752	0	1776	198	0
5	Q	1752	0	1776	217	0
6	F	705	0	731	88	0
6	R	705	0	731	79	0
7	G	1340	0	1357	154	0
7	S	1340	0	1357	212	0
8	H	1076	0	1046	178	0
8	T	1076	0	1046	163	0
9	I	971	0	929	128	0
9	U	971	0	929	137	0
10	J	532	0	542	98	0
10	V	532	0	542	98	0
11	K	919	0	929	84	0
11	W	919	0	929	88	0
12	L	363	0	387	89	0
12	X	363	0	387	89	0
13	1	368	0	203	25	0
13	4	368	0	203	23	0
14	2	117	0	70	13	0
14	5	117	0	70	11	0
15	3	230	0	121	8	0
15	6	230	0	121	8	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
16	M	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	N	1	0	0	0	0
16	O	1	0	0	0	0
16	U	2	0	0	0	0
16	V	1	0	0	0	0
16	X	1	0	0	0	0
All	All	63664	0	63254	7250	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 57.

All (7250) 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:N:510:LYS:HG3	2:N:511:PRO:HD3	1.21	1.17
1:A:855:THR:HG21	1:A:857:ARG:HE	1.08	1.16
9:U:111:THR:HG22	9:U:113:ASP:H	1.05	1.15
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.23	1.15
5:Q:124:VAL:HG13	5:Q:132:ILE:HB	1.28	1.15
8:H:4:THR:HA	8:H:60:ALA:HB2	1.26	1.14
1:M:855:THR:HG21	1:M:857:ARG:HE	1.03	1.14
9:I:111:THR:HG22	9:I:113:ASP:H	1.05	1.14
3:O:57:VAL:HG11	10:V:60:PHE:HB3	1.26	1.14
2:N:102:VAL:HG23	2:N:112:LEU:HB2	1.30	1.14
8:T:4:THR:HA	8:T:60:ALA:HB2	1.27	1.13
1:A:53:LEU:HD23	1:A:54:ASN:H	1.03	1.12
2:B:508:LEU:N	14:2:1:DA:HO5'	1.49	1.10
1:M:1420:ASP:HB3	1:M:1422:ARG:HG3	1.33	1.10
2:N:710:LEU:HA	2:N:733:HIS:HB3	1.33	1.09
1:M:351:THR:HG22	2:N:1103:ILE:HA	1.35	1.09
3:C:177:GLU:HG3	3:C:231:ASN:HB3	1.33	1.09
1:A:567:LYS:HB3	8:H:96:VAL:H	1.12	1.08
2:B:559:SER:HA	2:B:563:MET:HB3	1.33	1.08
1:M:1161:THR:HG22	1:M:1163:ILE:H	1.12	1.08
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.35	1.07
1:M:41:MET:HB3	1:M:49:LYS:HA	1.33	1.07
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.31	1.07
2:N:559:SER:HA	2:N:563:MET:HB3	1.34	1.07
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.33	1.07
7:G:111:THR:HG23	7:G:114:LEU:HB2	1.35	1.07
13:1:25:DG:H2''	13:1:26:DT:H71	1.31	1.07
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.33	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:4:25:DG:H2"	13:4:26:DT:H71	1.30	1.06
1:M:53:LEU:HD23	1:M:54:ASN:N	1.69	1.06
2:N:622:LYS:HE2	9:U:59:VAL:HG22	1.34	1.06
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.12	1.06
5:Q:197:LYS:HE2	5:Q:199:ILE:HD11	1.36	1.06
1:A:41:MET:HB3	1:A:49:LYS:HA	1.33	1.06
1:A:107:CYS:HA	1:A:171:GLN:HE22	1.18	1.06
1:M:53:LEU:CD2	1:M:54:ASN:H	1.68	1.05
1:M:108:MET:HA	1:M:210:ILE:HD13	1.37	1.05
1:M:567:LYS:HB3	8:T:96:VAL:H	1.18	1.05
2:N:521:LEU:HD22	2:N:633:VAL:HG12	1.35	1.05
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.33	1.05
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.36	1.05
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.30	1.04
5:E:197:LYS:HE2	5:E:199:ILE:HD11	1.37	1.04
12:L:26:THR:HG22	12:L:27:LEU:H	1.21	1.04
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.38	1.04
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.37	1.04
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.37	1.03
1:M:53:LEU:HD23	1:M:54:ASN:H	0.87	1.03
1:M:353:ILE:HG21	1:M:487:MET:HG3	1.41	1.03
5:E:117:THR:HG22	5:E:119:SER:H	1.23	1.02
2:N:516:ASN:H	2:N:516:ASN:HD22	1.04	1.02
2:N:114:PRO:HG3	2:N:181:LEU:HD11	1.36	1.02
2:N:516:ASN:HD22	2:N:516:ASN:N	1.57	1.02
2:N:583:ASN:HD21	2:N:628:THR:HG22	1.19	1.01
12:X:26:THR:HG22	12:X:27:LEU:H	1.21	1.01
1:A:671:ALA:HB3	1:A:676:MET:HE2	1.39	1.01
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.24	1.01
1:M:297:GLN:HA	1:M:297:GLN:HE21	1.23	1.01
2:N:577:ALA:HB1	2:N:589:VAL:HG11	1.39	1.01
3:O:177:GLU:HG3	3:O:231:ASN:HB3	1.43	1.01
2:B:510:LYS:CG	2:B:511:PRO:HD3	1.91	1.01
7:S:1:MET:HE1	7:S:79:PHE:HA	1.39	1.01
1:A:53:LEU:CD2	1:A:54:ASN:H	1.73	1.00
1:M:1385:THR:HG22	1:M:1387:HIS:H	1.24	1.00
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.24	1.00
1:M:705:LYS:HB2	1:M:708:MET:HE3	1.41	1.00
1:A:297:GLN:HA	1:A:297:GLN:HE21	1.25	1.00
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.44	1.00
12:L:40:LEU:HD13	12:L:44:ASP:HB3	1.44	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:93:LYS:HD3	9:U:93:LYS:H	1.25	0.99
5:E:56:LYS:HE2	5:E:84:ASP:HB2	1.44	0.99
1:A:524:VAL:HG12	1:A:525:GLN:H	1.28	0.99
8:T:130:ARG:HB2	8:T:130:ARG:HH11	1.26	0.98
8:T:95:TYR:HE2	8:T:97:MET:HG3	1.26	0.98
8:H:59:ILE:HG22	8:H:60:ALA:H	1.28	0.98
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.41	0.98
1:A:344:ARG:HB3	1:A:344:ARG:HH11	1.25	0.98
1:M:1255:GLU:HG3	1:M:1258:HIS:HD2	1.28	0.98
2:B:516:ASN:HD22	2:B:516:ASN:H	1.12	0.98
2:B:510:LYS:HG3	2:B:511:PRO:CD	1.92	0.98
2:B:744:HIS:HD2	2:B:745:PRO:HD2	1.24	0.97
5:Q:56:LYS:HE2	5:Q:84:ASP:HB2	1.45	0.97
2:N:789:MET:HE2	2:N:953:LEU:HD22	1.45	0.97
4:P:118:THR:HB	4:P:121:LYS:HB2	1.46	0.97
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.46	0.97
2:N:429:PHE:HA	2:N:432:MET:HE3	1.46	0.97
5:Q:14:ARG:HH21	5:Q:141:VAL:HG12	1.26	0.97
3:C:7:GLN:HE21	11:K:104:ASN:ND2	1.61	0.97
10:V:5:VAL:HG12	10:V:6:ARG:HG3	1.45	0.97
2:B:615:MET:HB3	2:B:626:ILE:HG12	1.45	0.97
2:B:789:MET:HE2	2:B:953:LEU:HD22	1.46	0.97
8:T:84:ALA:HB2	8:T:87:ARG:HD2	1.45	0.97
2:B:957:ASN:HD21	2:B:961:LEU:HB2	1.26	0.97
9:I:6:PHE:HB3	9:I:12:ASN:O	1.64	0.97
1:M:903:ASN:HD22	1:M:904:THR:N	1.62	0.97
4:P:56:ARG:HA	4:P:148:LEU:HD13	1.46	0.97
4:P:159:THR:O	4:P:163:VAL:HG23	1.64	0.96
1:M:1006:ILE:HD11	5:Q:163:GLU:HG3	1.46	0.96
1:A:90:VAL:HB	1:A:297:GLN:NE2	1.81	0.96
6:F:103:MET:HE2	7:G:66:GLY:H	1.26	0.96
1:M:779:PHE:CE1	1:M:785:PRO:HD3	2.01	0.96
8:T:59:ILE:HG22	8:T:60:ALA:H	1.31	0.96
1:A:53:LEU:HD23	1:A:54:ASN:N	1.79	0.96
1:A:1329:THR:HG22	1:A:1331:SER:H	1.28	0.96
1:A:34:LYS:HD2	4:P:187:THR:HG21	1.45	0.95
5:E:153:HIS:O	5:E:154:ILE:HG13	1.64	0.95
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.01	0.95
2:N:510:LYS:CG	2:N:511:PRO:HD3	1.96	0.95
5:Q:153:HIS:O	5:Q:154:ILE:HG13	1.67	0.95
1:A:1116:LEU:N	1:A:1308:THR:HG22	1.80	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:41:MET:CB	1:M:49:LYS:HA	1.96	0.95
2:N:880:THR:HB	2:N:934:LYS:HD2	1.49	0.95
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.45	0.95
2:B:516:ASN:HD22	2:B:516:ASN:N	1.64	0.95
3:C:238:ILE:HG22	3:C:243:VAL:HG23	1.49	0.95
3:O:47:ASP:HA	12:X:69:ALA:HB3	1.47	0.95
9:U:26:LEU:HD23	9:U:37:GLU:HA	1.45	0.95
9:U:6:PHE:HB3	9:U:12:ASN:O	1.67	0.95
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.45	0.95
1:M:855:THR:CG2	1:M:857:ARG:HE	1.80	0.95
1:M:108:MET:HE3	1:M:210:ILE:HD12	1.46	0.95
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.45	0.94
2:B:510:LYS:HG3	2:B:511:PRO:HD3	0.97	0.94
1:A:63:ARG:HA	1:A:74:MET:HE2	1.49	0.94
1:A:472:LEU:O	1:A:475:THR:HB	1.68	0.94
10:J:64:ASN:HB3	10:J:65:PRO:CD	1.97	0.94
2:B:806:THR:HG22	2:B:808:ALA:H	1.31	0.94
10:V:64:ASN:HB3	10:V:65:PRO:CD	1.98	0.94
2:N:289:LEU:HD13	2:N:375:ALA:HB2	1.49	0.94
4:P:14:ARG:HH22	4:P:16:LYS:HD2	1.29	0.94
1:A:308:ILE:HG22	1:A:309:ALA:H	1.33	0.94
1:A:770:VAL:HG12	1:A:771:GLU:HG3	1.49	0.94
2:N:1007:VAL:HG22	2:N:1008:PRO:HD2	1.50	0.94
1:A:108:MET:HA	1:A:210:ILE:HD13	1.47	0.93
7:S:91:VAL:HG23	7:S:143:ILE:HD11	1.46	0.93
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.03	0.93
2:N:806:THR:HG22	2:N:808:ALA:H	1.31	0.93
6:R:93:ILE:HD11	6:R:134:ILE:HD11	1.50	0.93
7:G:139:ILE:HG23	7:G:140:LYS:HG3	1.46	0.93
1:M:1364:ASN:OD1	1:M:1366:ARG:HG2	1.69	0.93
2:B:289:LEU:HD13	2:B:375:ALA:HB2	1.48	0.93
5:Q:114:ASN:O	5:Q:115:ASN:HB3	1.65	0.93
6:R:103:MET:CE	7:S:66:GLY:H	1.80	0.93
12:X:40:LEU:HD13	12:X:44:ASP:HB3	1.48	0.93
1:M:14:VAL:H	1:M:1432:GLN:HE22	1.07	0.93
12:X:55:ILE:HG12	12:X:56:LEU:H	1.34	0.93
2:N:508:LEU:N	14:5:1:DA:HO5'	1.65	0.93
1:A:903:ASN:ND2	1:A:905:ASP:H	1.66	0.93
3:C:123:ASN:ND2	3:C:125:MET:HG2	1.84	0.93
1:M:344:ARG:HB3	1:M:344:ARG:HH11	1.34	0.93
9:I:93:LYS:H	9:I:93:LYS:HD3	1.29	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:55:ILE:HD13	12:L:55:ILE:H	1.33	0.92
10:V:3:VAL:HG21	10:V:18:TRP:HB2	1.50	0.92
2:B:288:ALA:HB1	2:B:331:LEU:HD12	1.50	0.92
1:M:1036:ARG:HG2	1:M:1036:ARG:HH11	1.34	0.92
6:F:103:MET:CE	7:G:66:GLY:H	1.82	0.92
1:M:855:THR:HG21	1:M:857:ARG:NE	1.83	0.92
2:N:778:MET:HE1	2:N:1094:ARG:HD3	1.49	0.92
7:S:91:VAL:CG2	7:S:143:ILE:HD11	2.00	0.92
6:R:103:MET:HE2	7:S:66:GLY:H	1.32	0.92
1:M:503:GLN:HE21	6:R:90:ARG:HH21	1.17	0.92
1:A:41:MET:CB	1:A:49:LYS:HA	2.00	0.92
1:M:90:VAL:HB	1:M:297:GLN:NE2	1.84	0.92
1:M:563:PRO:HG3	1:M:572:TRP:CZ2	2.04	0.92
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.00	0.91
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.50	0.91
1:A:7:SER:HB3	2:B:1193:GLN:HE22	1.32	0.91
1:A:503:GLN:HE21	6:F:90:ARG:HH21	1.04	0.91
1:M:1116:LEU:N	1:M:1308:THR:HG22	1.84	0.91
1:M:1444:MET:HG3	7:S:60:ARG:HA	1.50	0.91
5:E:9:ILE:HD11	5:E:53:PRO:HD3	1.52	0.91
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.52	0.91
6:R:82:THR:HG22	6:R:84:TYR:H	1.35	0.91
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.52	0.91
10:J:63:TYR:O	10:J:64:ASN:HB2	1.71	0.91
1:M:961:ARG:HG2	1:M:965:GLN:HE21	1.35	0.91
1:A:567:LYS:HB3	8:H:96:VAL:N	1.86	0.91
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.53	0.91
5:E:114:ASN:O	5:E:115:ASN:HB3	1.69	0.91
7:G:97:HIS:CD2	7:S:95:SER:HB3	2.05	0.91
1:M:288:ALA:HA	1:M:291:GLU:CD	1.96	0.91
7:G:151:ILE:HG21	7:S:113:HIS:O	1.70	0.90
2:N:217:ARG:HE	2:N:405:ARG:HB2	1.32	0.90
11:W:65:HIS:CD2	11:W:67:PHE:H	1.89	0.90
4:D:118:THR:HB	4:D:121:LYS:HB2	1.52	0.90
3:O:123:ASN:ND2	3:O:125:MET:HG2	1.84	0.90
8:H:82:PRO:C	8:H:84:ALA:H	1.78	0.90
2:B:737:THR:HG21	9:I:66:PRO:HA	1.53	0.90
4:P:154:PHE:CD1	4:P:163:VAL:HG21	2.06	0.90
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.36	0.90
2:B:579:ARG:HB2	2:B:586:TRP:NE1	1.86	0.90
2:N:863:GLU:OE2	2:N:873:THR:HA	1.71	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:82:PRO:C	8:T:84:ALA:H	1.78	0.90
2:N:427:ASP:HA	2:N:430:ARG:HD2	1.54	0.89
2:B:999:MET:HA	2:B:999:MET:HE3	1.55	0.89
10:V:48:ARG:HG2	10:V:48:ARG:HH11	1.36	0.89
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.35	0.89
13:1:22:DC:H2''	13:1:23:BRU:H5'	1.52	0.89
1:M:316:GLN:HE21	1:M:317:LYS:HE3	1.36	0.89
1:M:1255:GLU:HG3	1:M:1258:HIS:CD2	2.06	0.89
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.10	0.89
8:T:130:ARG:HB2	8:T:130:ARG:NH1	1.88	0.89
2:B:744:HIS:CD2	2:B:745:PRO:HD2	2.08	0.89
1:M:567:LYS:NZ	8:T:46:LEU:HB2	1.87	0.89
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.07	0.89
2:B:890:TYR:O	2:B:893:LEU:HB2	1.73	0.89
7:S:13:LEU:HD21	7:S:17:PHE:HB2	1.54	0.89
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.07	0.88
1:A:687:LYS:O	1:A:690:VAL:HG12	1.72	0.88
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.53	0.88
2:B:805:THR:HG22	2:B:806:THR:H	1.36	0.88
2:N:800:GLN:HB3	10:V:52:THR:CG2	2.02	0.88
13:4:22:DC:H2''	13:4:23:BRU:H5'	1.53	0.88
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.52	0.88
9:I:111:THR:CG2	9:I:113:ASP:H	1.87	0.88
1:M:1224:LEU:HD11	1:M:1240:CYS:HB3	1.55	0.88
4:P:188:ALA:HB3	4:P:204:ASP:OD1	1.74	0.88
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.02	0.88
13:1:13:DT:H2''	13:1:14:DA:OP2	1.72	0.88
1:M:308:ILE:HG22	1:M:309:ALA:H	1.39	0.88
4:P:156:ASP:HB3	4:P:158:GLU:OE1	1.73	0.88
1:A:629:LEU:O	1:A:633:VAL:HG23	1.74	0.88
1:A:913:LEU:HD12	1:A:914:GLU:H	1.36	0.88
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.54	0.88
1:A:1398:MET:HB2	1:A:1426:GLU:OE2	1.74	0.88
1:M:687:LYS:O	1:M:690:VAL:HG12	1.72	0.88
1:M:903:ASN:ND2	1:M:905:ASP:H	1.72	0.88
2:N:168:GLY:H	2:N:450:ALA:HB1	1.37	0.87
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.56	0.87
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.53	0.87
12:L:55:ILE:HG12	12:L:56:LEU:H	1.39	0.87
2:N:273:LEU:HD12	2:N:280:ILE:HD12	1.55	0.87
1:M:902:LEU:HG	1:M:926:GLN:HG3	1.53	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:64:ASN:HD22	10:V:65:PRO:HD3	1.39	0.87
1:A:705:LYS:HB2	1:A:708:MET:HE3	1.57	0.87
5:Q:117:THR:HG22	5:Q:119:SER:H	1.38	0.87
2:B:168:GLY:H	2:B:450:ALA:HB1	1.37	0.87
2:B:597:MET:HA	2:B:597:MET:HE3	1.56	0.87
2:B:1095:LEU:H	2:B:1095:LEU:HD12	1.37	0.87
8:H:84:ALA:HB2	8:H:87:ARG:HD2	1.55	0.87
2:N:957:ASN:HD21	2:N:961:LEU:HB2	1.38	0.87
1:M:399:HIS:HB3	1:M:400:PRO:HD3	1.54	0.87
5:Q:94:LYS:HE2	5:Q:98:ILE:HD11	1.57	0.87
2:B:792:MET:HE2	2:B:857:ARG:HH22	1.38	0.87
1:M:316:GLN:NE2	1:M:317:LYS:HE3	1.90	0.87
4:P:156:ASP:HB2	4:P:159:THR:HG23	1.55	0.87
10:V:63:TYR:O	10:V:64:ASN:HB2	1.75	0.87
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.54	0.86
1:A:1036:ARG:HG2	1:A:1036:ARG:HH11	1.40	0.86
8:H:100:THR:HG23	8:H:138:GLU:HA	1.56	0.86
2:N:226:PHE:HA	2:N:395:GLN:HG3	1.55	0.86
9:U:50:THR:HG22	9:U:51:ASN:H	1.39	0.86
1:M:768:GLN:HG2	1:M:816:HIS:HA	1.56	0.86
1:A:710:LEU:H	1:A:710:LEU:HD12	1.38	0.86
2:B:473:MET:HE3	2:B:474:SER:HA	1.57	0.86
7:G:26:LEU:HD12	7:G:56:ILE:HD11	1.55	0.86
13:4:13:DT:H2"	13:4:14:DA:OP2	1.73	0.86
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.11	0.86
3:O:66:ARG:NH1	10:V:2:ILE:HG21	1.91	0.86
2:B:880:THR:HB	2:B:934:LYS:HD2	1.58	0.86
2:N:805:THR:HG22	2:N:806:THR:H	1.39	0.86
2:N:1065:GLN:HE21	2:N:1067:ARG:H	1.17	0.86
11:W:65:HIS:HD2	11:W:67:PHE:H	1.21	0.86
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.58	0.86
1:A:1341:ILE:HD12	1:A:1379:GLY:O	1.75	0.86
1:M:381:THR:HG22	1:M:383:TYR:H	1.41	0.86
1:M:853:ASP:OD1	1:M:855:THR:HB	1.76	0.86
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.55	0.85
5:E:117:THR:HB	5:E:120:ALA:HB2	1.57	0.85
8:H:59:ILE:HG22	8:H:60:ALA:N	1.90	0.85
1:M:90:VAL:HB	1:M:297:GLN:HE22	1.41	0.85
1:M:961:ARG:HG2	1:M:965:GLN:NE2	1.90	0.85
2:N:241:ARG:HG2	2:N:253:THR:CG2	2.05	0.85
1:M:265:LYS:CA	1:M:265:LYS:HE3	2.05	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:672:ASP:HB3	1:M:736:ASN:HD21	1.41	0.85
12:X:32:ALA:CB	12:X:55:ILE:HG13	2.06	0.85
1:A:903:ASN:HD22	1:A:904:THR:N	1.71	0.85
1:M:249:SER:O	1:M:250:ILE:HG13	1.74	0.85
1:M:285:PRO:HG2	1:M:288:ALA:HB3	1.58	0.85
9:U:111:THR:HG22	9:U:113:ASP:N	1.90	0.85
1:M:629:LEU:O	1:M:633:VAL:HG23	1.76	0.85
4:P:71:LYS:HA	4:P:74:GLN:HG3	1.59	0.85
2:B:583:ASN:HD21	2:B:628:THR:CG2	1.88	0.85
1:M:54:ASN:HB3	1:M:247:ARG:HH12	1.41	0.85
2:N:510:LYS:HG3	2:N:511:PRO:CD	2.05	0.85
7:S:116:PRO:HD2	7:S:119:LEU:HD23	1.59	0.85
1:A:1364:ASN:OD1	1:A:1366:ARG:HG2	1.77	0.85
2:B:430:ARG:HB3	2:B:430:ARG:HH11	1.39	0.85
2:B:792:MET:HE2	2:B:857:ARG:NH2	1.91	0.85
1:A:855:THR:HG21	1:A:857:ARG:NE	1.92	0.85
2:B:744:HIS:HD2	2:B:745:PRO:CD	1.89	0.85
9:I:111:THR:HG22	9:I:113:ASP:N	1.91	0.85
1:M:1341:ILE:HD12	1:M:1379:GLY:O	1.76	0.85
4:P:208:GLU:O	4:P:212:LYS:HG3	1.77	0.85
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.59	0.85
1:M:567:LYS:HB2	1:M:568:PRO:HD2	1.58	0.85
2:N:705:MET:H	2:N:710:LEU:HD12	1.42	0.85
2:N:758:PHE:CE2	2:N:1044:ALA:HA	2.11	0.85
1:M:288:ALA:HA	1:M:291:GLU:OE1	1.77	0.85
1:M:567:LYS:HB3	8:T:96:VAL:N	1.92	0.85
8:T:59:ILE:HG22	8:T:60:ALA:N	1.90	0.85
10:J:1:MET:H1	10:J:57:ILE:H	1.24	0.84
2:B:824:ILE:HG12	10:J:48:ARG:HH12	1.42	0.84
3:C:50:GLU:OE1	12:L:64:LEU:HD22	1.77	0.84
2:N:241:ARG:HG2	2:N:253:THR:HG22	1.56	0.84
2:N:890:TYR:O	2:N:893:LEU:HB2	1.78	0.84
3:O:56:THR:HG21	3:O:145:CYS:SG	2.17	0.84
2:B:294:ASP:O	2:B:296:GLU:N	2.10	0.84
2:N:428:ILE:HG22	2:N:432:MET:HE2	1.58	0.84
3:O:37:MET:HE3	3:O:176:ILE:HD13	1.59	0.84
1:A:667:GLY:HA2	1:A:670:ILE:HD11	1.58	0.84
1:A:754:SER:H	1:A:757:ASN:HD22	1.22	0.84
2:B:65:GLU:OE1	2:B:418:LYS:HE3	1.77	0.84
5:Q:116:ILE:HB	5:Q:121:MET:HE2	1.60	0.84
7:S:115:MET:HB3	7:S:116:PRO:HD2	1.59	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:138:THR:HG22	7:S:139:ILE:HG22	1.57	0.84
6:F:79:ARG:HA	6:F:144:GLU:OE1	1.78	0.84
1:M:754:SER:H	1:M:757:ASN:HD22	1.23	0.84
2:N:261:ARG:HB3	2:N:261:ARG:HH11	1.43	0.84
5:Q:15:ALA:O	5:Q:19:VAL:HG23	1.76	0.84
8:T:89:LEU:C	8:T:91:ASP:H	1.84	0.84
2:B:295:GLY:H	2:B:298:LEU:HD23	1.42	0.84
1:M:858:ASN:ND2	1:M:860:LEU:H	1.76	0.84
1:M:1202:MET:HE1	1:M:1212:VAL:HG21	1.58	0.84
2:N:244:LEU:HD11	2:N:366:GLN:HE22	1.43	0.84
7:S:122:ASN:ND2	7:S:125:SER:HB3	1.93	0.84
1:M:145:LYS:HE3	1:M:145:LYS:HA	1.60	0.83
2:N:473:MET:HE3	2:N:474:SER:HA	1.58	0.83
3:O:73:GLN:HE21	3:O:75:MET:H	1.25	0.83
1:A:1385:THR:HG22	1:A:1387:HIS:H	1.42	0.83
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.60	0.83
6:F:82:THR:HG22	6:F:84:TYR:H	1.42	0.83
1:A:107:CYS:HA	1:A:171:GLN:NE2	1.93	0.83
2:B:878:GLN:HB2	2:B:879:ARG:HD2	1.61	0.83
8:H:89:LEU:C	8:H:91:ASP:H	1.85	0.83
11:K:65:HIS:CD2	11:K:67:PHE:H	1.95	0.83
12:L:30:ILE:O	12:L:56:LEU:HA	1.77	0.83
7:S:34:VAL:HG11	7:S:74:TYR:HE1	1.42	0.83
13:4:25:DG:C2'	13:4:26:DT:H71	2.07	0.83
7:G:97:HIS:HD2	7:S:95:SER:HB3	1.44	0.83
1:M:567:LYS:HD2	1:M:568:PRO:HD2	1.58	0.83
11:W:58:PHE:HB3	11:W:76:GLN:HB3	1.59	0.83
1:A:43:GLU:HG3	1:A:46:THR:HB	1.59	0.83
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.13	0.83
2:B:642:ASP:HA	2:B:649:LYS:HA	1.60	0.83
2:B:705:MET:HA	2:B:705:MET:HE3	1.60	0.83
1:M:1110:ASN:HD22	1:M:1110:ASN:N	1.76	0.83
7:S:13:LEU:CD2	7:S:17:PHE:HB2	2.08	0.83
2:N:542:MET:HG2	2:N:747:MET:HE3	1.58	0.83
2:N:879:ARG:H	2:N:879:ARG:CZ	1.90	0.83
4:P:14:ARG:NH2	4:P:16:LYS:HD2	1.93	0.83
8:T:100:THR:HG23	8:T:138:GLU:HA	1.59	0.83
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.61	0.83
1:M:43:GLU:HG3	1:M:46:THR:HB	1.61	0.83
1:M:567:LYS:CG	1:M:568:PRO:HD2	2.09	0.83
13:4:12:DG:H4'	13:4:13:DT:OP1	1.78	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ARG:HB2	1:A:487:MET:SD	2.18	0.83
1:M:157:ASP:OD2	1:M:159:THR:HB	1.79	0.83
1:M:341:MET:HE3	2:N:1135:ARG:NH1	1.94	0.83
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.60	0.83
2:B:292:ILE:HD11	2:B:327:ARG:H	1.43	0.83
1:M:591:PHE:HA	1:M:595:THR:HG21	1.60	0.83
2:N:292:ILE:HD11	2:N:327:ARG:H	1.43	0.83
5:Q:117:THR:HB	5:Q:120:ALA:HB2	1.61	0.83
1:A:1445:ILE:H	1:A:1445:ILE:HD12	1.41	0.83
1:M:87:ALA:HB3	1:M:276:LEU:HD23	1.61	0.83
2:N:465:ASN:HD22	2:N:465:ASN:N	1.74	0.83
2:N:999:MET:HG3	2:N:1000:PRO:HD2	1.60	0.83
4:P:158:GLU:H	4:P:158:GLU:CD	1.86	0.83
1:A:265:LYS:CA	1:A:265:LYS:HE3	2.09	0.82
2:B:705:MET:H	2:B:710:LEU:HD12	1.43	0.82
12:L:32:ALA:CB	12:L:55:ILE:HG13	2.09	0.82
2:N:862:GLN:HG2	2:N:963:PHE:HD1	1.42	0.82
6:R:111:LEU:H	6:R:111:LEU:HD12	1.43	0.82
1:A:1158:PRO:O	1:A:1159:ARG:HG3	1.79	0.82
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.61	0.82
3:C:33:LEU:HG	3:C:37:MET:HE2	1.60	0.82
2:N:763:GLN:HG2	2:N:765:PRO:HD2	1.61	0.82
7:S:7:LEU:HB2	7:S:74:TYR:CE2	2.15	0.82
10:V:64:ASN:HB3	10:V:65:PRO:HD3	1.62	0.82
1:A:33:ALA:HA	1:A:57:ARG:HH12	1.43	0.82
2:B:429:PHE:HA	2:B:432:MET:HE3	1.60	0.82
1:M:414:ASP:OD1	1:M:416:ARG:HG2	1.79	0.82
2:N:751:VAL:HG13	2:N:812:LEU:HD22	1.60	0.82
1:A:1161:THR:HG22	1:A:1163:ILE:N	1.94	0.82
1:M:710:LEU:H	1:M:710:LEU:HD12	1.45	0.82
5:Q:180:ARG:HH21	5:Q:192:ARG:HB2	1.44	0.82
2:B:745:PRO:O	2:B:748:ILE:HG12	1.79	0.82
1:M:66:LYS:HD3	1:M:67:CYS:N	1.95	0.82
2:N:642:ASP:HA	2:N:649:LYS:HA	1.61	0.82
8:T:109:LYS:HG2	8:T:110:ASP:OD1	1.80	0.82
2:B:515:HIS:H	2:B:518:HIS:HD2	1.27	0.82
1:M:541:ILE:HD13	1:M:549:MET:HE1	1.60	0.82
2:N:1072:MET:CE	2:N:1085:ILE:HB	2.09	0.82
6:R:90:ARG:HD3	6:R:155:LEU:HD13	1.62	0.82
2:B:295:GLY:N	2:B:298:LEU:HD23	1.94	0.82
4:D:192:LYS:HD2	4:D:199:ASN:HA	1.59	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:12:DG:H4'	13:1:13:DT:OP1	1.79	0.82
2:N:1095:LEU:H	2:N:1095:LEU:HD12	1.45	0.82
2:N:1201:LYS:HE2	2:N:1205:GLN:OE1	1.79	0.82
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.60	0.82
1:M:265:LYS:HE3	1:M:265:LYS:HA	1.61	0.82
3:O:148:ARG:NH1	3:O:149:LYS:HE3	1.93	0.82
1:A:90:VAL:HB	1:A:297:GLN:HE22	1.41	0.82
2:B:469:GLN:O	2:B:472:ALA:HB3	1.80	0.82
2:N:393:LYS:HE3	2:N:393:LYS:HA	1.61	0.82
4:P:56:ARG:HH21	4:P:155:ARG:HG2	1.45	0.82
4:P:119:ARG:HB2	4:P:221:TYR:CE1	2.15	0.82
5:Q:19:VAL:O	5:Q:23:VAL:HG23	1.79	0.81
12:X:30:ILE:O	12:X:56:LEU:HA	1.79	0.81
1:A:157:ASP:OD2	1:A:159:THR:HB	1.81	0.81
1:A:265:LYS:HE3	1:A:265:LYS:N	1.95	0.81
2:B:390:LEU:O	2:B:392:ARG:HG3	1.80	0.81
7:G:13:LEU:CD2	7:G:17:PHE:HB2	2.11	0.81
1:M:244:PRO:HB2	1:M:245:PRO:HD3	1.62	0.81
3:O:128:ASN:O	3:O:129:ILE:HG13	1.80	0.81
3:O:244:VAL:O	3:O:248:ILE:HG13	1.79	0.81
4:P:146:GLN:O	4:P:149:THR:HG22	1.79	0.81
9:U:93:LYS:H	9:U:93:LYS:CD	1.93	0.81
1:A:858:ASN:ND2	1:A:860:LEU:H	1.78	0.81
2:B:879:ARG:H	2:B:879:ARG:CZ	1.93	0.81
2:B:1187:ASN:HD21	2:B:1190:ASP:HB3	1.46	0.81
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.60	0.81
8:T:40:LEU:HD23	8:T:42:ILE:HD11	1.61	0.81
1:A:470:LEU:HD23	1:A:470:LEU:H	1.45	0.81
1:A:1329:THR:HG22	1:A:1331:SER:N	1.94	0.81
13:1:25:DG:C2'	13:1:26:DT:H71	2.09	0.81
1:A:288:ALA:HA	1:A:291:GLU:CD	2.06	0.81
2:B:622:LYS:HE2	9:I:59:VAL:CG2	2.10	0.81
2:B:996:ARG:HH12	3:C:174:ALA:HA	1.44	0.81
5:E:19:VAL:O	5:E:23:VAL:HG23	1.80	0.81
10:V:1:MET:N	10:V:57:ILE:H	1.78	0.81
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.61	0.81
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.61	0.81
2:N:65:GLU:OE1	2:N:418:LYS:HE3	1.80	0.81
3:O:238:ILE:HG22	3:O:243:VAL:HG23	1.61	0.81
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.63	0.81
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.63	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1100:ASP:OD2	11:K:1:MET:HB3	1.80	0.81
9:I:50:THR:HG22	9:I:51:ASN:H	1.44	0.81
13:1:23:BRU:H6	13:1:23:BRU:H5''	1.61	0.81
1:M:524:VAL:HG12	1:M:525:GLN:H	1.45	0.81
7:S:126:ASN:HD22	7:S:127:PRO:HA	1.46	0.81
8:T:84:ALA:CB	8:T:87:ARG:HD2	2.11	0.81
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.63	0.80
3:O:252:GLN:HG3	11:W:95:ILE:HG23	1.63	0.80
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.79	0.80
7:G:122:ASN:ND2	7:G:125:SER:HB3	1.95	0.80
1:M:567:LYS:HB2	1:M:568:PRO:CD	2.11	0.80
1:M:1161:THR:HG22	1:M:1163:ILE:N	1.94	0.80
1:M:1259:MET:HA	1:M:1262:LYS:HD2	1.63	0.80
9:U:76:PRO:HD2	9:U:108:HIS:HD2	1.46	0.80
13:4:16:DT:H5'	13:4:16:DT:H6	1.46	0.80
2:B:370:PHE:HD2	2:B:373:ARG:HD3	1.46	0.80
5:E:15:ALA:O	5:E:19:VAL:HG23	1.82	0.80
7:G:138:THR:HG22	7:G:139:ILE:N	1.96	0.80
1:M:202:LEU:HB3	1:M:207:ILE:HD11	1.64	0.80
8:H:40:LEU:HD12	8:H:123:MET:HB2	1.63	0.80
1:M:472:LEU:O	1:M:475:THR:HB	1.80	0.80
1:M:1155:ASP:OD2	1:M:1161:THR:HG23	1.80	0.80
2:N:810:GLU:HB2	2:N:815:ARG:HH22	1.45	0.80
5:Q:48:ASP:HB3	5:Q:54:GLN:NE2	1.96	0.80
1:A:858:ASN:C	1:A:858:ASN:HD22	1.88	0.80
2:B:583:ASN:ND2	2:B:628:THR:HG22	1.97	0.80
2:N:583:ASN:ND2	2:N:628:THR:HG22	1.97	0.80
2:N:766:ARG:HH21	2:N:1020:ARG:CD	1.94	0.80
1:A:344:ARG:HB3	1:A:344:ARG:NH1	1.96	0.80
2:B:261:ARG:HH11	2:B:261:ARG:HB3	1.45	0.80
1:M:1170:ILE:H	1:M:1170:ILE:HD12	1.47	0.80
2:N:800:GLN:HB3	10:V:52:THR:HG21	1.64	0.80
3:O:147:LEU:HB2	3:O:151:GLN:HB2	1.62	0.80
9:U:105:SER:O	9:U:106:CYS:HB3	1.80	0.80
1:A:855:THR:CG2	1:A:857:ARG:HE	1.93	0.80
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.63	0.80
3:C:73:GLN:HE21	3:C:75:MET:H	1.30	0.80
5:E:48:ASP:CG	5:E:49:SER:H	1.86	0.80
13:1:16:DT:H5'	13:1:16:DT:H6	1.46	0.80
1:M:14:VAL:N	1:M:1432:GLN:HE22	1.81	0.80
2:B:955:THR:HG22	2:B:956:THR:O	1.81	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:GLN:NE2	3:C:75:MET:HB2	1.97	0.79
10:J:1:MET:N	10:J:57:ILE:H	1.80	0.79
4:P:176:GLU:OE2	4:P:197:SER:HB2	1.80	0.79
4:P:214:LEU:HD13	4:P:214:LEU:O	1.82	0.79
1:M:1387:HIS:O	1:M:1391:ARG:HG3	1.82	0.79
1:M:167:CYS:HB2	1:M:169:ASN:HD21	1.45	0.79
1:M:1214:GLU:O	1:M:1218:GLN:HG2	1.82	0.79
2:N:351:TYR:O	2:N:355:ILE:HG13	1.82	0.79
2:N:469:GLN:O	2:N:472:ALA:HB3	1.82	0.79
3:O:50:GLU:OE1	12:X:64:LEU:HD22	1.83	0.79
10:V:57:ILE:HA	10:V:60:PHE:HD2	1.46	0.79
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.46	0.79
1:M:534:LEU:O	1:M:574:GLY:HA3	1.82	0.79
9:U:50:THR:HG22	9:U:51:ASN:N	1.98	0.79
1:A:372:LYS:HA	1:A:435:HIS:HD1	1.47	0.79
2:B:552:MET:HA	2:B:552:MET:HE3	1.64	0.79
6:F:111:LEU:HD12	6:F:111:LEU:N	1.98	0.79
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.62	0.79
9:I:105:SER:O	9:I:106:CYS:HB3	1.79	0.79
1:M:93:VAL:HG13	1:M:301:ALA:HB1	1.63	0.79
9:U:93:LYS:HD3	9:U:93:LYS:N	1.97	0.79
2:N:583:ASN:HD21	2:N:628:THR:CG2	1.95	0.79
6:R:77:ASP:O	6:R:78:GLN:HB2	1.81	0.79
1:A:7:SER:HB3	2:B:1193:GLN:NE2	1.98	0.79
2:B:309:GLN:HG3	9:I:52:ILE:HD11	1.64	0.79
1:M:535:THR:HG21	1:M:616:VAL:HA	1.63	0.79
1:M:567:LYS:CB	1:M:568:PRO:HD2	2.12	0.79
2:B:1224:PHE:CE1	5:E:171:LYS:HG3	2.17	0.79
12:X:61:THR:CG2	12:X:63:ARG:HG3	2.13	0.79
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.12	0.79
3:C:6:PRO:HB2	3:C:25:VAL:HG22	1.65	0.79
4:P:66:ARG:HD2	4:P:133:THR:HB	1.65	0.79
1:A:40:THR:HG22	1:A:41:MET:HG3	1.63	0.79
1:A:722:LEU:H	1:A:722:LEU:HD12	1.48	0.79
4:D:208:GLU:O	4:D:212:LYS:HG3	1.83	0.79
6:F:90:ARG:HD3	6:F:155:LEU:HD13	1.63	0.79
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.47	0.79
1:M:858:ASN:HD22	1:M:858:ASN:C	1.87	0.79
2:N:603:LEU:HD13	2:N:608:ASP:HB2	1.65	0.79
2:N:658:ILE:HG22	2:N:662:MET:HE2	1.65	0.79
8:T:58:THR:HG22	8:T:59:ILE:H	1.48	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:GLN:NE2	6:F:90:ARG:HH21	1.80	0.78
9:I:93:LYS:H	9:I:93:LYS:CD	1.96	0.78
1:M:1308:THR:HG23	1:M:1309:ASP:N	1.97	0.78
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.16	0.78
1:A:697:ALA:HB2	1:A:702:LEU:HD11	1.65	0.78
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.48	0.78
1:M:1291:VAL:HG22	1:M:1292:PRO:HD2	1.64	0.78
1:M:1323:ASP:OD1	1:M:1325:THR:HG22	1.84	0.78
13:4:23:BRU:H6	13:4:23:BRU:H5''	1.63	0.78
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.81	0.78
1:A:1308:THR:HG23	1:A:1309:ASP:N	1.98	0.78
1:M:225:ASN:ND2	1:M:228:PHE:H	1.81	0.78
1:M:1259:MET:HE2	1:M:1263:ILE:HG13	1.62	0.78
1:A:390:GLN:HE21	1:A:394:ASN:HD22	1.31	0.78
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.65	0.78
5:E:48:ASP:HB3	5:E:54:GLN:NE2	1.99	0.78
8:H:58:THR:HG22	8:H:59:ILE:H	1.49	0.78
1:M:693:VAL:HG21	1:M:721:PHE:HE1	1.48	0.78
6:R:111:LEU:HD12	6:R:111:LEU:N	1.98	0.78
2:B:862:GLN:HG2	2:B:963:PHE:HD1	1.48	0.78
4:D:159:THR:O	4:D:163:VAL:HG23	1.84	0.78
1:M:1081:LEU:HD11	1:M:1097:GLY:HA3	1.66	0.78
4:P:194:LEU:HD13	7:S:86:VAL:HG11	1.65	0.78
9:U:111:THR:CG2	9:U:113:ASP:H	1.92	0.78
1:A:714:PHE:HB2	9:I:97:MET:HE1	1.66	0.78
1:A:913:LEU:HD12	1:A:914:GLU:N	1.98	0.78
2:B:603:LEU:HD13	2:B:608:ASP:HB2	1.66	0.78
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.65	0.78
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.46	0.78
2:N:737:THR:HG21	9:U:66:PRO:HA	1.64	0.78
1:M:830:LYS:O	1:M:834:THR:HB	1.84	0.78
1:M:981:LEU:HD21	1:M:1039:LYS:HA	1.66	0.78
4:P:47:LEU:HD13	4:P:48:ILE:N	1.99	0.78
7:S:34:VAL:HG11	7:S:74:TYR:CE1	2.19	0.78
7:S:119:LEU:HD11	7:S:130:TYR:HB3	1.66	0.78
8:T:17:PRO:HB3	8:T:24:CYS:SG	2.23	0.78
1:A:225:ASN:ND2	1:A:228:PHE:H	1.80	0.78
1:A:591:PHE:HA	1:A:595:THR:HG21	1.66	0.78
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.19	0.78
1:M:1094:VAL:HG13	1:M:1113:THR:CG2	2.14	0.78
1:M:1259:MET:HE3	1:M:1262:LYS:HB2	1.66	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:745:PRO:O	2:N:748:ILE:HG12	1.84	0.78
2:N:824:ILE:HG12	10:V:48:ARG:HH12	1.49	0.78
3:O:148:ARG:HD3	3:O:149:LYS:HG3	1.66	0.78
1:A:934:LYS:O	1:A:937:VAL:HG12	1.83	0.78
2:B:199:MET:HE2	2:B:492:LEU:CD2	2.14	0.78
2:B:294:ASP:C	2:B:296:GLU:H	1.91	0.78
2:B:751:VAL:HG13	2:B:812:LEU:HD22	1.63	0.78
2:N:865:LYS:HB2	2:N:961:LEU:HD11	1.64	0.78
7:S:129:SER:HB2	7:S:138:THR:OG1	1.84	0.78
2:B:857:ARG:HD2	2:B:945:GLU:OE1	1.83	0.78
5:E:84:ASP:O	5:E:86:PRO:HD3	1.84	0.78
1:M:503:GLN:NE2	6:R:90:ARG:HH21	1.81	0.78
1:M:567:LYS:CD	1:M:568:PRO:HD2	2.12	0.78
7:S:115:MET:HB3	7:S:119:LEU:HD23	1.65	0.78
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.64	0.77
9:U:80:SER:OG	9:U:105:SER:HB2	1.83	0.77
1:M:741:ASN:HD22	1:M:742:ASN:N	1.83	0.77
5:Q:22:MET:HE3	5:Q:26:ARG:NE	1.98	0.77
1:A:62:ASP:O	1:A:63:ARG:C	2.28	0.77
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.20	0.77
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.64	0.77
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.00	0.77
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.13	0.77
9:I:80:SER:OG	9:I:105:SER:HB2	1.84	0.77
9:U:74:GLU:HB3	9:U:81:ARG:HD2	1.65	0.77
10:V:3:VAL:HG21	10:V:18:TRP:CB	2.13	0.77
14:2:5:DC:C2'	14:2:6:DT:H72	2.15	0.77
1:M:855:THR:HG23	1:M:857:ARG:HG3	1.66	0.77
2:N:999:MET:HA	2:N:999:MET:HE3	1.64	0.77
11:W:47:ARG:HB3	11:W:47:ARG:HH11	1.50	0.77
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	1.85	0.77
4:D:146:GLN:O	4:D:149:THR:HG22	1.83	0.77
1:M:62:ASP:O	1:M:63:ARG:C	2.28	0.77
1:M:93:VAL:HG22	1:M:301:ALA:HA	1.64	0.77
1:M:590:ARG:O	1:M:591:PHE:HB2	1.84	0.77
1:M:899:VAL:HB	1:M:929:LEU:HD12	1.65	0.77
2:N:294:ASP:O	2:N:296:GLU:N	2.16	0.77
2:N:615:MET:HB3	2:N:626:ILE:HG12	1.65	0.77
7:S:53:ASN:HD22	7:S:53:ASN:N	1.81	0.77
7:S:85:GLU:HG2	7:S:87:VAL:HG12	1.66	0.77
1:A:287:HIS:HA	1:A:290:GLU:HG2	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.65	0.77
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.20	0.77
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.66	0.77
1:M:407:ARG:HD2	1:M:413:ILE:HD11	1.65	0.77
1:M:565:ILE:HG23	1:M:567:LYS:HG2	1.66	0.77
1:M:596:THR:O	1:M:598:LEU:N	2.17	0.77
8:T:40:LEU:HD13	8:T:123:MET:HE3	1.65	0.77
8:T:127:GLY:O	8:T:128:ASN:HB2	1.82	0.77
1:M:537:ARG:HD2	8:T:20:TYR:CE1	2.20	0.77
14:5:5:DC:C2'	14:5:6:DT:H72	2.15	0.77
4:D:187:THR:HG21	1:M:34:LYS:NZ	2.00	0.77
6:F:111:LEU:HD12	6:F:111:LEU:H	1.50	0.77
1:M:821:ARG:HH11	1:M:821:ARG:HB2	1.48	0.77
1:M:1094:VAL:HG13	1:M:1113:THR:HG21	1.66	0.77
2:N:313:MET:HE2	2:N:390:LEU:HD11	1.67	0.77
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.67	0.77
1:M:714:PHE:HB2	9:U:97:MET:HE1	1.67	0.77
1:M:1095:THR:HG21	1:M:1112:LYS:HB2	1.66	0.77
1:M:1293:SER:OG	1:M:1295:THR:HG23	1.84	0.77
2:N:579:ARG:HB2	2:N:586:TRP:HE1	1.48	0.77
2:N:766:ARG:HH21	2:N:1020:ARG:HD3	1.48	0.77
5:Q:176:PRO:O	5:Q:212:ARG:HA	1.85	0.77
12:X:32:ALA:HB2	12:X:55:ILE:HG13	1.64	0.77
12:X:47:ARG:HH11	12:X:47:ARG:HB2	1.50	0.77
2:B:273:LEU:HD21	2:B:360:PHE:HD1	1.49	0.76
8:H:40:LEU:HD23	8:H:42:ILE:HD11	1.66	0.76
1:M:172:PRO:HB3	1:M:185:TRP:CE2	2.20	0.76
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.67	0.76
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.13	0.76
1:M:184:SER:HB3	1:M:199:LEU:HD23	1.65	0.76
2:N:294:ASP:C	2:N:296:GLU:H	1.93	0.76
7:S:106:MET:HG2	7:S:107:LYS:N	1.98	0.76
8:T:15:VAL:HG22	8:T:26:ILE:HG12	1.67	0.76
8:T:130:ARG:HH11	8:T:130:ARG:CB	1.99	0.76
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.50	0.76
12:L:53:HIS:HB3	12:L:55:ILE:CD1	2.15	0.76
1:M:310:GLY:O	1:M:312:PRO:HD2	1.84	0.76
5:Q:84:ASP:O	5:Q:86:PRO:HD3	1.86	0.76
2:B:863:GLU:OE2	2:B:873:THR:HA	1.84	0.76
5:E:117:THR:HB	5:E:120:ALA:CB	2.15	0.76
1:M:913:LEU:HD12	1:M:914:GLU:H	1.48	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:69:LEU:H	3:O:69:LEU:HD12	1.50	0.76
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.66	0.76
1:A:541:ILE:HD13	1:A:549:MET:CE	2.15	0.76
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.68	0.76
1:A:1385:THR:CG2	1:A:1387:HIS:H	1.98	0.76
3:O:51:VAL:HG22	3:O:155:LEU:HD22	1.67	0.76
1:A:963:ILE:HD13	1:A:1049:ILE:HG13	1.65	0.76
2:B:1069:PHE:H	2:B:1069:PHE:HD1	1.30	0.76
1:M:541:ILE:HD13	1:M:549:MET:CE	2.15	0.76
1:M:770:VAL:HG12	1:M:771:GLU:HG3	1.68	0.76
1:M:822:GLU:HG3	2:N:513:GLN:NE2	2.00	0.76
1:M:905:ASP:C	1:M:906:HIS:HD1	1.94	0.76
2:N:792:MET:HE2	2:N:857:ARG:HH22	1.50	0.76
3:O:11:ARG:HE	3:O:21:ILE:HD11	1.51	0.76
4:P:138:ASN:C	4:P:142:LYS:HE2	2.11	0.76
1:A:824:LEU:O	1:A:827:THR:HG22	1.85	0.76
2:B:579:ARG:HG2	2:B:579:ARG:HH11	1.48	0.76
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.86	0.76
4:D:154:PHE:HE2	4:D:218:GLU:HA	1.51	0.76
2:N:172:ILE:HD13	2:N:178:ASN:HD22	1.50	0.76
2:N:617:ARG:HE	2:N:619:ILE:HG12	1.50	0.76
1:M:89:PRO:O	1:M:204:THR:HG21	1.85	0.76
1:M:794:PRO:HG2	1:M:795:GLU:OE2	1.86	0.76
1:M:1006:ILE:HD11	5:Q:163:GLU:CG	2.16	0.76
8:T:95:TYR:CE2	8:T:97:MET:HG3	2.16	0.76
1:A:353:ILE:HG21	1:A:487:MET:CG	2.14	0.76
1:M:164:ARG:HG3	1:M:165:GLY:H	1.51	0.76
1:M:535:THR:CG2	1:M:616:VAL:HA	2.14	0.76
11:W:65:HIS:HD2	11:W:67:PHE:N	1.84	0.76
1:A:534:LEU:O	1:A:574:GLY:HA3	1.85	0.76
1:A:1387:HIS:O	1:A:1391:ARG:HG3	1.85	0.76
3:C:93:ASP:OD1	3:C:122:SER:HB2	1.86	0.76
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.68	0.75
1:A:341:MET:HE3	2:B:1135:ARG:NH1	2.00	0.75
2:B:737:THR:CG2	9:I:66:PRO:HA	2.15	0.75
2:N:792:MET:HE2	2:N:857:ARG:NH2	2.01	0.75
5:Q:9:ILE:HD11	5:Q:53:PRO:HD3	1.66	0.75
1:A:1223:ASP:HA	1:A:1243:VAL:CG2	2.15	0.75
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.66	0.75
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.86	0.75
1:M:846:GLU:OE2	1:M:1398:MET:HE2	1.86	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:HIS:C	1:A:282:ASN:HD22	1.94	0.75
1:A:869:GLY:O	5:E:204:THR:HG21	1.87	0.75
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.68	0.75
7:S:83:LYS:HG3	7:S:148:GLU:O	1.86	0.75
8:T:40:LEU:HD12	8:T:123:MET:HB2	1.67	0.75
1:A:567:LYS:HB2	8:H:95:TYR:HA	1.66	0.75
3:C:56:THR:HG22	3:C:57:VAL:H	1.51	0.75
1:M:108:MET:CA	1:M:210:ILE:HD13	2.15	0.75
2:N:60:GLN:O	2:N:63:ILE:HG22	1.86	0.75
3:O:56:THR:HG22	3:O:57:VAL:H	1.50	0.75
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.68	0.75
13:1:22:DC:H2''	13:1:23:BRU:C5'	2.14	0.75
1:M:842:VAL:HG11	2:N:1136:ASP:OD2	1.87	0.75
2:N:25:ILE:CG2	2:N:658:ILE:HD12	2.16	0.75
2:N:744:HIS:CD2	2:N:745:PRO:HD2	2.22	0.75
5:Q:117:THR:HB	5:Q:120:ALA:CB	2.16	0.75
9:U:50:THR:CG2	9:U:52:ILE:HG12	2.17	0.75
9:U:65:ASP:HB3	9:U:68:LEU:HD12	1.68	0.75
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.22	0.75
2:B:36:ALA:HA	2:B:39:ARG:HD2	1.69	0.75
5:E:202:SER:OG	5:E:204:THR:HG22	1.87	0.75
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.51	0.75
1:M:1218:GLN:O	1:M:1221:LYS:HE3	1.86	0.75
4:P:14:ARG:HB3	4:P:14:ARG:HH11	1.50	0.75
1:M:1336:MET:HE2	1:M:1381:LEU:HG	1.67	0.75
2:N:35:SER:HA	2:N:811:TYR:HE2	1.51	0.75
3:O:183:TRP:O	3:O:185:LYS:N	2.19	0.75
7:S:115:MET:O	7:S:164:LYS:HD3	1.87	0.75
1:A:34:LYS:CD	4:P:187:THR:HG21	2.17	0.75
3:C:183:TRP:O	3:C:185:LYS:N	2.19	0.75
2:N:744:HIS:HD2	2:N:745:PRO:CD	2.00	0.75
1:A:107:CYS:CA	1:A:171:GLN:HE22	1.99	0.75
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	1.68	0.75
2:B:800:GLN:HB3	10:J:52:THR:HG22	1.69	0.75
4:D:66:ARG:HD2	4:D:133:THR:HB	1.68	0.75
2:N:1187:ASN:HD21	2:N:1190:ASP:HB3	1.52	0.75
5:Q:48:ASP:CG	5:Q:49:SER:H	1.93	0.75
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.21	0.74
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.69	0.74
4:D:71:LYS:HA	4:D:74:GLN:HB2	1.68	0.74
1:M:973:ILE:HD13	1:M:1037:LEU:HA	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:129:PHE:HE2	2:N:166:PHE:HB2	1.52	0.74
2:N:917:PRO:O	2:N:918:ILE:HG13	1.86	0.74
3:C:238:ILE:CG2	3:C:243:VAL:HG23	2.16	0.74
1:M:167:CYS:HB2	1:M:169:ASN:ND2	2.01	0.74
1:M:869:GLY:O	5:Q:204:THR:HG21	1.87	0.74
1:M:1255:GLU:O	1:M:1255:GLU:HG2	1.87	0.74
2:N:955:THR:HG22	2:N:956:THR:O	1.87	0.74
8:T:130:ARG:HD3	8:T:130:ARG:N	2.01	0.74
9:U:55:THR:HG23	9:U:100:PHE:CD2	2.22	0.74
12:X:61:THR:HG22	12:X:63:ARG:HG3	1.69	0.74
1:A:1353:TYR:HD2	1:A:1353:TYR:C	1.94	0.74
3:C:244:VAL:O	3:C:248:ILE:HG13	1.87	0.74
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.69	0.74
12:L:38:LEU:HD13	12:L:49:LYS:HE2	1.69	0.74
1:M:37:PHE:CD1	1:M:37:PHE:N	2.53	0.74
1:M:446:ARG:HB2	1:M:487:MET:SD	2.26	0.74
7:S:95:SER:OG	7:S:96:GLN:N	2.15	0.74
2:N:345:LYS:O	2:N:347:LYS:HG2	1.87	0.74
2:N:1224:PHE:CZ	5:Q:171:LYS:HG3	2.22	0.74
8:T:8:ASP:OD2	8:T:9:ILE:N	2.19	0.74
2:B:549:THR:HB	2:B:628:THR:OG1	1.87	0.74
12:L:26:THR:HG22	12:L:27:LEU:N	2.01	0.74
1:M:451:HIS:CD2	1:M:1074:GLU:HG3	2.23	0.74
2:N:261:ARG:HB3	2:N:261:ARG:NH1	2.02	0.74
3:O:147:LEU:HD23	3:O:147:LEU:N	2.03	0.74
4:P:12:ARG:HH11	4:P:12:ARG:HG2	1.52	0.74
7:S:18:PHE:HA	7:S:22:MET:HE3	1.69	0.74
12:X:55:ILE:HD13	12:X:55:ILE:H	1.53	0.74
13:4:22:DC:H2''	13:4:23:BRU:C5'	2.15	0.74
1:A:537:ARG:HD2	8:H:20:TYR:CE1	2.22	0.74
3:C:7:GLN:HE21	11:K:104:ASN:HD21	1.34	0.74
1:M:1015:VAL:HG12	1:M:1019:CYS:SG	2.27	0.74
1:A:866:PHE:C	1:A:867:ILE:HD12	2.12	0.74
1:A:903:ASN:HD22	1:A:903:ASN:C	1.91	0.74
1:A:470:LEU:HD23	1:A:470:LEU:N	2.02	0.74
1:A:1293:SER:OG	1:A:1295:THR:HG23	1.88	0.74
2:B:345:LYS:O	2:B:347:LYS:HG2	1.87	0.74
6:F:90:ARG:HD3	6:F:155:LEU:CD1	2.18	0.74
1:M:55:ASP:C	1:M:57:ARG:H	1.94	0.74
9:I:111:THR:CG2	9:I:112:SER:N	2.50	0.74
1:M:1105:LEU:HD22	1:M:1384:VAL:HG21	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:309:GLN:HG3	9:U:52:ILE:HD11	1.70	0.74
1:A:69:THR:O	1:A:71:GLN:N	2.21	0.74
4:D:29:LEU:HD22	4:D:29:LEU:N	2.03	0.74
1:M:353:ILE:HG21	1:M:487:MET:CG	2.17	0.74
3:O:183:TRP:CZ2	3:O:207:CYS:HB3	2.23	0.74
4:P:190:GLU:HA	7:S:167:TYR:CD1	2.22	0.74
9:U:50:THR:HG22	9:U:52:ILE:H	1.52	0.74
12:X:49:LYS:O	12:X:50:ASP:HB2	1.86	0.74
1:A:596:THR:O	1:A:598:LEU:N	2.20	0.73
6:F:147:SER:OG	6:F:150:GLU:HG3	1.88	0.73
7:G:26:LEU:HD12	7:G:56:ILE:CD1	2.17	0.73
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.18	0.73
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.68	0.73
1:A:590:ARG:O	1:A:591:PHE:HB2	1.88	0.73
2:B:798:TYR:CD1	10:J:4:PRO:HG3	2.23	0.73
2:B:865:LYS:HB2	2:B:961:LEU:HD11	1.69	0.73
1:M:287:HIS:HA	1:M:290:GLU:HG2	1.68	0.73
2:N:659:ALA:HA	2:N:662:MET:HE3	1.68	0.73
1:A:853:ASP:OD1	1:A:855:THR:HB	1.87	0.73
1:A:901:LEU:H	1:A:926:GLN:NE2	1.85	0.73
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.69	0.73
2:B:241:ARG:HG2	2:B:253:THR:HG22	1.69	0.73
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.70	0.73
7:G:53:ASN:HD22	7:G:53:ASN:N	1.84	0.73
8:H:127:GLY:O	8:H:128:ASN:HB2	1.85	0.73
2:N:1072:MET:HE3	2:N:1085:ILE:HB	1.69	0.73
9:U:74:GLU:HB3	9:U:81:ARG:CD	2.18	0.73
11:W:45:LEU:HG	11:W:94:ILE:HD13	1.70	0.73
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.70	0.73
2:B:277:LYS:HG2	2:B:336:ARG:HB3	1.70	0.73
6:F:69:LEU:HB3	6:F:71:GLU:OE1	1.88	0.73
1:M:1202:MET:HE1	1:M:1212:VAL:CG2	2.18	0.73
2:N:806:THR:HG22	2:N:808:ALA:N	2.04	0.73
12:X:26:THR:HG22	12:X:27:LEU:N	2.02	0.73
1:A:1107:VAL:HG12	1:A:1107:VAL:O	1.87	0.73
3:C:203:GLN:HG2	3:C:207:CYS:SG	2.29	0.73
12:L:60:ARG:HG2	12:L:61:THR:H	1.53	0.73
12:X:30:ILE:HD11	12:X:59:ALA:HB2	1.68	0.73
1:A:33:ALA:HA	1:A:57:ARG:NH1	2.03	0.73
1:M:590:ARG:HG2	1:M:590:ARG:HH11	1.52	0.73
1:M:896:ARG:HD3	1:M:897:TYR:CE1	2.23	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:364:ILE:HG13	2:N:585:VAL:HG13	1.70	0.73
2:N:613:VAL:HG13	2:N:627:PHE:O	1.89	0.73
2:N:800:GLN:HB3	10:V:52:THR:HG22	1.70	0.73
7:S:51:TYR:O	7:S:54:ILE:HG13	1.88	0.73
12:X:47:ARG:HG3	12:X:52:GLY:O	1.87	0.73
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.02	0.73
1:A:567:LYS:CB	8:H:95:TYR:HA	2.17	0.73
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.27	0.73
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.24	0.73
8:H:84:ALA:CB	8:H:87:ARG:HD2	2.17	0.73
2:N:308:TRP:CH2	9:U:45:ARG:HG2	2.24	0.73
2:N:1065:GLN:HE21	2:N:1067:ARG:N	1.86	0.73
4:P:141:LEU:O	4:P:145:MET:HG2	1.89	0.73
1:M:66:LYS:NZ	1:M:68:GLN:H	1.87	0.73
1:M:567:LYS:HB2	8:T:95:TYR:HA	1.69	0.73
2:N:333:PHE:O	2:N:334:ILE:HG13	1.89	0.73
7:S:129:SER:HB2	7:S:138:THR:HG1	1.54	0.73
1:A:250:ILE:O	1:A:250:ILE:HG22	1.87	0.73
2:B:313:MET:HE2	2:B:390:LEU:HD11	1.69	0.73
3:C:11:ARG:HH12	3:C:205:LYS:HZ3	1.37	0.73
5:E:116:ILE:HB	5:E:121:MET:HE2	1.69	0.73
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.71	0.73
9:I:50:THR:HG22	9:I:51:ASN:N	2.04	0.73
1:M:69:THR:O	1:M:71:GLN:N	2.22	0.73
1:M:107:CYS:HA	1:M:171:GLN:HE22	1.54	0.73
1:M:321:PRO:O	1:M:322:VAL:HG12	1.89	0.73
1:M:1223:ASP:HA	1:M:1243:VAL:HG22	1.70	0.73
10:V:1:MET:H2	10:V:57:ILE:H	1.35	0.73
1:A:70:CYS:O	1:A:72:GLU:HG2	1.89	0.73
1:A:1353:TYR:C	1:A:1353:TYR:CD2	2.65	0.73
3:C:66:ARG:NH1	10:J:2:ILE:HG21	2.04	0.73
1:M:225:ASN:ND2	1:M:227:VAL:H	1.86	0.73
1:M:337:ARG:HD3	2:N:1132:GLU:OE1	1.89	0.73
2:N:579:ARG:HB2	2:N:586:TRP:NE1	2.03	0.73
2:N:589:VAL:HG12	2:N:590:HIS:H	1.52	0.73
2:N:879:ARG:H	2:N:879:ARG:NH1	1.86	0.73
4:P:189:ASP:O	4:P:193:THR:HB	1.89	0.73
4:P:207:LEU:O	4:P:211:LEU:HD12	1.89	0.73
1:A:62:ASP:O	1:A:64:ASN:HB2	1.89	0.72
1:A:535:THR:HG21	1:A:616:VAL:HA	1.71	0.72
1:A:901:LEU:HA	1:A:907:THR:OG1	1.88	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:176:PRO:O	5:E:212:ARG:HA	1.89	0.72
6:F:109:VAL:HG12	6:F:110:ASP:H	1.54	0.72
1:M:11:LEU:O	1:M:11:LEU:HD23	1.89	0.72
2:N:644:GLU:HB3	2:N:648:HIS:O	1.89	0.72
3:O:16:ASP:C	3:O:240:VAL:HG11	2.14	0.72
1:A:829:VAL:HG21	2:B:508:LEU:HD13	1.69	0.72
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.24	0.72
4:D:154:PHE:CE2	4:D:218:GLU:HA	2.24	0.72
6:F:109:VAL:HG12	6:F:110:ASP:N	2.02	0.72
1:M:1394:THR:HG21	1:M:1398:MET:SD	2.28	0.72
2:N:911:ILE:HD11	2:N:941:LEU:HD13	1.71	0.72
3:O:263:THR:O	3:O:266:ASP:HB2	1.89	0.72
7:S:116:PRO:HG2	7:S:119:LEU:CB	2.19	0.72
1:A:40:THR:HG23	1:A:54:ASN:HD21	1.54	0.72
7:G:18:PHE:HA	7:G:22:MET:HE3	1.70	0.72
1:M:66:LYS:HD3	1:M:67:CYS:H	1.52	0.72
1:M:667:GLY:HA2	1:M:670:ILE:HD11	1.70	0.72
1:M:860:LEU:HD11	1:M:1393:ASN:HB2	1.71	0.72
2:N:542:MET:HG2	2:N:747:MET:CE	2.18	0.72
6:R:109:VAL:HG12	6:R:110:ASP:N	2.02	0.72
1:A:297:GLN:HE21	1:A:297:GLN:CA	2.02	0.72
1:M:89:PRO:C	1:M:204:THR:HG21	2.13	0.72
2:N:549:THR:HG22	2:N:550:ASP:N	2.05	0.72
2:N:582:VAL:HG23	2:N:626:ILE:HB	1.70	0.72
2:N:1016:ALA:O	2:N:1020:ARG:HG3	1.89	0.72
7:S:1:MET:SD	7:S:2:PHE:N	2.63	0.72
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.71	0.72
1:A:55:ASP:C	1:A:57:ARG:H	1.95	0.72
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.18	0.72
2:B:292:ILE:HD11	2:B:327:ARG:N	2.03	0.72
2:B:1095:LEU:HD12	2:B:1095:LEU:N	2.04	0.72
1:M:341:MET:HE3	2:N:1135:ARG:HH11	1.54	0.72
2:N:287:ARG:HG2	2:N:292:ILE:HA	1.72	0.72
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.55	0.72
2:B:589:VAL:HG12	2:B:590:HIS:H	1.53	0.72
2:B:600:LEU:O	2:B:609:ILE:HD11	1.90	0.72
1:M:445:ASN:HB2	1:M:455:MET:HG2	1.70	0.72
2:B:724:ASP:OD2	2:B:727:LYS:HG3	1.90	0.72
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.54	0.72
1:M:332:LYS:HG2	1:M:333:GLU:HG2	1.72	0.72
1:M:866:PHE:C	1:M:867:ILE:HD12	2.15	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:1183:LYS:N	2:N:1183:LYS:HE3	2.04	0.72
7:S:87:VAL:CG2	7:S:103:VAL:HG21	2.19	0.72
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.20	0.72
5:E:23:VAL:O	5:E:28:TYR:HB2	1.90	0.72
2:N:622:LYS:NZ	9:U:59:VAL:HG13	2.05	0.72
2:N:1096:ARG:O	2:N:1097:HIS:HB2	1.90	0.72
3:O:36:VAL:HG21	3:O:251:LEU:HD13	1.72	0.72
1:A:601:LYS:HB2	1:A:603:ASN:ND2	2.05	0.72
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.89	0.72
5:E:14:ARG:HH21	5:E:141:VAL:HG12	1.54	0.72
1:A:310:GLY:O	1:A:312:PRO:HD2	1.89	0.72
1:A:1094:VAL:HG13	1:A:1113:THR:CG2	2.19	0.72
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.72	0.72
2:B:278:GLN:HG2	2:B:279:ASP:H	1.54	0.72
2:B:549:THR:HG22	2:B:550:ASP:N	2.04	0.72
1:M:7:SER:OG	2:N:1161:HIS:HE1	1.72	0.72
1:M:517:ASN:HD22	1:M:1364:ASN:HD22	1.38	0.72
1:M:1385:THR:HG22	1:M:1387:HIS:N	2.04	0.72
2:N:56:ASP:HB3	2:N:57:TYR:CD1	2.25	0.72
2:N:1224:PHE:CE1	5:Q:171:LYS:HG3	2.25	0.72
3:O:8:VAL:O	3:O:9:LYS:HG3	1.90	0.72
9:U:111:THR:CG2	9:U:112:SER:N	2.52	0.72
1:M:231:PRO:HA	1:M:234:MET:HE2	1.71	0.71
1:M:889:SER:HB3	1:M:1297:GLU:HG3	1.72	0.71
2:N:336:ARG:HH11	2:N:336:ARG:HG3	1.56	0.71
2:N:766:ARG:HH22	2:N:1020:ARG:HH11	1.38	0.71
7:S:153:GLN:HG2	7:S:154:VAL:HG23	1.71	0.71
10:J:48:ARG:HG2	10:J:48:ARG:HH11	1.54	0.71
1:M:470:LEU:H	1:M:470:LEU:HD23	1.55	0.71
2:N:56:ASP:HB3	2:N:57:TYR:HD1	1.55	0.71
2:N:289:LEU:HD13	2:N:375:ALA:CB	2.20	0.71
3:O:166:GLU:HG3	11:W:10:PHE:HZ	1.55	0.71
8:T:24:CYS:HB2	8:T:44:VAL:HG21	1.72	0.71
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.20	0.71
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.72	0.71
3:O:165:LYS:O	11:W:6:ARG:NH1	2.22	0.71
1:A:37:PHE:N	1:A:37:PHE:CD1	2.56	0.71
1:A:68:GLN:OE1	1:A:68:GLN:O	2.09	0.71
1:A:517:ASN:HD22	1:A:1364:ASN:HD22	1.37	0.71
1:A:1223:ASP:HA	1:A:1243:VAL:HG22	1.72	0.71
2:B:56:ASP:HB3	2:B:57:TYR:CD1	2.25	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:LEU:HD22	3:C:230:MET:HE1	1.70	0.71
4:D:138:ASN:HD21	7:G:35:GLU:HB3	1.55	0.71
6:F:77:ASP:O	6:F:78:GLN:HB2	1.90	0.71
8:H:130:ARG:HD3	8:H:130:ARG:N	2.06	0.71
1:M:239:LEU:HD12	1:M:240:PRO:HD2	1.71	0.71
1:M:1116:LEU:H	1:M:1308:THR:HG22	1.55	0.71
2:N:953:LEU:HD21	2:N:965:LYS:HB2	1.71	0.71
5:Q:50:MET:HG2	5:Q:52:ARG:HH21	1.55	0.71
1:A:1202:MET:HE1	1:A:1212:VAL:HG21	1.72	0.71
2:B:427:ASP:HA	2:B:430:ARG:HD2	1.73	0.71
1:M:549:MET:HE1	1:M:656:TRP:HD1	1.55	0.71
2:N:515:HIS:HD2	2:N:517:THR:H	1.37	0.71
5:Q:23:VAL:O	5:Q:28:TYR:HB2	1.90	0.71
1:A:316:GLN:HG2	1:A:317:LYS:HG2	1.71	0.71
1:A:709:THR:HG22	1:A:710:LEU:N	2.04	0.71
4:D:8:PHE:CE1	4:D:37:GLN:HB2	2.26	0.71
12:L:32:ALA:HB2	12:L:55:ILE:HG13	1.72	0.71
1:M:115:LEU:HD12	1:M:142:CYS:HB3	1.71	0.71
1:M:709:THR:HG22	1:M:710:LEU:N	2.05	0.71
2:N:295:GLY:N	2:N:298:LEU:HD23	2.06	0.71
2:N:563:MET:HE1	2:N:580:VAL:HB	1.73	0.71
1:A:37:PHE:N	1:A:37:PHE:HD1	1.89	0.71
2:B:1016:ALA:O	2:B:1020:ARG:HG3	1.91	0.71
1:M:1189:SER:O	1:M:1241:ARG:HD3	1.91	0.71
2:N:705:MET:N	2:N:710:LEU:HD12	2.06	0.71
9:U:34:TYR:CD2	9:U:35:VAL:N	2.59	0.71
2:B:60:GLN:O	2:B:63:ILE:HG22	1.89	0.71
2:B:659:ALA:HA	2:B:662:MET:HE3	1.73	0.71
7:G:13:LEU:HD22	7:G:17:PHE:HB2	1.70	0.71
12:L:47:ARG:HB2	12:L:47:ARG:HH11	1.56	0.71
12:L:47:ARG:HG3	12:L:52:GLY:O	1.91	0.71
1:M:390:GLN:HE21	1:M:394:ASN:HD22	1.39	0.71
1:M:722:LEU:H	1:M:722:LEU:HD12	1.55	0.71
1:M:767:GLN:NE2	1:M:774:ARG:HB3	2.05	0.71
2:N:467:GLY:N	2:N:475:SER:HB3	2.06	0.71
2:N:515:HIS:CD2	2:N:517:THR:HG23	2.26	0.71
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	1.90	0.71
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.21	0.71
9:I:93:LYS:HD3	9:I:93:LYS:N	2.04	0.71
1:M:671:ALA:HB3	1:M:676:MET:HE2	1.73	0.71
1:M:1011:GLN:HE22	1:M:1015:VAL:HG21	1.56	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1353:TYR:C	1:M:1353:TYR:CD2	2.68	0.71
2:N:25:ILE:HG21	2:N:658:ILE:HD12	1.73	0.71
2:N:620:ARG:NH1	9:U:68:LEU:HD21	2.05	0.71
5:Q:16:PHE:CZ	5:Q:20:LYS:HE2	2.26	0.71
1:A:253:ASN:ND2	2:B:884:ARG:HD2	2.05	0.70
1:A:1207:LEU:HD13	1:A:1273:LEU:HD23	1.73	0.70
2:B:226:PHE:HA	2:B:395:GLN:CG	2.20	0.70
2:B:384:ARG:HH12	2:B:393:LYS:HD3	1.55	0.70
2:B:898:LEU:HD13	2:B:952:VAL:HG11	1.72	0.70
2:B:917:PRO:O	2:B:918:ILE:HG13	1.90	0.70
1:M:157:ASP:OD2	1:M:160:GLN:HG3	1.91	0.70
1:M:1121:GLU:CG	1:M:1122:PRO:HD2	2.20	0.70
2:N:217:ARG:NE	2:N:405:ARG:HB2	2.06	0.70
7:S:52:ASP:C	7:S:53:ASN:HD22	1.98	0.70
7:S:99:PHE:O	7:S:110:VAL:HG23	1.90	0.70
1:A:71:GLN:O	1:A:73:GLY:N	2.23	0.70
1:A:225:ASN:HD22	1:A:228:PHE:H	1.37	0.70
1:A:523:ILE:CG1	1:A:622:VAL:HG22	2.21	0.70
1:M:1118:VAL:HG23	1:M:1306:LEU:HB2	1.72	0.70
2:N:756:ILE:O	2:N:759:PRO:HD3	1.91	0.70
4:P:8:PHE:HE1	4:P:37:GLN:HB2	1.55	0.70
2:B:873:THR:O	2:B:914:LYS:HA	1.91	0.70
3:C:147:LEU:N	3:C:147:LEU:HD23	2.07	0.70
1:M:49:LYS:HZ3	1:M:61:ILE:HG13	1.56	0.70
1:M:254:GLU:HB2	2:N:935:ARG:NH2	2.06	0.70
1:M:916:GLY:O	1:M:919:ILE:HG22	1.91	0.70
1:M:1293:SER:OG	1:M:1294:PRO:HD2	1.91	0.70
2:N:38:PHE:HD1	2:N:811:TYR:CD2	2.09	0.70
2:N:873:THR:O	2:N:914:LYS:HA	1.91	0.70
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.73	0.70
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	1.91	0.70
2:B:309:GLN:HG3	9:I:52:ILE:CD1	2.21	0.70
2:B:1004:GLU:HG3	10:J:42:LYS:NZ	2.05	0.70
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.21	0.70
1:M:216:VAL:O	1:M:219:PHE:HB2	1.91	0.70
2:N:604:ARG:HB2	2:N:609:ILE:HG13	1.73	0.70
4:P:29:LEU:HD12	7:S:82:PHE:CZ	2.26	0.70
10:V:44:TYR:HA	10:V:47:ARG:HB2	1.74	0.70
11:W:60:ALA:O	11:W:73:LEU:HD12	1.90	0.70
1:A:249:SER:O	1:A:250:ILE:HG13	1.90	0.70
1:A:626:ASN:O	1:A:631:HIS:HD2	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.74	0.70
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.71	0.70
2:B:168:GLY:HA2	2:B:454:THR:OG1	1.91	0.70
2:B:642:ASP:O	2:B:644:GLU:N	2.21	0.70
3:C:101:LEU:HD13	3:C:118:LEU:CD2	2.20	0.70
4:D:130:LEU:HD13	4:D:142:LYS:HG2	1.72	0.70
5:E:10:SER:O	5:E:13:TRP:HB3	1.92	0.70
7:G:126:ASN:HD22	7:G:127:PRO:CA	2.05	0.70
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.31	0.70
1:M:541:ILE:HG22	1:M:546:VAL:HG23	1.73	0.70
2:N:240:ILE:CG2	2:N:254:LEU:HB3	2.22	0.70
2:N:288:ALA:HB1	2:N:331:LEU:HD12	1.71	0.70
6:R:130:ILE:HB	6:R:148:VAL:HG21	1.72	0.70
10:V:53:HIS:CD2	10:V:54:VAL:N	2.59	0.70
1:A:388:LEU:O	1:A:392:VAL:HG23	1.92	0.70
1:A:908:LEU:HD11	1:A:983:ILE:HD11	1.74	0.70
2:B:428:ILE:HG22	2:B:432:MET:HE2	1.73	0.70
2:B:542:MET:HE2	2:B:747:MET:HE2	1.72	0.70
1:M:567:LYS:CB	8:T:95:TYR:HA	2.20	0.70
4:P:70:PHE:O	4:P:74:GLN:HG3	1.91	0.70
4:P:151:PHE:N	4:P:151:PHE:CD1	2.58	0.70
5:Q:180:ARG:NH2	5:Q:192:ARG:HB2	2.05	0.70
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.57	0.70
2:B:847:ASP:C	2:B:849:GLY:H	1.98	0.70
3:C:16:ASP:C	3:C:240:VAL:HG11	2.16	0.70
1:M:122:MET:HA	1:M:141:LEU:CD1	2.22	0.70
1:M:1409:LEU:HD13	2:N:1207:LEU:HD11	1.73	0.70
2:N:600:LEU:O	2:N:609:ILE:HD11	1.90	0.70
2:N:846:ILE:HG23	2:N:974:PRO:HG2	1.72	0.70
4:P:120:GLU:O	4:P:124:GLU:OE2	2.09	0.70
2:B:247:GLY:H	2:B:249:ARG:HH21	1.37	0.70
2:B:705:MET:H	2:B:710:LEU:CD1	2.04	0.70
8:H:8:ASP:OD2	8:H:9:ILE:N	2.24	0.70
10:J:53:HIS:CD2	10:J:54:VAL:N	2.60	0.70
1:M:40:THR:HG22	1:M:41:MET:HG3	1.72	0.70
2:N:129:PHE:CE2	2:N:166:PHE:HB2	2.27	0.70
2:N:642:ASP:CA	2:N:649:LYS:HG3	2.22	0.70
7:S:138:THR:HG22	7:S:139:ILE:N	2.06	0.70
1:A:595:THR:O	1:A:596:THR:HG23	1.92	0.70
1:A:1293:SER:OG	1:A:1294:PRO:HD2	1.90	0.70
1:M:236:LEU:HD11	1:M:304:MET:HE1	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:768:GLN:CG	1:M:816:HIS:HA	2.22	0.70
1:M:1006:ILE:CD1	5:Q:163:GLU:HG3	2.21	0.70
4:P:134:THR:HG23	4:P:141:LEU:HD23	1.74	0.70
5:Q:202:SER:OG	5:Q:204:THR:HG22	1.92	0.70
2:B:245:GLU:O	2:B:246:LYS:HG3	1.91	0.70
5:E:147:HIS:HD2	5:E:149:LEU:H	1.39	0.70
11:K:65:HIS:HD2	11:K:67:PHE:H	1.38	0.70
1:M:372:LYS:HA	1:M:435:HIS:ND1	2.07	0.70
2:N:345:LYS:CG	2:N:346:GLU:H	2.05	0.70
2:N:705:MET:H	2:N:710:LEU:CD1	2.04	0.70
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.88	0.69
1:A:794:PRO:HG2	1:A:795:GLU:OE2	1.91	0.69
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.27	0.69
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.73	0.69
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.05	0.69
2:B:559:SER:CA	2:B:563:MET:HB3	2.19	0.69
4:D:35:LEU:H	4:D:35:LEU:HD12	1.56	0.69
7:G:139:ILE:HG23	7:G:140:LYS:N	2.07	0.69
10:J:64:ASN:HB3	10:J:65:PRO:HD2	1.74	0.69
1:M:34:LYS:HZ1	1:M:57:ARG:NH2	1.89	0.69
1:M:672:ASP:HB3	1:M:736:ASN:ND2	2.07	0.69
1:M:722:LEU:HD21	1:M:794:PRO:HB3	1.72	0.69
1:A:225:ASN:ND2	1:A:227:VAL:H	1.90	0.69
1:A:1210:GLY:O	1:A:1214:GLU:HG2	1.92	0.69
1:M:351:THR:HG22	2:N:1103:ILE:CA	2.20	0.69
2:N:199:MET:HE2	2:N:492:LEU:HD23	1.74	0.69
3:O:33:LEU:O	3:O:37:MET:HG3	1.92	0.69
9:U:4:PHE:HE1	9:U:13:MET:HG3	1.58	0.69
11:W:57:LEU:HB2	11:W:76:GLN:HG2	1.73	0.69
11:W:101:LEU:HD23	11:W:101:LEU:O	1.92	0.69
1:A:288:ALA:HA	1:A:291:GLU:OE1	1.91	0.69
1:A:535:THR:CG2	1:A:616:VAL:HA	2.23	0.69
2:B:114:PRO:HG2	2:B:115:GLN:H	1.57	0.69
1:M:399:HIS:O	1:M:401:GLY:N	2.25	0.69
5:Q:94:LYS:O	5:Q:98:ILE:HG13	1.92	0.69
7:S:94:CYS:SG	7:S:128:PRO:HB2	2.32	0.69
1:A:425:GLN:OE1	1:A:425:GLN:N	2.25	0.69
1:A:960:ILE:O	1:A:963:ILE:HG22	1.92	0.69
2:B:542:MET:HG2	2:B:747:MET:CE	2.22	0.69
2:B:957:ASN:ND2	2:B:961:LEU:HB2	2.03	0.69
1:M:1236:LEU:C	1:M:1237:ILE:HD12	2.15	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:39:ALA:HA	3:O:164:ALA:HB3	1.74	0.69
5:Q:124:VAL:CG1	5:Q:132:ILE:HB	2.16	0.69
8:T:84:ALA:HB1	8:T:87:ARG:HB2	1.74	0.69
2:B:165:VAL:HG11	2:B:448:ILE:HD13	1.73	0.69
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.08	0.69
3:C:165:LYS:O	11:K:6:ARG:NH1	2.25	0.69
2:N:996:ARG:HH12	3:O:174:ALA:HA	1.58	0.69
3:O:66:ARG:NH2	10:V:3:VAL:O	2.25	0.69
11:W:46:ILE:O	11:W:50:LEU:HB2	1.92	0.69
2:B:96:TYR:HB2	2:B:129:PHE:HB2	1.73	0.69
3:C:66:ARG:NH2	10:J:3:VAL:O	2.26	0.69
1:M:42:ASP:O	1:M:44:THR:N	2.26	0.69
1:M:115:LEU:CD1	1:M:142:CYS:HB3	2.22	0.69
1:M:537:ARG:HD2	8:T:20:TYR:HE1	1.56	0.69
1:M:1011:GLN:HE22	1:M:1015:VAL:CG2	2.06	0.69
2:N:357:GLN:O	2:N:366:GLN:HA	1.91	0.69
2:N:737:THR:CG2	9:U:66:PRO:HA	2.22	0.69
4:P:160:VAL:O	4:P:164:ILE:HG13	1.92	0.69
6:R:89:GLU:O	6:R:93:ILE:HD12	1.92	0.69
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.27	0.69
7:G:14:HIS:CD2	7:G:16:SER:H	2.10	0.69
9:I:50:THR:HG22	9:I:52:ILE:H	1.58	0.69
1:M:596:THR:C	1:M:598:LEU:H	2.01	0.69
1:M:698:GLN:HA	9:U:97:MET:O	1.92	0.69
1:M:822:GLU:HG3	2:N:513:GLN:HE21	1.57	0.69
2:N:473:MET:HE3	2:N:474:SER:CA	2.23	0.69
7:S:90:THR:HG22	7:S:91:VAL:O	1.92	0.69
7:S:121:PHE:CE2	7:S:123:ALA:HB2	2.28	0.69
1:A:567:LYS:HZ1	8:H:43:ASN:HB3	1.57	0.69
1:A:828:ALA:HB1	2:B:530:GLY:HA2	1.73	0.69
2:B:241:ARG:HG2	2:B:253:THR:CG2	2.23	0.69
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.08	0.69
7:G:125:SER:OG	7:G:128:PRO:HA	1.93	0.69
9:I:111:THR:HG23	9:I:112:SER:H	1.57	0.69
1:M:122:MET:HA	1:M:141:LEU:HD11	1.74	0.69
1:M:332:LYS:C	1:M:334:GLY:H	2.01	0.69
1:M:741:ASN:HD22	1:M:741:ASN:C	1.99	0.69
1:M:1223:ASP:HA	1:M:1243:VAL:CG2	2.22	0.69
2:N:642:ASP:O	2:N:644:GLU:N	2.23	0.69
2:N:710:LEU:CA	2:N:733:HIS:HB3	2.17	0.69
4:P:59:ILE:HG21	4:P:145:MET:SD	2.33	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:81:PRO:CB	8:T:82:PRO:HD2	2.22	0.69
11:W:113:THR:O	11:W:114:LEU:HB2	1.93	0.69
2:B:616:ILE:HD12	2:B:616:ILE:N	2.07	0.69
12:L:32:ALA:HB3	12:L:55:ILE:HG13	1.74	0.69
1:M:1353:TYR:C	1:M:1353:TYR:HD2	2.01	0.69
2:N:36:ALA:HA	2:N:39:ARG:HD2	1.74	0.69
2:N:834:ASN:HB3	2:N:840:ILE:HG13	1.73	0.69
7:S:95:SER:O	7:S:130:TYR:OH	2.07	0.69
1:A:1112:LYS:O	1:A:1114:PRO:HD3	1.92	0.69
2:B:582:VAL:HG23	2:B:626:ILE:HB	1.73	0.69
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.74	0.69
4:D:187:THR:HG21	1:M:34:LYS:HZ3	1.56	0.69
1:M:381:THR:HG23	1:M:382:PRO:HD2	1.75	0.69
4:P:158:GLU:CD	4:P:158:GLU:N	2.51	0.69
9:U:26:LEU:CD2	9:U:37:GLU:HA	2.19	0.69
2:B:707:PRO:HG2	2:B:708:GLU:H	1.57	0.68
2:B:1181:GLU:HA	2:B:1187:ASN:O	1.92	0.68
2:N:559:SER:CA	2:N:563:MET:HB3	2.20	0.68
2:N:770:GLN:CD	2:N:983:ARG:HA	2.18	0.68
6:R:103:MET:HE2	7:S:66:GLY:N	2.08	0.68
8:T:82:PRO:C	8:T:84:ALA:N	2.52	0.68
9:U:55:THR:HG23	9:U:100:PHE:HD2	1.57	0.68
12:X:47:ARG:HB2	12:X:47:ARG:NH1	2.07	0.68
1:A:709:THR:HG22	1:A:710:LEU:H	1.58	0.68
1:A:1148:ILE:HD11	1:A:1198:ASP:HA	1.75	0.68
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.75	0.68
2:B:168:GLY:N	2:B:450:ALA:HB1	2.08	0.68
2:B:357:GLN:O	2:B:366:GLN:HA	1.92	0.68
2:B:653:VAL:HG23	2:B:689:LEU:HB3	1.76	0.68
2:B:705:MET:N	2:B:710:LEU:HD12	2.09	0.68
2:B:797:TYR:C	2:B:798:TYR:HD2	2.01	0.68
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.73	0.68
1:M:903:ASN:HD22	1:M:903:ASN:C	2.00	0.68
2:N:1113:VAL:CG2	15:6:1:C:H4'	2.23	0.68
7:S:112:LYS:HB3	7:S:113:HIS:CE1	2.28	0.68
11:W:108:GLU:O	11:W:112:GLN:HG2	1.93	0.68
1:A:185:TRP:HE3	1:A:185:TRP:H	1.41	0.68
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.74	0.68
1:A:1207:LEU:CD1	1:A:1273:LEU:HD23	2.24	0.68
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.29	0.68
2:B:378:LEU:O	2:B:382:ILE:HG13	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:130:ARG:NH1	8:H:130:ARG:HB2	2.08	0.68
10:J:1:MET:H1	10:J:57:ILE:N	1.91	0.68
11:K:63:VAL:HG23	11:K:63:VAL:O	1.94	0.68
12:L:26:THR:CG2	12:L:27:LEU:H	2.02	0.68
2:N:744:HIS:HD2	2:N:745:PRO:HD2	1.55	0.68
2:B:955:THR:OG1	12:L:55:ILE:HA	1.93	0.68
2:B:1183:LYS:N	2:B:1183:LYS:HE3	2.08	0.68
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.74	0.68
1:M:1036:ARG:HG2	1:M:1036:ARG:NH1	2.05	0.68
1:M:1195:LEU:HD11	1:M:1267:MET:CE	2.23	0.68
2:N:244:LEU:HD11	2:N:366:GLN:NE2	2.08	0.68
7:S:128:PRO:O	7:S:138:THR:HG23	1.94	0.68
8:T:12:VAL:HA	8:T:28:ALA:HB2	1.74	0.68
1:A:503:GLN:HE21	6:F:90:ARG:NH2	1.87	0.68
1:A:524:VAL:HG12	1:A:525:GLN:N	2.06	0.68
2:B:806:THR:N	2:B:809:MET:HE3	2.08	0.68
1:M:875:ALA:HB2	1:M:1366:ARG:HD2	1.76	0.68
2:N:778:MET:CE	2:N:1094:ARG:HD3	2.21	0.68
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	1.74	0.68
1:A:1325:THR:O	5:E:148:GLU:HB2	1.94	0.68
3:C:56:THR:HG21	3:C:145:CYS:SG	2.33	0.68
6:F:103:MET:HE2	7:G:66:GLY:N	2.05	0.68
8:H:61:SER:HB3	8:H:139:ASN:HB3	1.74	0.68
1:M:150:THR:HG23	1:M:166:GLY:HA2	1.76	0.68
1:M:913:LEU:HD12	1:M:914:GLU:N	2.09	0.68
2:N:69:LEU:HB3	2:N:429:PHE:CE1	2.28	0.68
2:N:708:GLU:O	2:N:710:LEU:N	2.27	0.68
3:O:3:GLU:HB3	11:W:104:ASN:OD1	1.93	0.68
3:O:93:ASP:OD1	3:O:122:SER:HB2	1.92	0.68
3:O:181:ASP:CG	3:O:186:LEU:HD13	2.18	0.68
1:A:830:LYS:O	1:A:834:THR:HB	1.94	0.68
3:C:69:LEU:HB3	10:J:6:ARG:HD3	1.76	0.68
10:J:64:ASN:HD22	10:J:65:PRO:HD3	1.58	0.68
1:M:1325:THR:O	5:Q:148:GLU:HB2	1.94	0.68
2:N:309:GLN:OE1	9:U:52:ILE:HD11	1.92	0.68
4:P:59:ILE:HG22	4:P:60:LYS:N	2.07	0.68
4:P:153:ARG:O	4:P:154:PHE:HD2	1.76	0.68
7:S:111:THR:HG22	7:S:114:LEU:HB2	1.75	0.68
1:A:66:LYS:HD3	1:A:67:CYS:H	1.59	0.68
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	1.94	0.68
1:A:413:ILE:HG21	1:A:424:ILE:HD11	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:THR:C	1:A:598:LEU:H	2.02	0.68
4:D:14:ARG:HB3	4:D:14:ARG:HH11	1.58	0.68
8:H:12:VAL:HA	8:H:28:ALA:HB2	1.75	0.68
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.28	0.68
1:M:1420:ASP:CB	1:M:1422:ARG:HG3	2.19	0.68
2:N:836:GLU:O	2:N:837:ASP:HB2	1.93	0.68
4:P:4:SER:O	4:P:5:THR:HB	1.94	0.68
4:P:138:ASN:HB3	4:P:141:LEU:HB3	1.75	0.68
5:Q:147:HIS:HB3	5:Q:150:VAL:HG23	1.76	0.68
8:T:99:GLY:HA3	8:T:118:PHE:HD2	1.58	0.68
1:A:49:LYS:NZ	1:A:60:SER:HA	2.09	0.68
2:B:34:ILE:HG23	2:B:542:MET:HE2	1.76	0.68
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.75	0.68
5:E:50:MET:HG2	5:E:52:ARG:HH21	1.59	0.68
6:F:116:ASP:HB3	6:F:119:ARG:HB2	1.76	0.68
10:J:16:ASP:OD1	10:J:17:LYS:HD2	1.93	0.68
14:2:5:DC:H2''	14:2:6:DT:C7	2.24	0.68
2:N:226:PHE:HA	2:N:395:GLN:CG	2.24	0.68
2:N:597:MET:HA	2:N:597:MET:CE	2.24	0.68
4:P:35:LEU:HD12	4:P:35:LEU:N	2.09	0.68
9:U:76:PRO:HD2	9:U:108:HIS:CD2	2.28	0.68
1:A:567:LYS:CB	8:H:96:VAL:H	1.98	0.68
2:B:34:ILE:HG12	2:B:542:MET:HE1	1.75	0.68
4:D:18:VAL:O	4:D:19:GLU:HB2	1.94	0.68
7:G:1:MET:SD	7:G:79:PHE:CD1	2.87	0.68
2:N:100:PRO:HG3	2:N:172:ILE:HD12	1.75	0.68
2:N:857:ARG:HD2	2:N:945:GLU:OE1	1.92	0.68
1:A:332:LYS:C	1:A:334:GLY:H	2.02	0.67
2:B:345:LYS:HA	2:B:348:ARG:HE	1.59	0.67
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.86	0.67
4:D:29:LEU:HD22	4:D:29:LEU:H	1.57	0.67
5:E:144:ILE:HG13	5:E:145:THR:N	2.09	0.67
1:M:1195:LEU:HD11	1:M:1267:MET:HE1	1.76	0.67
2:N:807:ARG:HG2	2:N:1045:SER:OG	1.94	0.67
2:N:897:GLY:O	2:N:898:LEU:HD23	1.93	0.67
4:P:71:LYS:HA	4:P:74:GLN:HB2	1.75	0.67
1:A:42:ASP:O	1:A:44:THR:N	2.27	0.67
4:D:71:LYS:HG2	4:D:74:GLN:HG3	1.75	0.67
1:M:50:ILE:C	1:M:52:GLY:H	2.02	0.67
1:M:382:PRO:CA	1:M:428:TYR:HE2	2.07	0.67
1:M:852:TYR:CD2	1:M:1060:PRO:HB2	2.29	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:579:ARG:HG2	2:N:579:ARG:HH11	1.59	0.67
9:U:61:ASP:C	9:U:63:GLY:H	2.00	0.67
2:B:243:ALA:HA	2:B:250:PHE:O	1.93	0.67
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.56	0.67
3:C:186:LEU:HD21	3:C:225:ALA:HB2	1.76	0.67
4:D:146:GLN:HA	4:D:149:THR:HG22	1.76	0.67
1:M:433:GLU:OE1	2:N:1108:ARG:NH2	2.27	0.67
1:M:868:TYR:CD2	1:M:1058:VAL:HG21	2.30	0.67
2:N:20:ASP:O	2:N:22:SER:N	2.23	0.67
2:N:657:HIS:CE1	2:N:689:LEU:HD11	2.30	0.67
4:P:144:THR:O	4:P:148:LEU:HB2	1.94	0.67
12:X:53:HIS:HB3	12:X:55:ILE:CD1	2.23	0.67
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.76	0.67
2:B:199:MET:HE2	2:B:492:LEU:HD23	1.76	0.67
2:B:589:VAL:HG12	2:B:590:HIS:N	2.09	0.67
4:D:54:GLU:O	4:D:58:VAL:HG23	1.95	0.67
1:M:897:TYR:HB3	1:M:936:LEU:HD12	1.77	0.67
1:M:901:LEU:H	1:M:926:GLN:NE2	1.93	0.67
2:N:291:ILE:HD13	2:N:300:HIS:CD2	2.29	0.67
2:N:309:GLN:HG3	9:U:52:ILE:CD1	2.24	0.67
2:N:622:LYS:HE2	9:U:59:VAL:CG2	2.19	0.67
3:O:186:LEU:HD21	3:O:225:ALA:HB2	1.77	0.67
4:P:153:ARG:C	4:P:154:PHE:CD2	2.73	0.67
1:A:768:GLN:CG	1:A:816:HIS:HA	2.22	0.67
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.77	0.67
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.76	0.67
2:B:563:MET:HE1	2:B:580:VAL:HB	1.76	0.67
2:B:868:MET:O	2:B:870:ILE:HG13	1.95	0.67
1:M:903:ASN:ND2	1:M:904:THR:N	2.39	0.67
2:N:168:GLY:N	2:N:450:ALA:HB1	2.10	0.67
2:N:254:LEU:HD12	2:N:272:THR:O	1.94	0.67
2:N:345:LYS:N	2:N:347:LYS:HE2	2.10	0.67
3:O:124:LEU:O	3:O:127:ARG:HG2	1.94	0.67
1:A:205:GLU:H	1:A:205:GLU:CD	2.01	0.67
1:A:265:LYS:HE3	1:A:265:LYS:HA	1.74	0.67
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.10	0.67
2:B:363:HIS:O	2:B:364:ILE:HB	1.95	0.67
2:B:580:VAL:HG22	2:B:624:LEU:HB3	1.75	0.67
5:E:177:ARG:HD3	5:E:215:MET:SD	2.34	0.67
8:H:15:VAL:HG22	8:H:26:ILE:HD11	1.75	0.67
9:I:111:THR:HG21	9:I:113:ASP:HB2	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1141:THR:CG2	1:M:1205:LYS:HD3	2.25	0.67
2:N:165:VAL:HG11	2:N:448:ILE:HD13	1.76	0.67
2:N:562:GLY:HA3	2:N:590:HIS:CE1	2.30	0.67
2:N:618:ASP:CG	2:N:621:GLU:HB3	2.20	0.67
4:P:18:VAL:O	4:P:19:GLU:HB2	1.95	0.67
4:P:156:ASP:HB2	4:P:159:THR:CG2	2.24	0.67
5:Q:4:GLU:HB3	5:Q:7:ARG:HE	1.59	0.67
9:U:40:SER:OG	9:U:41:PRO:HD2	1.94	0.67
1:A:512:VAL:HA	1:A:519:PRO:HA	1.75	0.67
5:E:98:ILE:HG22	5:E:102:GLU:HG3	1.76	0.67
9:I:61:ASP:C	9:I:63:GLY:H	2.00	0.67
1:M:34:LYS:NZ	1:M:57:ARG:NH2	2.43	0.67
1:M:492:PRO:CB	1:M:497:THR:HG22	2.25	0.67
1:M:852:TYR:CE2	1:M:1060:PRO:HB2	2.30	0.67
2:N:309:GLN:CD	9:U:52:ILE:HD11	2.19	0.67
2:N:724:ASP:OD2	2:N:727:LYS:HG3	1.95	0.67
4:P:8:PHE:CE1	4:P:37:GLN:HB2	2.29	0.67
5:Q:94:LYS:HE2	5:Q:98:ILE:CD1	2.25	0.67
7:S:116:PRO:HG2	7:S:119:LEU:HB2	1.77	0.67
14:5:5:DC:H2"	14:5:6:DT:C7	2.25	0.67
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.60	0.67
2:B:1202:LEU:O	2:B:1206:GLU:HG3	1.95	0.67
2:B:1224:PHE:CZ	5:E:171:LYS:HG3	2.29	0.67
1:M:595:THR:O	1:M:596:THR:HG23	1.95	0.67
2:N:1124:ARG:NH1	15:6:2:G:OP2	2.28	0.67
12:X:38:LEU:CD1	12:X:49:LYS:HE2	2.25	0.67
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.10	0.67
2:B:217:ARG:HD2	2:B:217:ARG:C	2.20	0.67
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.25	0.67
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.77	0.67
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.75	0.67
4:D:4:SER:O	4:D:5:THR:HB	1.95	0.67
6:F:89:GLU:HG2	6:F:134:ILE:HD13	1.77	0.67
8:H:58:THR:HB	8:H:143:LEU:HD13	1.76	0.67
10:J:1:MET:N	10:J:56:LEU:N	2.43	0.67
1:M:185:TRP:H	1:M:185:TRP:HE3	1.42	0.67
1:M:284:ALA:O	1:M:286:HIS:N	2.27	0.67
1:M:567:LYS:HZ2	8:T:46:LEU:HB2	1.59	0.67
1:M:1144:LYS:HB2	1:M:1268:LEU:O	1.94	0.67
2:N:589:VAL:HG12	2:N:590:HIS:N	2.10	0.67
2:N:593:PRO:HG2	2:N:617:ARG:NH1	2.10	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:48:ILE:O	4:P:48:ILE:HG22	1.94	0.67
5:Q:100:ILE:HG23	5:Q:105:PHE:HB2	1.77	0.67
5:Q:157:SER:OG	5:Q:160:GLU:HG3	1.95	0.67
7:S:34:VAL:HG12	7:S:45:ILE:HG21	1.76	0.67
7:S:45:ILE:HA	7:S:78:VAL:HG12	1.77	0.67
9:U:44:TYR:CD1	9:U:45:ARG:N	2.62	0.67
11:W:63:VAL:O	11:W:63:VAL:HG23	1.95	0.67
1:A:34:LYS:HZ2	1:A:57:ARG:NH2	1.93	0.67
1:A:1147:THR:HB	9:I:48:LEU:HD12	1.77	0.67
2:B:261:ARG:HB3	2:B:261:ARG:NH1	2.09	0.67
2:B:806:THR:HG22	2:B:808:ALA:N	2.06	0.67
10:J:16:ASP:OD1	10:J:17:LYS:N	2.28	0.67
1:M:164:ARG:HG3	1:M:165:GLY:N	2.09	0.67
1:M:407:ARG:HG2	1:M:430:TRP:CZ2	2.29	0.67
1:M:492:PRO:HB2	1:M:497:THR:HG22	1.76	0.67
1:M:688:LYS:HG3	1:M:691:LEU:HD23	1.76	0.67
7:S:142:ARG:C	7:S:143:ILE:HG12	2.19	0.67
12:X:47:ARG:HG2	12:X:48:CYS:H	1.59	0.67
1:A:675:THR:O	1:A:679:ILE:HG13	1.95	0.66
2:B:227:LYS:H	2:B:395:GLN:CD	2.03	0.66
7:G:126:ASN:HD22	7:G:127:PRO:HA	1.59	0.66
1:M:66:LYS:HZ2	1:M:68:GLN:H	1.42	0.66
2:N:34:ILE:HG12	2:N:542:MET:HE1	1.76	0.66
2:N:515:HIS:CD2	2:N:517:THR:H	2.12	0.66
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.24	0.66
1:A:1255:GLU:HG3	1:A:1258:HIS:CD2	2.30	0.66
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.30	0.66
2:B:708:GLU:O	2:B:710:LEU:N	2.28	0.66
2:B:879:ARG:H	2:B:879:ARG:NE	1.93	0.66
2:N:868:MET:O	2:N:870:ILE:HG13	1.95	0.66
6:R:96:THR:O	6:R:100:GLN:HG3	1.95	0.66
1:A:122:MET:HA	1:A:141:LEU:CD1	2.25	0.66
1:A:698:GLN:HA	9:I:97:MET:O	1.95	0.66
1:A:977:LYS:HB3	1:A:978:PRO:HD2	1.77	0.66
2:B:805:THR:HG22	2:B:806:THR:N	2.10	0.66
2:B:955:THR:CG2	2:B:956:THR:N	2.57	0.66
12:L:40:LEU:HD13	12:L:44:ASP:CB	2.21	0.66
1:M:535:THR:HG21	1:M:617:VAL:H	1.60	0.66
1:M:870:GLU:HG2	5:Q:208:TYR:CG	2.30	0.66
1:A:1081:LEU:HD11	1:A:1098:VAL:H	1.60	0.66
1:A:1167:GLU:O	1:A:1170:ILE:HD12	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:604:ARG:HB2	2:B:609:ILE:HG13	1.77	0.66
7:G:1:MET:HE1	7:G:79:PHE:HA	1.77	0.66
7:G:115:MET:HB3	7:G:116:PRO:HD2	1.77	0.66
1:M:55:ASP:N	1:M:56:PRO:HD3	2.09	0.66
1:M:463:ILE:HB	1:M:464:PRO:HD2	1.78	0.66
1:M:828:ALA:HB1	2:N:530:GLY:HA2	1.76	0.66
2:N:658:ILE:CG2	2:N:662:MET:HE2	2.25	0.66
2:N:1037:LEU:HD21	2:N:1064:TYR:HE1	1.61	0.66
3:O:69:LEU:HB3	10:V:6:ARG:HD3	1.78	0.66
7:S:111:THR:HG22	7:S:114:LEU:HD13	1.77	0.66
9:U:8:ARG:HG3	9:U:34:TYR:HE1	1.60	0.66
1:A:203:SER:O	1:A:207:ILE:HG12	1.96	0.66
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.96	0.66
1:A:1076:ALA:HA	1:A:1079:MET:HG3	1.77	0.66
1:A:1116:LEU:HB3	1:A:1308:THR:HG21	1.78	0.66
1:A:1130:GLN:O	1:A:1134:ILE:HG13	1.96	0.66
2:B:345:LYS:HG2	2:B:346:GLU:H	1.61	0.66
2:B:553:PRO:O	2:B:557:PHE:HB2	1.95	0.66
6:F:111:LEU:O	6:F:113:GLY:N	2.23	0.66
7:G:7:LEU:HB2	7:G:74:TYR:HE2	1.60	0.66
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.76	0.66
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.26	0.66
14:2:5:DC:H2"	14:2:6:DT:H72	1.78	0.66
1:M:203:SER:O	1:M:207:ILE:HG12	1.96	0.66
2:N:516:ASN:H	2:N:516:ASN:ND2	1.81	0.66
2:N:562:GLY:HA3	2:N:590:HIS:ND1	2.11	0.66
2:N:911:ILE:HD11	2:N:941:LEU:CD1	2.24	0.66
8:T:95:TYR:HE2	8:T:97:MET:CG	2.05	0.66
9:U:19:ASP:HB3	9:U:24:ARG:HG2	1.77	0.66
1:A:710:LEU:H	1:A:710:LEU:CD1	2.08	0.66
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.25	0.66
1:A:1202:MET:HE1	1:A:1212:VAL:CG2	2.26	0.66
1:A:1258:HIS:O	1:A:1262:LYS:HE3	1.96	0.66
2:B:644:GLU:HB3	2:B:648:HIS:O	1.95	0.66
4:D:134:THR:HG22	4:D:135:GLY:N	2.10	0.66
12:L:38:LEU:CD1	12:L:49:LYS:HE2	2.25	0.66
1:M:66:LYS:O	1:M:67:CYS:HB2	1.93	0.66
2:N:1138:MET:HE2	2:N:1146:PHE:CD2	2.31	0.66
5:Q:14:ARG:HH21	5:Q:141:VAL:CG1	2.02	0.66
7:S:111:THR:CG2	7:S:114:LEU:HD13	2.26	0.66
1:A:50:ILE:C	1:A:52:GLY:H	2.03	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ILE:HG22	1:A:309:ALA:N	2.09	0.66
1:A:710:LEU:HD12	1:A:710:LEU:N	2.11	0.66
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.78	0.66
8:H:14:GLU:HG2	8:H:15:VAL:N	2.11	0.66
11:K:113:THR:O	11:K:114:LEU:HB2	1.96	0.66
2:N:847:ASP:C	2:N:849:GLY:H	2.02	0.66
9:U:73:ARG:HH12	9:U:112:SER:HB3	1.59	0.66
2:B:64:CYS:HA	2:B:67:SER:OG	1.95	0.66
1:M:71:GLN:O	1:M:73:GLY:N	2.28	0.66
1:M:268:ASP:HB3	1:M:299:HIS:CE1	2.31	0.66
1:M:463:ILE:HD11	1:M:469:ARG:HG3	1.78	0.66
1:M:1004:ASN:ND2	5:Q:167:ARG:HD2	2.10	0.66
4:P:71:LYS:HA	4:P:74:GLN:CG	2.24	0.66
4:P:118:THR:HB	4:P:121:LYS:CB	2.23	0.66
4:P:124:GLU:O	4:P:128:VAL:HG23	1.96	0.66
1:A:321:PRO:O	1:A:322:VAL:HG12	1.96	0.66
1:A:626:ASN:O	1:A:631:HIS:CD2	2.49	0.66
1:A:897:TYR:HB3	1:A:936:LEU:HD12	1.78	0.66
1:A:1342:GLU:CG	5:E:198:ILE:HD13	2.25	0.66
2:B:819:ALA:O	2:B:1093:GLN:HG2	1.95	0.66
7:G:116:PRO:HG2	7:G:119:LEU:HB2	1.77	0.66
10:J:23:ASN:C	10:J:25:LEU:H	2.04	0.66
2:N:295:GLY:H	2:N:298:LEU:HD23	1.59	0.66
4:P:139:LYS:HA	4:P:142:LYS:HD2	1.78	0.66
9:U:111:THR:CG2	9:U:112:SER:H	2.09	0.66
1:A:973:ILE:HD13	1:A:1037:LEU:HA	1.77	0.66
1:A:1036:ARG:HG2	1:A:1036:ARG:NH1	2.10	0.66
2:B:384:ARG:NH1	2:B:393:LYS:HD3	2.11	0.66
2:B:955:THR:HG22	2:B:956:THR:N	2.11	0.66
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.78	0.66
4:D:119:ARG:HG3	4:D:221:TYR:CZ	2.30	0.66
1:M:982:THR:O	1:M:985:ASP:HB2	1.96	0.66
7:S:13:LEU:HD21	7:S:17:PHE:CB	2.24	0.66
9:U:7:CYS:SG	9:U:8:ARG:O	2.54	0.66
10:V:1:MET:N	10:V:56:LEU:N	2.44	0.66
12:X:32:ALA:HB3	12:X:55:ILE:HG13	1.77	0.66
1:A:1095:THR:HG21	1:A:1112:LYS:HD2	1.77	0.65
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.78	0.65
2:B:287:ARG:NH1	2:B:324:ILE:O	2.28	0.65
2:B:418:LYS:HE2	2:B:422:LYS:NZ	2.10	0.65
5:E:2:ASP:O	5:E:3:GLN:HG2	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:64:ASN:CB	10:J:65:PRO:CD	2.74	0.65
12:L:61:THR:CG2	12:L:63:ARG:HG3	2.26	0.65
1:M:858:ASN:ND2	1:M:858:ASN:C	2.54	0.65
5:Q:197:LYS:HE2	5:Q:199:ILE:CD1	2.21	0.65
2:B:560:GLU:O	2:B:561:TRP:CD1	2.50	0.65
2:B:953:LEU:CD2	2:B:965:LYS:HB2	2.26	0.65
1:M:37:PHE:N	1:M:37:PHE:HD1	1.93	0.65
1:M:512:VAL:HA	1:M:519:PRO:HA	1.76	0.65
1:M:1241:ARG:O	1:M:1242:VAL:HB	1.95	0.65
2:N:1073:TYR:CE2	2:N:1080:LYS:HG2	2.31	0.65
4:P:50:LEU:HD13	4:P:55:ALA:HA	1.77	0.65
1:A:399:HIS:O	1:A:401:GLY:N	2.28	0.65
1:A:1170:ILE:HG22	1:A:1174:PHE:CE1	2.32	0.65
2:B:277:LYS:HE2	2:B:336:ARG:C	2.20	0.65
2:B:831:SER:HB2	2:B:833:TYR:HD1	1.61	0.65
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.96	0.65
3:C:69:LEU:N	3:C:69:LEU:HD12	2.11	0.65
1:M:37:PHE:HD1	1:M:37:PHE:H	1.44	0.65
1:M:1242:VAL:CG1	1:M:1243:VAL:N	2.59	0.65
2:N:167:ILE:HA	2:N:450:ALA:CB	2.26	0.65
2:N:243:ALA:HA	2:N:250:PHE:O	1.95	0.65
2:N:361:LEU:HD21	2:N:377:PHE:CD2	2.31	0.65
2:N:649:LYS:HD3	2:N:736:THR:O	1.96	0.65
3:O:238:ILE:HD11	3:O:246:ARG:NH1	2.12	0.65
5:Q:44:ALA:O	5:Q:45:LYS:HB2	1.95	0.65
7:S:139:ILE:HG12	7:S:140:LYS:HG3	1.77	0.65
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.79	0.65
1:A:1120:LEU:HD22	1:A:1125:ALA:HA	1.78	0.65
2:B:842:ASN:HD22	2:B:845:SER:H	1.42	0.65
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.78	0.65
1:M:14:VAL:H	1:M:1432:GLN:NE2	1.89	0.65
7:S:15:PRO:HA	7:S:18:PHE:CD1	2.31	0.65
8:H:139:ASN:O	8:H:140:ALA:HB2	1.96	0.65
2:N:69:LEU:HB3	2:N:429:PHE:HE1	1.61	0.65
2:N:425:THR:HA	2:N:428:ILE:HD12	1.78	0.65
8:T:139:ASN:O	8:T:140:ALA:HB2	1.96	0.65
10:V:23:ASN:C	10:V:25:LEU:H	2.05	0.65
10:V:24:LEU:O	10:V:30:LEU:HB2	1.95	0.65
14:5:5:DC:H2"	14:5:6:DT:H72	1.79	0.65
2:B:770:GLN:CD	2:B:983:ARG:HA	2.21	0.65
3:C:101:LEU:C	3:C:102:GLN:HG2	2.21	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:8:PHE:HE1	4:D:37:GLN:HB2	1.61	0.65
10:J:14:VAL:O	10:J:14:VAL:HG12	1.97	0.65
1:M:265:LYS:HE3	1:M:265:LYS:N	2.12	0.65
2:N:244:LEU:HD21	2:N:366:GLN:NE2	2.11	0.65
2:N:805:THR:HG22	2:N:806:THR:N	2.12	0.65
2:N:969:ARG:NH1	3:O:61:GLU:OE1	2.30	0.65
3:O:58:LEU:N	3:O:58:LEU:HD23	2.11	0.65
7:S:34:VAL:CG1	7:S:45:ILE:HG21	2.26	0.65
9:U:50:THR:CG2	9:U:51:ASN:H	2.10	0.65
10:V:21:TYR:HB2	10:V:39:LEU:HD11	1.77	0.65
2:B:613:VAL:HG13	2:B:627:PHE:O	1.97	0.65
2:B:780:VAL:HG21	10:J:56:LEU:HD11	1.78	0.65
2:N:292:ILE:HD11	2:N:327:ARG:N	2.12	0.65
4:P:12:ARG:HG2	4:P:12:ARG:NH1	2.12	0.65
5:E:9:ILE:CD1	5:E:53:PRO:HD3	2.25	0.65
5:E:56:LYS:CE	5:E:84:ASP:HB2	2.22	0.65
12:L:34:CYS:HB3	12:L:51:CYS:SG	2.37	0.65
2:N:431:TYR:CD1	2:N:447:ALA:HB2	2.32	0.65
2:N:707:PRO:HG2	2:N:708:GLU:H	1.62	0.65
4:P:119:ARG:HG3	4:P:221:TYR:CZ	2.32	0.65
4:P:155:ARG:NH1	4:P:155:ARG:HB2	2.11	0.65
6:R:111:LEU:H	6:R:111:LEU:CD1	2.10	0.65
1:A:335:ARG:HH12	2:B:1206:GLU:CD	2.04	0.65
2:B:20:ASP:O	2:B:22:SER:N	2.25	0.65
2:B:289:LEU:HD13	2:B:375:ALA:CB	2.23	0.65
9:I:73:ARG:HD2	9:I:101:PHE:CE2	2.32	0.65
10:J:44:TYR:H	10:J:44:TYR:HD2	1.43	0.65
1:M:134:ARG:HD2	1:M:221:SER:O	1.97	0.65
1:M:250:ILE:O	1:M:250:ILE:HG22	1.96	0.65
1:M:335:ARG:HA	1:M:339:ASN:HD22	1.62	0.65
1:M:1116:LEU:HB3	1:M:1308:THR:HG21	1.79	0.65
1:M:1121:GLU:HG2	1:M:1122:PRO:HD2	1.79	0.65
2:N:770:GLN:HG2	2:N:983:ARG:O	1.96	0.65
1:A:284:ALA:O	1:A:286:HIS:N	2.28	0.65
2:B:483:LEU:HD11	2:B:491:THR:HG22	1.78	0.65
2:B:497:ARG:NH2	2:B:775:LYS:NZ	2.45	0.65
2:B:1174:LYS:O	2:B:1176:ASN:N	2.30	0.65
8:H:15:VAL:HG22	8:H:26:ILE:CD1	2.26	0.65
1:M:626:ASN:O	1:M:631:HIS:HD2	1.80	0.65
1:M:1242:VAL:HG12	1:M:1243:VAL:N	2.11	0.65
2:N:123:THR:HG21	2:N:458:LYS:HE2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:12:ARG:NH1	4:P:14:ARG:HA	2.11	0.65
5:Q:78:LEU:HD12	5:Q:107:THR:HG21	1.78	0.65
2:B:167:ILE:HA	2:B:450:ALA:CB	2.27	0.64
2:N:364:ILE:O	2:N:365:THR:HB	1.96	0.64
2:N:515:HIS:H	2:N:518:HIS:HD2	1.45	0.64
2:N:521:LEU:CD2	2:N:633:VAL:HG12	2.19	0.64
5:Q:9:ILE:CD1	5:Q:53:PRO:HD3	2.27	0.64
8:T:139:ASN:O	8:T:140:ALA:CB	2.45	0.64
2:B:309:GLN:CG	9:I:52:ILE:HD11	2.27	0.64
3:C:73:GLN:NE2	3:C:75:MET:H	1.94	0.64
4:D:7:THR:O	4:D:9:GLN:N	2.29	0.64
5:E:117:THR:HG22	5:E:119:SER:N	2.04	0.64
9:I:52:ILE:HG13	9:I:52:ILE:O	1.98	0.64
1:M:106:VAL:HG12	1:M:107:CYS:N	2.12	0.64
2:N:205:ILE:HD12	2:N:205:ILE:N	2.12	0.64
5:Q:98:ILE:O	5:Q:102:GLU:HG3	1.97	0.64
6:R:147:SER:OG	6:R:150:GLU:HG3	1.96	0.64
9:U:50:THR:HG21	9:U:52:ILE:HG12	1.78	0.64
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.36	0.64
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.27	0.64
2:B:549:THR:HG22	2:B:550:ASP:H	1.60	0.64
8:H:32:THR:HG22	8:H:33:GLN:OE1	1.96	0.64
8:H:84:ALA:CA	8:H:87:ARG:HB2	2.26	0.64
12:L:40:LEU:HD22	12:L:44:ASP:CG	2.22	0.64
1:M:833:GLU:OE2	1:M:1102:LYS:HE3	1.97	0.64
2:N:217:ARG:HD2	2:N:217:ARG:C	2.22	0.64
2:N:309:GLN:CG	9:U:52:ILE:HD11	2.28	0.64
2:N:705:MET:HE3	2:N:705:MET:HA	1.80	0.64
2:N:957:ASN:ND2	2:N:961:LEU:HB2	2.11	0.64
4:P:56:ARG:CA	4:P:148:LEU:HD13	2.24	0.64
4:P:156:ASP:O	4:P:160:VAL:HG23	1.96	0.64
1:A:741:ASN:ND2	1:A:744:LYS:H	1.95	0.64
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.33	0.64
2:B:56:ASP:HB3	2:B:57:TYR:HD1	1.62	0.64
2:B:465:ASN:N	2:B:465:ASN:ND2	2.43	0.64
2:B:1072:MET:HE3	2:B:1085:ILE:CB	2.15	0.64
3:C:69:LEU:HD12	3:C:69:LEU:H	1.62	0.64
6:F:111:LEU:C	6:F:113:GLY:H	2.05	0.64
1:M:385:ILE:HD11	1:M:426:LEU:HB2	1.80	0.64
1:M:425:GLN:OE1	1:M:425:GLN:N	2.30	0.64
1:M:1258:HIS:O	1:M:1262:LYS:HE3	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.61	0.64
1:A:1333:ILE:O	1:A:1337:GLU:HG3	1.97	0.64
2:B:622:LYS:NZ	9:I:59:VAL:HG13	2.12	0.64
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.79	0.64
1:M:172:PRO:HB3	1:M:185:TRP:CD2	2.32	0.64
1:M:1041:ALA:O	1:M:1045:VAL:HG23	1.97	0.64
1:M:1112:LYS:O	1:M:1114:PRO:HD3	1.97	0.64
1:M:1345:ARG:HG2	1:M:1372:VAL:HG12	1.79	0.64
2:N:515:HIS:H	2:N:518:HIS:CD2	2.16	0.64
2:N:916:THR:O	2:N:935:ARG:HG2	1.97	0.64
3:O:11:ARG:HH12	3:O:205:LYS:NZ	1.95	0.64
5:Q:112:TYR:O	5:Q:137:GLU:HG3	1.97	0.64
10:V:48:ARG:HG2	10:V:48:ARG:NH1	2.09	0.64
11:W:49:GLU:HG3	11:W:94:ILE:HG13	1.80	0.64
2:B:272:THR:HG23	2:B:279:ASP:OD1	1.97	0.64
2:B:364:ILE:O	2:B:365:THR:HB	1.95	0.64
4:D:52:LEU:O	4:D:54:GLU:N	2.31	0.64
7:G:137:ILE:HG23	7:G:143:ILE:HD11	1.79	0.64
1:M:577:ILE:O	1:M:580:VAL:HG23	1.96	0.64
1:M:934:LYS:O	1:M:937:VAL:HG12	1.97	0.64
2:N:611:PRO:HB3	2:N:685:LEU:HD11	1.80	0.64
2:N:806:THR:N	2:N:809:MET:HE3	2.13	0.64
4:P:162:ALA:HB1	4:P:217:LEU:HD13	1.78	0.64
4:P:163:VAL:O	4:P:167:LEU:HG	1.97	0.64
1:A:523:ILE:HG12	1:A:622:VAL:HG22	1.79	0.64
1:A:916:GLY:O	1:A:919:ILE:HG22	1.97	0.64
1:A:1144:LYS:HB2	1:A:1268:LEU:O	1.97	0.64
2:B:225:VAL:HG11	2:B:385:LEU:HA	1.80	0.64
2:B:515:HIS:H	2:B:518:HIS:CD2	2.12	0.64
3:C:238:ILE:HD11	3:C:246:ARG:CZ	2.28	0.64
12:L:53:HIS:HB3	12:L:55:ILE:HD11	1.78	0.64
1:M:129:LYS:O	1:M:130:ASP:HB2	1.95	0.64
2:N:115:GLN:HG2	2:N:193:LYS:HB2	1.80	0.64
2:N:582:VAL:CG2	2:N:626:ILE:HB	2.28	0.64
4:P:154:PHE:HD1	4:P:163:VAL:HG21	1.63	0.64
5:Q:69:ILE:HD12	5:Q:69:ILE:N	2.12	0.64
5:Q:144:ILE:HG13	5:Q:145:THR:H	1.62	0.64
9:U:17:ARG:HH21	9:U:30:ARG:NE	1.96	0.64
1:A:341:MET:HE3	2:B:1135:ARG:HH11	1.60	0.64
1:A:351:THR:CG2	2:B:1103:ILE:HA	2.22	0.64
1:A:1011:GLN:HE22	1:A:1015:VAL:CG2	2.11	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:MET:HE2	2:B:492:LEU:HD21	1.78	0.64
2:B:345:LYS:CG	2:B:346:GLU:H	2.11	0.64
3:C:43:THR:CG2	3:C:44:LEU:N	2.60	0.64
4:D:14:ARG:HB3	4:D:14:ARG:NH1	2.12	0.64
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.80	0.64
2:N:23:ALA:HB1	2:N:24:PRO:HD2	1.80	0.64
3:O:73:GLN:NE2	3:O:75:MET:HB2	2.13	0.64
7:S:87:VAL:HG21	7:S:103:VAL:HG11	1.79	0.64
11:W:45:LEU:HG	11:W:94:ILE:CD1	2.27	0.64
1:A:1139:GLU:O	1:A:1139:GLU:HG2	1.96	0.64
2:B:57:TYR:HD1	2:B:57:TYR:N	1.96	0.64
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.80	0.64
7:G:1:MET:SD	7:G:2:PHE:N	2.70	0.64
8:H:139:ASN:O	8:H:140:ALA:CB	2.46	0.64
11:K:90:ALA:O	11:K:94:ILE:HG13	1.97	0.64
12:L:47:ARG:HB2	12:L:47:ARG:NH1	2.12	0.64
1:M:22:PHE:HB2	2:N:1211:ASN:ND2	2.13	0.64
1:M:518:LYS:HE2	1:M:624:SER:O	1.98	0.64
1:M:567:LYS:CB	8:T:96:VAL:H	2.02	0.64
2:N:780:VAL:HG21	10:V:56:LEU:HD11	1.80	0.64
4:P:163:VAL:O	4:P:166:LEU:HB3	1.98	0.64
5:Q:56:LYS:CE	5:Q:84:ASP:HB2	2.24	0.64
7:S:81:PRO:HG3	7:S:106:MET:SD	2.38	0.64
9:U:78:CYS:SG	9:U:106:CYS:HB3	2.38	0.64
1:A:741:ASN:HD22	1:A:744:LYS:H	1.44	0.64
1:A:1029:ARG:HH11	1:A:1029:ARG:HG3	1.63	0.64
2:B:123:THR:HG21	2:B:458:LYS:HE2	1.79	0.64
2:B:1037:LEU:HD21	2:B:1064:TYR:HE1	1.63	0.64
2:B:1115:THR:O	2:B:1116:ARG:HB2	1.98	0.64
11:K:21:ILE:CG2	11:K:31:VAL:HG11	2.28	0.64
1:M:79:GLY:HA3	1:M:243:PRO:HG3	1.78	0.64
1:M:331:GLY:O	1:M:332:LYS:O	2.15	0.64
1:M:567:LYS:CB	1:M:568:PRO:CD	2.72	0.64
1:M:1385:THR:CG2	1:M:1387:HIS:H	2.05	0.64
2:N:120:ARG:NH1	12:X:54:ARG:HH11	1.96	0.64
2:N:549:THR:HB	2:N:628:THR:OG1	1.97	0.64
2:N:1100:ASP:OD2	11:W:1:MET:HB3	1.98	0.64
3:O:148:ARG:N	3:O:151:GLN:HG3	2.12	0.64
5:Q:144:ILE:HG13	5:Q:145:THR:N	2.13	0.64
6:R:69:LEU:HB3	6:R:71:GLU:OE1	1.98	0.64
12:X:34:CYS:HB3	12:X:51:CYS:HG	1.63	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:LYS:H	1:A:773:LYS:HD2	1.63	0.63
2:B:577:ALA:CB	2:B:589:VAL:HG11	2.21	0.63
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.33	0.63
8:H:130:ARG:HB2	8:H:130:ARG:HH11	1.62	0.63
9:I:58:VAL:HG13	9:I:62:ILE:HD13	1.80	0.63
2:N:31:TRP:CZ3	2:N:34:ILE:HD12	2.33	0.63
2:N:186:GLU:HG2	10:V:62:ARG:HH22	1.63	0.63
2:N:553:PRO:O	2:N:557:PHE:HB2	1.97	0.63
2:N:955:THR:HG22	2:N:956:THR:N	2.11	0.63
10:V:64:ASN:ND2	10:V:65:PRO:HD3	2.12	0.63
12:X:34:CYS:HB3	12:X:51:CYS:SG	2.38	0.63
1:A:670:ILE:HG23	1:A:805:LEU:HD21	1.78	0.63
2:B:554:ILE:HD11	2:B:609:ILE:HG22	1.79	0.63
2:B:562:GLY:HA3	2:B:590:HIS:ND1	2.12	0.63
3:C:11:ARG:HH12	3:C:205:LYS:NZ	1.95	0.63
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.80	0.63
13:1:22:DC:C2'	13:1:23:BRU:H5'	2.25	0.63
1:M:335:ARG:HH12	2:N:1206:GLU:CD	2.06	0.63
1:M:883:LEU:HD23	1:M:1021:LEU:HD13	1.80	0.63
2:N:126:SER:OG	2:N:172:ILE:HD11	1.98	0.63
2:N:1072:MET:HE2	2:N:1085:ILE:HB	1.79	0.63
8:T:14:GLU:HG2	8:T:15:VAL:N	2.13	0.63
11:W:21:ILE:HG23	11:W:33:ILE:HG12	1.80	0.63
1:A:252:PHE:HB2	1:A:256:GLN:NE2	2.14	0.63
2:B:102:VAL:HG21	2:B:112:LEU:HD13	1.80	0.63
2:B:484:ASN:O	2:B:491:THR:HG23	1.99	0.63
3:C:124:LEU:O	3:C:127:ARG:HG2	1.99	0.63
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.81	0.63
12:L:38:LEU:HG	12:L:39:SER:H	1.64	0.63
1:M:107:CYS:HA	1:M:171:GLN:NE2	2.13	0.63
4:P:14:ARG:O	4:P:16:LYS:N	2.25	0.63
7:S:111:THR:O	7:S:114:LEU:HB2	1.98	0.63
1:A:216:VAL:O	1:A:219:PHE:HB2	1.99	0.63
1:A:489:LEU:HD12	1:A:490:HIS:N	2.13	0.63
1:A:961:ARG:HH11	1:A:961:ARG:HB2	1.63	0.63
2:B:282:ILE:O	2:B:286:PHE:HD1	1.81	0.63
2:B:798:TYR:HD1	10:J:4:PRO:HG3	1.64	0.63
2:B:886:LYS:HE2	2:B:940:PRO:HD3	1.80	0.63
6:F:75:PRO:O	6:F:77:ASP:O	2.16	0.63
6:F:119:ARG:HH11	6:F:119:ARG:CG	2.11	0.63
8:H:100:THR:OG1	8:H:138:GLU:HG2	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:31:VAL:HG12	11:K:32:VAL:N	2.12	0.63
1:M:626:ASN:O	1:M:631:HIS:CD2	2.52	0.63
1:M:903:ASN:ND2	1:M:903:ASN:C	2.56	0.63
2:N:370:PHE:HD2	2:N:373:ARG:CD	2.11	0.63
2:N:955:THR:OG1	12:X:55:ILE:HA	1.97	0.63
4:P:219:THR:HG22	4:P:220:LEU:O	1.98	0.63
5:Q:39:LEU:HG	5:Q:43:LYS:HE3	1.79	0.63
5:Q:178:ILE:HG22	5:Q:213:ILE:O	1.98	0.63
5:Q:180:ARG:HB2	5:Q:215:MET:OXT	1.97	0.63
1:A:1410:PHE:HA	2:B:1212:ILE:HD11	1.80	0.63
2:B:284:ILE:HD13	2:B:333:PHE:HD2	1.64	0.63
2:B:465:ASN:N	2:B:465:ASN:HD22	1.94	0.63
2:B:1113:VAL:HG23	15:3:1:C:H4'	1.80	0.63
5:E:157:SER:OG	5:E:160:GLU:HG3	1.99	0.63
12:L:60:ARG:HG2	12:L:61:THR:N	2.13	0.63
1:M:87:ALA:CB	1:M:276:LEU:HD23	2.28	0.63
1:M:252:PHE:O	1:M:256:GLN:NE2	2.30	0.63
1:M:873:MET:C	1:M:1058:VAL:HG23	2.24	0.63
2:N:193:LYS:NZ	12:X:32:ALA:HB1	2.13	0.63
2:N:575:PRO:HG2	2:N:576:ASP:H	1.62	0.63
2:N:1065:GLN:NE2	2:N:1067:ARG:H	1.94	0.63
4:P:155:ARG:HH21	4:P:221:TYR:HD1	1.43	0.63
1:A:67:CYS:C	1:A:68:GLN:HG3	2.22	0.63
1:A:1006:ILE:CD1	5:E:163:GLU:HG3	2.29	0.63
1:A:1338:VAL:HG12	1:A:1339:LEU:HD23	1.81	0.63
2:B:789:MET:HE3	2:B:965:LYS:HB3	1.81	0.63
3:C:261:ALA:HA	3:C:264:GLN:OE1	1.99	0.63
4:D:14:ARG:NH2	4:D:16:LYS:HD2	2.14	0.63
1:M:325:ILE:HG22	2:N:1210:MET:HE2	1.80	0.63
1:M:567:LYS:NZ	8:T:43:ASN:HB3	2.14	0.63
1:M:949:ASP:OD1	1:M:951:GLU:HB2	1.99	0.63
2:N:422:LYS:O	2:N:426:LYS:HG2	1.97	0.63
2:N:465:ASN:N	2:N:465:ASN:ND2	2.44	0.63
2:N:1001:PHE:CE1	2:N:1073:TYR:HB2	2.33	0.63
5:Q:46:TYR:CD2	5:Q:58:MET:HG2	2.34	0.63
8:T:38:LEU:HD12	8:T:39:THR:H	1.64	0.63
1:A:666:ILE:HD12	1:A:667:GLY:H	1.62	0.63
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.32	0.63
1:A:1170:ILE:HD12	1:A:1170:ILE:H	1.62	0.63
2:B:293:PRO:HD2	2:B:296:GLU:OE1	1.99	0.63
2:B:370:PHE:HD2	2:B:373:ARG:CD	2.12	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:806:THR:H	2:B:809:MET:HE3	1.63	0.63
5:E:153:HIS:O	5:E:154:ILE:CG1	2.45	0.63
9:I:76:PRO:HD2	9:I:108:HIS:CD2	2.32	0.63
12:L:28:LYS:HE3	12:L:39:SER:OG	1.97	0.63
1:M:297:GLN:HE21	1:M:297:GLN:CA	2.02	0.63
1:M:903:ASN:HD22	1:M:904:THR:H	1.45	0.63
1:M:993:LEU:HD22	1:M:1046:LEU:HD22	1.81	0.63
2:N:284:ILE:HD13	2:N:333:PHE:HD2	1.63	0.63
3:O:148:ARG:H	3:O:151:GLN:HG3	1.63	0.63
4:P:14:ARG:HB3	4:P:14:ARG:NH1	2.13	0.63
4:P:35:LEU:HD11	4:P:173:HIS:CD2	2.34	0.63
4:P:71:LYS:HG2	4:P:74:GLN:NE2	2.14	0.63
15:6:2:G:O2'	15:6:3:A:H5'	1.99	0.63
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.33	0.63
2:B:751:VAL:HG13	2:B:812:LEU:CD2	2.27	0.63
2:B:1096:ARG:HB2	2:B:1096:ARG:HH11	1.64	0.63
9:I:34:TYR:CD2	9:I:35:VAL:N	2.67	0.63
15:3:2:G:O2'	15:3:3:A:H5'	1.99	0.63
1:M:666:ILE:HD12	1:M:667:GLY:H	1.63	0.63
1:M:697:ALA:HB2	1:M:702:LEU:HD11	1.81	0.63
1:M:977:LYS:HB3	1:M:978:PRO:HD2	1.80	0.63
2:N:1113:VAL:HG23	15:6:1:C:H4'	1.80	0.63
5:Q:22:MET:HE3	5:Q:26:ARG:CZ	2.28	0.63
7:S:106:MET:HG2	7:S:107:LYS:H	1.64	0.63
8:T:99:GLY:HA3	8:T:118:PHE:CD2	2.33	0.63
1:A:44:THR:O	1:A:45:GLN:HB2	1.98	0.63
1:A:961:ARG:HG2	1:A:965:GLN:HE21	1.63	0.63
2:B:597:MET:HA	2:B:597:MET:CE	2.27	0.63
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.81	0.63
8:H:127:GLY:O	8:H:128:ASN:CB	2.47	0.63
12:L:61:THR:HG22	12:L:63:ARG:HG3	1.80	0.63
1:M:1076:ALA:HA	1:M:1079:MET:HG3	1.80	0.63
2:N:1017:ILE:HB	2:N:1018:PRO:HD3	1.81	0.63
9:U:111:THR:HG22	9:U:112:SER:N	2.13	0.63
2:B:649:LYS:HD3	2:B:736:THR:O	1.99	0.62
7:G:51:TYR:O	7:G:54:ILE:HG13	1.99	0.62
2:N:464:GLY:O	2:N:477:ALA:HA	1.99	0.62
2:N:654:ARG:HG3	2:N:654:ARG:HH11	1.64	0.62
2:N:789:MET:CE	2:N:953:LEU:HD22	2.26	0.62
2:N:1095:LEU:HD12	2:N:1095:LEU:N	2.14	0.62
7:S:21:ARG:HD2	7:S:24:GLN:CB	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:64:ASN:CB	10:V:65:PRO:CD	2.75	0.62
12:X:58:LYS:O	12:X:59:ALA:O	2.17	0.62
1:A:71:GLN:C	1:A:73:GLY:H	2.06	0.62
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.62	0.62
2:B:370:PHE:CD2	2:B:373:ARG:HD3	2.33	0.62
2:B:1084:GLN:N	2:B:1084:GLN:NE2	2.47	0.62
1:M:67:CYS:C	1:M:68:GLN:HG3	2.24	0.62
1:M:270:LEU:O	1:M:274:ILE:HG13	1.98	0.62
1:M:789:LYS:HE3	9:U:67:THR:OG1	1.97	0.62
2:N:233:PRO:HG2	2:N:234:ILE:HD13	1.80	0.62
2:N:644:GLU:OE2	2:N:646:LEU:HB3	1.98	0.62
2:N:941:LEU:HD21	2:N:946:ASN:HA	1.80	0.62
3:O:66:ARG:HA	3:O:69:LEU:HD13	1.80	0.62
9:U:111:THR:HG23	9:U:112:SER:H	1.63	0.62
1:A:635:ARG:HA	1:A:635:ARG:NH1	2.14	0.62
2:B:579:ARG:HD2	2:B:586:TRP:CZ2	2.34	0.62
2:B:822:ASN:ND2	10:J:52:THR:HG21	2.14	0.62
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.28	0.62
7:G:52:ASP:C	7:G:53:ASN:HD22	2.07	0.62
12:L:58:LYS:O	12:L:59:ALA:O	2.17	0.62
1:M:33:ALA:HA	1:M:57:ARG:NH1	2.14	0.62
1:M:335:ARG:O	1:M:339:ASN:HB2	1.98	0.62
1:M:709:THR:HB	1:M:712:GLU:HG3	1.81	0.62
1:M:782:ARG:NH2	2:N:699:GLU:O	2.32	0.62
2:N:102:VAL:HG21	2:N:112:LEU:HD13	1.81	0.62
2:N:815:ARG:HH11	2:N:815:ARG:HB2	1.65	0.62
3:O:241:ASP:O	3:O:245:VAL:HG23	1.98	0.62
6:R:69:LEU:O	6:R:71:GLU:HG3	1.98	0.62
1:A:252:PHE:O	1:A:256:GLN:NE2	2.32	0.62
2:B:57:TYR:CD1	2:B:57:TYR:N	2.67	0.62
2:B:126:SER:OG	2:B:172:ILE:HD11	1.99	0.62
2:B:365:THR:HG21	2:B:370:PHE:CG	2.34	0.62
2:B:398:ARG:CB	2:B:398:ARG:HH11	2.12	0.62
2:B:766:ARG:HH21	2:B:1020:ARG:HD3	1.63	0.62
3:C:73:GLN:HE21	3:C:75:MET:HB2	1.63	0.62
6:F:111:LEU:H	6:F:111:LEU:CD1	2.11	0.62
7:G:126:ASN:HD22	7:G:127:PRO:N	1.97	0.62
9:I:78:CYS:SG	9:I:106:CYS:HB3	2.40	0.62
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.81	0.62
2:N:64:CYS:HA	2:N:67:SER:OG	1.99	0.62
2:N:516:ASN:N	2:N:516:ASN:ND2	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:216:ASN:C	4:P:218:GLU:N	2.54	0.62
13:4:22:DC:C2'	13:4:23:BRU:H5'	2.26	0.62
1:A:567:LYS:HZ2	8:H:46:LEU:HB2	1.63	0.62
2:B:43:LEU:HD11	2:B:811:TYR:O	1.99	0.62
1:M:93:VAL:CG2	1:M:301:ALA:HA	2.28	0.62
1:M:1127:ASP:HB3	1:M:1130:GLN:HB3	1.79	0.62
7:S:150:CYS:SG	7:S:159:ALA:HB2	2.39	0.62
1:A:351:THR:HG21	2:B:1103:ILE:HG13	1.80	0.62
2:B:408:LEU:HD11	2:B:545:ILE:HD13	1.82	0.62
2:B:916:THR:O	2:B:935:ARG:HG2	1.99	0.62
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.64	0.62
2:N:168:GLY:HA2	2:N:454:THR:OG1	1.99	0.62
2:N:427:ASP:HA	2:N:430:ARG:CD	2.29	0.62
3:O:251:LEU:O	3:O:255:VAL:HG23	1.99	0.62
4:P:134:THR:HG22	4:P:135:GLY:N	2.15	0.62
5:Q:56:LYS:HZ3	5:Q:84:ASP:N	1.98	0.62
12:X:64:LEU:H	12:X:64:LEU:HD12	1.64	0.62
1:A:714:PHE:CB	9:I:97:MET:HE1	2.30	0.62
2:B:345:LYS:CE	2:B:349:ILE:HD11	2.29	0.62
2:B:557:PHE:CE1	2:B:603:LEU:HD11	2.35	0.62
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.81	0.62
1:M:98:LYS:O	1:M:102:VAL:HG23	2.00	0.62
1:M:1254:ALA:O	1:M:1255:GLU:HB3	2.00	0.62
1:M:1394:THR:CG2	1:M:1398:MET:SD	2.87	0.62
2:N:39:ARG:HH11	2:N:39:ARG:HG2	1.63	0.62
2:N:597:MET:HA	2:N:597:MET:HE3	1.81	0.62
5:Q:98:ILE:HG22	5:Q:102:GLU:HG3	1.82	0.62
7:S:35:GLU:HG2	7:S:48:VAL:HG23	1.82	0.62
8:T:127:GLY:O	8:T:128:ASN:CB	2.48	0.62
1:A:55:ASP:N	1:A:56:PRO:HD3	2.13	0.62
1:A:671:ALA:CB	1:A:676:MET:HE2	2.23	0.62
1:A:1141:THR:CG2	1:A:1205:LYS:HD3	2.30	0.62
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.81	0.62
2:B:470:LYS:C	2:B:472:ALA:N	2.57	0.62
2:B:1115:THR:CG2	2:B:1117:GLN:HB2	2.29	0.62
3:C:8:VAL:O	3:C:9:LYS:HG3	2.00	0.62
4:D:155:ARG:NH2	4:D:221:TYR:HD1	1.98	0.62
5:E:128:PRO:HA	5:E:129:PRO:C	2.23	0.62
1:M:78:PRO:HA	2:N:1201:LYS:HZ1	1.65	0.62
1:M:888:GLY:O	1:M:940:ARG:NH2	2.33	0.62
2:N:1174:LYS:O	2:N:1176:ASN:N	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:111:LEU:C	6:R:113:GLY:H	2.07	0.62
10:V:16:ASP:OD1	10:V:17:LYS:HD2	1.98	0.62
1:A:49:LYS:CD	1:A:55:ASP:HB3	2.30	0.62
1:A:535:THR:HG21	1:A:617:VAL:H	1.65	0.62
1:A:675:THR:HG21	1:A:736:ASN:CB	2.30	0.62
1:A:690:VAL:CG2	1:A:718:VAL:HG13	2.30	0.62
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.82	0.62
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.15	0.62
1:A:1259:MET:HE2	1:A:1263:ILE:HG13	1.81	0.62
1:A:1385:THR:HG22	1:A:1387:HIS:N	2.12	0.62
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.15	0.62
2:B:810:GLU:HB2	2:B:815:ARG:HH22	1.63	0.62
2:B:941:LEU:HD21	2:B:946:ASN:HA	1.82	0.62
3:C:184:ASN:ND2	3:C:189:THR:HB	2.14	0.62
3:C:265:MET:HE1	11:K:19:LEU:HB2	1.82	0.62
4:D:13:ARG:C	4:D:15:LEU:H	2.06	0.62
5:E:44:ALA:O	5:E:45:LYS:HB2	2.00	0.62
9:I:111:THR:CG2	9:I:112:SER:H	2.11	0.62
12:L:34:CYS:O	12:L:34:CYS:SG	2.57	0.62
1:M:38:PRO:HA	1:M:270:LEU:HD23	1.81	0.62
1:M:399:HIS:HB3	1:M:400:PRO:CD	2.29	0.62
1:M:497:THR:HG23	2:N:1146:PHE:HD1	1.65	0.62
2:N:811:TYR:N	2:N:811:TYR:CD1	2.68	0.62
14:5:3:DT:H2"	14:5:4:DA:OP2	2.00	0.62
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.80	0.62
1:A:857:ARG:HD3	1:A:861:GLY:O	2.00	0.62
1:A:1445:ILE:HD12	1:A:1445:ILE:N	2.14	0.62
2:B:284:ILE:HD13	2:B:333:PHE:CD2	2.34	0.62
2:B:333:PHE:O	2:B:334:ILE:HG13	2.00	0.62
2:B:570:VAL:HG21	2:B:573:GLN:CD	2.25	0.62
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.80	0.62
7:G:115:MET:O	7:G:164:LYS:HD3	2.00	0.62
1:M:219:PHE:CE2	1:M:231:PRO:HD2	2.33	0.62
1:M:960:ILE:O	1:M:963:ILE:HG22	2.00	0.62
1:M:1118:VAL:CG2	1:M:1306:LEU:HB2	2.30	0.62
2:N:53:GLN:HG2	2:N:547:VAL:CG2	2.30	0.62
2:N:288:ALA:CB	2:N:331:LEU:HD12	2.30	0.62
2:N:470:LYS:C	2:N:472:ALA:N	2.57	0.62
2:N:652:LYS:HD2	2:N:688:GLY:O	2.00	0.62
4:P:185:CYS:SG	4:P:190:GLU:HG2	2.40	0.62
5:Q:56:LYS:HZ3	5:Q:84:ASP:H	1.48	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:87:VAL:CG2	7:S:103:VAL:HG11	2.30	0.62
1:A:268:ASP:HB3	1:A:299:HIS:ND1	2.15	0.61
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.29	0.61
2:B:345:LYS:HE3	2:B:349:ILE:HD11	1.81	0.61
2:B:1004:GLU:HG3	10:J:42:LYS:HZ1	1.62	0.61
2:B:1220:ARG:NH1	2:B:1220:ARG:HB3	2.15	0.61
6:F:97:ARG:NH2	6:F:108:PHE:HE1	1.98	0.61
11:K:65:HIS:HD2	11:K:67:PHE:N	1.97	0.61
1:M:99:ILE:HG23	1:M:211:PHE:HE2	1.64	0.61
1:M:427:GLN:HG3	1:M:430:TRP:CZ2	2.35	0.61
1:M:675:THR:O	1:M:679:ILE:HG13	2.00	0.61
1:M:803:SER:OG	1:M:806:ARG:HG3	1.99	0.61
2:N:247:GLY:C	2:N:249:ARG:H	2.08	0.61
2:N:886:LYS:HE2	2:N:940:PRO:HD3	1.82	0.61
2:N:953:LEU:CD2	2:N:965:LYS:HB2	2.30	0.61
3:O:69:LEU:HD12	3:O:69:LEU:N	2.14	0.61
8:T:130:ARG:HB3	8:T:134:ASN:H	1.66	0.61
1:A:63:ARG:HA	1:A:74:MET:CE	2.29	0.61
1:A:856:THR:HB	1:A:865:GLN:HB2	1.81	0.61
1:A:1111:MET:HE2	1:A:1113:THR:O	2.00	0.61
1:A:1200:ALA:HA	1:A:1203:ASN:HD22	1.65	0.61
2:B:326:ASP:OD2	2:B:328:GLU:HB3	2.01	0.61
2:B:334:ILE:HG22	2:B:334:ILE:O	1.98	0.61
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.81	0.61
2:B:758:PHE:HE1	2:B:1027:ILE:HG22	1.63	0.61
3:C:189:THR:HG22	3:C:190:ASP:N	2.15	0.61
4:D:71:LYS:HA	4:D:74:GLN:CB	2.29	0.61
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.66	0.61
1:M:56:PRO:O	1:M:57:ARG:HG3	2.00	0.61
1:M:78:PRO:HA	2:N:1201:LYS:NZ	2.15	0.61
1:M:364:VAL:HG13	1:M:364:VAL:O	1.99	0.61
1:M:1029:ARG:HG3	1:M:1029:ARG:HH11	1.65	0.61
2:N:129:PHE:HD2	2:N:166:PHE:HA	1.66	0.61
2:N:235:SER:OG	2:N:236:HIS:CD2	2.54	0.61
2:N:241:ARG:HG2	2:N:253:THR:HG21	1.82	0.61
2:N:287:ARG:NH1	2:N:324:ILE:O	2.32	0.61
2:N:549:THR:CG2	2:N:550:ASP:N	2.62	0.61
2:N:862:GLN:HG2	2:N:963:PHE:CD1	2.32	0.61
2:N:953:LEU:O	2:N:953:LEU:HD23	2.00	0.61
4:P:29:LEU:HD22	4:P:29:LEU:N	2.15	0.61
7:S:53:ASN:N	7:S:53:ASN:ND2	2.47	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.35	0.61
1:A:982:THR:O	1:A:985:ASP:HB2	2.00	0.61
2:B:35:SER:HA	2:B:811:TYR:HE2	1.65	0.61
3:C:143:LEU:HD21	3:C:146:LYS:CE	2.29	0.61
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.25	0.61
4:D:130:LEU:C	4:D:132:GLN:H	2.08	0.61
6:F:69:LEU:O	6:F:71:GLU:HG3	1.99	0.61
10:J:64:ASN:ND2	10:J:65:PRO:HD3	2.14	0.61
12:L:52:GLY:O	12:L:53:HIS:C	2.43	0.61
1:M:7:SER:OG	2:N:1161:HIS:CE1	2.52	0.61
1:M:70:CYS:O	1:M:72:GLU:HG2	2.00	0.61
1:M:960:ILE:HA	1:M:963:ILE:HG22	1.82	0.61
2:N:29:ASP:HB3	2:N:658:ILE:HD13	1.82	0.61
2:N:57:TYR:HD1	2:N:57:TYR:N	1.98	0.61
2:N:336:ARG:HG3	2:N:336:ARG:NH1	2.15	0.61
2:N:794:ASN:C	2:N:795:ILE:HD12	2.25	0.61
2:N:999:MET:HE2	2:N:1011:ILE:HD11	1.82	0.61
4:P:29:LEU:HD12	7:S:82:PHE:CE2	2.35	0.61
1:A:351:THR:CG2	2:B:1103:ILE:HG13	2.30	0.61
1:A:401:GLY:C	1:A:435:HIS:HD2	2.07	0.61
1:A:500:GLU:OE2	2:B:1145:SER:HB2	1.99	0.61
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.64	0.61
2:B:68:THR:HA	2:B:90:ILE:O	2.00	0.61
2:B:618:ASP:CG	2:B:621:GLU:HB3	2.25	0.61
2:N:192:LEU:O	2:N:193:LYS:HB2	2.00	0.61
2:N:418:LYS:HE2	2:N:422:LYS:NZ	2.15	0.61
2:N:577:ALA:CB	2:N:589:VAL:HG11	2.22	0.61
6:R:111:LEU:O	6:R:113:GLY:N	2.28	0.61
12:X:55:ILE:HG12	12:X:56:LEU:N	2.08	0.61
1:A:782:ARG:NH2	2:B:699:GLU:O	2.33	0.61
1:A:1241:ARG:O	1:A:1242:VAL:HG23	2.01	0.61
2:B:637:LEU:HD21	2:B:742:GLU:OE2	2.01	0.61
4:D:14:ARG:O	4:D:16:LYS:N	2.27	0.61
7:G:55:ASP:OD1	7:G:57:GLN:HG3	2.00	0.61
14:2:3:DT:H2"	14:2:4:DA:OP2	2.00	0.61
2:N:766:ARG:NH2	2:N:1020:ARG:CD	2.62	0.61
2:N:911:ILE:CG2	2:N:966:VAL:HG11	2.30	0.61
12:X:38:LEU:HD13	12:X:49:LYS:HE2	1.82	0.61
1:A:78:PRO:HA	2:B:1201:LYS:HZ1	1.66	0.61
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.34	0.61
1:A:317:LYS:O	1:A:318:SER:CB	2.49	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:ALA:O	1:A:687:LYS:HB2	2.01	0.61
1:A:710:LEU:HD22	9:I:96:SER:HA	1.82	0.61
1:A:1142:THR:O	1:A:1145:SER:OG	2.19	0.61
2:B:100:PRO:HB2	2:B:180:TYR:HE1	1.65	0.61
2:B:247:GLY:C	2:B:249:ARG:H	2.09	0.61
2:B:464:GLY:O	2:B:477:ALA:HA	2.00	0.61
2:B:652:LYS:HB3	2:B:689:LEU:HD23	1.81	0.61
8:H:130:ARG:HH11	8:H:130:ARG:H	1.47	0.61
12:L:49:LYS:O	12:L:50:ASP:HB2	2.00	0.61
1:M:1120:LEU:O	1:M:1323:ASP:HB2	2.01	0.61
4:P:13:ARG:C	4:P:15:LEU:H	2.07	0.61
4:P:52:LEU:O	4:P:54:GLU:N	2.34	0.61
8:T:11:GLN:HA	8:T:53:ASP:O	2.01	0.61
8:T:51:ALA:O	8:T:52:GLN:HB2	2.01	0.61
1:A:38:PRO:CA	1:A:270:LEU:HD23	2.30	0.61
2:B:787:VAL:O	2:B:787:VAL:HG12	1.98	0.61
2:B:815:ARG:HD3	2:B:1041:GLU:OE2	2.00	0.61
2:B:864:LYS:HG3	2:B:872:GLU:OE1	1.99	0.61
2:B:1096:ARG:HB2	2:B:1096:ARG:NH1	2.15	0.61
3:C:6:PRO:CB	3:C:25:VAL:HG22	2.30	0.61
5:E:29:PHE:O	5:E:30:ILE:HG13	2.00	0.61
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.82	0.61
7:G:21:ARG:HD2	7:G:24:GLN:CB	2.31	0.61
11:K:46:ILE:O	11:K:50:LEU:HB2	2.00	0.61
1:M:40:THR:HG23	1:M:54:ASN:HD21	1.66	0.61
1:M:598:LEU:HD23	1:M:598:LEU:O	2.01	0.61
1:M:1436:ILE:O	1:M:1437:GLY:C	2.43	0.61
2:N:68:THR:HA	2:N:90:ILE:O	2.00	0.61
2:N:345:LYS:HE3	2:N:349:ILE:HD11	1.83	0.61
4:P:71:LYS:HA	4:P:74:GLN:CB	2.30	0.61
8:T:44:VAL:HG13	8:T:48:PRO:HA	1.82	0.61
1:A:1255:GLU:HG3	1:A:1258:HIS:HD2	1.62	0.61
2:B:53:GLN:HG2	2:B:547:VAL:CG2	2.31	0.61
2:B:425:THR:HA	2:B:428:ILE:HD12	1.82	0.61
2:B:839:MET:CE	2:B:980:PHE:HB2	2.29	0.61
2:B:1138:MET:HE2	2:B:1146:PHE:CD2	2.36	0.61
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.81	0.61
8:H:128:ASN:ND2	8:H:131:ASN:OD1	2.33	0.61
2:N:167:ILE:HG22	2:N:453:ILE:HD12	1.82	0.61
2:N:221:ASN:OD1	2:N:242:SER:HA	2.01	0.61
2:N:857:ARG:HH21	2:N:942:ARG:CZ	2.13	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:918:ILE:HD12	2:N:935:ARG:NH1	2.16	0.61
2:N:1220:ARG:HB3	2:N:1220:ARG:NH1	2.16	0.61
4:P:7:THR:O	4:P:9:GLN:N	2.33	0.61
1:A:325:ILE:HG22	2:B:1210:MET:HE2	1.83	0.61
2:B:398:ARG:NH1	2:B:398:ARG:HB2	2.15	0.61
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.83	0.61
3:C:215:GLU:O	3:C:216:GLY:C	2.44	0.61
4:D:25:ALA:HB1	4:D:196:PRO:HG2	1.83	0.61
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.31	0.61
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.36	0.61
10:J:24:LEU:N	10:J:24:LEU:HD23	2.15	0.61
2:N:1181:GLU:HA	2:N:1187:ASN:O	2.00	0.61
8:T:123:MET:HE1	8:T:142:LEU:HD13	1.82	0.61
9:U:111:THR:HG21	9:U:113:ASP:HB2	1.82	0.61
1:A:1116:LEU:HB2	1:A:1329:THR:OG1	2.00	0.61
2:B:192:LEU:O	2:B:193:LYS:HB2	2.01	0.61
2:B:309:GLN:OE1	9:I:52:ILE:HD11	2.01	0.61
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.31	0.61
3:C:148:ARG:NH1	3:C:149:LYS:HE3	2.16	0.61
4:D:216:ASN:C	4:D:218:GLU:N	2.57	0.61
5:E:65:THR:O	5:E:69:ILE:HD12	2.01	0.61
2:N:902:GLY:O	12:X:65:VAL:HG11	2.00	0.61
2:N:955:THR:CG2	2:N:956:THR:N	2.63	0.61
3:O:8:VAL:HG12	3:O:9:LYS:N	2.16	0.61
10:V:1:MET:H1	10:V:56:LEU:N	1.99	0.61
2:B:516:ASN:N	2:B:516:ASN:ND2	2.35	0.60
2:B:575:PRO:HG2	2:B:576:ASP:H	1.64	0.60
7:G:34:VAL:HG11	7:G:74:TYR:CE1	2.32	0.60
1:M:821:ARG:HB2	1:M:821:ARG:NH1	2.15	0.60
1:M:866:PHE:O	1:M:867:ILE:HD12	2.00	0.60
1:M:1291:VAL:HG22	1:M:1292:PRO:CD	2.31	0.60
2:N:240:ILE:HG23	2:N:254:LEU:HB3	1.83	0.60
2:N:549:THR:CG2	2:N:550:ASP:H	2.14	0.60
3:O:248:ILE:HD13	11:W:101:LEU:HD22	1.83	0.60
3:O:261:ALA:HA	3:O:264:GLN:OE1	2.00	0.60
5:Q:78:LEU:HB2	5:Q:107:THR:HB	1.83	0.60
6:R:69:LEU:HB3	6:R:71:GLU:CD	2.26	0.60
8:T:89:LEU:C	8:T:91:ASP:N	2.52	0.60
1:A:150:THR:HG23	1:A:166:GLY:HA2	1.83	0.60
1:A:598:LEU:CD1	8:H:124:ARG:HB2	2.31	0.60
1:A:939:ASP:OD2	1:A:1023:ARG:NH1	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:ILE:HD13	2:B:178:ASN:HD22	1.66	0.60
2:B:1147:LEU:HD22	2:B:1151:LEU:HD22	1.82	0.60
7:G:138:THR:HG22	7:G:139:ILE:H	1.63	0.60
1:M:332:LYS:O	1:M:333:GLU:HB2	2.00	0.60
1:M:593:GLU:C	1:M:595:THR:H	2.09	0.60
1:M:828:ALA:CB	2:N:530:GLY:HA2	2.31	0.60
1:M:857:ARG:CZ	6:R:139:PRO:HG3	2.31	0.60
2:N:39:ARG:NH2	2:N:665:GLU:HG2	2.16	0.60
2:N:57:TYR:CD1	2:N:57:TYR:N	2.69	0.60
2:N:123:THR:O	2:N:125:SER:N	2.34	0.60
2:N:291:ILE:HD13	2:N:300:HIS:NE2	2.16	0.60
7:S:115:MET:HB3	7:S:116:PRO:CD	2.30	0.60
1:A:231:PRO:HA	1:A:234:MET:HE2	1.84	0.60
2:B:473:MET:HE3	2:B:474:SER:CA	2.30	0.60
2:B:797:TYR:HE1	2:B:854:LEU:CD2	2.15	0.60
4:D:12:ARG:NH1	4:D:14:ARG:HA	2.17	0.60
8:H:89:LEU:HB2	8:H:91:ASP:CG	2.26	0.60
9:I:101:PHE:N	9:I:101:PHE:CD1	2.69	0.60
1:M:573:SER:O	1:M:576:GLN:HB2	2.01	0.60
1:M:1206:ASP:O	1:M:1274:ARG:CZ	2.49	0.60
2:N:359:GLU:O	2:N:362:PRO:HD3	2.02	0.60
2:N:653:VAL:CG2	2:N:689:LEU:HB3	2.31	0.60
2:N:865:LYS:HG2	2:N:961:LEU:HD21	1.82	0.60
2:N:983:ARG:NH1	2:N:1028:GLU:OE1	2.35	0.60
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.31	0.60
1:A:427:GLN:O	1:A:428:TYR:C	2.43	0.60
1:A:920:LEU:HD23	1:A:921:GLY:N	2.16	0.60
6:F:89:GLU:O	6:F:93:ILE:HD12	2.02	0.60
12:L:68:GLU:H	12:L:68:GLU:CD	2.10	0.60
1:M:1277:GLU:C	1:M:1279:ILE:H	2.09	0.60
1:M:1420:ASP:O	1:M:1421:CYS:HB2	2.00	0.60
2:N:39:ARG:HG2	2:N:39:ARG:NH1	2.17	0.60
2:N:189:LEU:O	2:N:192:LEU:N	2.32	0.60
2:N:227:LYS:H	2:N:395:GLN:CD	2.08	0.60
2:N:662:MET:HA	2:N:665:GLU:HG3	1.83	0.60
3:O:172:PRO:O	3:O:235:VAL:HG23	2.02	0.60
3:O:189:THR:HG22	3:O:190:ASP:N	2.16	0.60
3:O:215:GLU:O	3:O:216:GLY:C	2.45	0.60
1:A:873:MET:HE3	1:A:957:PRO:HG3	1.84	0.60
1:A:1215:ARG:NH1	1:A:1272:THR:O	2.34	0.60
4:D:71:LYS:HA	4:D:74:GLN:CG	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:44:THR:O	1:M:45:GLN:HB2	2.01	0.60
1:M:65:LEU:O	1:M:66:LYS:C	2.43	0.60
1:M:590:ARG:HG2	1:M:590:ARG:NH1	2.16	0.60
1:M:709:THR:HG22	1:M:710:LEU:H	1.66	0.60
1:M:870:GLU:HG2	5:Q:208:TYR:CD2	2.36	0.60
1:M:1208:THR:HG22	1:M:1210:GLY:H	1.66	0.60
2:N:102:VAL:HG22	2:N:112:LEU:HD22	1.83	0.60
4:P:151:PHE:HD1	4:P:151:PHE:H	1.48	0.60
4:P:193:THR:HG22	4:P:194:LEU:N	2.16	0.60
12:X:52:GLY:O	12:X:53:HIS:C	2.44	0.60
1:A:65:LEU:O	1:A:66:LYS:C	2.44	0.60
1:A:129:LYS:O	1:A:130:ASP:CB	2.49	0.60
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.36	0.60
2:B:120:ARG:NH1	12:L:54:ARG:NH1	2.50	0.60
2:B:171:PRO:HD2	2:B:457:LEU:HD12	1.82	0.60
2:B:547:VAL:HG12	2:B:612:GLU:OE2	2.02	0.60
10:J:24:LEU:O	10:J:30:LEU:HB2	2.01	0.60
12:L:47:ARG:HG2	12:L:48:CYS:H	1.65	0.60
1:M:427:GLN:O	1:M:428:TYR:C	2.44	0.60
2:N:25:ILE:HG22	2:N:658:ILE:HD12	1.83	0.60
2:N:235:SER:C	2:N:236:HIS:HD2	2.09	0.60
4:P:130:LEU:C	4:P:132:GLN:H	2.10	0.60
1:A:145:LYS:HA	1:A:145:LYS:HE3	1.82	0.60
1:A:567:LYS:CB	1:A:568:PRO:CD	2.74	0.60
1:A:1438:THR:HG22	6:F:92:ARG:HD2	1.84	0.60
2:B:235:SER:C	2:B:236:HIS:HD2	2.10	0.60
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.84	0.60
2:B:1116:ARG:HG3	2:B:1198:TYR:CG	2.37	0.60
1:M:675:THR:HG21	1:M:736:ASN:CB	2.32	0.60
1:M:709:THR:HG22	1:M:711:ARG:H	1.66	0.60
4:P:63:LEU:HD22	4:P:133:THR:OG1	2.01	0.60
4:P:154:PHE:CE1	4:P:163:VAL:HG21	2.35	0.60
4:P:162:ALA:CB	4:P:217:LEU:HD13	2.32	0.60
4:P:209:ARG:NH1	4:P:209:ARG:HG2	2.17	0.60
6:R:116:ASP:HB3	6:R:119:ARG:HB2	1.84	0.60
8:T:56:THR:HB	8:T:145:ARG:HG2	1.82	0.60
10:V:27:GLU:C	10:V:29:GLU:H	2.10	0.60
1:A:690:VAL:HG21	1:A:718:VAL:HG13	1.82	0.60
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.32	0.60
2:B:123:THR:HG23	2:B:205:ILE:HA	1.82	0.60
8:H:11:GLN:C	8:H:28:ALA:HB1	2.26	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:79:GLY:HA3	1:M:243:PRO:CG	2.32	0.60
1:M:225:ASN:HD22	1:M:228:PHE:H	1.46	0.60
1:M:831:THR:O	1:M:834:THR:HG22	2.02	0.60
2:N:797:TYR:O	10:V:1:MET:HG2	2.02	0.60
7:S:116:PRO:HG2	7:S:119:LEU:HB3	1.84	0.60
8:T:100:THR:OG1	8:T:138:GLU:HG2	2.00	0.60
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.28	0.60
2:B:307:ASP:OD2	2:B:310:MET:HB2	2.01	0.60
2:B:308:TRP:CH2	9:I:45:ARG:HG2	2.36	0.60
2:B:542:MET:HG2	2:B:747:MET:HE2	1.83	0.60
2:B:579:ARG:HG2	2:B:579:ARG:NH1	2.17	0.60
5:E:185:ALA:O	5:E:190:LEU:HG	2.02	0.60
8:H:89:LEU:C	8:H:91:ASP:N	2.54	0.60
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.83	0.60
11:K:51:LEU:CD1	11:K:59:ALA:HB3	2.31	0.60
1:M:598:LEU:O	1:M:599:SER:C	2.44	0.60
1:M:1149:ALA:HB2	9:U:47:GLU:HA	1.83	0.60
2:N:798:TYR:HE2	3:O:62:PHE:CZ	2.19	0.60
3:O:203:GLN:HG2	3:O:207:CYS:SG	2.42	0.60
5:Q:128:PRO:HA	5:Q:129:PRO:C	2.26	0.60
12:X:61:THR:HG21	12:X:63:ARG:HG3	1.84	0.60
1:A:172:PRO:HD3	1:A:185:TRP:NE1	2.17	0.60
1:A:1308:THR:HG23	1:A:1310:GLY:H	1.67	0.60
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.84	0.60
2:B:120:ARG:NH1	12:L:54:ARG:HH11	2.00	0.60
3:C:101:LEU:CD1	3:C:118:LEU:HD23	2.27	0.60
9:I:111:THR:HG22	9:I:112:SER:N	2.17	0.60
1:M:7:SER:HB3	2:N:1193:GLN:HE22	1.67	0.60
1:M:33:ALA:HA	1:M:57:ARG:HH12	1.66	0.60
1:M:35:ILE:O	1:M:35:ILE:HG22	2.00	0.60
2:N:102:VAL:CG2	2:N:112:LEU:HB2	2.18	0.60
2:N:1096:ARG:O	2:N:1097:HIS:CB	2.49	0.60
2:N:1202:LEU:O	2:N:1206:GLU:HG3	2.01	0.60
4:P:188:ALA:O	4:P:192:LYS:HG2	2.02	0.60
4:P:194:LEU:HB3	7:S:86:VAL:HG21	1.83	0.60
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.85	0.59
1:A:605:MET:HE1	1:A:612:ILE:HG23	1.84	0.59
1:A:1294:PRO:HG2	1:A:1295:THR:HG22	1.83	0.59
2:B:278:GLN:CG	2:B:279:ASP:H	2.15	0.59
3:C:124:LEU:HD21	3:C:129:ILE:O	2.01	0.59
3:C:184:ASN:OD1	3:C:187:LYS:HA	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:138:THR:CG2	7:G:139:ILE:N	2.63	0.59
8:H:11:GLN:HA	8:H:53:ASP:O	2.02	0.59
2:N:96:TYR:N	2:N:129:PHE:O	2.30	0.59
2:N:236:HIS:CE1	2:N:389:ALA:HA	2.37	0.59
2:N:863:GLU:O	2:N:961:LEU:HD13	2.02	0.59
4:P:51:ASN:OD1	4:P:52:LEU:O	2.20	0.59
4:P:118:THR:HG21	4:P:121:LYS:HE3	1.83	0.59
5:Q:32:GLN:HG3	5:Q:36:GLU:OE2	2.02	0.59
1:A:253:ASN:HD22	2:B:884:ARG:HD2	1.66	0.59
1:A:337:ARG:HD3	2:B:1132:GLU:CD	2.26	0.59
1:A:628:GLY:O	1:A:632:VAL:HG23	2.02	0.59
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.84	0.59
2:B:863:GLU:O	2:B:961:LEU:HD13	2.02	0.59
2:B:902:GLY:O	12:L:65:VAL:HG11	2.01	0.59
8:H:82:PRO:O	8:H:84:ALA:N	2.34	0.59
1:M:1114:PRO:O	1:M:1311:VAL:HG23	2.02	0.59
2:N:29:ASP:HB3	2:N:658:ILE:CD1	2.32	0.59
2:N:34:ILE:HG12	2:N:542:MET:CE	2.33	0.59
4:P:144:THR:HG21	7:S:46:LEU:HD13	1.83	0.59
4:P:173:HIS:CE1	4:P:175:PHE:H	2.21	0.59
6:R:109:VAL:CG1	6:R:110:ASP:N	2.64	0.59
7:S:142:ARG:HB3	7:S:171:ILE:HD11	1.84	0.59
8:T:32:THR:HG22	8:T:33:GLN:OE1	2.01	0.59
1:A:56:PRO:O	1:A:57:ARG:HG3	2.02	0.59
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.84	0.59
1:A:285:PRO:CG	1:A:288:ALA:HB3	2.27	0.59
1:A:332:LYS:O	1:A:333:GLU:HB2	2.02	0.59
2:B:189:LEU:O	2:B:192:LEU:N	2.33	0.59
2:B:211:VAL:O	2:B:480:SER:HA	2.02	0.59
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.36	0.59
2:B:936:ASP:OD1	2:B:937:ALA:N	2.36	0.59
4:D:5:THR:O	4:D:5:THR:HG23	2.02	0.59
6:F:69:LEU:HB3	6:F:71:GLU:CD	2.27	0.59
7:G:26:LEU:CD1	7:G:56:ILE:HD11	2.30	0.59
7:G:81:PRO:HB3	7:G:106:MET:HE1	1.84	0.59
7:G:117:GLN:NE2	7:S:154:VAL:HG22	2.18	0.59
1:M:597:LEU:HD23	8:T:103:LYS:HD2	1.83	0.59
1:M:1210:GLY:O	1:M:1214:GLU:HG2	2.02	0.59
2:N:1181:GLU:HB2	2:N:1188:LYS:HG3	1.84	0.59
4:P:130:LEU:HD13	4:P:142:LYS:HG2	1.84	0.59
4:P:188:ALA:O	4:P:192:LYS:CG	2.51	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:126:ASN:HD22	7:S:127:PRO:CA	2.15	0.59
12:X:49:LYS:O	12:X:50:ASP:CB	2.50	0.59
1:A:283:GLY:O	1:A:285:PRO:HD3	2.02	0.59
1:A:297:GLN:HA	1:A:297:GLN:NE2	2.08	0.59
1:A:555:ASP:O	1:A:556:TRP:C	2.46	0.59
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.37	0.59
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.03	0.59
1:A:1171:GLN:OE1	1:A:1172:LEU:N	2.36	0.59
1:A:1436:ILE:O	1:A:1437:GLY:C	2.45	0.59
2:B:123:THR:O	2:B:125:SER:N	2.36	0.59
2:B:273:LEU:HD12	2:B:280:ILE:HD12	1.83	0.59
2:B:298:LEU:HD22	2:B:298:LEU:N	2.17	0.59
2:B:766:ARG:NH2	2:B:1020:ARG:CD	2.65	0.59
2:B:770:GLN:HG2	2:B:983:ARG:O	2.02	0.59
4:D:202:ILE:HG23	4:D:207:LEU:HB2	1.84	0.59
5:E:131:THR:HG21	5:E:191:LYS:NZ	2.18	0.59
8:H:130:ARG:HB3	8:H:134:ASN:H	1.68	0.59
1:M:105:CYS:SG	1:M:139:TRP:HA	2.42	0.59
2:N:334:ILE:O	2:N:334:ILE:HG22	2.02	0.59
2:N:1187:ASN:OD1	2:N:1188:LYS:N	2.35	0.59
3:O:66:ARG:NH1	10:V:2:ILE:CG2	2.64	0.59
6:R:99:LEU:O	6:R:103:MET:HG2	2.02	0.59
7:S:109:PHE:O	7:S:160:ILE:HG23	2.01	0.59
7:S:111:THR:HG22	7:S:114:LEU:HD22	1.84	0.59
8:T:11:GLN:C	8:T:28:ALA:HB1	2.26	0.59
8:T:42:ILE:HG23	8:T:95:TYR:CE1	2.37	0.59
1:A:331:GLY:O	1:A:332:LYS:O	2.20	0.59
2:B:549:THR:CG2	2:B:550:ASP:H	2.15	0.59
2:B:848:ARG:HH22	2:B:996:ARG:HD3	1.66	0.59
2:B:887:HIS:CD2	2:B:887:HIS:N	2.69	0.59
3:C:184:ASN:HD21	3:C:189:THR:HB	1.67	0.59
4:D:13:ARG:O	4:D:15:LEU:N	2.29	0.59
1:M:116:ASP:OD2	1:M:164:ARG:HD2	2.02	0.59
1:M:297:GLN:HA	1:M:297:GLN:NE2	2.06	0.59
1:M:492:PRO:C	1:M:493:GLN:HE21	2.11	0.59
1:M:528:LEU:HD23	1:M:751:SER:HA	1.84	0.59
1:M:1241:ARG:O	1:M:1242:VAL:CB	2.50	0.59
1:M:1259:MET:CE	1:M:1263:ILE:HG13	2.31	0.59
2:N:384:ARG:HH12	2:N:393:LYS:HD3	1.68	0.59
2:N:766:ARG:NH2	2:N:1020:ARG:HD2	2.18	0.59
2:N:941:LEU:CD1	2:N:968:VAL:HG21	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:254:LYS:HE2	11:W:42:LEU:HD13	1.85	0.59
5:Q:198:ILE:HD11	5:Q:212:ARG:HG3	1.83	0.59
8:T:84:ALA:CB	8:T:87:ARG:HB2	2.31	0.59
12:X:26:THR:C	12:X:27:LEU:HD23	2.27	0.59
2:B:244:LEU:HD21	2:B:366:GLN:NE2	2.17	0.59
2:B:615:MET:CB	2:B:626:ILE:HG12	2.26	0.59
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.32	0.59
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.37	0.59
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.84	0.59
1:M:675:THR:OG1	1:M:736:ASN:ND2	2.34	0.59
2:N:96:TYR:HB2	2:N:129:PHE:HB2	1.82	0.59
2:N:639:ILE:HD11	2:N:691:GLU:HB2	1.84	0.59
2:N:899:ILE:HD11	2:N:911:ILE:HA	1.84	0.59
3:O:39:ALA:O	3:O:164:ALA:HB3	2.02	0.59
9:U:52:ILE:O	9:U:52:ILE:HG13	2.02	0.59
11:W:82:ASP:OD1	11:W:84:LYS:N	2.35	0.59
1:A:110:CYS:HB3	1:A:167:CYS:SG	2.42	0.59
1:A:1208:THR:HG22	1:A:1210:GLY:N	2.18	0.59
2:B:224:GLN:HA	2:B:396:ASP:OD2	2.03	0.59
2:B:637:LEU:HD12	2:B:693:ILE:CD1	2.33	0.59
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.68	0.59
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.32	0.59
1:M:62:ASP:O	1:M:64:ASN:HB2	2.03	0.59
1:M:68:GLN:OE1	1:M:68:GLN:O	2.20	0.59
1:M:323:LYS:H	1:M:323:LYS:HD2	1.66	0.59
1:M:908:LEU:HD11	1:M:983:ILE:HD11	1.84	0.59
2:N:810:GLU:CB	2:N:815:ARG:HH22	2.14	0.59
7:S:51:TYR:C	7:S:51:TYR:CD2	2.81	0.59
9:U:73:ARG:HD2	9:U:101:PHE:CE2	2.37	0.59
1:A:69:THR:O	1:A:70:CYS:C	2.45	0.59
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.84	0.59
1:A:350:ARG:HB2	2:B:1128:LEU:CD1	2.32	0.59
1:A:593:GLU:C	1:A:595:THR:H	2.11	0.59
1:A:754:SER:N	1:A:757:ASN:HD22	1.96	0.59
3:C:8:VAL:CG1	3:C:9:LYS:N	2.66	0.59
3:C:43:THR:HG22	3:C:44:LEU:N	2.17	0.59
1:M:71:GLN:C	1:M:73:GLY:H	2.10	0.59
1:M:253:ASN:ND2	2:N:884:ARG:HD2	2.18	0.59
1:M:399:HIS:CB	1:M:400:PRO:HD3	2.30	0.59
1:M:444:PHE:CE2	1:M:487:MET:HE2	2.36	0.59
1:M:549:MET:HE1	1:M:656:TRP:CD1	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:718:VAL:O	1:M:722:LEU:HD12	2.03	0.59
1:M:804:TYR:OH	2:N:763:GLN:HA	2.03	0.59
1:M:1340:GLY:HA2	5:Q:183:PRO:HD2	1.84	0.59
2:N:806:THR:CG2	2:N:808:ALA:HB3	2.33	0.59
3:O:243:VAL:O	3:O:243:VAL:HG12	2.01	0.59
5:Q:177:ARG:HD3	5:Q:215:MET:SD	2.42	0.59
8:T:89:LEU:HB2	8:T:91:ASP:OD1	2.02	0.59
12:X:38:LEU:HG	12:X:39:SER:H	1.67	0.59
1:A:24:PRO:HG2	1:A:25:GLU:OE2	2.01	0.59
1:A:66:LYS:O	1:A:67:CYS:HB2	2.00	0.59
1:A:1152:ILE:HD12	1:A:1261:LYS:HE3	1.84	0.59
1:A:1214:GLU:O	1:A:1218:GLN:HG2	2.02	0.59
2:B:327:ARG:NH2	2:B:371:GLU:HG2	2.17	0.59
2:B:418:LYS:HE2	2:B:422:LYS:HZ2	1.67	0.59
2:B:597:MET:SD	2:B:624:LEU:HD11	2.43	0.59
2:B:638:PHE:HD2	2:B:690:VAL:HG12	1.68	0.59
7:G:21:ARG:HD2	7:G:24:GLN:HB2	1.85	0.59
8:H:27:GLU:HG2	8:H:39:THR:HA	1.85	0.59
1:M:1308:THR:HG23	1:M:1310:GLY:H	1.67	0.59
1:M:1441:PHE:CZ	6:R:89:GLU:HA	2.37	0.59
3:O:89:GLU:O	3:O:90:ASP:HB3	2.01	0.59
7:S:88:ASP:O	7:S:88:ASP:OD2	2.21	0.59
8:T:123:MET:HE1	8:T:142:LEU:CD1	2.33	0.59
9:U:59:VAL:C	9:U:61:ASP:H	2.10	0.59
11:W:50:LEU:HD11	11:W:75:ILE:CD1	2.33	0.59
2:B:879:ARG:CD	2:B:879:ARG:N	2.65	0.59
5:E:64:PRO:O	5:E:69:ILE:HD11	2.02	0.59
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.38	0.59
9:I:44:TYR:CD1	9:I:45:ARG:N	2.71	0.59
1:M:427:GLN:HG3	1:M:430:TRP:CE2	2.38	0.59
1:M:1141:THR:HG23	1:M:1205:LYS:HD3	1.84	0.59
1:M:1450:LEU:HD11	6:R:108:PHE:CZ	2.38	0.59
2:N:766:ARG:HH21	2:N:1020:ARG:HD2	1.67	0.59
4:P:126:ILE:HD13	4:P:145:MET:HE3	1.84	0.59
7:S:87:VAL:HG21	7:S:103:VAL:HG21	1.83	0.59
10:V:30:LEU:HD11	10:V:38:ARG:NH1	2.18	0.59
12:X:34:CYS:SG	12:X:51:CYS:SG	3.01	0.59
1:A:66:LYS:HD3	1:A:67:CYS:N	2.18	0.58
1:A:718:VAL:O	1:A:722:LEU:HD12	2.03	0.58
1:A:907:THR:HG23	1:A:908:LEU:N	2.18	0.58
1:A:982:THR:HB	1:A:985:ASP:H	1.65	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.84	0.58
1:A:1399:ARG:HB3	1:A:1408:ILE:HD13	1.84	0.58
2:B:273:LEU:CD2	2:B:360:PHE:HD1	2.16	0.58
2:B:642:ASP:CA	2:B:649:LYS:HG3	2.32	0.58
2:B:710:LEU:CA	2:B:733:HIS:HB3	2.20	0.58
4:D:25:ALA:HB1	4:D:196:PRO:CG	2.33	0.58
5:E:164:LEU:HD11	5:E:211:TYR:CE1	2.38	0.58
1:M:555:ASP:O	1:M:556:TRP:C	2.46	0.58
3:O:69:LEU:O	10:V:6:ARG:HD2	2.03	0.58
4:P:164:ILE:O	4:P:168:LYS:HG2	2.03	0.58
1:A:598:LEU:O	1:A:599:SER:C	2.46	0.58
2:B:262:GLU:HA	2:B:267:ARG:NH2	2.18	0.58
2:B:273:LEU:HD21	2:B:360:PHE:CD1	2.35	0.58
2:B:620:ARG:NH1	9:I:68:LEU:HD21	2.17	0.58
2:B:638:PHE:HB3	2:B:651:LEU:CD2	2.33	0.58
2:B:766:ARG:NH2	2:B:1020:ARG:HD2	2.18	0.58
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.02	0.58
2:B:842:ASN:ND2	2:B:845:SER:H	2.00	0.58
1:M:95:PHE:O	1:M:96:ILE:C	2.45	0.58
1:M:317:LYS:O	1:M:318:SER:CB	2.51	0.58
1:M:444:PHE:CE2	1:M:487:MET:CE	2.86	0.58
2:N:433:GLN:O	2:N:434:ARG:HG3	2.03	0.58
2:N:842:ASN:ND2	2:N:845:SER:OG	2.29	0.58
4:P:13:ARG:O	4:P:15:LEU:N	2.29	0.58
4:P:220:LEU:HD23	4:P:221:TYR:C	2.28	0.58
5:Q:29:PHE:O	5:Q:30:ILE:HG13	2.02	0.58
10:V:3:VAL:HG21	10:V:18:TRP:CG	2.38	0.58
1:A:1313:LEU:O	1:A:1315:GLU:N	2.36	0.58
2:B:816:GLU:O	2:B:817:LEU:HD23	2.02	0.58
9:I:59:VAL:C	9:I:61:ASP:H	2.11	0.58
1:M:420:ARG:O	1:M:424:ILE:HG13	2.04	0.58
1:M:684:ALA:O	1:M:687:LYS:HB2	2.04	0.58
2:N:637:LEU:HD22	2:N:741:CYS:O	2.02	0.58
2:N:815:ARG:HD3	2:N:1041:GLU:OE2	2.03	0.58
2:N:847:ASP:OD2	11:W:6:ARG:NH2	2.34	0.58
4:P:153:ARG:O	4:P:154:PHE:CD2	2.56	0.58
5:Q:212:ARG:HG3	5:Q:212:ARG:HH11	1.68	0.58
7:S:1:MET:HG3	7:S:85:GLU:OE2	2.03	0.58
10:V:21:TYR:HB2	10:V:39:LEU:CD1	2.33	0.58
12:X:34:CYS:CB	12:X:51:CYS:HG	2.17	0.58
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:LEU:HB3	2:B:429:PHE:CE1	2.38	0.58
2:B:96:TYR:N	2:B:129:PHE:O	2.31	0.58
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.85	0.58
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.33	0.58
9:I:74:GLU:HB3	9:I:81:ARG:CD	2.33	0.58
11:K:82:ASP:OD1	11:K:84:LYS:N	2.36	0.58
1:M:335:ARG:NH1	2:N:1206:GLU:CD	2.61	0.58
1:M:382:PRO:HA	1:M:428:TYR:HE2	1.68	0.58
1:M:693:VAL:HG21	1:M:721:PHE:CE1	2.35	0.58
1:M:774:ARG:NH2	1:M:797:LYS:HB2	2.19	0.58
1:M:1171:GLN:OE1	1:M:1172:LEU:HG	2.03	0.58
1:M:1171:GLN:OE1	1:M:1172:LEU:N	2.37	0.58
2:N:277:LYS:HG2	2:N:336:ARG:HB3	1.84	0.58
2:N:579:ARG:HA	2:N:589:VAL:HG13	1.85	0.58
3:O:32:SER:O	3:O:36:VAL:HG23	2.04	0.58
5:Q:10:SER:O	5:Q:13:TRP:HB3	2.03	0.58
5:Q:97:VAL:HG13	5:Q:127:ILE:HD13	1.84	0.58
7:S:15:PRO:HA	7:S:18:PHE:CE1	2.38	0.58
7:S:116:PRO:HD2	7:S:119:LEU:CD2	2.31	0.58
8:T:128:ASN:ND2	8:T:131:ASN:OD1	2.37	0.58
1:A:157:ASP:OD2	1:A:160:GLN:HG3	2.03	0.58
1:A:219:PHE:CE2	1:A:231:PRO:HD2	2.39	0.58
1:A:1225:PHE:CE2	1:A:1227:ILE:HD11	2.39	0.58
2:B:47:GLN:O	2:B:173:MET:HE1	2.04	0.58
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.03	0.58
2:B:756:ILE:O	2:B:759:PRO:HD3	2.04	0.58
4:D:161:GLY:O	4:D:165:GLN:HG3	2.03	0.58
1:M:89:PRO:HB2	1:M:204:THR:CG2	2.33	0.58
1:M:281:HIS:C	1:M:282:ASN:HD22	2.11	0.58
1:M:308:ILE:HG22	1:M:309:ALA:N	2.16	0.58
1:M:351:THR:CG2	2:N:1103:ILE:HG13	2.33	0.58
1:M:472:LEU:HD11	2:N:835:GLN:NE2	2.18	0.58
1:M:886:ILE:HG23	1:M:887:GLY:N	2.19	0.58
1:M:1118:VAL:O	1:M:1305:VAL:HG13	2.04	0.58
2:N:664:THR:HG23	2:N:678:GLU:N	2.19	0.58
2:N:824:ILE:HG12	10:V:48:ARG:NH1	2.17	0.58
2:N:957:ASN:O	2:N:959:ASP:N	2.36	0.58
2:N:975:GLN:HG2	2:N:976:ILE:H	1.68	0.58
3:O:238:ILE:HG23	3:O:242:GLN:HB2	1.85	0.58
8:T:143:LEU:N	8:T:143:LEU:HD12	2.19	0.58
1:A:886:ILE:HG23	1:A:887:GLY:N	2.19	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:ILE:H	2:B:429:PHE:HE1	1.51	0.58
2:B:205:ILE:N	2:B:205:ILE:HD12	2.18	0.58
2:B:313:MET:O	2:B:316:PRO:HD2	2.03	0.58
2:B:865:LYS:HG2	2:B:961:LEU:HD21	1.85	0.58
9:I:92:ARG:HG2	9:I:93:LYS:HE2	1.84	0.58
1:M:344:ARG:HB3	1:M:344:ARG:NH1	2.14	0.58
1:M:1166:ASP:HA	1:M:1169:ILE:HD12	1.85	0.58
2:N:640:VAL:O	2:N:641:GLU:C	2.46	0.58
2:N:1115:THR:O	2:N:1116:ARG:HB2	2.02	0.58
4:P:146:GLN:O	4:P:147:TYR:C	2.46	0.58
8:T:95:TYR:CE2	8:T:97:MET:HE2	2.38	0.58
10:V:14:VAL:O	10:V:14:VAL:HG12	2.01	0.58
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.67	0.58
1:A:567:LYS:NZ	8:H:43:ASN:HB3	2.18	0.58
1:A:883:LEU:HD23	1:A:1021:LEU:HD13	1.86	0.58
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.86	0.58
2:B:110:HIS:HB3	12:L:54:ARG:HH22	1.69	0.58
2:B:251:ILE:O	2:B:251:ILE:HG22	2.04	0.58
2:B:846:ILE:CG2	2:B:974:PRO:HG2	2.32	0.58
8:H:95:TYR:HE2	8:H:97:MET:HG3	1.68	0.58
9:I:55:THR:HG23	9:I:100:PHE:CD2	2.38	0.58
1:M:41:MET:O	1:M:42:ASP:C	2.46	0.58
1:M:500:GLU:OE2	2:N:1145:SER:HB2	2.03	0.58
2:N:46:GLN:HG3	2:N:47:GLN:H	1.68	0.58
2:N:120:ARG:NH1	12:X:54:ARG:NH1	2.52	0.58
2:N:244:LEU:HD21	2:N:366:GLN:HE21	1.68	0.58
2:N:361:LEU:HD21	2:N:377:PHE:HD2	1.69	0.58
1:A:93:VAL:HG23	1:A:304:MET:HE3	1.85	0.58
1:A:1259:MET:CE	1:A:1263:ILE:HG13	2.34	0.58
2:B:613:VAL:HG13	2:B:628:THR:HA	1.85	0.58
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.84	0.58
2:B:916:THR:HB	2:B:935:ARG:HD2	1.86	0.58
2:B:1161:HIS:NE2	2:B:1175:LEU:HD21	2.19	0.58
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.39	0.58
8:H:15:VAL:HG22	8:H:26:ILE:HG13	1.86	0.58
1:M:689:LYS:HE2	1:M:721:PHE:CE2	2.39	0.58
1:M:1342:GLU:CG	5:Q:198:ILE:HD13	2.33	0.58
4:P:25:ALA:HB1	4:P:196:PRO:HG2	1.86	0.58
4:P:52:LEU:HD21	4:P:147:TYR:CE2	2.38	0.58
7:S:94:CYS:SG	7:S:94:CYS:O	2.59	0.58
7:S:138:THR:HG22	7:S:139:ILE:H	1.69	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:82:PRO:O	8:T:84:ALA:N	2.35	0.58
10:V:16:ASP:OD1	10:V:17:LYS:N	2.36	0.58
2:B:185:THR:H	2:B:188:ASP:HB2	1.69	0.58
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.51	0.58
5:E:69:ILE:HD12	5:E:69:ILE:H	1.69	0.58
5:E:204:THR:HG23	5:E:205:SER:N	2.19	0.58
5:E:212:ARG:HG3	5:E:212:ARG:HH11	1.69	0.58
10:J:23:ASN:O	10:J:25:LEU:N	2.37	0.58
10:J:27:GLU:C	10:J:29:GLU:H	2.12	0.58
12:L:27:LEU:HD13	12:L:37:LYS:HD2	1.86	0.58
12:L:30:ILE:HG22	12:L:31:CYS:N	2.18	0.58
1:M:1227:ILE:HG22	1:M:1228:TRP:H	1.69	0.58
2:N:273:LEU:HB2	2:N:276:ILE:HD12	1.86	0.58
6:R:75:PRO:O	6:R:77:ASP:O	2.22	0.58
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.84	0.58
1:A:901:LEU:H	1:A:926:GLN:CD	2.12	0.58
1:A:1277:GLU:C	1:A:1279:ILE:H	2.12	0.58
2:B:359:GLU:O	2:B:362:PRO:HD3	2.04	0.58
3:C:241:ASP:O	3:C:245:VAL:HG23	2.04	0.58
5:E:207:ARG:HB3	5:E:207:ARG:HH11	1.69	0.58
7:G:1:MET:C	7:G:1:MET:HE2	2.29	0.58
1:M:69:THR:O	1:M:70:CYS:C	2.47	0.58
1:M:399:HIS:O	1:M:400:PRO:C	2.41	0.58
2:N:98:THR:O	2:N:126:SER:HB2	2.03	0.58
2:N:284:ILE:HD13	2:N:333:PHE:CD2	2.39	0.58
2:N:293:PRO:HD2	2:N:296:GLU:OE1	2.03	0.58
2:N:1084:GLN:NE2	2:N:1084:GLN:N	2.52	0.58
2:N:1183:LYS:N	2:N:1183:LYS:CE	2.67	0.58
3:O:43:THR:CG2	3:O:44:LEU:N	2.67	0.58
5:Q:50:MET:HG2	5:Q:52:ARG:NH2	2.19	0.58
9:U:84:VAL:O	9:U:84:VAL:HG13	2.02	0.58
1:A:252:PHE:HB2	1:A:256:GLN:CD	2.28	0.57
1:A:278:THR:O	1:A:278:THR:HG22	2.04	0.57
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.86	0.57
1:A:1173:HIS:ND1	1:A:1173:HIS:O	2.37	0.57
1:A:1437:GLY:O	1:A:1439:GLY:N	2.37	0.57
2:B:638:PHE:HB3	2:B:651:LEU:HD22	1.86	0.57
2:B:1056:SER:HB3	2:B:1066:SER:OG	2.02	0.57
3:C:193:TYR:C	3:C:193:TYR:CD1	2.81	0.57
8:H:40:LEU:HD23	8:H:42:ILE:CD1	2.34	0.57
1:M:34:LYS:HB2	1:M:36:ARG:CZ	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:493:GLN:HE21	1:M:493:GLN:CA	2.16	0.57
2:N:235:SER:O	2:N:236:HIS:HD2	1.87	0.57
3:O:73:GLN:HE21	3:O:75:MET:N	1.99	0.57
12:X:47:ARG:HD3	12:X:52:GLY:HA2	1.86	0.57
1:A:311:GLN:O	1:A:313:GLN:N	2.36	0.57
1:A:470:LEU:N	1:A:470:LEU:CD2	2.67	0.57
1:A:720:ARG:O	1:A:724:GLU:HB3	2.03	0.57
2:B:129:PHE:HA	2:B:165:VAL:O	2.05	0.57
2:B:508:LEU:N	14:2:1:DA:O5'	2.28	0.57
2:B:604:ARG:NH2	2:B:614:SER:HA	2.19	0.57
2:B:654:ARG:HH11	2:B:654:ARG:HG3	1.67	0.57
3:C:39:ALA:O	3:C:164:ALA:HB3	2.04	0.57
3:C:243:VAL:O	3:C:243:VAL:HG12	2.03	0.57
4:D:50:LEU:HD11	7:G:4:ILE:HD11	1.85	0.57
4:D:202:ILE:CG2	4:D:207:LEU:HB2	2.34	0.57
4:D:209:ARG:HA	4:D:212:LYS:CE	2.34	0.57
5:E:78:LEU:HB2	5:E:107:THR:HB	1.86	0.57
7:G:137:ILE:CG2	7:G:143:ILE:HD11	2.34	0.57
2:N:878:GLN:O	2:N:879:ARG:C	2.47	0.57
2:N:880:THR:HG21	2:N:934:LYS:HE3	1.86	0.57
2:N:1172:ILE:O	2:N:1172:ILE:HG22	2.02	0.57
4:P:130:LEU:HD11	4:P:142:LYS:HA	1.86	0.57
8:T:44:VAL:O	8:T:44:VAL:HG12	2.03	0.57
12:X:60:ARG:HG2	12:X:61:THR:H	1.70	0.57
1:A:444:PHE:CE2	1:A:487:MET:HE3	2.39	0.57
1:A:523:ILE:HG13	1:A:622:VAL:HG22	1.86	0.57
1:A:1242:VAL:CG1	1:A:1243:VAL:N	2.67	0.57
2:B:640:VAL:O	2:B:641:GLU:C	2.46	0.57
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.33	0.57
2:B:1115:THR:HG22	2:B:1117:GLN:HB2	1.85	0.57
5:E:62:ALA:HB3	5:E:78:LEU:HD22	1.86	0.57
7:G:126:ASN:HD22	7:G:126:ASN:C	2.12	0.57
8:H:143:LEU:HD12	8:H:143:LEU:N	2.20	0.57
1:M:313:GLN:O	1:M:314:ALA:C	2.47	0.57
1:M:440:ASP:O	1:M:460:VAL:HG23	2.04	0.57
2:N:199:MET:HE2	2:N:492:LEU:CD2	2.34	0.57
2:N:390:LEU:HD13	2:N:392:ARG:NH2	2.19	0.57
2:N:398:ARG:HB3	2:N:398:ARG:HH11	1.70	0.57
2:N:638:PHE:HD2	2:N:690:VAL:HG12	1.69	0.57
2:N:824:ILE:CG1	10:V:48:ARG:HH12	2.15	0.57
2:N:1008:PRO:HB3	2:N:1087:PHE:HE2	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:11:ARG:HH12	3:O:205:LYS:HZ3	1.51	0.57
3:O:44:LEU:HD21	3:O:159:ALA:HB1	1.86	0.57
5:Q:153:HIS:O	5:Q:154:ILE:CG1	2.48	0.57
8:T:106:GLU:HA	8:T:112:ILE:HD12	1.84	0.57
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.85	0.57
1:A:335:ARG:O	1:A:339:ASN:HB2	2.03	0.57
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.05	0.57
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.85	0.57
1:A:1438:THR:HG23	6:F:92:ARG:HB2	1.86	0.57
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.39	0.57
9:I:58:VAL:O	9:I:58:VAL:HG12	2.05	0.57
1:M:107:CYS:CA	1:M:171:GLN:HE22	2.17	0.57
1:M:369:SER:HB3	11:W:2:ASN:OD1	2.04	0.57
2:N:276:ILE:HG22	2:N:276:ILE:O	2.02	0.57
2:N:282:ILE:O	2:N:286:PHE:HD1	1.88	0.57
2:N:773:MET:CE	2:N:985:GLY:HA2	2.35	0.57
1:A:1349:TYR:C	1:A:1349:TYR:CD2	2.82	0.57
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.39	0.57
2:B:58:THR:O	2:B:62:ILE:HG13	2.04	0.57
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.37	0.57
3:C:32:SER:O	3:C:36:VAL:HG23	2.05	0.57
5:E:158:SER:O	5:E:162:ARG:HD3	2.04	0.57
1:M:873:MET:HE3	1:M:957:PRO:HG3	1.87	0.57
1:M:993:LEU:HD22	1:M:1046:LEU:CD2	2.34	0.57
1:M:1100:ARG:HH21	1:M:1351:GLU:CG	2.18	0.57
2:N:189:LEU:HA	2:N:192:LEU:HD12	1.87	0.57
2:N:526:GLU:HG3	2:N:771:SER:HB3	1.85	0.57
2:N:797:TYR:HE1	2:N:854:LEU:HD23	1.69	0.57
3:O:36:VAL:CG2	3:O:251:LEU:HD13	2.35	0.57
4:P:154:PHE:HZ	4:P:214:LEU:HD11	1.69	0.57
5:Q:99:HIS:CE1	5:Q:103:LYS:HG3	2.39	0.57
7:S:136:VAL:O	7:S:136:VAL:HG12	2.04	0.57
10:V:23:ASN:O	10:V:25:LEU:N	2.37	0.57
2:B:309:GLN:CD	9:I:52:ILE:HD11	2.30	0.57
2:B:862:GLN:HG2	2:B:963:PHE:CD1	2.36	0.57
6:F:119:ARG:CG	6:F:119:ARG:NH1	2.68	0.57
8:H:15:VAL:HG22	8:H:26:ILE:CG1	2.34	0.57
1:M:61:ILE:HG22	1:M:62:ASP:H	1.69	0.57
1:M:973:ILE:CD1	1:M:1037:LEU:HA	2.34	0.57
2:N:120:ARG:HH11	12:X:54:ARG:HH11	1.53	0.57
2:N:211:VAL:O	2:N:480:SER:HA	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:313:MET:SD	2:N:390:LEU:HD21	2.45	0.57
1:A:41:MET:HB2	1:A:48:ALA:O	2.05	0.57
1:A:1118:VAL:O	1:A:1305:VAL:HG13	2.05	0.57
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.87	0.57
2:B:315:LYS:N	2:B:316:PRO:HD2	2.19	0.57
10:J:23:ASN:C	10:J:25:LEU:N	2.60	0.57
1:M:129:LYS:O	1:M:130:ASP:CB	2.52	0.57
1:M:794:PRO:C	1:M:796:SER:H	2.12	0.57
1:M:1121:GLU:HB3	1:M:1124:HIS:NE2	2.20	0.57
2:N:100:PRO:HB2	2:N:180:TYR:HE1	1.69	0.57
2:N:357:GLN:CD	2:N:368:GLU:HA	2.30	0.57
2:N:408:LEU:N	2:N:408:LEU:HD12	2.20	0.57
2:N:1177:HIS:HB3	2:N:1179:GLN:NE2	2.19	0.57
7:S:125:SER:OG	7:S:128:PRO:HA	2.05	0.57
1:A:427:GLN:HG3	1:A:430:TRP:CE2	2.39	0.57
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.39	0.57
2:B:1190:ASP:C	2:B:1191:ILE:HG13	2.30	0.57
4:D:204:ASP:O	4:D:208:GLU:HB2	2.04	0.57
1:M:523:ILE:CG1	1:M:622:VAL:HG22	2.35	0.57
2:N:622:LYS:HZ3	9:U:59:VAL:HG13	1.69	0.57
2:N:857:ARG:HH21	2:N:942:ARG:NH2	2.03	0.57
4:P:195:ILE:O	4:P:198:LEU:HG	2.03	0.57
8:T:89:LEU:HB2	8:T:91:ASP:CG	2.30	0.57
1:A:34:LYS:NZ	1:A:57:ARG:NH2	2.53	0.57
1:A:709:THR:HB	1:A:712:GLU:HG3	1.87	0.57
1:A:888:GLY:O	1:A:940:ARG:NH2	2.38	0.57
1:A:1268:LEU:O	1:A:1269:GLU:HG3	2.05	0.57
2:B:402:GLY:HA2	2:B:695:ALA:HB3	1.86	0.57
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.34	0.57
3:C:238:ILE:HD11	3:C:246:ARG:NH1	2.19	0.57
4:D:144:THR:O	4:D:148:LEU:HB2	2.05	0.57
8:H:7:ASP:O	8:H:8:ASP:HB2	2.05	0.57
9:I:111:THR:CG2	9:I:113:ASP:HB2	2.34	0.57
1:M:49:LYS:HE2	1:M:61:ILE:HD12	1.86	0.57
1:M:1259:MET:HE2	1:M:1263:ILE:CG1	2.34	0.57
1:M:1294:PRO:HG2	1:M:1295:THR:HG22	1.86	0.57
2:N:39:ARG:NH2	2:N:665:GLU:CG	2.68	0.57
2:N:193:LYS:HZ1	12:X:32:ALA:HB1	1.70	0.57
2:N:580:VAL:HG22	2:N:624:LEU:HB3	1.87	0.57
2:N:642:ASP:HA	2:N:649:LYS:HG3	1.86	0.57
3:O:193:TYR:CD1	3:O:193:TYR:C	2.82	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:106:MET:CG	7:S:107:LYS:N	2.67	0.57
1:A:556:TRP:CZ2	1:A:558:GLY:HA2	2.40	0.57
2:B:519:TRP:C	2:B:519:TRP:CD1	2.83	0.57
2:B:542:MET:HG2	2:B:747:MET:HE3	1.86	0.57
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.87	0.57
6:F:79:ARG:HG3	6:F:144:GLU:OE1	2.04	0.57
6:F:111:LEU:N	6:F:111:LEU:CD1	2.67	0.57
8:H:81:PRO:HB2	8:H:82:PRO:HD2	1.84	0.57
1:M:93:VAL:CG1	1:M:301:ALA:HB1	2.35	0.57
1:M:152:VAL:HG13	1:M:153:PRO:HD2	1.87	0.57
3:O:184:ASN:HD21	3:O:189:THR:HB	1.70	0.57
4:P:209:ARG:HG2	4:P:209:ARG:HH11	1.69	0.57
8:T:4:THR:HG22	8:T:5:LEU:N	2.20	0.57
9:U:62:ILE:O	9:U:62:ILE:HG12	2.03	0.57
1:A:42:ASP:HA	1:A:46:THR:O	2.05	0.56
2:B:167:ILE:HA	2:B:450:ALA:HB2	1.87	0.56
5:E:55:ARG:HG3	5:E:55:ARG:HH11	1.70	0.56
5:E:100:ILE:CG2	5:E:105:PHE:HB2	2.35	0.56
10:J:36:LEU:HB2	10:J:47:ARG:HH12	1.70	0.56
1:M:699:ALA:HB3	1:M:701:LEU:HG	1.87	0.56
2:N:254:LEU:HD23	2:N:381:MET:HE1	1.86	0.56
2:N:313:MET:CE	2:N:386:LEU:HD22	2.35	0.56
1:A:492:PRO:CB	1:A:497:THR:HG22	2.34	0.56
1:A:898:ARG:HD2	1:A:899:VAL:H	1.70	0.56
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.20	0.56
2:B:508:LEU:O	2:B:509:ALA:HB3	2.05	0.56
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.86	0.56
7:G:151:ILE:HG12	7:S:114:LEU:HD12	1.86	0.56
12:L:55:ILE:HG12	12:L:56:LEU:N	2.13	0.56
2:N:345:LYS:CG	2:N:346:GLU:N	2.65	0.56
2:N:810:GLU:HB2	2:N:815:ARG:NH2	2.19	0.56
2:N:1084:GLN:HG2	3:O:201:TRP:CZ2	2.40	0.56
4:P:155:ARG:NH1	4:P:155:ARG:CB	2.68	0.56
7:S:14:HIS:CD2	7:S:16:SER:H	2.23	0.56
8:T:104:PHE:CE2	8:T:136:LYS:HG3	2.40	0.56
1:A:41:MET:O	1:A:42:ASP:C	2.48	0.56
1:A:256:GLN:O	1:A:257:ARG:HB2	2.04	0.56
1:A:382:PRO:HA	1:A:428:TYR:HE2	1.69	0.56
1:A:441:PRO:HG3	1:A:498:ARG:HB2	1.88	0.56
1:A:475:THR:CG2	1:A:476:SER:N	2.67	0.56
1:A:666:ILE:HD12	1:A:666:ILE:N	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:MET:C	1:A:1058:VAL:HG23	2.30	0.56
2:B:336:ARG:HH11	2:B:336:ARG:HG3	1.70	0.56
2:B:957:ASN:O	2:B:959:ASP:N	2.38	0.56
3:C:148:ARG:N	3:C:151:GLN:HG3	2.19	0.56
3:C:177:GLU:CG	3:C:231:ASN:HB3	2.21	0.56
4:D:14:ARG:HH12	4:D:16:LYS:NZ	2.04	0.56
7:G:128:PRO:O	7:G:138:THR:HG23	2.04	0.56
8:H:104:PHE:CE2	8:H:136:LYS:HG3	2.40	0.56
1:M:311:GLN:O	1:M:313:GLN:N	2.38	0.56
1:M:500:GLU:OE2	1:M:1438:THR:HG21	2.05	0.56
1:M:744:LYS:HD3	1:M:748:MET:HE2	1.87	0.56
1:M:786:HIS:CD2	1:M:786:HIS:N	2.73	0.56
1:M:818:MET:HE3	2:N:514:LEU:O	2.04	0.56
2:N:345:LYS:CE	2:N:349:ILE:HD11	2.35	0.56
3:O:259:LEU:HD21	11:W:91:CYS:HB3	1.87	0.56
4:P:155:ARG:NE	4:P:221:TYR:HE1	2.04	0.56
5:Q:19:VAL:HG22	5:Q:140:LEU:HD12	1.87	0.56
5:Q:79:TRP:HE1	5:Q:81:GLU:HB2	1.71	0.56
5:Q:145:THR:HG21	5:Q:187:TYR:CD2	2.40	0.56
6:R:69:LEU:HD13	6:R:71:GLU:OE1	2.04	0.56
9:U:50:THR:HG22	9:U:52:ILE:N	2.19	0.56
10:V:23:ASN:C	10:V:25:LEU:N	2.61	0.56
1:A:55:ASP:CG	1:A:55:ASP:O	2.46	0.56
1:A:830:LYS:HE3	1:A:1081:LEU:HD12	1.86	0.56
1:A:1316:VAL:O	1:A:1316:VAL:HG12	2.05	0.56
2:B:497:ARG:NH2	2:B:775:LYS:HZ3	2.04	0.56
2:B:731:VAL:HG12	2:B:732:SER:N	2.20	0.56
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.33	0.56
3:C:148:ARG:H	3:C:151:GLN:HG3	1.70	0.56
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.87	0.56
5:E:112:TYR:CE1	5:E:136:ASN:HA	2.40	0.56
9:I:84:VAL:HG13	9:I:84:VAL:O	2.04	0.56
1:M:99:ILE:HG23	1:M:211:PHE:CE2	2.41	0.56
1:M:705:LYS:CB	1:M:708:MET:HE3	2.27	0.56
1:M:853:ASP:OD1	1:M:855:THR:CB	2.52	0.56
1:M:1433:MET:HE3	7:S:63:PRO:HB2	1.85	0.56
2:N:20:ASP:C	2:N:22:SER:H	2.12	0.56
2:N:434:ARG:O	2:N:436:VAL:HG23	2.05	0.56
2:N:898:LEU:HD13	2:N:952:VAL:HG11	1.87	0.56
3:O:213:PRO:O	3:O:214:ASN:HB3	2.06	0.56
8:T:84:ALA:O	8:T:85:GLY:C	2.49	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLU:CG	1:A:46:THR:HB	2.31	0.56
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.41	0.56
2:B:288:ALA:HB1	2:B:331:LEU:CD1	2.32	0.56
2:B:842:ASN:ND2	2:B:845:SER:OG	2.37	0.56
2:B:906:SER:O	2:B:907:GLY:C	2.48	0.56
2:B:1098:MET:HE3	2:B:1101:ASP:OD2	2.05	0.56
3:C:91:HIS:C	3:C:91:HIS:CD2	2.82	0.56
4:D:12:ARG:HG2	4:D:12:ARG:HH11	1.71	0.56
1:M:710:LEU:HD22	9:U:96:SER:HA	1.88	0.56
1:M:852:TYR:CD1	6:R:136:ARG:HB3	2.40	0.56
1:M:962:ARG:O	1:M:964:ILE:N	2.39	0.56
1:M:1130:GLN:O	1:M:1134:ILE:HG13	2.05	0.56
1:M:1315:GLU:C	1:M:1317:MET:H	2.13	0.56
2:N:167:ILE:HA	2:N:450:ALA:HB2	1.87	0.56
2:N:430:ARG:HB3	2:N:434:ARG:NH2	2.21	0.56
2:N:614:SER:HB2	2:N:697:GLU:OE1	2.05	0.56
2:N:848:ARG:HD3	10:V:11:GLY:HA2	1.86	0.56
3:O:174:ALA:O	3:O:175:ALA:HB3	2.06	0.56
4:P:154:PHE:CE2	4:P:218:GLU:HA	2.40	0.56
1:A:195:ASP:O	1:A:196:GLU:HB3	2.05	0.56
1:A:1141:THR:HA	1:A:1205:LYS:HZ3	1.70	0.56
1:A:1255:GLU:HG2	1:A:1258:HIS:HB2	1.86	0.56
2:B:594:ALA:HB2	2:B:617:ARG:HH12	1.71	0.56
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.88	0.56
2:B:805:THR:HG23	2:B:809:MET:SD	2.45	0.56
4:D:155:ARG:NE	4:D:221:TYR:CE1	2.74	0.56
1:M:283:GLY:O	1:M:285:PRO:CD	2.53	0.56
1:M:401:GLY:CA	1:M:435:HIS:HD2	2.19	0.56
1:M:883:LEU:HD11	1:M:1017:LEU:HD11	1.86	0.56
2:N:115:GLN:HG2	2:N:193:LYS:CB	2.36	0.56
2:N:361:LEU:O	2:N:363:HIS:O	2.24	0.56
2:N:418:LYS:HE2	2:N:422:LYS:HZ2	1.70	0.56
2:N:486:TYR:N	2:N:486:TYR:CD2	2.71	0.56
2:N:613:VAL:HG13	2:N:628:THR:HA	1.86	0.56
2:N:686:ASN:C	2:N:688:GLY:H	2.13	0.56
3:O:44:LEU:HD21	3:O:159:ALA:CB	2.36	0.56
5:Q:28:TYR:CE1	5:Q:78:LEU:HD13	2.41	0.56
5:Q:28:TYR:HE1	5:Q:78:LEU:HD13	1.71	0.56
5:Q:124:VAL:HB	5:Q:125:PRO:HD3	1.87	0.56
5:Q:190:LEU:C	5:Q:191:LYS:HG2	2.30	0.56
8:T:59:ILE:CG2	8:T:60:ALA:N	2.64	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:55:LYS:HB2	11:W:81:TYR:CE1	2.41	0.56
1:A:10:PRO:HG2	2:B:1192:TYR:HD2	1.71	0.56
2:B:434:ARG:O	2:B:436:VAL:HG23	2.05	0.56
2:B:640:VAL:O	2:B:640:VAL:HG12	2.04	0.56
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.87	0.56
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.87	0.56
10:J:7:CYS:CB	10:J:49:MET:HE3	2.35	0.56
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.35	0.56
1:M:598:LEU:HD23	8:T:25:ARG:NH1	2.20	0.56
1:M:929:LEU:HD21	1:M:983:ILE:HG21	1.87	0.56
2:N:560:GLU:O	2:N:561:TRP:CD1	2.59	0.56
2:N:638:PHE:HB3	2:N:651:LEU:HD22	1.88	0.56
2:N:906:SER:O	2:N:907:GLY:C	2.48	0.56
1:A:399:HIS:O	1:A:400:PRO:C	2.49	0.56
2:B:361:LEU:O	2:B:363:HIS:O	2.24	0.56
2:B:516:ASN:H	2:B:516:ASN:ND2	1.90	0.56
2:B:801:LYS:O	10:J:52:THR:HG23	2.05	0.56
2:B:842:ASN:HD22	2:B:845:SER:N	2.03	0.56
2:B:865:LYS:NZ	2:B:869:SER:HA	2.21	0.56
5:E:46:TYR:CD2	5:E:58:MET:HG2	2.41	0.56
7:G:112:LYS:HA	7:G:115:MET:HE3	1.87	0.56
8:H:80:ARG:HD2	8:H:87:ARG:HH22	1.71	0.56
1:M:367:PRO:HG2	1:M:370:ILE:HD12	1.88	0.56
1:M:666:ILE:O	1:M:670:ILE:HD13	2.06	0.56
1:M:993:LEU:HD23	1:M:1022:LEU:HD21	1.88	0.56
1:M:1173:HIS:ND1	1:M:1173:HIS:O	2.39	0.56
2:N:39:ARG:HH21	2:N:665:GLU:CD	2.13	0.56
2:N:424:LEU:O	2:N:428:ILE:HG13	2.05	0.56
2:N:508:LEU:O	2:N:509:ALA:HB3	2.06	0.56
3:O:179:GLU:HG2	3:O:180:TYR:N	2.21	0.56
5:Q:121:MET:C	5:Q:123:LEU:H	2.12	0.56
1:A:89:PRO:C	1:A:204:THR:HG21	2.30	0.56
1:A:401:GLY:CA	1:A:435:HIS:HD2	2.18	0.56
1:A:608:ILE:HG13	1:A:613:ILE:HD12	1.88	0.56
1:A:794:PRO:C	1:A:796:SER:H	2.14	0.56
1:A:1241:ARG:O	1:A:1242:VAL:CB	2.53	0.56
2:B:679:TYR:CE1	2:B:683:SER:HB2	2.41	0.56
3:C:99:LEU:N	3:C:99:LEU:CD2	2.68	0.56
5:E:136:ASN:OD1	5:E:138:ALA:N	2.39	0.56
5:E:169:ARG:HD3	6:F:140:ASP:CG	2.30	0.56
7:G:117:GLN:HE21	7:S:153:GLN:HG3	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:360:GLU:HB2	1:M:363:GLN:HG3	1.88	0.56
1:M:535:THR:HG21	1:M:617:VAL:N	2.21	0.56
1:M:672:ASP:CB	1:M:736:ASN:HD21	2.14	0.56
1:M:981:LEU:CD2	1:M:1039:LYS:HA	2.35	0.56
1:M:1207:LEU:HD13	1:M:1273:LEU:HD23	1.88	0.56
2:N:365:THR:HG21	2:N:370:PHE:CG	2.41	0.56
2:N:796:LEU:HD21	2:N:821:GLN:HE21	1.70	0.56
3:O:91:HIS:C	3:O:91:HIS:CD2	2.83	0.56
7:S:55:ASP:OD1	7:S:57:GLN:HG3	2.06	0.56
8:T:7:ASP:O	8:T:8:ASP:HB2	2.06	0.56
8:T:101:ALA:HB2	8:T:116:TYR:CE2	2.41	0.56
1:A:547:LEU:HD21	1:A:560:ILE:HD13	1.89	0.56
1:A:738:LYS:H	1:A:738:LYS:HD3	1.71	0.56
1:A:834:THR:HG22	1:A:835:GLY:N	2.21	0.56
2:B:878:GLN:O	2:B:879:ARG:C	2.49	0.56
2:B:1167:GLY:HA3	2:B:1216:LEU:H	1.70	0.56
3:C:166:GLU:CG	11:K:10:PHE:HZ	2.19	0.56
5:E:48:ASP:CG	5:E:49:SER:N	2.59	0.56
6:F:97:ARG:NH2	6:F:108:PHE:CE1	2.73	0.56
7:G:114:LEU:HG	7:G:162:SER:HB3	1.88	0.56
9:I:74:GLU:HB3	9:I:81:ARG:NE	2.21	0.56
11:K:93:SER:O	11:K:97:LYS:HG3	2.05	0.56
1:M:836:TYR:CE2	1:M:840:ARG:HD2	2.40	0.56
2:N:278:GLN:HG2	2:N:279:ASP:H	1.70	0.56
2:N:1180:PHE:HB3	2:N:1191:ILE:HD13	1.88	0.56
4:P:56:ARG:HG2	4:P:56:ARG:HH11	1.71	0.56
4:P:202:ILE:HD13	4:P:207:LEU:HB2	1.87	0.56
5:Q:79:TRP:HB2	5:Q:105:PHE:CE1	2.41	0.56
1:A:117:GLU:H	1:A:117:GLU:CD	2.14	0.55
1:A:993:LEU:HD21	1:A:1049:ILE:HG21	1.87	0.55
2:B:126:SER:CB	2:B:172:ILE:HD11	2.36	0.55
2:B:240:ILE:HG23	2:B:254:LEU:HB3	1.88	0.55
2:B:300:HIS:O	2:B:303:TYR:HE2	1.88	0.55
2:B:430:ARG:HH11	2:B:430:ARG:CB	2.15	0.55
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.36	0.55
3:C:248:ILE:CD1	11:K:101:LEU:HD22	2.36	0.55
4:D:12:ARG:NH1	4:D:12:ARG:HG2	2.19	0.55
4:D:14:ARG:HH12	4:D:16:LYS:HZ2	1.52	0.55
5:E:112:TYR:C	5:E:112:TYR:CD1	2.84	0.55
8:H:40:LEU:HD12	8:H:123:MET:CB	2.35	0.55
8:H:51:ALA:O	8:H:52:GLN:HB2	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:23:SER:HB3	1:M:233:TRP:CZ2	2.42	0.55
1:M:547:LEU:HD22	11:W:58:PHE:CE1	2.42	0.55
1:M:567:LYS:HZ1	8:T:46:LEU:HB2	1.69	0.55
1:M:852:TYR:CD2	1:M:1060:PRO:CB	2.89	0.55
1:M:1220:PHE:O	1:M:1221:LYS:HB2	2.05	0.55
2:N:398:ARG:HH11	2:N:398:ARG:CB	2.18	0.55
2:N:766:ARG:NH2	2:N:1020:ARG:HD3	2.20	0.55
4:P:71:LYS:CG	4:P:74:GLN:HE21	2.19	0.55
4:P:154:PHE:HE1	4:P:163:VAL:HG11	1.71	0.55
7:S:21:ARG:HD2	7:S:24:GLN:HB2	1.89	0.55
8:T:81:PRO:HB3	8:T:82:PRO:HD2	1.86	0.55
1:A:67:CYS:O	1:A:68:GLN:C	2.49	0.55
1:A:148:CYS:HB3	1:A:167:CYS:O	2.05	0.55
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.36	0.55
2:B:102:VAL:HG13	2:B:958:GLN:HE21	1.71	0.55
2:B:549:THR:CG2	2:B:550:ASP:N	2.68	0.55
2:B:911:ILE:HG21	2:B:966:VAL:HG11	1.88	0.55
2:B:950:ASP:HB3	2:B:967:ARG:O	2.07	0.55
2:B:999:MET:HA	2:B:999:MET:CE	2.33	0.55
8:H:123:MET:HG2	8:H:124:ARG:N	2.20	0.55
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.20	0.55
11:K:47:ARG:C	11:K:47:ARG:HD2	2.32	0.55
1:M:42:ASP:HB3	1:M:45:GLN:HA	1.87	0.55
1:M:768:GLN:HG2	1:M:816:HIS:CA	2.34	0.55
2:N:39:ARG:HH21	2:N:665:GLU:CG	2.19	0.55
2:N:48:LEU:HD23	2:N:173:MET:SD	2.47	0.55
2:N:118:ARG:HH11	2:N:204:ILE:HD11	1.70	0.55
2:N:185:THR:O	2:N:186:GLU:C	2.49	0.55
4:P:15:LEU:O	4:P:17:LYS:HG3	2.06	0.55
4:P:155:ARG:CB	4:P:155:ARG:HH11	2.19	0.55
5:Q:16:PHE:CE2	5:Q:20:LYS:HE2	2.41	0.55
5:Q:204:THR:HG23	5:Q:205:SER:N	2.22	0.55
7:S:9:LEU:HD12	7:S:10:ASN:H	1.71	0.55
11:W:47:ARG:HD3	11:W:59:ALA:O	2.06	0.55
15:6:5:C:H2'	15:6:6:A:C8	2.40	0.55
1:A:528:LEU:HD23	1:A:751:SER:HA	1.89	0.55
1:A:666:ILE:O	1:A:670:ILE:HD13	2.06	0.55
1:A:858:ASN:ND2	1:A:858:ASN:C	2.55	0.55
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.88	0.55
2:B:327:ARG:HH22	2:B:371:GLU:HG2	1.71	0.55
12:L:26:THR:HG23	12:L:62:LYS:NZ	2.20	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:42:ASP:HA	1:M:46:THR:O	2.07	0.55
1:M:61:ILE:HG22	1:M:62:ASP:N	2.21	0.55
2:N:347:LYS:HG3	2:N:348:ARG:H	1.72	0.55
2:N:637:LEU:CD2	2:N:742:GLU:HA	2.36	0.55
3:O:116:LYS:HD3	3:O:140:ASN:HA	1.89	0.55
5:Q:56:LYS:NZ	5:Q:84:ASP:H	2.04	0.55
5:Q:207:ARG:HB3	5:Q:207:ARG:HH11	1.71	0.55
1:A:89:PRO:O	1:A:204:THR:HG21	2.07	0.55
1:A:115:LEU:HG	1:A:142:CYS:HB3	1.89	0.55
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.88	0.55
1:A:1239:ARG:HH12	1:A:1241:ARG:HH12	1.54	0.55
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.06	0.55
2:B:258:LEU:HG	2:B:258:LEU:O	2.05	0.55
2:B:531:GLN:HG2	2:B:532:ALA:H	1.69	0.55
2:B:1124:ARG:NH1	15:3:2:G:OP2	2.37	0.55
3:C:174:ALA:O	3:C:175:ALA:HB3	2.07	0.55
4:D:220:LEU:HG	4:D:221:TYR:H	1.71	0.55
9:I:86:PHE:CE1	9:I:100:PHE:HB2	2.41	0.55
1:M:351:THR:HG21	2:N:1103:ILE:HG13	1.89	0.55
1:M:824:LEU:O	1:M:827:THR:HG22	2.06	0.55
2:N:300:HIS:O	2:N:303:TYR:HE2	1.89	0.55
2:N:378:LEU:O	2:N:382:ILE:HG13	2.06	0.55
3:O:36:VAL:HG21	3:O:251:LEU:HB2	1.89	0.55
3:O:51:VAL:HG22	3:O:155:LEU:CD2	2.35	0.55
4:P:4:SER:O	4:P:5:THR:CB	2.53	0.55
12:X:27:LEU:O	12:X:28:LYS:HB2	2.05	0.55
12:X:30:ILE:HG22	12:X:31:CYS:N	2.21	0.55
13:4:15:DG:C2'	13:4:16:DT:H71	2.37	0.55
1:A:313:GLN:O	1:A:314:ALA:C	2.49	0.55
1:A:903:ASN:HD22	1:A:905:ASP:H	1.48	0.55
1:A:1171:GLN:OE1	1:A:1172:LEU:HG	2.06	0.55
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.42	0.55
2:B:244:LEU:HD11	2:B:366:GLN:HE22	1.70	0.55
2:B:345:LYS:HG2	2:B:346:GLU:N	2.21	0.55
2:B:657:HIS:CE1	2:B:689:LEU:HD11	2.42	0.55
2:B:918:ILE:HG21	2:B:935:ARG:NH2	2.21	0.55
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.40	0.55
1:M:41:MET:HB2	1:M:49:LYS:HA	1.86	0.55
1:M:711:ARG:NH1	9:U:95:THR:HB	2.21	0.55
1:M:1095:THR:CG2	1:M:1112:LYS:HB2	2.33	0.55
1:M:1454:MET:HG3	1:M:1454:MET:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:174:LEU:HD22	2:N:202:TYR:CE1	2.41	0.55
2:N:308:TRP:HB2	9:U:2:THR:HG22	1.89	0.55
2:N:422:LYS:HA	2:N:425:THR:HB	1.87	0.55
2:N:461:LEU:HD12	2:N:461:LEU:N	2.21	0.55
3:O:75:MET:HB3	3:O:128:ASN:HB3	1.88	0.55
3:O:148:ARG:NH1	10:V:64:ASN:HA	2.22	0.55
4:P:155:ARG:NE	4:P:221:TYR:CE1	2.73	0.55
1:A:28:ARG:HH21	1:A:238:CYS:HB2	1.71	0.55
1:A:699:ALA:HB3	1:A:701:LEU:HG	1.89	0.55
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.89	0.55
2:B:686:ASN:C	2:B:688:GLY:H	2.14	0.55
2:B:836:GLU:O	2:B:837:ASP:HB2	2.05	0.55
11:K:12:LEU:HD12	11:K:37:LYS:CG	2.37	0.55
1:M:2:VAL:CG1	2:N:1157:ALA:O	2.54	0.55
1:M:347:PHE:HE2	1:M:375:THR:CG2	2.19	0.55
1:M:512:VAL:O	1:M:512:VAL:HG12	2.07	0.55
1:M:535:THR:O	1:M:575:LYS:HE3	2.05	0.55
2:N:731:VAL:HG12	2:N:732:SER:N	2.20	0.55
4:P:216:ASN:C	4:P:218:GLU:H	2.13	0.55
5:Q:169:ARG:HD3	6:R:140:ASP:CG	2.31	0.55
5:Q:192:ARG:HG3	5:Q:192:ARG:NH1	2.22	0.55
9:U:8:ARG:HG3	9:U:34:TYR:CE1	2.42	0.55
11:W:23:PRO:HA	11:W:31:VAL:HG13	1.89	0.55
1:A:60:SER:OG	1:A:61:ILE:N	2.39	0.55
1:A:207:ILE:HG22	1:A:211:PHE:CE2	2.42	0.55
1:A:382:PRO:CA	1:A:428:TYR:HE2	2.20	0.55
1:A:639:PRO:HG2	1:A:640:GLN:NE2	2.22	0.55
1:A:1329:THR:CG2	1:A:1331:SER:H	2.13	0.55
1:A:1444:MET:CG	7:G:60:ARG:HA	2.34	0.55
2:B:165:VAL:HG11	2:B:448:ILE:CD1	2.37	0.55
2:B:860:MET:HG2	2:B:861:ASP:H	1.71	0.55
3:C:73:GLN:HE21	3:C:75:MET:CB	2.19	0.55
8:H:12:VAL:HG13	8:H:26:ILE:HG12	1.87	0.55
8:H:18:GLY:O	8:H:19:ARG:HB2	2.07	0.55
8:H:47:PHE:HB3	8:H:95:TYR:HD1	1.71	0.55
12:L:38:LEU:O	12:L:39:SER:HB3	2.06	0.55
1:M:252:PHE:HB2	1:M:256:GLN:CD	2.31	0.55
1:M:605:MET:HE1	1:M:612:ILE:HG23	1.89	0.55
1:M:1308:THR:HG21	1:M:1310:GLY:O	2.07	0.55
2:N:118:ARG:HH22	2:N:194:GLU:CD	2.14	0.55
2:N:364:ILE:CG1	2:N:585:VAL:HG13	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:22:LEU:HD11	11:W:101:LEU:HD11	1.87	0.55
4:P:56:ARG:HD3	4:P:149:THR:HA	1.89	0.55
5:Q:22:MET:HE3	5:Q:26:ARG:HE	1.69	0.55
1:A:323:LYS:H	1:A:323:LYS:HD2	1.72	0.55
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.65	0.55
1:A:960:ILE:HA	1:A:963:ILE:HG22	1.88	0.55
1:A:1308:THR:HG21	1:A:1310:GLY:O	2.07	0.55
2:B:20:ASP:C	2:B:22:SER:H	2.14	0.55
2:B:66:ASP:OD2	2:B:422:LYS:HG2	2.07	0.55
2:B:579:ARG:HA	2:B:589:VAL:HG13	1.89	0.55
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.88	0.55
2:B:794:ASN:C	2:B:795:ILE:HD12	2.32	0.55
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.39	0.55
7:G:139:ILE:CG2	7:G:140:LYS:HG3	2.31	0.55
12:L:49:LYS:O	12:L:50:ASP:CB	2.54	0.55
13:1:15:DG:C2'	13:1:16:DT:H71	2.37	0.55
1:M:145:LYS:HA	1:M:145:LYS:CE	2.35	0.55
1:M:836:TYR:CZ	1:M:840:ARG:HD2	2.42	0.55
1:M:1155:ASP:OD2	1:M:1161:THR:HA	2.07	0.55
1:M:1348:LEU:O	1:M:1352:VAL:HG23	2.07	0.55
2:N:770:GLN:OE1	2:N:983:ARG:HA	2.06	0.55
4:P:8:PHE:HD2	7:S:6:ASP:O	1.90	0.55
1:A:106:VAL:HG12	1:A:107:CYS:N	2.22	0.55
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.88	0.55
2:B:185:THR:O	2:B:186:GLU:C	2.50	0.55
2:B:637:LEU:HD11	2:B:703:ILE:HD13	1.89	0.55
2:B:1063:GLY:O	3:C:202:PRO:HG2	2.06	0.55
3:C:114:TYR:CG	3:C:140:ASN:HB3	2.41	0.55
5:E:99:HIS:CE1	5:E:103:LYS:HG3	2.42	0.55
7:G:138:THR:CG2	7:G:139:ILE:H	2.19	0.55
9:I:19:ASP:HB3	9:I:24:ARG:HG2	1.88	0.55
9:I:50:THR:HG21	9:I:52:ILE:HG12	1.87	0.55
1:M:7:SER:HB3	2:N:1193:GLN:NE2	2.22	0.55
1:M:1329:THR:HG22	1:M:1335:ILE:HG13	1.88	0.55
1:M:1403:GLU:O	13:4:16:DT:OP1	2.24	0.55
1:M:1438:THR:HB	2:N:1144:ALA:HB3	1.87	0.55
2:N:38:PHE:CD1	2:N:811:TYR:CD2	2.93	0.55
2:N:313:MET:HE3	2:N:386:LEU:HD22	1.89	0.55
2:N:637:LEU:HD12	2:N:693:ILE:HD12	1.88	0.55
2:N:652:LYS:HB3	2:N:689:LEU:HD23	1.89	0.55
2:N:1197:PRO:O	2:N:1200:ALA:N	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:114:TYR:CG	3:O:140:ASN:HB3	2.42	0.55
7:S:34:VAL:HG13	7:S:45:ILE:HD13	1.89	0.55
2:B:526:GLU:OE1	2:B:752:ALA:HB3	2.07	0.55
2:B:1162:ILE:HD13	2:B:1194:ILE:HD13	1.88	0.55
4:D:146:GLN:CA	4:D:149:THR:HG22	2.37	0.55
5:E:155:ARG:HG2	5:E:155:ARG:HH11	1.71	0.55
5:E:156:LEU:HA	5:E:160:GLU:OE1	2.07	0.55
7:G:30:LEU:HD22	7:G:72:VAL:HG11	1.89	0.55
10:J:52:THR:HG22	10:J:52:THR:O	2.07	0.55
1:M:337:ARG:HD3	2:N:1132:GLU:CD	2.32	0.55
1:M:850:VAL:HG21	1:M:1058:VAL:HG11	1.88	0.55
1:M:973:ILE:HG22	1:M:973:ILE:O	2.05	0.55
1:M:1263:ILE:O	1:M:1267:MET:HG3	2.07	0.55
2:N:402:GLY:HA2	2:N:695:ALA:HB3	1.88	0.55
3:O:35:ARG:HH12	11:W:41:THR:H	1.55	0.55
5:Q:55:ARG:HA	5:Q:58:MET:HG3	1.88	0.55
5:Q:64:PRO:HB2	5:Q:69:ILE:HD11	1.89	0.55
5:Q:111:VAL:HG12	5:Q:137:GLU:HG2	1.87	0.55
11:W:93:SER:O	11:W:97:LYS:HG3	2.06	0.55
1:A:549:MET:CE	1:A:656:TRP:HD1	2.20	0.54
1:A:556:TRP:CH2	1:A:558:GLY:HA2	2.42	0.54
5:E:179:GLN:HB2	5:E:182:ASP:HB2	1.89	0.54
7:G:117:GLN:HE22	7:S:154:VAL:HG22	1.69	0.54
8:H:59:ILE:CG2	8:H:60:ALA:N	2.63	0.54
1:M:265:LYS:HE2	1:M:268:ASP:OD2	2.07	0.54
1:M:470:LEU:HD23	1:M:470:LEU:N	2.21	0.54
1:M:475:THR:CG2	1:M:476:SER:N	2.69	0.54
1:M:503:GLN:HE21	6:R:90:ARG:NH2	1.98	0.54
1:M:1120:LEU:HD22	1:M:1125:ALA:HA	1.89	0.54
1:M:1152:ILE:HD12	1:M:1261:LYS:HE3	1.89	0.54
1:M:1450:LEU:HD11	6:R:108:PHE:HZ	1.71	0.54
2:N:185:THR:H	2:N:188:ASP:HB2	1.71	0.54
2:N:273:LEU:CB	2:N:276:ILE:HD12	2.37	0.54
2:N:351:TYR:CE1	2:N:355:ILE:HD11	2.42	0.54
2:N:613:VAL:HG22	2:N:628:THR:HA	1.89	0.54
2:N:640:VAL:O	2:N:640:VAL:HG12	2.05	0.54
4:P:207:LEU:O	4:P:207:LEU:HD12	2.06	0.54
9:U:10:CYS:SG	9:U:32:CYS:HB3	2.47	0.54
10:V:52:THR:HG22	10:V:52:THR:O	2.07	0.54
1:A:289:ILE:HG22	1:A:290:GLU:N	2.23	0.54
1:A:353:ILE:HD13	1:A:487:MET:HG3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:LEU:HG	1:A:1308:THR:HB	1.89	0.54
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.75	0.54
2:B:398:ARG:CB	2:B:398:ARG:NH1	2.70	0.54
2:B:848:ARG:HA	3:C:69:LEU:HD21	1.87	0.54
4:D:134:THR:CG2	4:D:135:GLY:N	2.69	0.54
7:G:111:THR:HG22	7:G:114:LEU:HD22	1.88	0.54
12:L:61:THR:HG22	12:L:63:ARG:H	1.72	0.54
1:M:441:PRO:HG3	1:M:498:ARG:HB2	1.89	0.54
1:M:475:THR:HG23	1:M:476:SER:N	2.22	0.54
1:M:1205:LYS:O	1:M:1207:LEU:HG	2.07	0.54
2:N:604:ARG:NH1	2:N:691:GLU:OE2	2.38	0.54
2:N:936:ASP:OD1	2:N:937:ALA:N	2.40	0.54
2:N:1147:LEU:HD22	2:N:1151:LEU:HD22	1.88	0.54
2:N:1167:GLY:HA3	2:N:1216:LEU:H	1.70	0.54
3:O:114:TYR:CD2	3:O:140:ASN:HB3	2.43	0.54
4:P:69:ALA:C	4:P:71:LYS:H	2.15	0.54
5:Q:192:ARG:HG3	5:Q:192:ARG:HH11	1.71	0.54
8:T:15:VAL:HG22	8:T:26:ILE:CG1	2.36	0.54
12:X:26:THR:CG2	12:X:27:LEU:H	2.03	0.54
1:A:385:ILE:HG22	1:A:386:ASP:N	2.21	0.54
4:D:146:GLN:O	4:D:147:TYR:C	2.50	0.54
11:K:47:ARG:HD2	11:K:47:ARG:O	2.08	0.54
12:L:53:HIS:O	12:L:55:ILE:HD13	2.08	0.54
1:M:41:MET:HB2	1:M:48:ALA:O	2.08	0.54
1:M:332:LYS:C	1:M:334:GLY:N	2.64	0.54
1:M:567:LYS:HZ3	8:T:43:ASN:HB3	1.70	0.54
1:M:874:ASP:C	1:M:874:ASP:OD1	2.49	0.54
1:M:1015:VAL:HG12	1:M:1015:VAL:O	2.07	0.54
2:N:806:THR:H	2:N:809:MET:HE3	1.70	0.54
4:P:193:THR:HG23	4:P:194:LEU:HD23	1.88	0.54
8:T:58:THR:HG22	8:T:59:ILE:N	2.20	0.54
10:V:9:SER:HB2	10:V:45:CYS:HB2	1.90	0.54
1:A:351:THR:HG22	2:B:1103:ILE:CA	2.23	0.54
1:A:518:LYS:HE2	1:A:624:SER:O	2.08	0.54
1:A:534:LEU:O	1:A:534:LEU:HG	2.07	0.54
2:B:34:ILE:HG12	2:B:542:MET:CE	2.37	0.54
2:B:552:MET:HA	2:B:552:MET:CE	2.34	0.54
4:D:209:ARG:HA	4:D:212:LYS:HE3	1.89	0.54
10:J:7:CYS:HB2	10:J:49:MET:HE3	1.89	0.54
12:L:66:GLN:HG2	12:L:67:PHE:N	2.22	0.54
1:M:153:PRO:HB3	1:M:161:LEU:HD22	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:289:ILE:HG22	1:M:290:GLU:N	2.23	0.54
1:M:489:LEU:HD12	1:M:490:HIS:N	2.22	0.54
1:M:541:ILE:HG22	1:M:546:VAL:CG2	2.37	0.54
1:M:868:TYR:HD2	1:M:1058:VAL:HG21	1.72	0.54
1:M:979:SER:OG	1:M:980:ASP:N	2.37	0.54
1:M:1072:ILE:O	1:M:1075:PRO:HG2	2.07	0.54
1:M:1142:THR:O	1:M:1145:SER:OG	2.21	0.54
2:N:114:PRO:HG2	2:N:115:GLN:H	1.73	0.54
2:N:123:THR:HG23	2:N:205:ILE:HA	1.89	0.54
2:N:467:GLY:CA	2:N:475:SER:HB3	2.38	0.54
2:N:766:ARG:NH2	2:N:1020:ARG:HH11	2.03	0.54
2:N:950:ASP:HB3	2:N:967:ARG:O	2.08	0.54
5:Q:42:PHE:HE1	5:Q:58:MET:HE3	1.73	0.54
7:S:55:ASP:HB3	7:S:73:LYS:HB2	1.89	0.54
12:X:47:ARG:CG	12:X:48:CYS:H	2.20	0.54
1:A:401:GLY:C	1:A:435:HIS:CD2	2.85	0.54
1:A:438:ASP:O	1:A:439:ASN:HB2	2.05	0.54
1:A:883:LEU:HD11	1:A:1017:LEU:HD11	1.88	0.54
1:A:1315:GLU:C	1:A:1317:MET:H	2.15	0.54
2:B:658:ILE:CG2	2:B:662:MET:HE2	2.37	0.54
2:B:797:TYR:O	10:J:1:MET:HG2	2.07	0.54
5:E:79:TRP:HB2	5:E:105:PHE:CE1	2.43	0.54
5:E:129:PRO:O	5:E:130:ALA:C	2.51	0.54
6:F:110:ASP:O	6:F:123:LYS:HE3	2.07	0.54
7:G:115:MET:HG2	7:G:163:ILE:HD11	1.89	0.54
8:H:130:ARG:HD3	8:H:130:ARG:H	1.70	0.54
10:J:25:LEU:O	10:J:29:GLU:HA	2.08	0.54
12:L:31:CYS:HB2	12:L:48:CYS:SG	2.47	0.54
1:M:1206:ASP:O	1:M:1274:ARG:NH2	2.40	0.54
1:M:1317:MET:O	1:M:1322:ILE:HD11	2.08	0.54
2:N:129:PHE:HA	2:N:165:VAL:O	2.08	0.54
2:N:315:LYS:N	2:N:316:PRO:HD2	2.23	0.54
2:N:859:TYR:CZ	2:N:941:LEU:HD12	2.43	0.54
4:P:220:LEU:HG	4:P:221:TYR:H	1.73	0.54
5:Q:64:PRO:O	5:Q:69:ILE:HD11	2.07	0.54
5:Q:98:ILE:HG22	5:Q:102:GLU:CG	2.37	0.54
7:S:112:LYS:HB3	7:S:113:HIS:ND1	2.22	0.54
7:S:115:MET:HE1	7:S:130:TYR:CE2	2.42	0.54
9:U:17:ARG:HH21	9:U:30:ARG:CZ	2.20	0.54
1:A:489:LEU:HD12	1:A:489:LEU:C	2.32	0.54
1:A:962:ARG:O	1:A:964:ILE:N	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.07	0.54
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.89	0.54
2:B:866:TYR:CG	2:B:870:ILE:HB	2.42	0.54
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.23	0.54
3:C:25:VAL:HG12	3:C:26:ASP:N	2.23	0.54
3:C:104:PHE:HE2	3:C:150:GLY:HA2	1.73	0.54
4:D:7:THR:O	4:D:7:THR:HG23	2.08	0.54
4:D:216:ASN:C	4:D:218:GLU:H	2.16	0.54
5:E:121:MET:C	5:E:123:LEU:H	2.14	0.54
6:F:99:LEU:O	6:F:103:MET:HG2	2.08	0.54
11:K:55:LYS:HB2	11:K:81:TYR:CE1	2.43	0.54
1:M:35:ILE:CD1	1:M:241:VAL:HG11	2.37	0.54
1:M:283:GLY:O	1:M:285:PRO:HD3	2.06	0.54
1:M:1121:GLU:HG3	1:M:1122:PRO:HD2	1.90	0.54
2:N:185:THR:O	2:N:188:ASP:HB2	2.07	0.54
2:N:276:ILE:HA	2:N:336:ARG:O	2.07	0.54
2:N:449:ASN:C	2:N:451:LYS:H	2.16	0.54
5:Q:198:ILE:CD1	5:Q:212:ARG:HG3	2.38	0.54
7:S:129:SER:OG	7:S:130:TYR:N	2.36	0.54
12:X:58:LYS:O	12:X:58:LYS:HG2	2.07	0.54
1:A:34:LYS:HG3	1:A:36:ARG:NH2	2.22	0.54
1:A:105:CYS:SG	1:A:139:TRP:HA	2.48	0.54
1:A:332:LYS:HG2	1:A:333:GLU:HG2	1.90	0.54
5:E:17:ARG:O	5:E:21:GLU:HG3	2.08	0.54
5:E:177:ARG:HB3	5:E:215:MET:HG2	1.90	0.54
8:H:40:LEU:HD11	8:H:142:LEU:CD2	2.38	0.54
8:H:89:LEU:HB2	8:H:91:ASP:OD1	2.08	0.54
10:J:1:MET:H1	10:J:56:LEU:N	2.06	0.54
11:K:21:ILE:HG23	11:K:31:VAL:HG11	1.89	0.54
1:M:130:ASP:OD2	1:M:133:LYS:HG3	2.08	0.54
1:M:468:PHE:CE2	1:M:489:LEU:HD23	2.43	0.54
1:M:770:VAL:HA	1:M:822:GLU:OE1	2.08	0.54
1:M:779:PHE:HE1	1:M:785:PRO:HD3	1.69	0.54
2:N:616:ILE:HD12	2:N:616:ILE:N	2.21	0.54
2:N:650:GLU:HG3	2:N:654:ARG:HH21	1.73	0.54
2:N:684:LEU:O	2:N:689:LEU:HB2	2.08	0.54
2:N:773:MET:HE2	2:N:985:GLY:HA2	1.90	0.54
3:O:88:CYS:SG	3:O:91:HIS:HA	2.48	0.54
4:P:50:LEU:HD22	4:P:54:GLU:HG2	1.89	0.54
5:Q:69:ILE:HD12	5:Q:69:ILE:H	1.70	0.54
12:X:38:LEU:O	12:X:39:SER:HB3	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:CD1	1:A:142:CYS:HB3	2.37	0.54
1:A:535:THR:HG21	1:A:617:VAL:N	2.23	0.54
1:A:973:ILE:HD11	1:A:1041:ALA:CB	2.38	0.54
1:A:979:SER:OG	1:A:980:ASP:N	2.39	0.54
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.33	0.54
1:A:1155:ASP:OD2	1:A:1161:THR:HA	2.07	0.54
3:C:148:ARG:NH1	10:J:64:ASN:HA	2.22	0.54
5:E:124:VAL:CG1	5:E:132:ILE:HB	2.21	0.54
8:H:106:GLU:C	8:H:108:SER:H	2.15	0.54
9:I:55:THR:HG23	9:I:100:PHE:HD2	1.72	0.54
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.90	0.54
1:M:401:GLY:C	1:M:435:HIS:HD2	2.15	0.54
1:M:556:TRP:CH2	1:M:558:GLY:HA2	2.43	0.54
1:M:565:ILE:HG23	1:M:567:LYS:CG	2.38	0.54
1:M:710:LEU:H	1:M:710:LEU:CD1	2.18	0.54
1:M:1445:ILE:H	1:M:1445:ILE:HD12	1.73	0.54
2:N:114:PRO:CG	2:N:181:LEU:HD11	2.25	0.54
2:N:205:ILE:N	2:N:205:ILE:CD1	2.71	0.54
2:N:526:GLU:OE1	2:N:752:ALA:HB3	2.08	0.54
2:N:570:VAL:HG21	2:N:573:GLN:CD	2.33	0.54
3:O:67:LEU:HD11	3:O:155:LEU:HD13	1.89	0.54
1:A:381:THR:HG22	1:A:383:TYR:H	1.73	0.54
1:A:512:VAL:O	1:A:512:VAL:HG12	2.07	0.54
1:A:1421:CYS:HA	1:A:1426:GLU:HG3	1.89	0.54
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.71	0.54
2:B:955:THR:HG1	12:L:55:ILE:HA	1.72	0.54
3:C:44:LEU:HD21	3:C:159:ALA:CB	2.38	0.54
8:H:123:MET:HE3	8:H:142:LEU:HD22	1.90	0.54
9:I:8:ARG:HG3	9:I:34:TYR:HE1	1.71	0.54
9:I:73:ARG:HH12	9:I:112:SER:HB3	1.72	0.54
1:M:385:ILE:CD1	1:M:426:LEU:HB2	2.37	0.54
1:M:610:GLY:O	1:M:611:GLN:NE2	2.41	0.54
1:M:1011:GLN:NE2	1:M:1015:VAL:CG2	2.71	0.54
2:N:531:GLN:CG	2:N:532:ALA:H	2.20	0.54
2:N:995:ARG:HB3	2:N:997:GLU:OE2	2.07	0.54
3:O:56:THR:HG22	3:O:57:VAL:N	2.21	0.54
6:R:119:ARG:HH11	6:R:119:ARG:HG3	1.73	0.54
12:X:43:THR:O	12:X:43:THR:HG22	2.08	0.54
2:B:642:ASP:HA	2:B:649:LYS:HG3	1.90	0.54
2:B:898:LEU:HD13	2:B:952:VAL:CG1	2.38	0.54
3:C:148:ARG:HD3	3:C:149:LYS:HG3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:144:ILE:HG13	5:E:145:THR:H	1.70	0.54
12:L:55:ILE:HD13	12:L:55:ILE:N	2.15	0.54
1:M:438:ASP:O	1:M:439:ASN:HB2	2.07	0.54
1:M:565:ILE:HG21	1:M:567:LYS:HE2	1.90	0.54
1:M:697:ALA:HA	1:M:702:LEU:HG	1.90	0.54
1:M:963:ILE:HD11	1:M:1048:ASN:HB2	1.89	0.54
2:N:167:ILE:HG21	2:N:424:LEU:CD2	2.38	0.54
2:N:805:THR:HG23	2:N:809:MET:SD	2.48	0.54
3:O:35:ARG:NH1	11:W:41:THR:H	2.06	0.54
3:O:66:ARG:NH2	10:V:5:VAL:HG23	2.23	0.54
4:P:56:ARG:NH2	4:P:155:ARG:HG2	2.21	0.54
8:T:106:GLU:C	8:T:108:SER:H	2.15	0.54
11:W:51:LEU:HD13	11:W:59:ALA:HB3	1.90	0.54
1:A:129:LYS:O	1:A:130:ASP:HB2	2.08	0.53
1:A:838:GLN:O	1:A:842:VAL:HG23	2.08	0.53
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.43	0.53
5:E:42:PHE:CE1	5:E:58:MET:HE3	2.43	0.53
8:H:4:THR:HG22	8:H:5:LEU:N	2.23	0.53
8:H:15:VAL:HG21	8:H:49:VAL:O	2.07	0.53
8:H:84:ALA:O	8:H:85:GLY:C	2.52	0.53
12:L:29:TYR:O	12:L:30:ILE:HG13	2.08	0.53
1:M:537:ARG:NH1	8:T:120:GLY:O	2.41	0.53
1:M:920:LEU:HD23	1:M:921:GLY:N	2.23	0.53
1:M:1141:THR:OG1	1:M:1205:LYS:HD3	2.08	0.53
1:M:1313:LEU:O	1:M:1315:GLU:N	2.41	0.53
2:N:398:ARG:CB	2:N:398:ARG:NH1	2.71	0.53
2:N:642:ASP:HB3	2:N:649:LYS:CD	2.38	0.53
2:N:661:LEU:HD11	2:N:684:LEU:HD11	1.90	0.53
2:N:1115:THR:HG22	2:N:1117:GLN:HG3	1.90	0.53
4:P:35:LEU:N	4:P:35:LEU:CD1	2.70	0.53
5:Q:177:ARG:C	5:Q:212:ARG:HD3	2.33	0.53
1:A:341:MET:HE2	1:A:843:LYS:HZ1	1.73	0.53
1:A:597:LEU:HD12	1:A:597:LEU:N	2.23	0.53
1:A:714:PHE:O	1:A:718:VAL:HG23	2.08	0.53
2:B:308:TRP:HB2	9:I:2:THR:HG22	1.89	0.53
2:B:1004:GLU:OE1	10:J:42:LYS:HE2	2.08	0.53
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.91	0.53
4:D:29:LEU:H	4:D:29:LEU:CD2	2.22	0.53
7:G:106:MET:HG2	7:G:107:LYS:N	2.23	0.53
1:M:381:THR:CG2	1:M:382:PRO:HD2	2.38	0.53
1:M:598:LEU:HA	8:T:122:LEU:HD13	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:901:LEU:H	1:M:926:GLN:CD	2.16	0.53
1:M:1215:ARG:NH1	1:M:1272:THR:O	2.40	0.53
2:N:273:LEU:O	2:N:276:ILE:HB	2.08	0.53
2:N:809:MET:O	2:N:812:LEU:N	2.40	0.53
2:N:1177:HIS:HB3	2:N:1179:GLN:HE21	1.73	0.53
3:O:184:ASN:ND2	3:O:189:THR:HB	2.22	0.53
8:T:76:THR:O	8:T:77:ARG:HB2	2.07	0.53
8:T:91:ASP:C	8:T:93:TYR:H	2.16	0.53
1:A:573:SER:O	1:A:576:GLN:HB2	2.07	0.53
1:A:687:LYS:HE2	1:A:795:GLU:OE2	2.09	0.53
1:A:907:THR:CG2	1:A:908:LEU:N	2.71	0.53
2:B:56:ASP:C	2:B:57:TYR:HD1	2.16	0.53
2:B:809:MET:O	2:B:812:LEU:N	2.40	0.53
2:B:885:MET:HA	2:B:936:ASP:HB2	1.91	0.53
4:D:4:SER:O	4:D:5:THR:CB	2.55	0.53
5:E:79:TRP:HE1	5:E:81:GLU:HB2	1.73	0.53
5:E:180:ARG:HB2	5:E:215:MET:OXT	2.07	0.53
7:G:1:MET:O	7:G:2:PHE:C	2.51	0.53
7:G:102:GLN:HG3	7:G:106:MET:O	2.09	0.53
9:I:74:GLU:HB3	9:I:81:ARG:HD2	1.89	0.53
10:J:48:ARG:HG2	10:J:48:ARG:NH1	2.23	0.53
11:K:107:THR:O	11:K:111:LEU:HG	2.09	0.53
1:M:337:ARG:CD	2:N:1132:GLU:OE1	2.56	0.53
1:M:590:ARG:HH12	1:M:592:ASP:CG	2.16	0.53
1:M:1412:ALA:HA	1:M:1417:GLU:OE2	2.09	0.53
2:N:66:ASP:OD2	2:N:422:LYS:HG2	2.08	0.53
2:N:847:ASP:C	2:N:849:GLY:N	2.66	0.53
8:T:38:LEU:HD12	8:T:39:THR:N	2.24	0.53
12:X:66:GLN:HG2	12:X:67:PHE:N	2.23	0.53
1:A:353:ILE:HD13	1:A:487:MET:CG	2.39	0.53
1:A:370:ILE:CG2	1:A:374:LEU:HD12	2.38	0.53
1:A:493:GLN:N	1:A:493:GLN:HE21	2.06	0.53
8:H:58:THR:HG22	8:H:59:ILE:N	2.21	0.53
8:H:91:ASP:C	8:H:93:TYR:H	2.17	0.53
1:M:168:GLY:O	1:M:169:ASN:C	2.50	0.53
1:M:756:ILE:O	1:M:759:ALA:HB3	2.08	0.53
1:M:853:ASP:O	1:M:854:ASN:HB2	2.07	0.53
2:N:190:TYR:CZ	2:N:196:PRO:HG3	2.44	0.53
2:N:277:LYS:HG3	2:N:336:ARG:HG2	1.90	0.53
2:N:393:LYS:HA	2:N:393:LYS:CE	2.35	0.53
2:N:1001:PHE:CZ	2:N:1073:TYR:HB2	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:101:ILE:HD13	6:R:120:ILE:CG2	2.39	0.53
8:T:130:ARG:HD3	8:T:130:ARG:H	1.72	0.53
9:U:106:CYS:O	9:U:107:SER:HB2	2.09	0.53
10:V:14:VAL:O	10:V:14:VAL:CG1	2.56	0.53
10:V:53:HIS:HD2	10:V:54:VAL:H	1.55	0.53
1:A:69:THR:C	1:A:71:GLN:N	2.65	0.53
1:A:335:ARG:NH1	2:B:1206:GLU:CD	2.66	0.53
1:A:697:ALA:CB	1:A:702:LEU:HD11	2.36	0.53
1:A:1141:THR:HA	1:A:1205:LYS:NZ	2.24	0.53
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.73	0.53
3:C:104:PHE:HD2	3:C:105:GLY:N	2.06	0.53
7:G:53:ASN:N	7:G:53:ASN:ND2	2.55	0.53
9:I:50:THR:CG2	9:I:51:ASN:H	2.16	0.53
1:M:720:ARG:O	1:M:720:ARG:HG2	2.08	0.53
2:N:398:ARG:NH1	2:N:398:ARG:HB2	2.24	0.53
8:T:15:VAL:HG21	8:T:49:VAL:O	2.08	0.53
1:A:347:PHE:HE2	1:A:375:THR:HG22	1.73	0.53
1:A:597:LEU:HD23	8:H:103:LYS:HD2	1.89	0.53
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.90	0.53
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.92	0.53
1:A:961:ARG:HG2	1:A:965:GLN:NE2	2.24	0.53
1:A:1025:ARG:HG3	1:A:1025:ARG:HH11	1.72	0.53
1:A:1433:MET:HE3	7:G:63:PRO:HB2	1.90	0.53
2:B:766:ARG:HH21	2:B:1020:ARG:CD	2.19	0.53
3:C:133:ILE:CD1	3:C:236:GLY:C	2.82	0.53
7:G:139:ILE:HG23	7:G:140:LYS:H	1.72	0.53
8:H:76:THR:O	8:H:77:ARG:HB2	2.07	0.53
9:I:61:ASP:C	9:I:63:GLY:N	2.66	0.53
10:J:30:LEU:HD21	10:J:38:ARG:HH12	1.74	0.53
12:L:26:THR:C	12:L:27:LEU:HD23	2.34	0.53
1:M:35:ILE:HD13	1:M:241:VAL:HG11	1.89	0.53
1:M:198:GLU:O	1:M:198:GLU:HG2	2.07	0.53
1:M:913:LEU:HD13	1:M:981:LEU:O	2.09	0.53
1:M:1148:ILE:HD11	1:M:1198:ASP:HA	1.89	0.53
1:M:1450:LEU:HG	1:M:1450:LEU:O	2.08	0.53
2:N:53:GLN:HG2	2:N:547:VAL:HG22	1.90	0.53
2:N:90:ILE:CD1	2:N:432:MET:SD	2.96	0.53
2:N:696:GLU:O	2:N:699:GLU:HB2	2.09	0.53
2:N:1065:GLN:NE2	2:N:1066:SER:N	2.56	0.53
2:N:1161:HIS:NE2	2:N:1175:LEU:HD21	2.23	0.53
9:U:61:ASP:C	9:U:63:GLY:N	2.66	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:427:ASP:HA	2:B:430:ARG:HG3	1.90	0.53
3:C:172:PRO:O	3:C:235:VAL:HG23	2.09	0.53
3:C:221:TYR:CD2	8:H:46:LEU:HD22	2.44	0.53
6:F:108:PHE:O	6:F:129:LYS:HD3	2.07	0.53
1:M:186:LYS:NZ	1:M:197:PRO:HD3	2.23	0.53
1:M:323:LYS:HD2	1:M:323:LYS:N	2.23	0.53
1:M:518:LYS:HB2	1:M:519:PRO:HD2	1.91	0.53
1:M:549:MET:CE	1:M:656:TRP:HD1	2.21	0.53
2:N:798:TYR:HE2	3:O:62:PHE:CE2	2.27	0.53
2:N:1110:PRO:HB2	2:N:1119:VAL:HG11	1.91	0.53
3:O:44:LEU:CD2	3:O:159:ALA:HB1	2.39	0.53
3:O:252:GLN:HE21	11:W:95:ILE:HG22	1.74	0.53
3:O:252:GLN:CG	11:W:95:ILE:HG23	2.35	0.53
4:P:190:GLU:O	4:P:193:THR:HG22	2.09	0.53
5:Q:129:PRO:O	5:Q:130:ALA:C	2.52	0.53
10:V:51:LEU:HD12	10:V:51:LEU:O	2.09	0.53
1:A:95:PHE:O	1:A:96:ILE:C	2.51	0.53
1:A:332:LYS:C	1:A:334:GLY:N	2.66	0.53
1:A:675:THR:HG21	1:A:736:ASN:HB2	1.90	0.53
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.43	0.53
2:B:171:PRO:HD2	2:B:457:LEU:CD1	2.39	0.53
3:C:181:ASP:OD1	3:C:186:LEU:HD13	2.09	0.53
3:C:251:LEU:O	3:C:255:VAL:HG23	2.08	0.53
7:G:35:GLU:CG	7:G:48:VAL:HG23	2.38	0.53
1:M:310:GLY:O	1:M:312:PRO:CD	2.56	0.53
1:M:493:GLN:HE21	1:M:493:GLN:N	2.06	0.53
1:M:967:ALA:HA	1:M:1044:TRP:CZ3	2.43	0.53
2:N:801:LYS:O	10:V:52:THR:HG23	2.09	0.53
2:N:807:ARG:HD3	2:N:1043:ASP:OD1	2.09	0.53
2:N:878:GLN:HB2	2:N:879:ARG:NH1	2.24	0.53
2:N:887:HIS:N	2:N:887:HIS:CD2	2.75	0.53
2:N:1004:GLU:HG3	10:V:42:LYS:NZ	2.24	0.53
4:P:12:ARG:HD3	4:P:14:ARG:HG2	1.90	0.53
9:U:34:TYR:HD2	9:U:35:VAL:N	2.05	0.53
1:A:186:LYS:NZ	1:A:197:PRO:HD3	2.24	0.53
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.91	0.53
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.49	0.53
2:B:37:PHE:HE2	2:B:542:MET:HA	1.74	0.53
2:B:288:ALA:CB	2:B:331:LEU:HD12	2.32	0.53
2:B:806:THR:HG21	2:B:808:ALA:HB3	1.91	0.53
2:B:860:MET:HG2	2:B:861:ASP:N	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:872:GLU:CD	2:B:914:LYS:HE2	2.34	0.53
3:C:22:LEU:HD22	3:C:230:MET:CE	2.37	0.53
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.91	0.53
3:C:133:ILE:HD12	3:C:237:SER:N	2.24	0.53
3:C:245:VAL:HG13	11:K:102:LYS:HG3	1.91	0.53
9:I:16:PRO:HB3	9:I:27:PHE:CE2	2.44	0.53
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.44	0.53
15:3:5:C:H2'	15:3:6:A:C8	2.42	0.53
1:M:62:ASP:O	1:M:64:ASN:N	2.41	0.53
1:M:524:VAL:HG12	1:M:525:GLN:N	2.22	0.53
2:N:225:VAL:HA	2:N:237:VAL:O	2.08	0.53
3:O:45:ALA:HA	3:O:72:LEU:HD12	1.89	0.53
4:P:150:ASN:HB2	4:P:151:PHE:CD1	2.44	0.53
1:A:1403:GLU:O	13:1:16:DT:OP1	2.27	0.53
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.90	0.53
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.24	0.53
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.74	0.53
4:D:155:ARG:HH21	4:D:221:TYR:HD1	1.56	0.53
1:M:598:LEU:CD1	8:T:124:ARG:HB2	2.40	0.53
1:M:608:ILE:HG13	1:M:613:ILE:HD12	1.91	0.53
1:M:709:THR:CG2	1:M:710:LEU:N	2.72	0.53
1:M:1018:PHE:O	1:M:1021:LEU:HB3	2.08	0.53
1:M:1139:GLU:HG2	1:M:1139:GLU:O	2.07	0.53
2:N:604:ARG:C	2:N:606:LYS:H	2.16	0.53
2:N:763:GLN:HG2	2:N:765:PRO:CD	2.34	0.53
2:N:1110:PRO:C	2:N:1119:VAL:HG13	2.34	0.53
3:O:10:ILE:HG22	3:O:11:ARG:O	2.09	0.53
3:O:242:GLN:C	3:O:244:VAL:H	2.16	0.53
5:Q:112:TYR:OH	5:Q:136:ASN:HB2	2.09	0.53
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.57	0.52
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.91	0.52
2:B:90:ILE:CD1	2:B:432:MET:SD	2.97	0.52
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.24	0.52
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.37	0.52
7:G:7:LEU:HD13	7:G:45:ILE:HD11	1.89	0.52
1:M:253:ASN:ND2	2:N:935:ARG:HB2	2.24	0.52
1:M:316:GLN:HE21	1:M:317:LYS:CE	2.17	0.52
1:M:982:THR:HB	1:M:985:ASP:H	1.72	0.52
1:M:1107:VAL:O	1:M:1107:VAL:HG12	2.08	0.52
2:N:620:ARG:HH12	9:U:68:LEU:HD21	1.73	0.52
2:N:680:THR:OG1	2:N:681:TRP:N	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:803:LEU:HD13	2:N:1032:SER:O	2.09	0.52
2:N:811:TYR:HD1	2:N:811:TYR:H	1.57	0.52
6:R:100:GLN:NE2	7:S:61:ILE:HD13	2.24	0.52
9:U:69:PRO:HB2	9:U:85:PHE:CZ	2.44	0.52
1:A:7:SER:OG	2:B:1161:HIS:CE1	2.62	0.52
1:A:62:ASP:O	1:A:64:ASN:N	2.42	0.52
1:A:537:ARG:NH1	8:H:120:GLY:O	2.42	0.52
1:A:946:VAL:HG12	1:A:947:PHE:CD2	2.44	0.52
1:A:1114:PRO:O	1:A:1311:VAL:HG23	2.09	0.52
1:A:1203:ASN:O	1:A:1204:ASP:C	2.52	0.52
1:A:1433:MET:CE	7:G:63:PRO:HB2	2.40	0.52
2:B:193:LYS:NZ	12:L:32:ALA:HB1	2.24	0.52
2:B:427:ASP:HA	2:B:430:ARG:CD	2.39	0.52
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.91	0.52
4:D:69:ALA:C	4:D:71:LYS:H	2.17	0.52
8:H:40:LEU:HD12	8:H:123:MET:HG3	1.91	0.52
8:H:135:LEU:HB2	8:H:137:GLN:HE21	1.75	0.52
1:M:523:ILE:HG12	1:M:622:VAL:HG22	1.90	0.52
1:M:556:TRP:CZ2	1:M:558:GLY:HA2	2.44	0.52
1:M:670:ILE:HG23	1:M:805:LEU:HD21	1.91	0.52
1:M:845:LEU:O	1:M:846:GLU:C	2.52	0.52
1:M:1116:LEU:C	1:M:1116:LEU:HD12	2.35	0.52
2:N:216:GLU:HA	2:N:406:LEU:HD23	1.92	0.52
2:N:519:TRP:CD1	2:N:519:TRP:C	2.87	0.52
2:N:546:SER:OG	2:N:631:GLY:N	2.43	0.52
2:N:733:HIS:O	2:N:735:ALA:N	2.41	0.52
3:O:179:GLU:HG2	3:O:180:TYR:H	1.74	0.52
3:O:242:GLN:OE1	3:O:242:GLN:HA	2.08	0.52
4:P:146:GLN:HA	4:P:149:THR:HG22	1.91	0.52
5:Q:156:LEU:HA	5:Q:160:GLU:OE1	2.09	0.52
1:A:544:ASP:CG	1:A:545:GLN:N	2.67	0.52
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	2.97	0.52
1:A:1313:LEU:C	1:A:1315:GLU:N	2.67	0.52
2:B:225:VAL:HA	2:B:237:VAL:O	2.09	0.52
2:B:235:SER:OG	2:B:236:HIS:CD2	2.63	0.52
2:B:498:THR:HG22	2:B:537:LYS:H	1.75	0.52
2:B:618:ASP:O	2:B:622:LYS:N	2.42	0.52
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.44	0.52
3:C:3:GLU:CD	3:C:4:GLU:HG3	2.35	0.52
5:E:2:ASP:C	5:E:3:GLN:HG2	2.35	0.52
5:E:178:ILE:HG22	5:E:213:ILE:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:74:ILE:HD12	6:F:144:GLU:HG2	1.90	0.52
8:H:95:TYR:HE2	8:H:97:MET:CG	2.22	0.52
1:M:929:LEU:HD21	1:M:983:ILE:CG2	2.40	0.52
1:M:1209:MET:CE	1:M:1236:LEU:HB3	2.38	0.52
2:N:479:VAL:O	2:N:480:SER:HB3	2.08	0.52
2:N:954:VAL:O	12:X:55:ILE:O	2.26	0.52
2:N:1056:SER:HB3	2:N:1066:SER:OG	2.09	0.52
7:S:21:ARG:HD2	7:S:24:GLN:HB3	1.89	0.52
7:S:45:ILE:O	7:S:45:ILE:HG22	2.10	0.52
11:W:21:ILE:HG22	11:W:31:VAL:HG11	1.92	0.52
1:A:845:LEU:O	1:A:846:GLU:C	2.52	0.52
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.91	0.52
1:A:1148:ILE:HG12	1:A:1198:ASP:HB2	1.90	0.52
2:B:278:GLN:HG2	2:B:279:ASP:N	2.22	0.52
2:B:449:ASN:C	2:B:451:LYS:H	2.17	0.52
2:B:865:LYS:HZ3	2:B:869:SER:HA	1.75	0.52
2:B:875:GLU:O	2:B:877:PRO:HD3	2.09	0.52
2:B:1079:LYS:HA	3:C:27:LEU:HD21	1.90	0.52
2:B:1187:ASN:OD1	2:B:1188:LYS:N	2.42	0.52
7:G:1:MET:CE	7:G:80:LYS:H	2.22	0.52
7:G:13:LEU:HD21	7:G:17:PHE:CB	2.39	0.52
7:G:88:ASP:HB3	7:G:144:ARG:HA	1.91	0.52
1:M:347:PHE:HE2	1:M:375:THR:HG23	1.74	0.52
2:N:95:ILE:HG13	2:N:130:VAL:HG22	1.91	0.52
2:N:167:ILE:N	2:N:167:ILE:HD12	2.24	0.52
2:N:552:MET:C	2:N:554:ILE:H	2.17	0.52
4:P:27:LEU:HG	4:P:197:SER:HB3	1.90	0.52
5:Q:30:ILE:HG23	5:Q:34:GLU:HG2	1.91	0.52
5:Q:114:ASN:O	5:Q:115:ASN:CB	2.47	0.52
7:S:27:LYS:O	7:S:31:LEU:HG	2.09	0.52
1:A:168:GLY:O	1:A:169:ASN:C	2.51	0.52
1:A:208:LEU:HD21	1:A:212:LYS:HE3	1.90	0.52
1:A:335:ARG:NH1	2:B:1202:LEU:HD13	2.24	0.52
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.75	0.52
1:A:549:MET:SD	1:A:577:ILE:HD12	2.49	0.52
1:A:852:TYR:CE1	6:F:136:ARG:HG2	2.45	0.52
1:A:1259:MET:HE3	1:A:1262:LYS:HB2	1.91	0.52
2:B:733:HIS:O	2:B:735:ALA:N	2.42	0.52
11:K:51:LEU:HD13	11:K:59:ALA:HB3	1.92	0.52
12:L:58:LYS:O	12:L:58:LYS:HG2	2.10	0.52
1:M:470:LEU:N	1:M:470:LEU:CD2	2.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1127:ASP:CG	1:M:1130:GLN:HB2	2.34	0.52
2:N:47:GLN:O	2:N:173:MET:HE1	2.09	0.52
2:N:521:LEU:HB3	2:N:633:VAL:HG11	1.91	0.52
2:N:801:LYS:O	10:V:52:THR:CG2	2.58	0.52
3:O:18:VAL:HG23	3:O:240:VAL:HB	1.90	0.52
5:Q:48:ASP:CG	5:Q:49:SER:N	2.64	0.52
1:A:964:ILE:O	1:A:967:ALA:HB3	2.09	0.52
1:A:1141:THR:OG1	1:A:1205:LYS:HD3	2.10	0.52
2:B:95:ILE:HG13	2:B:130:VAL:CG2	2.39	0.52
2:B:203:PHE:N	2:B:203:PHE:CD1	2.78	0.52
2:B:552:MET:C	2:B:554:ILE:H	2.17	0.52
2:B:616:ILE:HD12	2:B:625:LYS:O	2.10	0.52
2:B:684:LEU:O	2:B:689:LEU:HB2	2.10	0.52
2:B:916:THR:HB	2:B:935:ARG:CG	2.38	0.52
8:H:106:GLU:HA	8:H:112:ILE:HD12	1.92	0.52
1:M:458:HIS:NE2	1:M:478:TYR:OH	2.33	0.52
1:M:676:MET:HE1	1:M:762:SER:O	2.09	0.52
1:M:1081:LEU:CD1	1:M:1097:GLY:HA3	2.36	0.52
2:N:63:ILE:HD12	2:N:421:PHE:CE2	2.45	0.52
2:N:527:THR:OG1	2:N:528:PRO:HD2	2.10	0.52
2:N:911:ILE:HG22	2:N:966:VAL:HG21	1.92	0.52
4:P:14:ARG:NH1	4:P:14:ARG:CB	2.72	0.52
5:Q:153:HIS:C	5:Q:154:ILE:HG13	2.32	0.52
8:T:84:ALA:C	8:T:86:ASP:N	2.61	0.52
11:W:55:LYS:HB2	11:W:81:TYR:CD1	2.45	0.52
1:A:317:LYS:O	1:A:318:SER:HB3	2.10	0.52
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.90	0.52
1:A:1313:LEU:C	1:A:1315:GLU:H	2.17	0.52
2:B:398:ARG:HH11	2:B:398:ARG:HB3	1.74	0.52
2:B:486:TYR:CD2	2:B:486:TYR:N	2.76	0.52
2:B:758:PHE:CE1	2:B:1027:ILE:CG2	2.93	0.52
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.43	0.52
2:B:839:MET:HE1	2:B:980:PHE:CB	2.37	0.52
2:B:1084:GLN:NE2	2:B:1084:GLN:H	2.07	0.52
3:C:196:ASP:CG	3:C:199:LYS:HD3	2.35	0.52
9:I:50:THR:HG22	9:I:52:ILE:N	2.24	0.52
1:M:57:ARG:O	1:M:68:GLN:HG2	2.09	0.52
1:M:72:GLU:HB3	1:M:76:GLU:HG2	1.91	0.52
1:M:447:GLN:HA	1:M:448:PRO:C	2.33	0.52
1:M:503:GLN:NE2	6:R:90:ARG:NH2	2.53	0.52
1:M:710:LEU:HD12	1:M:710:LEU:N	2.21	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:820:GLY:O	1:M:822:GLU:N	2.43	0.52
2:N:102:VAL:CG2	2:N:112:LEU:HD13	2.39	0.52
2:N:273:LEU:CD2	2:N:360:PHE:HD1	2.22	0.52
2:N:579:ARG:HG2	2:N:579:ARG:NH1	2.23	0.52
2:N:1177:HIS:CB	2:N:1179:GLN:NE2	2.73	0.52
6:R:82:THR:HG22	6:R:84:TYR:N	2.15	0.52
7:S:49:LEU:HD11	7:S:77:VAL:HG23	1.91	0.52
9:U:19:ASP:CB	9:U:24:ARG:HG2	2.38	0.52
13:4:16:DT:H5'	13:4:16:DT:C6	2.37	0.52
15:6:5:C:H2'	15:6:6:A:H8	1.75	0.52
1:A:34:LYS:HZ2	1:A:57:ARG:HH22	1.58	0.52
1:A:41:MET:O	1:A:50:ILE:HG13	2.10	0.52
1:A:265:LYS:HA	1:A:265:LYS:CE	2.39	0.52
1:A:399:HIS:CB	1:A:400:PRO:CD	2.87	0.52
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.91	0.52
1:A:1120:LEU:CD2	1:A:1125:ALA:HA	2.40	0.52
1:A:1225:PHE:HE2	1:A:1227:ILE:HD11	1.73	0.52
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.25	0.52
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.90	0.52
2:B:601:ARG:HD3	2:B:605:ARG:CZ	2.40	0.52
2:B:617:ARG:HH22	9:I:61:ASP:CG	2.18	0.52
2:B:801:LYS:O	10:J:52:THR:CG2	2.58	0.52
4:D:120:GLU:OE1	4:D:120:GLU:O	2.27	0.52
6:F:97:ARG:HD3	6:F:130:ILE:HG23	1.92	0.52
13:1:23:BRU:H6	13:1:23:BRU:C5'	2.35	0.52
1:M:107:CYS:HB2	1:M:114:LEU:HD21	1.92	0.52
1:M:117:GLU:HA	1:M:123:ARG:HG3	1.90	0.52
1:M:682:THR:HG23	1:M:728:LYS:HE3	1.90	0.52
1:M:1149:ALA:CB	9:U:47:GLU:HA	2.40	0.52
1:M:1237:ILE:HG22	1:M:1238:ILE:N	2.23	0.52
1:M:1389:PHE:C	1:M:1391:ARG:H	2.18	0.52
1:M:1437:GLY:O	1:M:1439:GLY:N	2.43	0.52
2:N:277:LYS:HE2	2:N:336:ARG:C	2.35	0.52
2:N:466:TRP:CE3	2:N:466:TRP:HA	2.44	0.52
3:O:35:ARG:NH1	11:W:41:THR:OG1	2.43	0.52
4:P:5:THR:HG23	4:P:5:THR:O	2.09	0.52
4:P:32:GLU:O	7:S:5:LYS:NZ	2.30	0.52
4:P:193:THR:CG2	4:P:194:LEU:N	2.72	0.52
5:Q:60:PHE:CD1	5:Q:60:PHE:C	2.87	0.52
5:Q:112:TYR:CE1	5:Q:136:ASN:HA	2.45	0.52
5:Q:195:VAL:HG22	5:Q:213:ILE:HG13	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:139:ILE:HG12	7:S:140:LYS:CG	2.40	0.52
8:T:4:THR:HG22	8:T:6:PHE:H	1.74	0.52
2:B:98:THR:O	2:B:126:SER:HB2	2.09	0.52
2:B:126:SER:HB3	2:B:172:ILE:HD11	1.92	0.52
2:B:638:PHE:CD2	2:B:690:VAL:HG12	2.44	0.52
2:B:707:PRO:HG2	2:B:708:GLU:N	2.23	0.52
2:B:807:ARG:NH1	2:B:807:ARG:HB3	2.24	0.52
2:B:911:ILE:HG22	2:B:966:VAL:HG21	1.90	0.52
3:C:66:ARG:CZ	10:J:2:ILE:HG21	2.40	0.52
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.92	0.52
6:F:101:ILE:HD13	6:F:120:ILE:HG22	1.90	0.52
7:G:153:GLN:HG2	7:G:154:VAL:HG23	1.92	0.52
8:H:11:GLN:O	8:H:28:ALA:HB1	2.10	0.52
8:H:44:VAL:CG1	8:H:48:PRO:HA	2.40	0.52
8:H:59:ILE:O	8:H:60:ALA:HB3	2.10	0.52
13:1:23:BRU:H2''	13:1:24:DG:O5'	2.09	0.52
1:M:69:THR:C	1:M:71:GLN:N	2.67	0.52
1:M:148:CYS:HB3	1:M:167:CYS:O	2.09	0.52
1:M:1299:VAL:HG12	1:M:1300:LYS:N	2.25	0.52
2:N:707:PRO:O	2:N:708:GLU:O	2.27	0.52
3:O:112:ASN:HB3	3:O:114:TYR:CE1	2.45	0.52
4:P:185:CYS:SG	4:P:191:ALA:HA	2.50	0.52
4:P:187:THR:C	4:P:189:ASP:N	2.66	0.52
8:T:11:GLN:O	8:T:28:ALA:HB1	2.09	0.52
8:T:26:ILE:HD12	8:T:42:ILE:HD13	1.92	0.52
9:U:17:ARG:HG2	9:U:28:GLU:HG2	1.92	0.52
9:U:111:THR:CG2	9:U:113:ASP:HB2	2.39	0.52
10:V:30:LEU:HD22	10:V:34:THR:HB	1.92	0.52
1:A:390:GLN:O	1:A:394:ASN:HB2	2.10	0.52
1:A:826:ASP:O	1:A:830:LYS:HB2	2.09	0.52
1:A:898:ARG:HD2	1:A:899:VAL:N	2.24	0.52
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.40	0.52
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.44	0.52
2:B:43:LEU:N	2:B:43:LEU:HD23	2.25	0.52
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.18	0.52
2:B:345:LYS:CG	2:B:346:GLU:N	2.72	0.52
2:B:1115:THR:HG22	2:B:1117:GLN:CB	2.40	0.52
3:C:220:ASP:OD2	3:C:223:ALA:HB2	2.10	0.52
9:I:15:TYR:N	9:I:15:TYR:CD1	2.76	0.52
13:1:16:DT:H5'	13:1:16:DT:C6	2.37	0.52
1:M:222:LEU:O	1:M:224:PHE:HD1	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:754:SER:N	1:M:757:ASN:HD22	1.98	0.52
2:N:653:VAL:HG23	2:N:689:LEU:HB3	1.92	0.52
4:P:191:ALA:C	4:P:193:THR:H	2.18	0.52
1:A:108:MET:CA	1:A:210:ILE:HD13	2.28	0.51
1:A:157:ASP:C	1:A:159:THR:H	2.18	0.51
1:A:709:THR:CG2	1:A:710:LEU:N	2.73	0.51
2:B:102:VAL:CG2	2:B:112:LEU:HD13	2.40	0.51
2:B:604:ARG:HH21	2:B:614:SER:HA	1.75	0.51
2:B:642:ASP:CA	2:B:649:LYS:HA	2.38	0.51
2:B:954:VAL:O	12:L:55:ILE:O	2.27	0.51
3:C:73:GLN:HE21	3:C:75:MET:N	2.03	0.51
4:D:29:LEU:N	4:D:29:LEU:CD2	2.73	0.51
4:D:33:PHE:CE1	7:G:80:LYS:HD3	2.46	0.51
5:E:191:LYS:O	5:E:192:ARG:C	2.52	0.51
8:H:4:THR:HG22	8:H:6:PHE:H	1.73	0.51
1:M:962:ARG:C	1:M:964:ILE:N	2.68	0.51
2:N:120:ARG:NH1	12:X:54:ARG:HD2	2.24	0.51
2:N:390:LEU:O	2:N:392:ARG:HG3	2.10	0.51
2:N:557:PHE:CZ	2:N:603:LEU:HD11	2.45	0.51
2:N:601:ARG:O	2:N:605:ARG:HG3	2.11	0.51
2:N:837:ASP:OD2	2:N:1020:ARG:NH2	2.44	0.51
2:N:1063:GLY:O	3:O:202:PRO:HG2	2.09	0.51
4:P:29:LEU:N	4:P:29:LEU:CD2	2.73	0.51
4:P:118:THR:HG21	4:P:121:LYS:CD	2.40	0.51
5:Q:42:PHE:CE1	5:Q:58:MET:HE3	2.44	0.51
8:T:84:ALA:CA	8:T:87:ARG:HB2	2.39	0.51
8:T:99:GLY:CA	8:T:118:PHE:HD2	2.23	0.51
10:V:2:ILE:HG12	10:V:57:ILE:HD13	1.91	0.51
1:A:313:GLN:O	1:A:315:LEU:HD23	2.09	0.51
1:A:756:ILE:O	1:A:759:ALA:HB3	2.10	0.51
1:A:899:VAL:CG2	1:A:908:LEU:HD21	2.40	0.51
2:B:69:LEU:HB3	2:B:429:PHE:HE1	1.73	0.51
2:B:299:GLU:OE2	2:B:571:PRO:HG2	2.10	0.51
2:B:546:SER:OG	2:B:631:GLY:N	2.43	0.51
2:B:824:ILE:CG1	10:J:48:ARG:HH12	2.15	0.51
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.92	0.51
3:C:184:ASN:OD1	3:C:187:LYS:CA	2.58	0.51
5:E:124:VAL:HB	5:E:125:PRO:CD	2.40	0.51
6:F:109:VAL:HG13	6:F:127:GLU:OE1	2.09	0.51
9:I:82:GLU:OE2	9:I:104:LEU:HB2	2.10	0.51
1:M:38:PRO:CA	1:M:270:LEU:HD23	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:761:MET:HA	1:M:804:TYR:HB2	1.93	0.51
1:M:1120:LEU:CD2	1:M:1125:ALA:HA	2.40	0.51
2:N:473:MET:HE3	2:N:474:SER:N	2.24	0.51
2:N:916:THR:HB	2:N:935:ARG:HG3	1.92	0.51
3:O:212:PRO:HB3	3:O:213:PRO:HD2	1.92	0.51
4:P:202:ILE:HG23	4:P:202:ILE:O	2.09	0.51
4:P:214:LEU:O	4:P:218:GLU:HB2	2.11	0.51
5:Q:61:GLN:HG2	5:Q:62:ALA:N	2.24	0.51
5:Q:74:ASP:OD1	5:Q:74:ASP:N	2.43	0.51
7:S:91:VAL:CG1	7:S:92:VAL:N	2.72	0.51
13:4:23:BRU:H6	13:4:23:BRU:C5'	2.35	0.51
1:A:1241:ARG:O	1:A:1242:VAL:HB	2.09	0.51
1:A:1317:MET:O	1:A:1322:ILE:HD11	2.10	0.51
2:B:370:PHE:CD2	2:B:373:ARG:CD	2.93	0.51
2:B:604:ARG:C	2:B:606:LYS:H	2.18	0.51
2:B:878:GLN:CB	2:B:879:ARG:HH11	2.23	0.51
3:C:242:GLN:C	3:C:244:VAL:H	2.17	0.51
4:D:20:GLU:O	4:D:20:GLU:HG2	2.11	0.51
6:F:97:ARG:HH21	6:F:108:PHE:HE1	1.54	0.51
6:F:103:MET:O	6:F:104:ASN:HB2	2.10	0.51
7:G:106:MET:CG	7:G:107:LYS:N	2.72	0.51
8:H:30:SER:CB	8:H:36:CYS:HB3	2.41	0.51
8:H:130:ARG:HA	8:H:133:ASN:HB2	1.93	0.51
1:M:313:GLN:O	1:M:315:LEU:HD23	2.11	0.51
1:M:463:ILE:HD12	1:M:469:ARG:HD2	1.91	0.51
1:M:720:ARG:O	1:M:724:GLU:HB3	2.11	0.51
1:M:1325:THR:HG22	1:M:1326:ARG:HG3	1.91	0.51
2:N:235:SER:C	2:N:236:HIS:CD2	2.88	0.51
2:N:345:LYS:HG3	2:N:346:GLU:H	1.75	0.51
2:N:806:THR:HG21	2:N:808:ALA:HB3	1.92	0.51
3:O:186:LEU:CD2	3:O:225:ALA:HB2	2.41	0.51
4:P:194:LEU:C	4:P:195:ILE:HG13	2.34	0.51
5:Q:56:LYS:NZ	5:Q:84:ASP:N	2.58	0.51
6:R:75:PRO:HG3	6:R:78:GLN:OE1	2.10	0.51
8:T:59:ILE:O	8:T:60:ALA:HB3	2.10	0.51
8:T:89:LEU:O	8:T:91:ASP:N	2.43	0.51
12:X:47:ARG:CD	12:X:52:GLY:HA2	2.40	0.51
14:5:5:DC:H2'	14:5:6:DT:H72	1.91	0.51
1:A:153:PRO:HB3	1:A:161:LEU:HD22	1.91	0.51
1:A:347:PHE:HE2	1:A:375:THR:CG2	2.23	0.51
1:A:833:GLU:OE2	1:A:1102:LYS:HE3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1170:ILE:HG22	1:A:1174:PHE:HE1	1.75	0.51
1:A:1193:LEU:HD12	1:A:1193:LEU:C	2.35	0.51
2:B:63:ILE:HD12	2:B:421:PHE:CE2	2.46	0.51
2:B:273:LEU:O	2:B:276:ILE:HB	2.10	0.51
2:B:515:HIS:CD2	2:B:517:THR:HG23	2.46	0.51
2:B:603:LEU:HB3	2:B:609:ILE:HD11	1.92	0.51
2:B:984:HIS:NE2	2:B:1025:HIS:HA	2.25	0.51
3:C:10:ILE:HG22	3:C:11:ARG:O	2.10	0.51
3:C:252:GLN:HG3	11:K:95:ILE:HG23	1.93	0.51
1:M:106:VAL:HG21	1:M:214:ILE:CD1	2.40	0.51
1:M:567:LYS:CG	1:M:568:PRO:CD	2.85	0.51
1:M:740:LEU:HD12	1:M:741:ASN:N	2.25	0.51
1:M:963:ILE:HD11	1:M:1048:ASN:CB	2.40	0.51
2:N:258:LEU:HG	2:N:258:LEU:O	2.09	0.51
2:N:273:LEU:HD22	2:N:360:PHE:HD1	1.76	0.51
2:N:371:GLU:H	2:N:371:GLU:CD	2.18	0.51
2:N:549:THR:HG22	2:N:550:ASP:H	1.71	0.51
2:N:1167:GLY:HA3	2:N:1216:LEU:N	2.25	0.51
5:Q:161:LYS:HD2	5:Q:195:VAL:HG23	1.92	0.51
9:U:34:TYR:HE2	9:U:36:GLU:HB3	1.75	0.51
9:U:58:VAL:HG13	9:U:62:ILE:HD13	1.91	0.51
9:U:84:VAL:HG12	9:U:104:LEU:HD21	1.93	0.51
10:V:54:VAL:O	10:V:56:LEU:N	2.42	0.51
11:W:49:GLU:HG3	11:W:94:ILE:CG1	2.40	0.51
12:X:28:LYS:HE3	12:X:39:SER:OG	2.10	0.51
1:A:53:LEU:O	1:A:54:ASN:C	2.52	0.51
1:A:69:THR:HG21	2:B:1174:LYS:HZ3	1.75	0.51
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.93	0.51
2:B:37:PHE:HE1	2:B:41:LYS:HD3	1.75	0.51
2:B:558:LEU:O	2:B:561:TRP:N	2.44	0.51
2:B:879:ARG:NE	2:B:879:ARG:N	2.56	0.51
3:C:263:THR:O	3:C:266:ASP:HB2	2.10	0.51
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.93	0.51
11:K:47:ARG:HD3	11:K:59:ALA:O	2.11	0.51
1:M:857:ARG:HD3	1:M:861:GLY:O	2.11	0.51
1:M:901:LEU:HB2	1:M:926:GLN:HG2	1.91	0.51
1:M:1148:ILE:O	1:M:1149:ALA:HB2	2.10	0.51
1:M:1193:LEU:HD12	1:M:1194:ARG:N	2.26	0.51
1:M:1203:ASN:O	1:M:1204:ASP:C	2.53	0.51
2:N:345:LYS:HG2	2:N:346:GLU:H	1.73	0.51
2:N:594:ALA:N	2:N:617:ARG:HH12	2.08	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:83:CYS:SG	5:Q:85:GLU:HB2	2.51	0.51
5:Q:112:TYR:CD1	5:Q:112:TYR:C	2.89	0.51
8:T:18:GLY:O	8:T:19:ARG:HB2	2.11	0.51
10:V:25:LEU:O	10:V:29:GLU:HA	2.11	0.51
1:A:341:MET:HE2	1:A:843:LYS:NZ	2.26	0.51
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	1.92	0.51
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.91	0.51
2:B:37:PHE:HE1	2:B:41:LYS:CD	2.24	0.51
2:B:999:MET:HB3	2:B:1007:VAL:HG21	1.92	0.51
5:E:94:LYS:O	5:E:98:ILE:HG13	2.10	0.51
7:G:97:HIS:HE1	7:S:93:SER:HB2	1.75	0.51
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.41	0.51
8:H:89:LEU:O	8:H:91:ASP:N	2.43	0.51
10:J:54:VAL:O	10:J:56:LEU:N	2.42	0.51
1:M:157:ASP:C	1:M:159:THR:H	2.19	0.51
1:M:298:PHE:CZ	1:M:314:ALA:HB2	2.46	0.51
1:M:325:ILE:CG2	2:N:1210:MET:HE2	2.40	0.51
1:M:597:LEU:N	1:M:597:LEU:HD12	2.25	0.51
2:N:121:ASN:HD22	2:N:207:GLY:HA3	1.75	0.51
2:N:1037:LEU:HD21	2:N:1064:TYR:CE1	2.43	0.51
3:O:248:ILE:CD1	11:W:101:LEU:HD22	2.39	0.51
10:V:30:LEU:HD11	10:V:38:ARG:HH11	1.76	0.51
11:W:107:THR:O	11:W:111:LEU:HG	2.11	0.51
13:4:23:BRU:H2''	13:4:24:DG:O5'	2.10	0.51
1:A:49:LYS:HE2	1:A:61:ILE:CD1	2.38	0.51
1:A:224:PHE:HD2	1:A:229:SER:O	1.93	0.51
1:A:277:GLU:HG2	4:P:209:ARG:HH21	1.75	0.51
1:A:537:ARG:HD2	8:H:20:TYR:HE1	1.72	0.51
1:A:860:LEU:HD11	1:A:1393:ASN:HB2	1.92	0.51
1:A:1148:ILE:O	1:A:1149:ALA:HB2	2.10	0.51
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.76	0.51
2:B:259:TYR:HD1	2:B:259:TYR:H	1.59	0.51
2:B:276:ILE:HA	2:B:336:ARG:O	2.10	0.51
2:B:792:MET:HG2	2:B:855:PHE:HE1	1.76	0.51
4:D:130:LEU:O	4:D:132:GLN:N	2.41	0.51
5:E:32:GLN:HG3	5:E:36:GLU:OE2	2.11	0.51
1:M:67:CYS:O	1:M:70:CYS:HB3	2.11	0.51
1:M:67:CYS:O	1:M:68:GLN:C	2.51	0.51
1:M:154:SER:HB3	1:M:162:VAL:HG21	1.91	0.51
1:M:224:PHE:HD2	1:M:229:SER:O	1.94	0.51
1:M:253:ASN:HB2	2:N:884:ARG:NH1	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:915:SER:O	1:M:919:ILE:HB	2.11	0.51
1:M:1433:MET:CE	7:S:63:PRO:HB2	2.41	0.51
2:N:204:ILE:O	2:N:204:ILE:HG22	2.11	0.51
2:N:211:VAL:HG13	2:N:495:LEU:HD23	1.92	0.51
2:N:906:SER:N	2:N:909:ASP:OD2	2.43	0.51
3:O:39:ALA:HA	3:O:164:ALA:CB	2.39	0.51
7:S:91:VAL:HG12	7:S:92:VAL:N	2.24	0.51
7:S:109:PHE:O	7:S:160:ILE:HA	2.11	0.51
9:U:15:TYR:N	9:U:15:TYR:CD1	2.79	0.51
9:U:101:PHE:N	9:U:101:PHE:CD1	2.78	0.51
12:X:26:THR:HG23	12:X:62:LYS:NZ	2.26	0.51
1:A:222:LEU:O	1:A:224:PHE:HD1	1.94	0.51
1:A:541:ILE:CD1	1:A:549:MET:HE1	2.30	0.51
1:A:600:PRO:HA	8:H:25:ARG:NH1	2.25	0.51
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.43	0.51
2:B:422:LYS:HA	2:B:425:THR:HB	1.91	0.51
2:B:750:GLY:O	2:B:751:VAL:C	2.54	0.51
2:B:955:THR:CG2	2:B:956:THR:H	2.22	0.51
3:C:252:GLN:HE21	11:K:95:ILE:HG23	1.75	0.51
9:I:78:CYS:SG	9:I:105:SER:O	2.69	0.51
10:J:42:LYS:HD3	10:J:43:ARG:HD3	1.92	0.51
1:M:50:ILE:O	1:M:52:GLY:N	2.43	0.51
1:M:132:LYS:HE3	1:M:1411:GLU:HG3	1.93	0.51
1:M:399:HIS:CB	1:M:400:PRO:CD	2.88	0.51
1:M:856:THR:HB	1:M:865:GLN:HB2	1.92	0.51
1:M:886:ILE:CG2	1:M:887:GLY:N	2.74	0.51
2:N:390:LEU:O	2:N:391:ASP:C	2.54	0.51
2:N:918:ILE:HG21	2:N:935:ARG:NH2	2.25	0.51
2:N:1115:THR:HG22	2:N:1117:GLN:CG	2.40	0.51
4:P:118:THR:HG21	4:P:121:LYS:CE	2.40	0.51
6:R:138:LEU:HB3	6:R:139:PRO:HD2	1.91	0.51
7:S:138:THR:CG2	7:S:139:ILE:N	2.73	0.51
8:T:62:SER:OG	8:T:63:LEU:N	2.44	0.51
10:V:64:ASN:CB	10:V:65:PRO:HD3	2.36	0.51
11:W:50:LEU:HD11	11:W:75:ILE:HD13	1.93	0.51
1:A:549:MET:SD	1:A:577:ILE:CD1	2.99	0.51
1:A:598:LEU:HD23	8:H:25:ARG:NH2	2.26	0.51
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.46	0.51
1:A:1445:ILE:HD11	7:G:68:ALA:HB1	1.92	0.51
2:B:273:LEU:HB3	2:B:276:ILE:HD12	1.91	0.51
2:B:390:LEU:O	2:B:391:ASP:C	2.54	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:616:ILE:HD12	2:B:616:ILE:H	1.74	0.51
2:B:781:PHE:HE2	2:B:795:ILE:HD11	1.76	0.51
4:D:51:ASN:O	4:D:52:LEU:O	2.29	0.51
5:E:98:ILE:O	5:E:102:GLU:HG3	2.11	0.51
9:I:109:ILE:HG22	9:I:109:ILE:O	2.09	0.51
11:K:108:GLU:O	11:K:112:GLN:HG2	2.11	0.51
1:M:335:ARG:NH1	2:N:1206:GLU:OE1	2.44	0.51
1:M:1255:GLU:O	1:M:1255:GLU:CG	2.58	0.51
2:N:579:ARG:NH1	2:N:622:LYS:O	2.44	0.51
2:N:599:THR:HG22	2:N:600:LEU:N	2.25	0.51
3:O:22:LEU:HD22	3:O:230:MET:HE1	1.91	0.51
9:U:116:ASN:C	9:U:117:LYS:HD2	2.36	0.51
11:W:53:ASP:HB3	11:W:56:VAL:HG23	1.92	0.51
1:A:13:THR:HB	1:A:1432:GLN:NE2	2.26	0.51
1:A:56:PRO:O	1:A:57:ARG:CG	2.59	0.51
1:A:236:LEU:HD11	1:A:304:MET:HE1	1.92	0.51
1:A:493:GLN:HE21	1:A:493:GLN:CA	2.23	0.51
1:A:598:LEU:HD11	8:H:124:ARG:HB2	1.93	0.51
1:A:866:PHE:O	1:A:867:ILE:HD12	2.10	0.51
1:A:962:ARG:C	1:A:964:ILE:N	2.69	0.51
2:B:637:LEU:CD2	2:B:742:GLU:HA	2.41	0.51
2:B:839:MET:HE2	2:B:980:PHE:CD1	2.45	0.51
3:C:11:ARG:NH2	3:C:206:ASN:OD1	2.44	0.51
6:F:111:LEU:C	6:F:113:GLY:N	2.64	0.51
6:F:116:ASP:C	6:F:116:ASP:OD1	2.54	0.51
7:G:111:THR:CG2	7:G:114:LEU:HD22	2.40	0.51
8:H:84:ALA:C	8:H:86:ASP:N	2.63	0.51
8:H:95:TYR:HE2	8:H:97:MET:SD	2.34	0.51
11:K:22:ASP:C	11:K:31:VAL:HG13	2.36	0.51
1:M:114:LEU:HD21	1:M:171:GLN:HE21	1.75	0.51
1:M:200:ARG:HG2	1:M:200:ARG:HH11	1.75	0.51
1:M:443:LEU:HD12	2:N:1146:PHE:CE2	2.46	0.51
1:M:868:TYR:OH	1:M:1366:ARG:HD3	2.11	0.51
1:M:960:ILE:HA	1:M:963:ILE:CG2	2.41	0.51
1:M:967:ALA:O	1:M:971:PHE:HD1	1.92	0.51
2:N:96:TYR:HE1	2:N:131:ASP:OD1	1.94	0.51
2:N:165:VAL:HG11	2:N:448:ILE:CD1	2.41	0.51
2:N:237:VAL:HG22	2:N:257:LYS:HA	1.93	0.51
2:N:807:ARG:HB3	2:N:807:ARG:NH1	2.26	0.51
2:N:840:ILE:CG2	2:N:994:TYR:HD1	2.24	0.51
2:N:1068:GLY:O	2:N:1069:PHE:C	2.54	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:229:TYR:CD1	3:O:229:TYR:N	2.78	0.51
3:O:238:ILE:CG2	3:O:243:VAL:HG23	2.37	0.51
3:O:252:GLN:HE21	11:W:95:ILE:CG2	2.23	0.51
6:R:127:GLU:O	6:R:129:LYS:HG3	2.11	0.51
8:T:42:ILE:HG23	8:T:95:TYR:HE1	1.76	0.51
8:T:63:LEU:HD11	8:T:141:TYR:CD2	2.46	0.51
10:V:36:LEU:HD12	10:V:47:ARG:NH1	2.26	0.51
12:X:65:VAL:HG23	12:X:67:PHE:HE1	1.76	0.51
1:A:50:ILE:O	1:A:52:GLY:N	2.43	0.50
1:A:288:ALA:CA	1:A:291:GLU:HG3	2.40	0.50
1:A:562:THR:HB	8:H:98:TYR:CD2	2.46	0.50
1:A:694:THR:O	1:A:698:GLN:HG3	2.11	0.50
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.92	0.50
2:B:483:LEU:HD11	2:B:491:THR:CG2	2.40	0.50
3:C:177:GLU:HG3	3:C:231:ASN:CB	2.24	0.50
4:D:35:LEU:HA	4:D:47:LEU:HB2	1.93	0.50
7:G:126:ASN:HA	7:G:127:PRO:C	2.36	0.50
11:K:22:ASP:O	11:K:31:VAL:HG13	2.10	0.50
1:M:560:ILE:HD11	11:W:58:PHE:HD1	1.75	0.50
1:M:898:ARG:O	1:M:1029:ARG:NH1	2.44	0.50
1:M:1138:ILE:HG21	1:M:1316:VAL:HG13	1.92	0.50
2:N:33:VAL:HG21	2:N:638:PHE:HZ	1.76	0.50
2:N:638:PHE:CD2	2:N:690:VAL:HG12	2.46	0.50
2:N:654:ARG:O	2:N:657:HIS:N	2.44	0.50
2:N:791:THR:O	2:N:792:MET:HB2	2.10	0.50
2:N:847:ASP:HB3	3:O:167:HIS:CD2	2.45	0.50
2:N:1037:LEU:CD2	2:N:1064:TYR:HE1	2.23	0.50
2:N:1183:LYS:HE3	2:N:1183:LYS:O	2.12	0.50
4:P:20:GLU:HG2	4:P:20:GLU:O	2.11	0.50
4:P:155:ARG:NH2	4:P:221:TYR:CD1	2.76	0.50
7:S:139:ILE:HD11	7:S:140:LYS:HE3	1.94	0.50
10:V:44:TYR:H	10:V:44:TYR:HD2	1.54	0.50
12:X:59:ALA:O	12:X:60:ARG:O	2.30	0.50
1:A:283:GLY:O	1:A:285:PRO:CD	2.59	0.50
1:A:503:GLN:NE2	6:F:90:ARG:NH2	2.53	0.50
1:A:729:ALA:O	1:A:732:LEU:HB2	2.11	0.50
1:A:1168:GLU:O	1:A:1171:GLN:OE1	2.28	0.50
1:A:1236:LEU:C	1:A:1237:ILE:HD12	2.36	0.50
2:B:707:PRO:O	2:B:708:GLU:O	2.29	0.50
2:B:847:ASP:C	2:B:849:GLY:N	2.64	0.50
4:D:13:ARG:C	4:D:15:LEU:N	2.69	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:74:TYR:H	7:G:74:TYR:HD2	1.59	0.50
7:G:83:LYS:HG3	7:G:148:GLU:O	2.12	0.50
14:2:5:DC:H2'	14:2:6:DT:H72	1.92	0.50
1:M:162:VAL:HG12	1:M:163:SER:N	2.26	0.50
1:M:195:ASP:O	1:M:196:GLU:HB3	2.11	0.50
1:M:207:ILE:HG22	1:M:211:PHE:CE2	2.46	0.50
1:M:322:VAL:O	1:M:322:VAL:CG1	2.59	0.50
1:M:401:GLY:C	1:M:435:HIS:CD2	2.89	0.50
1:M:456:MET:HE3	1:M:478:TYR:CZ	2.46	0.50
1:M:826:ASP:O	1:M:830:LYS:HB2	2.11	0.50
1:M:909:ASP:OD1	1:M:911:SER:N	2.36	0.50
1:M:964:ILE:O	1:M:967:ALA:HB3	2.11	0.50
1:M:1339:LEU:HD13	5:Q:147:HIS:CD2	2.47	0.50
2:N:31:TRP:CD1	2:N:807:ARG:NH2	2.79	0.50
2:N:37:PHE:HE2	2:N:542:MET:HA	1.75	0.50
2:N:90:ILE:HD12	2:N:432:MET:SD	2.51	0.50
2:N:305:VAL:O	2:N:305:VAL:HG12	2.11	0.50
2:N:345:LYS:HG2	2:N:346:GLU:N	2.26	0.50
2:N:429:PHE:CA	2:N:432:MET:HE3	2.31	0.50
2:N:758:PHE:HE1	2:N:1027:ILE:HG22	1.76	0.50
3:O:123:ASN:HD22	3:O:125:MET:HG2	1.72	0.50
3:O:235:VAL:HG11	10:V:6:ARG:NH2	2.26	0.50
4:P:217:LEU:O	4:P:219:THR:N	2.43	0.50
5:Q:2:ASP:O	5:Q:3:GLN:HG2	2.10	0.50
5:Q:96:PHE:CE1	5:Q:100:ILE:HD11	2.46	0.50
8:T:84:ALA:HA	8:T:87:ARG:CG	2.41	0.50
9:U:78:CYS:SG	9:U:105:SER:O	2.69	0.50
1:A:101:LYS:HE2	1:A:139:TRP:CZ2	2.46	0.50
1:A:162:VAL:HG12	1:A:163:SER:H	1.76	0.50
1:A:595:THR:O	1:A:596:THR:CG2	2.59	0.50
1:A:701:LEU:HD21	9:I:114:GLN:HB2	1.94	0.50
1:A:786:HIS:N	1:A:786:HIS:CD2	2.79	0.50
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.94	0.50
2:B:368:GLU:O	2:B:370:PHE:N	2.43	0.50
2:B:696:GLU:O	2:B:699:GLU:HB2	2.11	0.50
3:C:243:VAL:O	3:C:243:VAL:CG1	2.59	0.50
4:D:51:ASN:C	4:D:52:LEU:O	2.51	0.50
4:D:203:SER:OG	4:D:206:GLU:HB2	2.11	0.50
1:M:49:LYS:HD2	1:M:55:ASP:HB3	1.91	0.50
1:M:53:LEU:O	1:M:54:ASN:C	2.53	0.50
1:M:1148:ILE:CG1	1:M:1198:ASP:HB2	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:298:LEU:HD22	2:N:298:LEU:N	2.27	0.50
3:O:22:LEU:HD22	3:O:230:MET:CE	2.41	0.50
5:Q:135:PHE:HD2	5:Q:140:LEU:HD21	1.76	0.50
5:Q:182:ASP:HB3	5:Q:185:ALA:HB2	1.93	0.50
7:S:1:MET:CE	7:S:2:PHE:HA	2.41	0.50
9:U:61:ASP:O	9:U:63:GLY:N	2.45	0.50
11:W:64:GLU:HA	11:W:64:GLU:OE2	2.11	0.50
1:A:64:ASN:O	1:A:66:LYS:N	2.44	0.50
1:A:427:GLN:HB2	1:A:430:TRP:CG	2.47	0.50
1:A:705:LYS:CB	1:A:708:MET:HE3	2.37	0.50
1:A:1206:ASP:O	1:A:1274:ARG:NH2	2.44	0.50
2:B:39:ARG:HH21	2:B:665:GLU:CG	2.24	0.50
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.47	0.50
2:B:431:TYR:CD1	2:B:447:ALA:HB2	2.47	0.50
2:B:563:MET:HE2	2:B:587:HIS:O	2.11	0.50
3:C:118:LEU:HB2	3:C:132:PRO:HG2	1.94	0.50
4:D:56:ARG:NH2	4:D:155:ARG:HA	2.26	0.50
4:D:162:ALA:HA	4:D:165:GLN:NE2	2.27	0.50
1:M:1036:ARG:NH1	1:M:1036:ARG:CG	2.69	0.50
1:M:1410:PHE:HD2	2:N:1212:ILE:CD1	2.24	0.50
2:N:259:TYR:H	2:N:259:TYR:HD1	1.60	0.50
2:N:272:THR:HG23	2:N:279:ASP:OD1	2.12	0.50
2:N:797:TYR:HE1	2:N:854:LEU:CD2	2.25	0.50
2:N:863:GLU:OE1	2:N:962:LYS:HB2	2.11	0.50
4:P:167:LEU:O	4:P:170:THR:HG23	2.12	0.50
7:S:92:VAL:HG21	7:S:102:GLN:HB2	1.93	0.50
12:X:36:SER:O	12:X:37:LYS:C	2.54	0.50
1:A:493:GLN:CA	1:A:493:GLN:NE2	2.73	0.50
1:A:596:THR:C	1:A:597:LEU:HD12	2.36	0.50
1:A:693:VAL:HG21	1:A:721:PHE:CE1	2.42	0.50
1:A:1124:HIS:HB2	1:A:1130:GLN:HG2	1.94	0.50
2:B:185:THR:O	2:B:188:ASP:HB2	2.11	0.50
2:B:622:LYS:CE	9:I:59:VAL:HG13	2.41	0.50
2:B:798:TYR:CE2	3:C:62:PHE:CZ	3.00	0.50
5:E:13:TRP:O	5:E:16:PHE:HB3	2.11	0.50
5:E:171:LYS:HG2	5:E:174:GLN:OE1	2.10	0.50
7:G:81:PRO:HD2	7:G:157:ILE:HD12	1.93	0.50
9:I:61:ASP:O	9:I:63:GLY:N	2.45	0.50
1:M:200:ARG:HG2	1:M:200:ARG:NH1	2.26	0.50
1:M:218:ASP:O	1:M:219:PHE:C	2.55	0.50
1:M:285:PRO:O	1:M:287:HIS:N	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:535:THR:HG21	1:M:616:VAL:CA	2.38	0.50
1:M:789:LYS:HD2	2:N:620:ARG:HH12	1.75	0.50
1:M:795:GLU:H	1:M:795:GLU:CD	2.19	0.50
1:M:1110:ASN:N	1:M:1110:ASN:ND2	2.49	0.50
1:M:1237:ILE:CG2	1:M:1238:ILE:N	2.74	0.50
1:M:1280:GLU:O	1:M:1281:ARG:C	2.54	0.50
2:N:63:ILE:HD12	2:N:421:PHE:CZ	2.47	0.50
2:N:209:GLU:OE2	2:N:485:ARG:NE	2.36	0.50
2:N:984:HIS:CD2	2:N:1025:HIS:HA	2.47	0.50
3:O:70:ILE:HG12	3:O:142:VAL:HG11	1.93	0.50
3:O:101:LEU:O	3:O:102:GLN:HG2	2.12	0.50
3:O:177:GLU:HG3	3:O:231:ASN:CB	2.30	0.50
3:O:209:TYR:HD1	3:O:209:TYR:H	1.58	0.50
5:Q:180:ARG:NH2	5:Q:192:ARG:HD2	2.27	0.50
1:A:72:GLU:HB3	1:A:76:GLU:HG2	1.92	0.50
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.94	0.50
1:A:1015:VAL:HG12	1:A:1015:VAL:O	2.11	0.50
1:A:1317:MET:HE1	1:A:1339:LEU:HD21	1.92	0.50
2:B:361:LEU:HD11	2:B:381:MET:HE1	1.93	0.50
2:B:611:PRO:O	2:B:692:TYR:HB2	2.12	0.50
2:B:773:MET:C	2:B:775:LYS:N	2.69	0.50
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.46	0.50
3:C:147:LEU:HD12	3:C:151:GLN:O	2.11	0.50
3:C:186:LEU:CD2	3:C:225:ALA:HB2	2.41	0.50
4:D:23:ASN:HA	4:D:28:GLN:O	2.12	0.50
4:D:51:ASN:HB3	4:D:178:ALA:O	2.11	0.50
12:L:47:ARG:HD3	12:L:52:GLY:HA2	1.92	0.50
1:M:196:GLU:HG3	1:M:197:PRO:HD2	1.94	0.50
1:M:409:SER:O	1:M:410:GLY:C	2.55	0.50
1:M:1021:LEU:O	1:M:1024:SER:HB3	2.12	0.50
1:M:1362:TYR:CD1	1:M:1363:VAL:N	2.79	0.50
2:N:95:ILE:CG1	2:N:130:VAL:HG22	2.41	0.50
2:N:773:MET:C	2:N:775:LYS:N	2.69	0.50
2:N:1117:GLN:HE21	2:N:1199:ALA:HB2	1.77	0.50
3:O:133:ILE:HD12	3:O:237:SER:N	2.26	0.50
4:P:36:LYS:HG2	4:P:44:GLU:OE1	2.12	0.50
4:P:120:GLU:O	4:P:120:GLU:OE1	2.30	0.50
9:U:6:PHE:CB	9:U:12:ASN:O	2.52	0.50
12:X:28:LYS:HB3	12:X:39:SER:HB2	1.93	0.50
1:A:973:ILE:HD11	1:A:1041:ALA:HB2	1.94	0.50
1:A:1280:GLU:O	1:A:1281:ARG:C	2.54	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1341:ILE:HD12	1:A:1379:GLY:C	2.36	0.50
2:B:245:GLU:C	2:B:246:LYS:HG3	2.37	0.50
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.47	0.50
2:B:1116:ARG:HG3	2:B:1198:TYR:CD2	2.47	0.50
4:D:8:PHE:HD2	7:G:6:ASP:O	1.94	0.50
7:G:14:HIS:CE1	7:G:15:PRO:HD2	2.46	0.50
7:G:126:ASN:C	7:G:126:ASN:ND2	2.67	0.50
8:H:106:GLU:O	8:H:108:SER:N	2.34	0.50
11:K:31:VAL:CG1	11:K:32:VAL:N	2.74	0.50
12:L:36:SER:O	12:L:37:LYS:C	2.54	0.50
1:M:171:GLN:OE1	1:M:171:GLN:HA	2.12	0.50
1:M:225:ASN:ND2	1:M:227:VAL:N	2.59	0.50
1:M:1095:THR:HG21	1:M:1112:LYS:HD2	1.94	0.50
1:M:1444:MET:HG3	7:S:60:ARG:CA	2.33	0.50
2:N:552:MET:HA	2:N:552:MET:HE3	1.92	0.50
2:N:599:THR:O	2:N:603:LEU:HB2	2.11	0.50
2:N:611:PRO:O	2:N:692:TYR:HB2	2.12	0.50
2:N:642:ASP:CA	2:N:649:LYS:HA	2.39	0.50
4:P:13:ARG:C	4:P:15:LEU:N	2.70	0.50
4:P:71:LYS:HG2	4:P:74:GLN:HE21	1.74	0.50
7:S:138:THR:O	7:S:140:LYS:N	2.45	0.50
14:5:2:DC:C5	14:5:3:DT:H73	2.46	0.50
1:A:306:ASN:ND2	1:A:322:VAL:HG12	2.26	0.50
1:A:645:LEU:HG	1:A:649:ILE:HD12	1.94	0.50
1:A:852:TYR:CD2	1:A:1060:PRO:CB	2.95	0.50
1:A:1255:GLU:HG2	1:A:1255:GLU:O	2.12	0.50
2:B:424:LEU:O	2:B:428:ILE:HG13	2.11	0.50
2:B:766:ARG:NH2	2:B:1020:ARG:HD3	2.26	0.50
1:M:567:LYS:CE	8:T:46:LEU:HB2	2.42	0.50
1:M:722:LEU:HB3	1:M:799:PHE:CE1	2.46	0.50
1:M:962:ARG:C	1:M:964:ILE:H	2.20	0.50
2:N:62:ILE:HG23	2:N:418:LYS:HG3	1.93	0.50
2:N:803:LEU:HD12	2:N:1032:SER:HB3	1.94	0.50
2:N:821:GLN:OE1	2:N:850:LEU:HD12	2.12	0.50
2:N:850:LEU:HD12	2:N:851:PHE:N	2.26	0.50
2:N:859:TYR:OH	2:N:941:LEU:HD12	2.12	0.50
3:O:147:LEU:N	3:O:147:LEU:CD2	2.74	0.50
4:P:130:LEU:O	4:P:132:GLN:N	2.41	0.50
10:V:64:ASN:HB3	10:V:65:PRO:HD2	1.89	0.50
13:4:16:DT:N3	13:4:17:DT:C4	2.80	0.50
1:A:1241:ARG:O	1:A:1242:VAL:CG2	2.60	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:641:GLU:C	2:B:643:ASP:H	2.19	0.50
2:B:893:LEU:HD22	2:B:897:GLY:HA2	1.94	0.50
2:B:1001:PHE:CE2	3:C:34:ARG:CZ	2.95	0.50
4:D:118:THR:HG22	4:D:118:THR:O	2.11	0.50
5:E:177:ARG:C	5:E:212:ARG:HD3	2.37	0.50
6:F:69:LEU:C	6:F:71:GLU:HG3	2.37	0.50
6:F:81:THR:HB	6:F:136:ARG:HH11	1.75	0.50
8:H:113:ALA:HA	8:H:125:LEU:O	2.11	0.50
1:M:64:ASN:O	1:M:65:LEU:C	2.55	0.50
1:M:133:LYS:O	1:M:136:ALA:HB3	2.12	0.50
1:M:567:LYS:HB3	8:T:95:TYR:HA	1.92	0.50
1:M:1035:TYR:O	1:M:1036:ARG:HB2	2.10	0.50
1:M:1324:PRO:HB2	5:Q:142:VAL:HG11	1.93	0.50
1:M:1399:ARG:HB3	1:M:1408:ILE:HD13	1.93	0.50
1:M:1421:CYS:HA	1:M:1426:GLU:HG3	1.93	0.50
2:N:313:MET:CE	2:N:390:LEU:HD11	2.38	0.50
2:N:618:ASP:O	2:N:622:LYS:N	2.45	0.50
2:N:751:VAL:HG13	2:N:812:LEU:CD2	2.37	0.50
2:N:789:MET:HE3	2:N:965:LYS:HB3	1.92	0.50
6:R:85:MET:HE2	6:R:93:ILE:HD13	1.94	0.50
7:S:106:MET:CG	7:S:107:LYS:H	2.25	0.50
7:S:113:HIS:ND1	7:S:113:HIS:N	2.56	0.50
1:A:349:ALA:HB2	1:A:374:LEU:HD11	1.94	0.49
1:A:562:THR:HB	8:H:98:TYR:HD2	1.75	0.49
1:A:807:GLY:HA2	2:B:760:ASP:O	2.11	0.49
1:A:903:ASN:ND2	1:A:903:ASN:C	2.62	0.49
1:A:1187:GLN:HG3	1:A:1188:GLN:H	1.76	0.49
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.75	0.49
1:A:1280:GLU:O	1:A:1281:ARG:O	2.30	0.49
1:A:1342:GLU:HG3	5:E:198:ILE:HD13	1.93	0.49
2:B:758:PHE:CE2	2:B:1044:ALA:CA	2.90	0.49
2:B:956:THR:HA	2:B:961:LEU:O	2.11	0.49
2:B:1103:ILE:HG23	2:B:1103:ILE:O	2.11	0.49
3:C:25:VAL:HG12	3:C:26:ASP:H	1.76	0.49
4:D:47:LEU:HD13	4:D:48:ILE:N	2.27	0.49
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.92	0.49
5:E:89:GLY:C	5:E:91:LYS:H	2.20	0.49
7:G:116:PRO:HG2	7:G:119:LEU:CB	2.42	0.49
7:G:138:THR:O	7:G:140:LYS:N	2.45	0.49
11:K:55:LYS:HD3	11:K:81:TYR:CE1	2.47	0.49
12:L:27:LEU:O	12:L:28:LYS:HB2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:34:CYS:O	12:L:35:SER:C	2.55	0.49
1:M:41:MET:O	1:M:42:ASP:O	2.29	0.49
1:M:117:GLU:CD	1:M:117:GLU:H	2.19	0.49
1:M:351:THR:CG2	2:N:1103:ILE:HA	2.22	0.49
1:M:1277:GLU:O	1:M:1279:ILE:N	2.44	0.49
2:N:203:PHE:HB3	2:N:205:ILE:CD1	2.42	0.49
2:N:327:ARG:O	2:N:331:LEU:HD13	2.12	0.49
2:N:916:THR:CG2	2:N:935:ARG:HD2	2.42	0.49
2:N:1147:LEU:CD2	2:N:1151:LEU:HD22	2.42	0.49
4:P:57:LEU:HD13	4:P:157:GLN:OE1	2.12	0.49
7:S:11:ILE:HD13	7:S:29:LYS:HB3	1.93	0.49
7:S:31:LEU:HD23	7:S:48:VAL:HG21	1.93	0.49
9:U:13:MET:HG2	9:U:14:LEU:N	2.27	0.49
9:U:73:ARG:HH12	9:U:112:SER:CB	2.25	0.49
1:A:445:ASN:CB	1:A:455:MET:HG2	2.35	0.49
1:A:456:MET:HE3	1:A:478:TYR:CZ	2.46	0.49
1:A:598:LEU:HD23	8:H:25:ARG:CZ	2.42	0.49
1:A:820:GLY:O	1:A:822:GLU:N	2.45	0.49
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.42	0.49
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.11	0.49
1:A:1242:VAL:CG1	1:A:1243:VAL:H	2.25	0.49
2:B:44:VAL:O	2:B:45:SER:C	2.54	0.49
2:B:167:ILE:HG21	2:B:424:LEU:CD2	2.42	0.49
2:B:282:ILE:HG21	2:B:382:ILE:CD1	2.42	0.49
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.27	0.49
2:B:1167:GLY:HA3	2:B:1216:LEU:N	2.27	0.49
5:E:78:LEU:HD23	5:E:78:LEU:C	2.37	0.49
8:H:42:ILE:HG23	8:H:95:TYR:CE1	2.47	0.49
8:H:58:THR:O	8:H:59:ILE:HG13	2.12	0.49
8:H:81:PRO:CB	8:H:82:PRO:CD	2.88	0.49
1:M:370:ILE:CG2	1:M:374:LEU:HD12	2.42	0.49
1:M:1254:ALA:O	1:M:1255:GLU:CB	2.60	0.49
2:N:168:GLY:HA2	2:N:450:ALA:O	2.12	0.49
2:N:431:TYR:CG	2:N:447:ALA:HB2	2.47	0.49
2:N:653:VAL:HA	2:N:689:LEU:HD22	1.94	0.49
2:N:770:GLN:HG2	2:N:983:ARG:C	2.37	0.49
2:N:885:MET:HA	2:N:936:ASP:HB2	1.94	0.49
3:O:65:HIS:O	3:O:69:LEU:HD12	2.11	0.49
3:O:258:ILE:HG23	11:W:19:LEU:HD11	1.94	0.49
4:P:175:PHE:O	4:P:178:ALA:HB3	2.11	0.49
12:X:48:CYS:HB3	12:X:51:CYS:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ASN:O	1:A:65:LEU:C	2.55	0.49
1:A:80:HIS:H	1:A:243:PRO:HB3	1.77	0.49
1:A:122:MET:HA	1:A:141:LEU:HD11	1.94	0.49
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.94	0.49
1:A:202:LEU:HA	1:A:206:GLU:OE1	2.13	0.49
1:A:399:HIS:CG	1:A:400:PRO:N	2.79	0.49
1:A:773:LYS:H	1:A:773:LYS:CD	2.23	0.49
1:A:1450:LEU:HD21	7:G:19:GLY:O	2.13	0.49
2:B:664:THR:HG1	2:B:678:GLU:N	2.10	0.49
2:B:728:ARG:HH12	2:B:1047:PHE:HB3	1.78	0.49
2:B:953:LEU:HD23	2:B:953:LEU:O	2.12	0.49
3:C:189:THR:CG2	3:C:190:ASP:N	2.74	0.49
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.95	0.49
7:G:121:PHE:HB2	7:G:130:TYR:CE2	2.48	0.49
12:L:38:LEU:HG	12:L:39:SER:N	2.28	0.49
1:M:50:ILE:C	1:M:52:GLY:N	2.68	0.49
1:M:1341:ILE:HD12	1:M:1379:GLY:C	2.37	0.49
1:M:1444:MET:HE1	6:R:135:ARG:HB2	1.94	0.49
2:N:31:TRP:CE3	2:N:34:ILE:HD12	2.46	0.49
2:N:108:VAL:HG23	2:N:109:THR:N	2.27	0.49
2:N:635:ARG:NH1	2:N:742:GLU:OE2	2.43	0.49
4:P:24:ALA:HA	7:S:83:LYS:O	2.12	0.49
7:S:77:VAL:O	7:S:77:VAL:HG12	2.11	0.49
1:A:164:ARG:HG3	1:A:165:GLY:N	2.26	0.49
1:A:967:ALA:HA	1:A:1044:TRP:CZ3	2.47	0.49
2:B:34:ILE:HG23	2:B:542:MET:CE	2.41	0.49
2:B:205:ILE:HD11	2:B:461:LEU:HD23	1.94	0.49
2:B:235:SER:O	2:B:236:HIS:HD2	1.95	0.49
2:B:244:LEU:HD12	2:B:250:PHE:HD1	1.77	0.49
5:E:114:ASN:O	5:E:115:ASN:CB	2.48	0.49
5:E:180:ARG:NH2	5:E:192:ARG:HB2	2.25	0.49
11:K:64:GLU:HA	11:K:64:GLU:OE2	2.12	0.49
1:M:285:PRO:CG	1:M:288:ALA:HB3	2.38	0.49
1:M:489:LEU:HD12	1:M:489:LEU:C	2.36	0.49
1:M:744:LYS:CD	1:M:748:MET:HE2	2.42	0.49
1:M:1100:ARG:NH2	1:M:1351:GLU:HG2	2.27	0.49
1:M:1163:ILE:HG22	1:M:1165:GLU:HG3	1.94	0.49
2:N:95:ILE:CB	2:N:130:VAL:HG22	2.43	0.49
2:N:110:HIS:HB3	12:X:54:ARG:HH22	1.78	0.49
2:N:848:ARG:HH22	2:N:996:ARG:HD3	1.77	0.49
2:N:956:THR:HA	2:N:961:LEU:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:118:LEU:HB2	3:O:132:PRO:HG2	1.94	0.49
5:Q:50:MET:O	5:Q:50:MET:HE3	2.13	0.49
1:A:385:ILE:CD1	1:A:426:LEU:HB2	2.42	0.49
1:A:447:GLN:HA	1:A:448:PRO:C	2.36	0.49
1:A:961:ARG:HH11	1:A:961:ARG:CB	2.26	0.49
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.93	0.49
2:B:240:ILE:HG21	2:B:381:MET:HE1	1.94	0.49
2:B:466:TRP:HA	2:B:466:TRP:CE3	2.46	0.49
4:D:146:GLN:C	4:D:149:THR:HG22	2.38	0.49
5:E:207:ARG:NH1	5:E:207:ARG:CB	2.75	0.49
9:I:7:CYS:HB2	9:I:34:TYR:CG	2.47	0.49
11:K:55:LYS:HB2	11:K:81:TYR:CD1	2.48	0.49
13:1:16:DT:N3	13:1:17:DT:C4	2.81	0.49
1:M:493:GLN:CA	1:M:493:GLN:NE2	2.75	0.49
1:M:714:PHE:O	1:M:718:VAL:HG23	2.12	0.49
2:N:221:ASN:N	2:N:241:ARG:O	2.40	0.49
2:N:244:LEU:CD1	2:N:366:GLN:HE22	2.18	0.49
2:N:307:ASP:OD2	2:N:310:MET:HB2	2.12	0.49
2:N:368:GLU:O	2:N:370:PHE:N	2.44	0.49
2:N:370:PHE:HD2	2:N:373:ARG:HD3	1.78	0.49
2:N:975:GLN:HG2	2:N:976:ILE:N	2.27	0.49
3:O:147:LEU:HD12	3:O:151:GLN:O	2.12	0.49
7:S:121:PHE:CZ	7:S:123:ALA:HA	2.48	0.49
9:U:44:TYR:HD1	9:U:45:ARG:H	1.61	0.49
1:A:134:ARG:HD2	1:A:221:SER:O	2.12	0.49
1:A:963:ILE:HD11	1:A:1048:ASN:HB2	1.93	0.49
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.76	0.49
2:B:282:ILE:HD11	2:B:317:CYS:SG	2.53	0.49
2:B:432:MET:C	2:B:434:ARG:H	2.20	0.49
2:B:497:ARG:HH21	2:B:775:LYS:NZ	2.10	0.49
2:B:578:THR:C	2:B:589:VAL:HG13	2.38	0.49
3:C:248:ILE:HD13	11:K:101:LEU:HD22	1.94	0.49
5:E:171:LYS:HG2	5:E:174:GLN:CD	2.38	0.49
7:G:160:ILE:HD11	7:S:111:THR:HG21	1.95	0.49
1:M:106:VAL:CG1	1:M:107:CYS:N	2.74	0.49
1:M:452:LYS:HB3	2:N:1141:HIS:CE1	2.47	0.49
1:M:679:ILE:HG23	1:M:729:ALA:HB1	1.95	0.49
2:N:190:TYR:CE1	2:N:196:PRO:HG3	2.48	0.49
2:N:558:LEU:O	2:N:561:TRP:N	2.45	0.49
2:N:955:THR:CG2	2:N:956:THR:H	2.25	0.49
2:N:999:MET:HA	2:N:999:MET:CE	2.38	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:109:SER:O	3:O:110:THR:C	2.55	0.49
4:P:155:ARG:NH2	4:P:221:TYR:HD1	2.08	0.49
4:P:220:LEU:HD23	4:P:221:TYR:N	2.28	0.49
7:S:1:MET:HE3	7:S:80:LYS:N	2.28	0.49
9:U:98:VAL:CG1	9:U:111:THR:HG23	2.43	0.49
12:X:34:CYS:SG	12:X:34:CYS:O	2.71	0.49
1:A:2:VAL:CG1	2:B:1157:ALA:O	2.60	0.49
1:A:440:ASP:O	1:A:460:VAL:HG23	2.13	0.49
2:B:209:GLU:CD	2:B:485:ARG:HE	2.21	0.49
2:B:263:GLY:O	2:B:264:SER:C	2.56	0.49
2:B:351:TYR:O	2:B:355:ILE:HG13	2.11	0.49
3:C:39:ALA:HA	3:C:164:ALA:CB	2.42	0.49
4:D:119:ARG:O	4:D:123:LEU:HD23	2.13	0.49
4:D:155:ARG:NE	4:D:221:TYR:HE1	2.10	0.49
5:E:48:ASP:HB3	5:E:54:GLN:CD	2.37	0.49
5:E:61:GLN:HG2	5:E:62:ALA:N	2.27	0.49
6:F:100:GLN:NE2	7:G:61:ILE:HD13	2.28	0.49
8:H:47:PHE:CB	8:H:95:TYR:HD1	2.26	0.49
9:I:92:ARG:HD2	9:I:94:ASP:OD2	2.12	0.49
14:2:2:DC:C5	14:2:3:DT:H73	2.47	0.49
1:M:145:LYS:HE3	1:M:145:LYS:CA	2.40	0.49
1:M:196:GLU:CG	1:M:197:PRO:HD2	2.43	0.49
1:M:563:PRO:HG3	1:M:572:TRP:CE2	2.44	0.49
1:M:597:LEU:HD23	8:T:103:LYS:CD	2.43	0.49
1:M:945:GLU:OE1	5:Q:201:LYS:NZ	2.45	0.49
1:M:1152:ILE:HD11	1:M:1261:LYS:HG3	1.93	0.49
2:N:313:MET:O	2:N:316:PRO:HD2	2.13	0.49
3:O:44:LEU:C	3:O:44:LEU:HD23	2.38	0.49
8:T:104:PHE:CZ	8:T:136:LYS:HA	2.47	0.49
10:V:5:VAL:C	10:V:6:ARG:HG3	2.37	0.49
1:A:50:ILE:C	1:A:52:GLY:N	2.69	0.49
1:A:67:CYS:O	1:A:70:CYS:HB3	2.12	0.49
1:A:288:ALA:HA	1:A:291:GLU:CG	2.42	0.49
1:A:451:HIS:O	1:A:452:LYS:C	2.56	0.49
2:B:351:TYR:CZ	2:B:355:ILE:HD11	2.47	0.49
2:B:492:LEU:HB2	2:B:751:VAL:HG11	1.95	0.49
4:D:167:LEU:O	4:D:170:THR:HG23	2.13	0.49
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.94	0.49
5:E:112:TYR:O	5:E:137:GLU:HG3	2.13	0.49
8:H:13:SER:HB3	8:H:27:GLU:O	2.13	0.49
9:I:58:VAL:HG13	9:I:62:ILE:HG21	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:55:ASP:C	1:M:57:ARG:N	2.64	0.49
1:M:64:ASN:O	1:M:66:LYS:N	2.46	0.49
1:M:547:LEU:HD22	11:W:58:PHE:CD1	2.47	0.49
1:M:663:SER:OG	1:M:664:THR:N	2.45	0.49
1:M:1313:LEU:C	1:M:1315:GLU:N	2.71	0.49
1:M:1410:PHE:HD2	2:N:1212:ILE:HD11	1.78	0.49
2:N:373:ARG:HA	2:N:566:LEU:CD2	2.42	0.49
2:N:373:ARG:HA	2:N:566:LEU:HD23	1.94	0.49
2:N:866:TYR:CG	2:N:870:ILE:HB	2.48	0.49
4:P:51:ASN:C	4:P:52:LEU:O	2.53	0.49
4:P:138:ASN:C	4:P:140:ASP:N	2.69	0.49
4:P:139:LYS:HG3	4:P:140:ASP:OD1	2.13	0.49
7:S:110:VAL:CG1	7:S:161:GLY:O	2.61	0.49
10:V:1:MET:H1	10:V:56:LEU:HB2	1.78	0.49
1:A:40:THR:HG23	1:A:54:ASN:ND2	2.27	0.49
1:A:106:VAL:HG12	1:A:107:CYS:H	1.76	0.49
1:A:265:LYS:CA	1:A:265:LYS:CE	2.89	0.49
1:A:316:GLN:HG2	1:A:317:LYS:N	2.28	0.49
1:A:460:VAL:HG12	1:A:461:LYS:N	2.27	0.49
1:A:886:ILE:CG2	1:A:887:GLY:N	2.76	0.49
1:A:962:ARG:C	1:A:964:ILE:H	2.21	0.49
2:B:118:ARG:NH2	2:B:194:GLU:OE1	2.42	0.49
2:B:235:SER:C	2:B:236:HIS:CD2	2.90	0.49
2:B:303:TYR:HH	2:B:586:TRP:HH2	1.59	0.49
2:B:371:GLU:OE1	2:B:371:GLU:N	2.45	0.49
2:B:614:SER:C	2:B:615:MET:HG3	2.38	0.49
2:B:629:ASP:HB3	2:B:632:ARG:HD3	1.94	0.49
2:B:805:THR:CG2	2:B:806:THR:H	2.16	0.49
5:E:88:VAL:HG21	5:E:110:PHE:CE1	2.47	0.49
8:H:44:VAL:O	8:H:44:VAL:HG12	2.13	0.49
8:H:130:ARG:HH11	8:H:130:ARG:CB	2.25	0.49
1:M:35:ILE:HA	1:M:52:GLY:O	2.13	0.49
1:M:42:ASP:HB3	1:M:45:GLN:CA	2.43	0.49
1:M:65:LEU:O	1:M:66:LYS:O	2.30	0.49
1:M:75:ASN:O	1:M:76:GLU:HB2	2.13	0.49
1:M:1170:ILE:HG22	1:M:1174:PHE:CE1	2.48	0.49
2:N:458:LYS:O	2:N:459:TYR:C	2.56	0.49
2:N:862:GLN:CG	2:N:963:PHE:HD1	2.19	0.49
2:N:1084:GLN:NE2	2:N:1084:GLN:H	2.09	0.49
2:N:1165:ILE:HG21	4:P:17:LYS:CG	2.43	0.49
3:O:44:LEU:HD13	3:O:129:ILE:HG23	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:26:ILE:HD13	8:T:49:VAL:HG11	1.94	0.49
10:V:30:LEU:CD1	10:V:38:ARG:HH11	2.26	0.49
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.48	0.49
1:A:37:PHE:HD1	1:A:37:PHE:H	1.58	0.49
1:A:57:ARG:O	1:A:68:GLN:HG2	2.12	0.49
1:A:407:ARG:HG2	1:A:430:TRP:CE2	2.48	0.49
1:A:831:THR:HG23	1:A:832:ALA:N	2.27	0.49
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.13	0.49
2:B:334:ILE:O	2:B:334:ILE:CG2	2.60	0.49
2:B:679:TYR:HE1	2:B:687:GLU:OE2	1.96	0.49
5:E:98:ILE:HG22	5:E:102:GLU:CG	2.42	0.49
5:E:153:HIS:C	5:E:154:ILE:HG13	2.37	0.49
5:E:157:SER:C	5:E:159:ASP:N	2.70	0.49
8:H:4:THR:HA	8:H:60:ALA:CB	2.19	0.49
8:H:40:LEU:HD23	8:H:42:ILE:CG1	2.43	0.49
12:L:53:HIS:C	12:L:55:ILE:HD13	2.38	0.49
1:M:30:ILE:HD11	2:N:1168:LEU:CD1	2.43	0.49
1:M:265:LYS:HA	1:M:265:LYS:CE	2.38	0.49
1:M:1118:VAL:HG12	1:M:1327:ILE:HG13	1.95	0.49
1:M:1147:THR:HB	9:U:48:LEU:HD12	1.94	0.49
1:M:1280:GLU:O	1:M:1281:ARG:O	2.31	0.49
1:M:1409:LEU:CD1	2:N:1207:LEU:HD11	2.42	0.49
2:N:131:ASP:HA	2:N:164:LYS:HB3	1.95	0.49
4:P:66:ARG:O	4:P:70:PHE:HB2	2.13	0.49
5:Q:37:LEU:CD1	5:Q:41:ASP:HB2	2.43	0.49
6:R:111:LEU:C	6:R:113:GLY:N	2.66	0.49
8:T:30:SER:CB	8:T:36:CYS:HB3	2.43	0.49
1:A:356:ASP:C	1:A:358:ASN:H	2.21	0.48
1:A:820:GLY:O	1:A:823:GLY:N	2.46	0.48
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.12	0.48
2:B:27:ALA:O	2:B:29:ASP:N	2.46	0.48
2:B:211:VAL:HG13	2:B:495:LEU:HD23	1.94	0.48
2:B:453:ILE:O	2:B:457:LEU:HG	2.12	0.48
2:B:531:GLN:CG	2:B:532:ALA:H	2.23	0.48
2:B:916:THR:CG2	2:B:935:ARG:HD2	2.43	0.48
3:C:8:VAL:HG12	3:C:9:LYS:N	2.28	0.48
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.46	0.48
3:C:219:PHE:CE2	3:C:221:TYR:HB3	2.48	0.48
3:C:242:GLN:OE1	3:C:242:GLN:HA	2.13	0.48
6:F:101:ILE:HD13	6:F:120:ILE:CG2	2.43	0.48
7:G:117:GLN:NE2	7:S:154:VAL:CG2	2.76	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:4:DA:H2''	14:2:5:DC:H6	1.78	0.48
1:M:716:ASP:C	1:M:716:ASP:OD1	2.56	0.48
2:N:120:ARG:HG2	2:N:955:THR:HG21	1.95	0.48
2:N:263:GLY:O	2:N:264:SER:C	2.56	0.48
2:N:331:LEU:O	2:N:334:ILE:HB	2.13	0.48
2:N:387:LEU:N	2:N:387:LEU:HD12	2.28	0.48
2:N:846:ILE:CG2	2:N:974:PRO:HG2	2.42	0.48
3:O:116:LYS:HG3	3:O:117:ASP:OD1	2.13	0.48
3:O:182:PRO:HD2	3:O:210:GLU:OE1	2.13	0.48
4:P:32:GLU:HG3	7:S:5:LYS:HE2	1.94	0.48
4:P:134:THR:CG2	4:P:141:LEU:HD23	2.42	0.48
4:P:214:LEU:HD13	4:P:214:LEU:C	2.38	0.48
8:T:106:GLU:O	8:T:108:SER:N	2.35	0.48
8:T:130:ARG:HA	8:T:133:ASN:HB2	1.95	0.48
14:5:4:DA:H2''	14:5:5:DC:H6	1.78	0.48
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.38	0.48
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.38	0.48
1:A:107:CYS:HB2	1:A:114:LEU:HD21	1.94	0.48
1:A:196:GLU:HG2	1:A:197:PRO:HD2	1.94	0.48
1:A:857:ARG:CZ	6:F:139:PRO:HG3	2.43	0.48
1:A:1376:THR:O	1:A:1377:THR:C	2.55	0.48
1:A:1389:PHE:C	1:A:1391:ARG:H	2.22	0.48
1:A:1402:PHE:CE2	1:A:1403:GLU:CG	2.95	0.48
2:B:244:LEU:HD11	2:B:366:GLN:NE2	2.28	0.48
2:B:487:THR:HG22	2:B:488:TYR:N	2.28	0.48
2:B:557:PHE:CZ	2:B:603:LEU:HD11	2.48	0.48
2:B:785:TYR:CD1	2:B:786:ASN:N	2.81	0.48
2:B:792:MET:HA	2:B:856:PHE:O	2.13	0.48
2:B:878:GLN:HB2	2:B:879:ARG:HH11	1.76	0.48
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.95	0.48
8:H:62:SER:OG	8:H:64:ASN:ND2	2.47	0.48
1:M:534:LEU:O	1:M:534:LEU:HG	2.12	0.48
1:M:595:THR:O	1:M:596:THR:CG2	2.61	0.48
1:M:1313:LEU:C	1:M:1315:GLU:H	2.21	0.48
1:M:1450:LEU:CD1	6:R:108:PHE:CZ	2.96	0.48
2:N:68:THR:HG22	2:N:91:SER:HA	1.94	0.48
2:N:436:VAL:O	2:N:436:VAL:HG12	2.13	0.48
2:N:594:ALA:N	2:N:617:ARG:NH1	2.61	0.48
2:N:798:TYR:CD1	10:V:4:PRO:HG3	2.48	0.48
2:N:1033:LYS:NZ	2:N:1070:GLU:OE1	2.36	0.48
3:O:35:ARG:NH1	11:W:41:THR:N	2.60	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:47:ASP:CG	3:O:47:ASP:O	2.57	0.48
7:S:22:MET:O	7:S:23:LYS:C	2.56	0.48
9:U:88:SER:HB3	9:U:95:THR:HG21	1.95	0.48
11:W:88:LYS:O	11:W:91:CYS:HB2	2.13	0.48
11:W:113:THR:O	11:W:114:LEU:CB	2.61	0.48
1:A:53:LEU:CD2	1:A:54:ASN:N	2.55	0.48
1:A:567:LYS:CE	8:H:46:LEU:HB2	2.43	0.48
1:A:1123:GLY:O	1:A:1125:ALA:N	2.46	0.48
2:B:39:ARG:NH2	2:B:665:GLU:CG	2.75	0.48
2:B:336:ARG:HG3	2:B:336:ARG:NH1	2.28	0.48
2:B:479:VAL:O	2:B:480:SER:HB3	2.12	0.48
2:B:806:THR:HG22	2:B:808:ALA:HB3	1.95	0.48
3:C:33:LEU:O	3:C:37:MET:HG3	2.12	0.48
4:D:12:ARG:HH12	4:D:14:ARG:HA	1.78	0.48
4:D:56:ARG:HD3	4:D:149:THR:HA	1.96	0.48
5:E:35:VAL:C	5:E:37:LEU:H	2.20	0.48
7:G:139:ILE:CG2	7:G:140:LYS:N	2.76	0.48
8:H:109:LYS:HG2	8:H:110:ASP:OD1	2.13	0.48
1:M:162:VAL:HG12	1:M:163:SER:H	1.78	0.48
1:M:316:GLN:O	1:M:317:LYS:C	2.56	0.48
1:M:390:GLN:O	1:M:394:ASN:HB2	2.12	0.48
1:M:946:VAL:HG22	5:Q:201:LYS:HD2	1.94	0.48
1:M:996:ASN:HA	1:M:998:LEU:CD1	2.44	0.48
3:O:114:TYR:HB2	3:O:116:LYS:HG2	1.94	0.48
3:O:213:PRO:HG2	3:O:214:ASN:H	1.78	0.48
4:P:185:CYS:SG	4:P:191:ALA:N	2.86	0.48
8:T:4:THR:HA	8:T:60:ALA:CB	2.20	0.48
1:A:463:ILE:HD11	1:A:469:ARG:HG3	1.96	0.48
1:A:476:SER:HB2	1:A:477:PRO:HD3	1.95	0.48
1:A:1011:GLN:NE2	1:A:1015:VAL:CG2	2.76	0.48
1:A:1148:ILE:CG1	1:A:1198:ASP:HB2	2.43	0.48
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.43	0.48
2:B:594:ALA:CA	2:B:617:ARG:NH1	2.76	0.48
2:B:889:THR:O	2:B:889:THR:HG22	2.13	0.48
2:B:918:ILE:HD12	2:B:935:ARG:NH1	2.28	0.48
5:E:96:PHE:CZ	5:E:100:ILE:HD11	2.49	0.48
9:I:7:CYS:SG	9:I:8:ARG:O	2.72	0.48
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.21	0.48
12:L:47:ARG:CG	12:L:48:CYS:H	2.26	0.48
12:L:59:ALA:O	12:L:60:ARG:O	2.32	0.48
1:M:370:ILE:HG22	1:M:374:LEU:HD12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:738:LYS:HD3	1:M:738:LYS:H	1.78	0.48
1:M:829:VAL:HG21	2:N:508:LEU:HD13	1.95	0.48
1:M:1124:HIS:HB2	1:M:1130:GLN:HG2	1.93	0.48
2:N:212:LEU:HD23	2:N:480:SER:HB2	1.95	0.48
2:N:432:MET:C	2:N:434:ARG:H	2.21	0.48
2:N:642:ASP:HB3	2:N:649:LYS:HG3	1.95	0.48
2:N:1116:ARG:HG3	2:N:1198:TYR:CG	2.48	0.48
3:O:177:GLU:CG	3:O:231:ASN:HB3	2.27	0.48
3:O:242:GLN:C	3:O:244:VAL:N	2.71	0.48
4:P:154:PHE:CE1	4:P:163:VAL:CG2	2.96	0.48
7:S:1:MET:HE2	7:S:3:PHE:CE1	2.48	0.48
8:T:81:PRO:CB	8:T:82:PRO:CD	2.88	0.48
1:A:55:ASP:C	1:A:57:ARG:N	2.65	0.48
1:A:332:LYS:O	1:A:333:GLU:CB	2.61	0.48
1:A:967:ALA:O	1:A:971:PHE:HD1	1.97	0.48
2:B:522:VAL:HG11	2:B:537:LYS:HB3	1.95	0.48
2:B:557:PHE:HD2	2:B:557:PHE:O	1.96	0.48
2:B:878:GLN:HA	2:B:885:MET:SD	2.53	0.48
3:C:63:ILE:HA	3:C:66:ARG:HG3	1.95	0.48
3:C:260:LEU:O	3:C:263:THR:HB	2.13	0.48
4:D:71:LYS:CA	4:D:74:GLN:HB2	2.39	0.48
4:D:156:ASP:CB	4:D:159:THR:HG23	2.44	0.48
8:H:143:LEU:C	8:H:144:ILE:HG13	2.37	0.48
12:L:30:ILE:CG2	12:L:31:CYS:N	2.76	0.48
1:M:392:VAL:HG13	1:M:415:LEU:HD11	1.95	0.48
1:M:593:GLU:C	1:M:595:THR:N	2.71	0.48
1:M:1259:MET:HA	1:M:1262:LYS:CD	2.37	0.48
2:N:1096:ARG:NH1	2:N:1096:ARG:HB2	2.28	0.48
2:N:1099:VAL:HG13	2:N:1100:ASP:N	2.29	0.48
4:P:139:LYS:O	4:P:143:ASN:ND2	2.46	0.48
4:P:189:ASP:OD2	7:S:167:TYR:HE1	1.96	0.48
7:S:116:PRO:CG	7:S:119:LEU:HB2	2.43	0.48
8:T:61:SER:HB3	8:T:139:ASN:HB3	1.96	0.48
12:X:38:LEU:HD11	12:X:49:LYS:HE2	1.96	0.48
1:A:65:LEU:O	1:A:66:LYS:O	2.31	0.48
1:A:321:PRO:O	1:A:322:VAL:CB	2.61	0.48
1:A:344:ARG:HH11	1:A:344:ARG:CB	2.12	0.48
1:A:523:ILE:HG13	1:A:622:VAL:CG2	2.43	0.48
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.47	0.48
1:A:1259:MET:HE2	1:A:1263:ILE:CG1	2.43	0.48
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:446:LEU:HG	2:B:446:LEU:O	2.13	0.48
2:B:552:MET:HE3	2:B:555:ILE:HB	1.95	0.48
3:C:44:LEU:HD21	3:C:159:ALA:HB1	1.95	0.48
3:C:166:GLU:C	11:K:6:ARG:NH1	2.72	0.48
3:C:236:GLY:O	3:C:238:ILE:N	2.46	0.48
4:D:56:ARG:CA	4:D:148:LEU:HD13	2.43	0.48
5:E:127:ILE:O	5:E:127:ILE:HG13	2.12	0.48
6:F:69:LEU:HB3	6:F:71:GLU:CG	2.44	0.48
8:H:61:SER:O	8:H:62:SER:HB2	2.13	0.48
14:2:4:DA:H2"	14:2:5:DC:C6	2.48	0.48
1:M:316:GLN:HG2	1:M:317:LYS:N	2.28	0.48
1:M:697:ALA:HB1	9:U:97:MET:HE3	1.96	0.48
1:M:821:ARG:O	1:M:825:ILE:HG13	2.13	0.48
1:M:1109:LYS:HG3	1:M:1110:ASN:ND2	2.28	0.48
1:M:1121:GLU:HB3	1:M:1124:HIS:CD2	2.48	0.48
2:N:780:VAL:HG11	10:V:56:LEU:HD13	1.96	0.48
2:N:1020:ARG:HB2	2:N:1022:THR:HG22	1.96	0.48
2:N:1072:MET:HE3	2:N:1085:ILE:CB	2.42	0.48
4:P:209:ARG:HA	4:P:212:LYS:CD	2.43	0.48
5:Q:28:TYR:C	5:Q:65:THR:HG23	2.39	0.48
7:S:43:GLY:HA2	7:S:157:ILE:HD11	1.95	0.48
8:T:24:CYS:HB2	8:T:44:VAL:CG2	2.42	0.48
9:U:77:LYS:O	9:U:79:HIS:N	2.46	0.48
11:W:53:ASP:HB3	11:W:56:VAL:CG2	2.44	0.48
1:A:41:MET:O	1:A:42:ASP:O	2.30	0.48
1:A:492:PRO:C	1:A:493:GLN:HE21	2.22	0.48
1:A:933:TYR:CD2	1:A:933:TYR:O	2.67	0.48
1:A:963:ILE:HD11	1:A:1049:ILE:N	2.29	0.48
1:A:1268:LEU:CD1	9:I:48:LEU:HD11	2.44	0.48
1:A:1315:GLU:O	1:A:1317:MET:N	2.46	0.48
1:A:1323:ASP:C	1:A:1325:THR:H	2.21	0.48
2:B:110:HIS:CB	12:L:54:ARG:HH22	2.25	0.48
2:B:221:ASN:OD1	2:B:242:SER:HA	2.14	0.48
2:B:798:TYR:CD2	2:B:798:TYR:N	2.81	0.48
3:C:109:SER:O	3:C:110:THR:C	2.56	0.48
4:D:29:LEU:HD12	7:G:82:PHE:CZ	2.49	0.48
5:E:55:ARG:CD	5:E:113:GLN:HE21	2.27	0.48
5:E:69:ILE:HD12	5:E:69:ILE:N	2.29	0.48
9:I:19:ASP:CB	9:I:24:ARG:HG2	2.42	0.48
10:J:44:TYR:CD2	10:J:44:TYR:N	2.74	0.48
11:K:40:HIS:O	11:K:41:THR:C	2.56	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:57:LEU:HD11	11:K:78:THR:HA	1.96	0.48
1:M:565:ILE:CG2	1:M:567:LYS:HE2	2.43	0.48
1:M:902:LEU:CG	1:M:926:GLN:HG3	2.34	0.48
1:M:1332:PHE:CE1	1:M:1381:LEU:HD13	2.49	0.48
2:N:110:HIS:CB	12:X:54:ARG:HH22	2.27	0.48
2:N:216:GLU:HB2	2:N:406:LEU:CD2	2.43	0.48
2:N:558:LEU:O	2:N:560:GLU:N	2.47	0.48
2:N:629:ASP:HB3	2:N:632:ARG:HD3	1.96	0.48
2:N:944:THR:HG21	2:N:1122:ARG:NH2	2.28	0.48
2:N:991:GLY:O	2:N:992:ILE:HB	2.12	0.48
3:O:97:VAL:HG21	3:O:129:ILE:CG2	2.44	0.48
3:O:98:VAL:HG13	3:O:157:CYS:O	2.14	0.48
3:O:226:ASP:O	3:O:227:THR:HB	2.14	0.48
4:P:209:ARG:HA	4:P:212:LYS:HE3	1.96	0.48
5:Q:94:LYS:HE2	5:Q:98:ILE:CG1	2.43	0.48
5:Q:102:GLU:C	5:Q:104:ASN:N	2.72	0.48
5:Q:191:LYS:O	5:Q:192:ARG:C	2.56	0.48
6:R:89:GLU:C	6:R:93:ILE:HD12	2.39	0.48
7:S:12:THR:O	7:S:12:THR:HG22	2.13	0.48
12:X:34:CYS:O	12:X:35:SER:C	2.56	0.48
12:X:38:LEU:HG	12:X:39:SER:N	2.29	0.48
1:A:676:MET:HE1	1:A:762:SER:O	2.13	0.48
1:A:709:THR:CG2	1:A:710:LEU:H	2.25	0.48
1:A:728:LYS:HA	1:A:731:ARG:CZ	2.43	0.48
1:A:929:LEU:HD21	1:A:983:ILE:CG2	2.43	0.48
1:A:1025:ARG:HG3	1:A:1025:ARG:NH1	2.28	0.48
1:A:1150:SER:O	1:A:1151:GLU:HG3	2.14	0.48
1:A:1254:ALA:O	1:A:1255:GLU:HB3	2.13	0.48
2:B:274:PRO:O	2:B:275:TYR:HB2	2.13	0.48
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.10	0.48
2:B:708:GLU:O	2:B:709:ASP:C	2.57	0.48
2:B:1095:LEU:C	2:B:1096:ARG:O	2.55	0.48
5:E:29:PHE:HA	5:E:65:THR:HG22	1.95	0.48
12:L:40:LEU:HD22	12:L:44:ASP:OD2	2.13	0.48
1:M:899:VAL:CG2	1:M:908:LEU:HD21	2.43	0.48
2:N:128:LEU:HB2	2:N:168:GLY:O	2.13	0.48
2:N:448:ILE:O	2:N:450:ALA:N	2.46	0.48
2:N:582:VAL:HG12	2:N:582:VAL:O	2.13	0.48
2:N:822:ASN:ND2	10:V:52:THR:HG21	2.29	0.48
2:N:996:ARG:NH1	3:O:174:ALA:HA	2.27	0.48
4:P:119:ARG:HB2	4:P:221:TYR:CZ	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:191:ALA:C	4:P:193:THR:N	2.72	0.48
5:Q:48:ASP:HB3	5:Q:54:GLN:CD	2.38	0.48
7:S:9:LEU:HD12	7:S:10:ASN:N	2.28	0.48
7:S:132:SER:HB3	7:S:135:ASP:H	1.79	0.48
8:T:135:LEU:HD13	8:T:137:GLN:NE2	2.29	0.48
1:A:250:ILE:O	1:A:250:ILE:CG2	2.59	0.48
1:A:541:ILE:HG21	1:A:549:MET:HE3	1.96	0.48
1:A:549:MET:HE1	1:A:656:TRP:CD1	2.48	0.48
1:A:598:LEU:O	1:A:598:LEU:HD23	2.13	0.48
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.95	0.48
2:B:654:ARG:O	2:B:657:HIS:N	2.47	0.48
2:B:805:THR:HA	2:B:809:MET:HE1	1.96	0.48
2:B:848:ARG:HD3	10:J:11:GLY:HA2	1.96	0.48
3:C:89:GLU:O	3:C:89:GLU:HG2	2.14	0.48
3:C:242:GLN:C	3:C:244:VAL:N	2.72	0.48
3:C:253:LYS:O	3:C:256:ALA:HB3	2.14	0.48
7:G:7:LEU:CB	7:G:74:TYR:HE2	2.26	0.48
9:I:4:PHE:CD1	9:I:4:PHE:C	2.92	0.48
1:M:164:ARG:CG	1:M:165:GLY:N	2.75	0.48
1:M:399:HIS:CG	1:M:400:PRO:N	2.81	0.48
1:M:451:HIS:O	1:M:452:LYS:C	2.56	0.48
1:M:477:PRO:CG	1:M:521:MET:HG2	2.43	0.48
1:M:1313:LEU:HD23	1:M:1338:VAL:HG21	1.95	0.48
1:M:1315:GLU:O	1:M:1317:MET:N	2.47	0.48
1:M:1333:ILE:O	1:M:1337:GLU:HG3	2.14	0.48
2:N:249:ARG:NH2	2:N:418:LYS:HZ2	2.12	0.48
2:N:750:GLY:O	2:N:751:VAL:C	2.56	0.48
2:N:853:SER:OG	2:N:1094:ARG:NH1	2.47	0.48
2:N:875:GLU:O	2:N:877:PRO:HD3	2.14	0.48
5:Q:116:ILE:HG22	5:Q:120:ALA:HB3	1.96	0.48
5:Q:177:ARG:HD3	5:Q:215:MET:CG	2.43	0.48
5:Q:207:ARG:CB	5:Q:207:ARG:NH1	2.77	0.48
7:S:7:LEU:HB2	7:S:74:TYR:HE2	1.74	0.48
8:T:128:ASN:HD22	8:T:128:ASN:C	2.22	0.48
10:V:6:ARG:HA	10:V:12:LYS:O	2.14	0.48
1:A:42:ASP:HB3	1:A:45:GLN:HA	1.95	0.48
1:A:175:ARG:HG2	1:A:182:VAL:HG12	1.96	0.48
1:A:504:LEU:CD1	6:F:91:ALA:HB2	2.44	0.48
2:B:221:ASN:N	2:B:241:ARG:O	2.40	0.48
2:B:237:VAL:HG22	2:B:257:LYS:HA	1.96	0.48
2:B:240:ILE:HG23	2:B:240:ILE:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1182:CYS:O	2:B:1182:CYS:SG	2.72	0.48
5:E:128:PRO:HA	5:E:129:PRO:O	2.14	0.48
6:F:69:LEU:HD22	6:F:71:GLU:OE1	2.14	0.48
10:J:42:LYS:HG2	10:J:43:ARG:N	2.28	0.48
10:J:64:ASN:CB	10:J:65:PRO:HD3	2.42	0.48
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.94	0.48
11:K:109:TRP:O	11:K:112:GLN:HB2	2.13	0.48
1:M:43:GLU:OE2	1:M:48:ALA:CB	2.62	0.48
1:M:102:VAL:CG1	1:M:211:PHE:HE1	2.27	0.48
1:M:385:ILE:HG22	1:M:386:ASP:N	2.29	0.48
1:M:846:GLU:OE1	1:M:1425:SER:OG	2.32	0.48
2:N:27:ALA:O	2:N:29:ASP:N	2.47	0.48
2:N:44:VAL:O	2:N:45:SER:C	2.56	0.48
2:N:708:GLU:O	2:N:709:ASP:C	2.57	0.48
2:N:806:THR:HG22	2:N:808:ALA:HB3	1.96	0.48
3:O:99:LEU:CD2	3:O:99:LEU:N	2.76	0.48
4:P:209:ARG:HA	4:P:212:LYS:CE	2.44	0.48
7:S:1:MET:O	7:S:3:PHE:CE2	2.67	0.48
7:S:13:LEU:HD22	7:S:17:PHE:HB2	1.90	0.48
7:S:26:LEU:HD12	7:S:56:ILE:CD1	2.43	0.48
1:A:524:VAL:O	1:A:525:GLN:C	2.57	0.47
1:A:822:GLU:HG3	2:B:513:GLN:HE21	1.79	0.47
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.28	0.47
1:A:1350:LYS:O	1:A:1354:ASN:ND2	2.46	0.47
2:B:433:GLN:O	2:B:434:ARG:HG3	2.14	0.47
2:B:886:LYS:HE2	2:B:940:PRO:CD	2.43	0.47
2:B:1156:ASP:HB3	2:B:1197:PRO:HA	1.96	0.47
4:D:217:LEU:O	4:D:219:THR:N	2.47	0.47
5:E:182:ASP:HB3	5:E:185:ALA:HB2	1.96	0.47
6:F:81:THR:HB	6:F:136:ARG:NH1	2.29	0.47
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.96	0.47
1:M:332:LYS:O	1:M:333:GLU:CB	2.59	0.47
1:M:1166:ASP:OD1	1:M:1194:ARG:NH2	2.45	0.47
1:M:1444:MET:HE2	1:M:1444:MET:N	2.28	0.47
2:N:244:LEU:CD1	2:N:250:PHE:HD1	2.27	0.47
2:N:642:ASP:HB3	2:N:649:LYS:HD2	1.96	0.47
2:N:889:THR:O	2:N:889:THR:HG22	2.13	0.47
4:P:122:GLU:HA	4:P:125:SER:OG	2.14	0.47
8:T:87:ARG:O	8:T:89:LEU:HD23	2.14	0.47
1:A:409:SER:O	1:A:410:GLY:C	2.57	0.47
1:A:565:ILE:HG23	1:A:567:LYS:CG	2.38	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:LYS:HG3	1:A:691:LEU:HD23	1.96	0.47
1:A:961:ARG:HH11	1:A:961:ARG:CG	2.27	0.47
1:A:1135:ARG:HG2	1:A:1136:SER:N	2.27	0.47
1:A:1217:LYS:O	1:A:1221:LYS:HA	2.13	0.47
2:B:278:GLN:CG	2:B:279:ASP:N	2.78	0.47
2:B:658:ILE:HG22	2:B:659:ALA:N	2.28	0.47
2:B:798:TYR:HE2	3:C:62:PHE:CZ	2.32	0.47
15:3:5:C:H2'	15:3:6:A:H8	1.80	0.47
1:M:55:ASP:O	1:M:55:ASP:CG	2.54	0.47
1:M:107:CYS:CB	1:M:171:GLN:HE22	2.27	0.47
1:M:690:VAL:CG2	1:M:718:VAL:HG13	2.44	0.47
1:M:902:LEU:CD2	1:M:923:LEU:HD23	2.45	0.47
1:M:946:VAL:HG22	5:Q:201:LYS:HB3	1.96	0.47
1:M:1121:GLU:O	1:M:1122:PRO:C	2.57	0.47
2:N:473:MET:CE	2:N:474:SER:HA	2.38	0.47
2:N:1009:ASP:C	2:N:1010:LEU:HD12	2.39	0.47
4:P:56:ARG:HH21	4:P:155:ARG:CG	2.21	0.47
4:P:126:ILE:HD13	4:P:145:MET:CE	2.44	0.47
4:P:173:HIS:ND1	4:P:175:PHE:N	2.46	0.47
5:Q:35:VAL:C	5:Q:37:LEU:H	2.22	0.47
9:U:7:CYS:HB2	9:U:34:TYR:CG	2.49	0.47
11:W:101:LEU:HD23	11:W:101:LEU:C	2.39	0.47
12:X:40:LEU:HD22	12:X:44:ASP:CG	2.38	0.47
14:5:4:DA:H2''	14:5:5:DC:C6	2.48	0.47
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.42	0.47
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.96	0.47
1:A:593:GLU:C	1:A:595:THR:N	2.72	0.47
1:A:1006:ILE:HD11	5:E:163:GLU:CG	2.41	0.47
1:A:1120:LEU:C	1:A:1120:LEU:HD12	2.39	0.47
1:A:1208:THR:O	1:A:1209:MET:C	2.56	0.47
1:A:1397:LEU:HB2	1:A:1426:GLU:OE1	2.14	0.47
2:B:131:ASP:HA	2:B:164:LYS:HB3	1.96	0.47
2:B:1006:ILE:H	2:B:1006:ILE:HG13	1.41	0.47
3:C:226:ASP:O	3:C:227:THR:HB	2.14	0.47
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.49	0.47
5:E:108:GLY:O	5:E:132:ILE:HG23	2.15	0.47
6:F:103:MET:HE3	7:G:15:PRO:HG2	1.96	0.47
9:I:88:SER:C	9:I:90:GLN:H	2.22	0.47
12:L:33:GLU:OE1	12:L:55:ILE:HD11	2.15	0.47
14:2:3:DT:C2	14:2:4:DA:N7	2.82	0.47
1:M:407:ARG:HG2	1:M:430:TRP:CH2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1048:ASN:N	1:M:1048:ASN:HD22	2.10	0.47
2:N:95:ILE:HG13	2:N:130:VAL:CG2	2.43	0.47
2:N:97:VAL:HG12	2:N:97:VAL:O	2.13	0.47
2:N:378:LEU:O	2:N:378:LEU:HD12	2.13	0.47
2:N:515:HIS:HD2	2:N:517:THR:HG23	1.76	0.47
3:O:184:ASN:OD1	3:O:187:LYS:HA	2.15	0.47
4:P:190:GLU:HA	7:S:167:TYR:CE1	2.48	0.47
5:Q:162:ARG:HG2	5:Q:162:ARG:HH11	1.78	0.47
7:S:74:TYR:H	7:S:74:TYR:HD2	1.62	0.47
1:A:568:PRO:CB	3:C:221:TYR:OH	2.62	0.47
1:A:761:MET:HA	1:A:804:TYR:HB2	1.96	0.47
1:A:789:LYS:HD2	2:B:620:ARG:HH12	1.79	0.47
1:A:1121:GLU:O	1:A:1122:PRO:C	2.57	0.47
2:B:33:VAL:O	2:B:36:ALA:HB3	2.14	0.47
2:B:244:LEU:CD1	2:B:250:PHE:HD1	2.27	0.47
2:B:408:LEU:HD12	2:B:408:LEU:N	2.29	0.47
2:B:1050:ILE:HG22	2:B:1051:THR:N	2.28	0.47
2:B:1197:PRO:O	2:B:1200:ALA:N	2.44	0.47
4:D:7:THR:HG21	4:D:32:GLU:CD	2.39	0.47
4:D:209:ARG:HA	4:D:212:LYS:CD	2.43	0.47
5:E:94:LYS:HE2	5:E:98:ILE:CD1	2.27	0.47
7:G:88:ASP:OD2	7:G:88:ASP:N	2.46	0.47
9:I:77:LYS:O	9:I:79:HIS:N	2.47	0.47
12:L:38:LEU:CG	12:L:39:SER:N	2.77	0.47
1:M:13:THR:HB	1:M:1432:GLN:NE2	2.29	0.47
1:M:63:ARG:HA	1:M:74:MET:HE2	1.96	0.47
1:M:353:ILE:HG22	1:M:468:PHE:HB2	1.96	0.47
1:M:472:LEU:O	1:M:475:THR:CB	2.58	0.47
1:M:1332:PHE:HE1	1:M:1381:LEU:HD13	1.79	0.47
2:N:35:SER:O	2:N:39:ARG:HG3	2.13	0.47
2:N:114:PRO:O	2:N:115:GLN:C	2.55	0.47
2:N:244:LEU:HD12	2:N:250:PHE:HD1	1.79	0.47
2:N:251:ILE:HG22	2:N:251:ILE:O	2.15	0.47
2:N:604:ARG:CB	2:N:609:ILE:HG13	2.44	0.47
2:N:1079:LYS:HA	3:O:27:LEU:HD21	1.96	0.47
2:N:1110:PRO:O	2:N:1119:VAL:HG13	2.14	0.47
2:N:1201:LYS:CE	2:N:1205:GLN:OE1	2.59	0.47
4:P:58:VAL:HG11	7:S:4:ILE:HD11	1.95	0.47
5:Q:145:THR:HG21	5:Q:187:TYR:CE2	2.49	0.47
7:S:146:LYS:HD2	7:S:165:GLU:HG3	1.95	0.47
12:X:38:LEU:CG	12:X:39:SER:N	2.77	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:HG22	1:A:62:ASP:H	1.79	0.47
1:A:285:PRO:O	1:A:287:HIS:N	2.47	0.47
1:A:381:THR:CG2	1:A:382:PRO:HD2	2.44	0.47
1:A:709:THR:HG23	9:I:94:ASP:HA	1.97	0.47
1:A:946:VAL:CG2	5:E:201:LYS:HD2	2.42	0.47
2:B:227:LYS:HE2	2:B:236:HIS:CE1	2.49	0.47
2:B:335:GLY:O	2:B:336:ARG:HG3	2.13	0.47
4:D:122:GLU:HA	4:D:125:SER:OG	2.15	0.47
7:G:51:TYR:C	7:G:51:TYR:CD2	2.93	0.47
8:H:128:ASN:ND2	8:H:128:ASN:C	2.71	0.47
10:J:30:LEU:HD21	10:J:38:ARG:NH1	2.29	0.47
1:M:335:ARG:NH1	2:N:1202:LEU:HD13	2.29	0.47
1:M:354:SER:HA	1:M:482:PHE:CD2	2.49	0.47
1:M:820:GLY:O	1:M:823:GLY:N	2.48	0.47
2:N:43:LEU:HD11	2:N:811:TYR:O	2.14	0.47
2:N:642:ASP:CB	2:N:649:LYS:HG3	2.44	0.47
2:N:805:THR:CG2	2:N:806:THR:H	2.18	0.47
2:N:831:SER:HB2	2:N:833:TYR:HD1	1.79	0.47
2:N:835:GLN:HE21	2:N:835:GLN:HB2	1.48	0.47
2:N:878:GLN:HA	2:N:885:MET:SD	2.55	0.47
3:O:99:LEU:N	3:O:99:LEU:HD22	2.30	0.47
4:P:7:THR:O	4:P:7:THR:HG23	2.15	0.47
4:P:12:ARG:HD3	4:P:14:ARG:CG	2.43	0.47
4:P:216:ASN:O	4:P:218:GLU:N	2.48	0.47
7:S:120:THR:HG23	7:S:131:GLN:O	2.14	0.47
8:T:128:ASN:ND2	8:T:128:ASN:C	2.72	0.47
1:A:741:ASN:HD22	1:A:741:ASN:C	2.22	0.47
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.15	0.47
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	2.30	0.47
2:B:357:GLN:CD	2:B:368:GLU:HA	2.40	0.47
3:C:27:LEU:O	3:C:28:ALA:C	2.58	0.47
3:C:196:ASP:OD1	3:C:198:ALA:HB3	2.15	0.47
6:F:152:ILE:HG22	6:F:153:VAL:N	2.29	0.47
7:G:87:VAL:HG23	7:G:103:VAL:HG21	1.97	0.47
8:H:81:PRO:HB3	8:H:82:PRO:HD2	1.96	0.47
9:I:10:CYS:O	9:I:11:ASN:C	2.58	0.47
10:J:53:HIS:CD2	10:J:54:VAL:H	2.31	0.47
1:M:12:ARG:HD2	2:N:1218:THR:HB	1.96	0.47
1:M:56:PRO:O	1:M:57:ARG:CG	2.61	0.47
1:M:60:SER:OG	1:M:61:ILE:N	2.48	0.47
1:M:255:SER:OG	2:N:918:ILE:HD13	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:121:ASN:ND2	2:N:207:GLY:HA3	2.28	0.47
2:N:211:VAL:HG23	2:N:483:LEU:HB2	1.97	0.47
2:N:247:GLY:H	2:N:249:ARG:HH21	1.63	0.47
2:N:785:TYR:CD1	2:N:786:ASN:N	2.82	0.47
3:O:254:LYS:O	3:O:258:ILE:HD13	2.15	0.47
4:P:67:ARG:HG2	4:P:67:ARG:O	2.15	0.47
12:X:33:GLU:OE1	12:X:55:ILE:HD11	2.15	0.47
1:A:71:GLN:C	1:A:73:GLY:N	2.68	0.47
1:A:75:ASN:O	1:A:76:GLU:HB2	2.15	0.47
1:A:137:ALA:O	1:A:138:ILE:C	2.57	0.47
1:A:139:TRP:O	1:A:140:THR:C	2.58	0.47
1:A:305:ASP:OD1	1:A:306:ASN:N	2.47	0.47
1:A:310:GLY:O	1:A:312:PRO:CD	2.60	0.47
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.49	0.47
1:A:765:VAL:HB	1:A:800:VAL:CG1	2.45	0.47
1:A:899:VAL:HG22	1:A:908:LEU:HD21	1.95	0.47
1:A:949:ASP:OD1	1:A:951:GLU:HB2	2.14	0.47
1:A:1050:GLU:O	1:A:1054:LEU:HD12	2.14	0.47
1:A:1193:LEU:HB2	1:A:1260:LEU:HD11	1.96	0.47
1:A:1280:GLU:HB3	1:A:1281:ARG:H	1.59	0.47
2:B:102:VAL:CG2	2:B:112:LEU:HD22	2.44	0.47
2:B:115:GLN:HG2	2:B:193:LYS:CB	2.44	0.47
2:B:189:LEU:HA	2:B:192:LEU:HD12	1.96	0.47
2:B:487:THR:CG2	2:B:488:TYR:N	2.78	0.47
2:B:558:LEU:O	2:B:560:GLU:N	2.48	0.47
2:B:594:ALA:HA	2:B:617:ARG:HH11	1.80	0.47
2:B:597:MET:SD	2:B:617:ARG:HB2	2.55	0.47
2:B:807:ARG:HD3	2:B:1043:ASP:OD1	2.15	0.47
2:B:953:LEU:O	2:B:964:VAL:HG23	2.14	0.47
2:B:996:ARG:NH1	3:C:174:ALA:HA	2.20	0.47
2:B:1068:GLY:O	2:B:1069:PHE:C	2.58	0.47
3:C:73:GLN:NE2	3:C:75:MET:N	2.62	0.47
3:C:89:GLU:O	3:C:90:ASP:HB3	2.14	0.47
3:C:213:PRO:HG2	3:C:214:ASN:H	1.80	0.47
4:D:12:ARG:NH1	4:D:14:ARG:CA	2.78	0.47
4:D:156:ASP:O	4:D:157:GLN:C	2.57	0.47
5:E:204:THR:CG2	5:E:205:SER:N	2.77	0.47
7:G:111:THR:CG2	7:G:114:LEU:HB2	2.25	0.47
9:I:10:CYS:SG	9:I:32:CYS:HB3	2.54	0.47
10:J:9:SER:CB	10:J:45:CYS:HB2	2.45	0.47
1:M:378:GLU:OE1	1:M:434:ARG:HD3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:401:GLY:N	1:M:435:HIS:HD2	2.13	0.47
1:M:460:VAL:HG12	1:M:461:LYS:N	2.30	0.47
1:M:675:THR:HG21	1:M:736:ASN:HB2	1.96	0.47
1:M:689:LYS:O	1:M:693:VAL:HG23	2.14	0.47
1:M:826:ASP:C	1:M:826:ASP:OD1	2.56	0.47
1:M:853:ASP:OD1	1:M:853:ASP:C	2.57	0.47
1:M:963:ILE:HD13	1:M:1049:ILE:HG13	1.96	0.47
1:M:1257:ASP:HA	1:M:1260:LEU:HB3	1.97	0.47
1:M:1342:GLU:OE2	5:Q:212:ARG:NH1	2.46	0.47
1:M:1345:ARG:HG2	1:M:1372:VAL:CG1	2.45	0.47
2:N:417:PHE:HE1	2:N:453:ILE:HG21	1.80	0.47
2:N:483:LEU:HD11	2:N:491:THR:CG2	2.45	0.47
2:N:578:THR:C	2:N:589:VAL:HG13	2.40	0.47
2:N:641:GLU:OE1	2:N:641:GLU:HA	2.15	0.47
2:N:661:LEU:HD23	2:N:679:TYR:O	2.14	0.47
2:N:889:THR:HG23	2:N:891:ASP:HB2	1.97	0.47
2:N:891:ASP:C	2:N:893:LEU:N	2.72	0.47
3:O:27:LEU:O	3:O:28:ALA:C	2.58	0.47
4:P:161:GLY:O	4:P:165:GLN:HG3	2.14	0.47
5:Q:89:GLY:C	5:Q:91:LYS:H	2.23	0.47
5:Q:157:SER:C	5:Q:159:ASP:N	2.71	0.47
6:R:119:ARG:HH11	6:R:119:ARG:CG	2.28	0.47
7:S:1:MET:O	7:S:2:PHE:C	2.57	0.47
8:T:113:ALA:HA	8:T:125:LEU:O	2.14	0.47
1:A:134:ARG:HG2	1:A:138:ILE:HD11	1.97	0.47
1:A:144:THR:O	1:A:146:MET:HG3	2.14	0.47
1:A:321:PRO:O	1:A:322:VAL:CG1	2.63	0.47
1:A:364:VAL:O	1:A:364:VAL:HG13	2.15	0.47
1:A:874:ASP:C	1:A:874:ASP:OD1	2.58	0.47
1:A:909:ASP:OD1	1:A:911:SER:N	2.41	0.47
2:B:435:THR:C	2:B:437:GLU:H	2.21	0.47
2:B:863:GLU:OE1	2:B:962:LYS:HB2	2.15	0.47
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.96	0.47
8:H:99:GLY:HA3	8:H:118:PHE:CD2	2.49	0.47
1:M:208:LEU:C	1:M:208:LEU:CD2	2.88	0.47
1:M:305:ASP:OD1	1:M:306:ASN:N	2.48	0.47
1:M:416:ARG:HG3	1:M:416:ARG:HH11	1.79	0.47
1:M:523:ILE:HG13	1:M:622:VAL:HG22	1.97	0.47
1:M:545:GLN:O	1:M:546:VAL:C	2.56	0.47
2:N:90:ILE:HD11	2:N:432:MET:SD	2.55	0.47
2:N:273:LEU:CD1	2:N:280:ILE:HD12	2.37	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:1039:GLY:HA2	10:V:51:LEU:HD22	1.97	0.47
3:O:3:GLU:OE1	3:O:4:GLU:N	2.47	0.47
6:R:103:MET:O	6:R:104:ASN:HB2	2.13	0.47
11:W:12:LEU:HD12	11:W:37:LYS:CG	2.45	0.47
1:A:100:LYS:HE2	1:A:104:GLU:OE2	2.14	0.47
1:A:477:PRO:CG	1:A:521:MET:HG2	2.45	0.47
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.47	0.47
1:A:1100:ARG:HH21	1:A:1351:GLU:CD	2.23	0.47
2:B:458:LYS:O	2:B:459:TYR:C	2.58	0.47
5:E:144:ILE:HD13	5:E:183:PRO:HB3	1.97	0.47
5:E:147:HIS:CD2	5:E:148:GLU:N	2.83	0.47
9:I:74:GLU:HA	9:I:80:SER:O	2.15	0.47
1:M:175:ARG:HG2	1:M:182:VAL:HG12	1.97	0.47
1:M:322:VAL:O	1:M:322:VAL:HG13	2.15	0.47
1:M:645:LEU:HD11	1:M:649:ILE:HD11	1.97	0.47
1:M:845:LEU:HD12	1:M:1069:ALA:HB2	1.96	0.47
2:N:58:THR:O	2:N:62:ILE:HG13	2.15	0.47
2:N:167:ILE:HA	2:N:450:ALA:HB1	1.94	0.47
2:N:224:GLN:HA	2:N:396:ASP:OD2	2.15	0.47
2:N:371:GLU:OE1	2:N:371:GLU:N	2.47	0.47
3:O:186:LEU:HD12	3:O:186:LEU:N	2.29	0.47
3:O:259:LEU:CD2	11:W:91:CYS:HB3	2.45	0.47
3:O:265:MET:HB2	3:O:265:MET:HE3	1.76	0.47
4:P:53:SER:C	4:P:55:ALA:N	2.70	0.47
4:P:154:PHE:HE1	4:P:163:VAL:CG1	2.26	0.47
5:Q:177:ARG:HB3	5:Q:215:MET:HG2	1.96	0.47
7:S:129:SER:C	7:S:130:TYR:CD1	2.93	0.47
11:W:47:ARG:HD2	11:W:47:ARG:C	2.39	0.47
1:A:67:CYS:O	1:A:68:GLN:HG3	2.15	0.47
1:A:75:ASN:HD22	2:B:1116:ARG:HH12	1.62	0.47
1:A:472:LEU:HD13	2:B:835:GLN:OE1	2.15	0.47
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.50	0.47
1:A:1189:SER:O	1:A:1241:ARG:HD3	2.15	0.47
1:A:1277:GLU:O	1:A:1279:ILE:N	2.47	0.47
1:A:1438:THR:CG2	6:F:92:ARG:HD2	2.43	0.47
2:B:172:ILE:HD13	2:B:178:ASN:ND2	2.30	0.47
2:B:222:ILE:N	2:B:240:ILE:HD12	2.30	0.47
2:B:886:LYS:HB2	2:B:890:TYR:OH	2.15	0.47
2:B:906:SER:O	2:B:941:LEU:HD23	2.15	0.47
3:C:147:LEU:N	3:C:147:LEU:CD2	2.75	0.47
4:D:148:LEU:O	4:D:152:SER:OG	2.16	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:26:ARG:HH12	5:E:133:GLU:CD	2.23	0.47
6:F:77:ASP:OD1	6:F:78:GLN:N	2.48	0.47
1:M:310:GLY:C	1:M:312:PRO:HD2	2.39	0.47
1:M:444:PHE:HE2	1:M:470:LEU:HD13	1.80	0.47
1:M:879:GLU:O	1:M:955:PRO:HA	2.15	0.47
1:M:1207:LEU:CD1	1:M:1273:LEU:HD23	2.45	0.47
2:N:186:GLU:CG	10:V:62:ARG:HH22	2.28	0.47
2:N:258:LEU:O	2:N:258:LEU:CG	2.63	0.47
2:N:525:ALA:O	2:N:768:THR:HG23	2.15	0.47
2:N:792:MET:HA	2:N:856:PHE:O	2.15	0.47
4:P:60:LYS:O	4:P:64:VAL:HG23	2.15	0.47
7:S:26:LEU:HD12	7:S:56:ILE:HD11	1.97	0.47
8:T:84:ALA:HA	8:T:87:ARG:HB2	1.97	0.47
1:A:35:ILE:O	1:A:35:ILE:HG22	2.16	0.46
1:A:984:LYS:HG2	1:A:988:LEU:HD12	1.97	0.46
1:A:1378:GLN:HG2	5:E:177:ARG:HH12	1.80	0.46
2:B:223:VAL:HG21	2:B:380:TYR:HE2	1.80	0.46
2:B:376:PHE:CZ	2:B:569:TYR:HD2	2.33	0.46
2:B:1027:ILE:C	2:B:1029:CYS:N	2.73	0.46
7:G:91:VAL:HG12	7:G:92:VAL:N	2.29	0.46
8:H:82:PRO:C	8:H:84:ALA:N	2.52	0.46
8:H:98:TYR:C	8:H:118:PHE:HD2	2.24	0.46
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.50	0.46
12:L:55:ILE:O	12:L:56:LEU:HB2	2.15	0.46
1:M:356:ASP:C	1:M:358:ASN:H	2.23	0.46
1:M:1148:ILE:O	1:M:1148:ILE:HG22	2.15	0.46
2:N:171:PRO:HD2	2:N:457:LEU:CD1	2.46	0.46
2:N:1156:ASP:HB3	2:N:1197:PRO:HA	1.96	0.46
4:P:187:THR:HB	4:P:189:ASP:HB3	1.96	0.46
6:R:101:ILE:HD13	6:R:120:ILE:HG22	1.97	0.46
9:U:88:SER:C	9:U:90:GLN:H	2.23	0.46
1:A:741:ASN:ND2	1:A:743:VAL:N	2.63	0.46
1:A:996:ASN:C	1:A:998:LEU:HD12	2.40	0.46
1:A:1029:ARG:HH11	1:A:1029:ARG:CG	2.25	0.46
2:B:470:LYS:O	2:B:472:ALA:N	2.48	0.46
2:B:707:PRO:CG	2:B:708:GLU:H	2.24	0.46
2:B:980:PHE:CA	2:B:1095:LEU:HD11	2.45	0.46
2:B:996:ARG:NH2	3:C:175:ALA:H	2.12	0.46
3:C:7:GLN:NE2	11:K:104:ASN:HD21	2.09	0.46
4:D:60:LYS:O	4:D:64:VAL:HG23	2.15	0.46
5:E:62:ALA:HB3	5:E:78:LEU:CD2	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:116:ILE:HG22	5:E:120:ALA:HB3	1.97	0.46
8:H:123:MET:HE3	8:H:142:LEU:CD2	2.44	0.46
9:I:106:CYS:O	9:I:107:SER:HB2	2.14	0.46
1:M:137:ALA:O	1:M:138:ILE:C	2.58	0.46
1:M:320:ARG:NE	1:M:323:LYS:NZ	2.64	0.46
1:M:413:ILE:HG21	1:M:424:ILE:HD11	1.98	0.46
1:M:977:LYS:HB3	1:M:978:PRO:CD	2.45	0.46
1:M:1293:SER:HB3	1:M:1297:GLU:OE1	2.16	0.46
1:M:1375:MET:HG2	1:M:1382:THR:O	2.15	0.46
2:N:274:PRO:CG	2:N:359:GLU:HB3	2.45	0.46
2:N:637:LEU:HD22	2:N:742:GLU:HA	1.98	0.46
2:N:1095:LEU:C	2:N:1096:ARG:O	2.57	0.46
3:O:18:VAL:O	3:O:20:PHE:HD2	1.98	0.46
3:O:236:GLY:O	3:O:238:ILE:N	2.48	0.46
4:P:139:LYS:N	4:P:142:LYS:HE2	2.29	0.46
5:Q:117:THR:HG22	5:Q:119:SER:N	2.19	0.46
7:S:137:ILE:O	7:S:138:THR:OG1	2.32	0.46
8:T:38:LEU:HD12	8:T:124:ARG:O	2.16	0.46
1:A:61:ILE:HG22	1:A:62:ASP:N	2.31	0.46
1:A:78:PRO:HA	2:B:1201:LYS:NZ	2.30	0.46
1:A:444:PHE:CB	1:A:458:HIS:HD2	2.28	0.46
2:B:96:TYR:HE1	2:B:131:ASP:OD1	1.97	0.46
2:B:617:ARG:HA	2:B:624:LEU:HD12	1.96	0.46
2:B:891:ASP:C	2:B:893:LEU:N	2.72	0.46
2:B:1116:ARG:HG3	2:B:1198:TYR:CD1	2.50	0.46
3:C:18:VAL:O	3:C:20:PHE:HD2	1.98	0.46
4:D:219:THR:HG22	4:D:220:LEU:O	2.15	0.46
5:E:192:ARG:NH1	5:E:215:MET:O	2.49	0.46
1:M:33:ALA:HB1	1:M:56:PRO:HB2	1.97	0.46
1:M:34:LYS:HG3	1:M:36:ARG:NH2	2.29	0.46
1:M:253:ASN:ND2	2:N:884:ARG:CD	2.78	0.46
1:M:482:PHE:C	1:M:484:GLY:H	2.24	0.46
1:M:570:PRO:O	1:M:571:LEU:HD12	2.16	0.46
2:N:193:LYS:HD3	2:N:787:VAL:HG11	1.96	0.46
2:N:231:PRO:HG2	2:N:231:PRO:O	2.15	0.46
2:N:371:GLU:CD	2:N:371:GLU:N	2.74	0.46
2:N:1068:GLY:O	2:N:1069:PHE:O	2.34	0.46
3:O:133:ILE:CD1	3:O:237:SER:HA	2.45	0.46
3:O:167:HIS:CE1	12:X:70:ARG:HA	2.50	0.46
3:O:258:ILE:HD12	3:O:258:ILE:N	2.30	0.46
5:Q:207:ARG:HB3	5:Q:207:ARG:NH1	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:123:MET:HG2	8:T:124:ARG:N	2.30	0.46
9:U:80:SER:HG	9:U:105:SER:HB2	1.79	0.46
11:W:55:LYS:CB	11:W:81:TYR:CD1	2.98	0.46
11:W:65:HIS:CD2	11:W:65:HIS:C	2.92	0.46
1:A:310:GLY:C	1:A:312:PRO:HD2	2.40	0.46
1:A:382:PRO:CA	1:A:428:TYR:CE2	2.99	0.46
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.97	0.46
1:A:591:PHE:CD2	1:A:595:THR:HB	2.50	0.46
1:A:1121:GLU:HB3	1:A:1124:HIS:CD2	2.51	0.46
1:A:1277:GLU:O	1:A:1279:ILE:HG12	2.15	0.46
1:A:1284:MET:HA	1:A:1306:LEU:HD23	1.98	0.46
1:A:1362:TYR:CD1	1:A:1362:TYR:C	2.92	0.46
2:B:90:ILE:HD12	2:B:432:MET:SD	2.56	0.46
2:B:91:SER:OG	2:B:133:LYS:HB2	2.15	0.46
2:B:105:SER:O	2:B:106:ASP:HB2	2.15	0.46
2:B:168:GLY:HA2	2:B:450:ALA:O	2.15	0.46
2:B:205:ILE:N	2:B:205:ILE:CD1	2.78	0.46
2:B:258:LEU:O	2:B:258:LEU:CG	2.62	0.46
2:B:282:ILE:HG21	2:B:382:ILE:HD13	1.97	0.46
2:B:305:VAL:O	2:B:305:VAL:HG12	2.15	0.46
2:B:431:TYR:CG	2:B:447:ALA:HB2	2.50	0.46
2:B:621:GLU:HG3	2:B:621:GLU:O	2.14	0.46
2:B:642:ASP:C	2:B:644:GLU:H	2.18	0.46
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.15	0.46
2:B:1156:ASP:O	2:B:1157:ALA:HB3	2.15	0.46
2:B:1183:LYS:HE3	2:B:1183:LYS:O	2.15	0.46
3:C:252:GLN:HE21	11:K:95:ILE:CG2	2.28	0.46
4:D:40:HIS:NE2	7:G:73:LYS:HG2	2.30	0.46
5:E:42:PHE:HE1	5:E:58:MET:HE3	1.81	0.46
5:E:50:MET:CG	5:E:52:ARG:HH21	2.26	0.46
10:J:21:TYR:HB2	10:J:39:LEU:CD1	2.45	0.46
1:M:254:GLU:HB2	2:N:935:ARG:HH21	1.77	0.46
1:M:427:GLN:HB2	1:M:430:TRP:CD1	2.50	0.46
1:M:427:GLN:HB2	1:M:430:TRP:CG	2.51	0.46
1:M:623:GLY:C	1:M:625:SER:H	2.24	0.46
1:M:722:LEU:HD23	1:M:799:PHE:CG	2.51	0.46
1:M:1123:GLY:O	1:M:1125:ALA:N	2.49	0.46
1:M:1255:GLU:HG2	1:M:1258:HIS:HB2	1.98	0.46
2:N:245:GLU:O	2:N:246:LYS:HG3	2.16	0.46
3:O:22:LEU:HG	3:O:25:VAL:HG21	1.98	0.46
4:P:12:ARG:NH1	4:P:14:ARG:CA	2.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:54:GLU:OE1	9:U:118:ARG:NH2	2.49	0.46
9:U:82:GLU:OE2	9:U:104:LEU:HB2	2.16	0.46
9:U:86:PHE:CE1	9:U:100:PHE:HB2	2.51	0.46
1:A:806:ARG:HH12	2:B:729:ILE:HD11	1.80	0.46
1:A:828:ALA:C	1:A:831:THR:HG22	2.41	0.46
2:B:35:SER:HA	2:B:811:TYR:CE2	2.49	0.46
2:B:293:PRO:C	2:B:294:ASP:O	2.56	0.46
2:B:599:THR:O	2:B:603:LEU:HB2	2.15	0.46
2:B:871:THR:HG22	2:B:872:GLU:N	2.30	0.46
4:D:15:LEU:O	4:D:15:LEU:HD12	2.16	0.46
8:H:47:PHE:HB3	8:H:95:TYR:CD1	2.49	0.46
1:M:49:LYS:CD	1:M:55:ASP:HB3	2.46	0.46
1:M:220:THR:O	1:M:221:SER:C	2.58	0.46
1:M:341:MET:HE2	1:M:843:LYS:HZ1	1.80	0.46
1:M:504:LEU:CD1	6:R:91:ALA:HB2	2.45	0.46
1:M:1315:GLU:C	1:M:1317:MET:N	2.72	0.46
1:M:1316:VAL:O	1:M:1316:VAL:HG12	2.14	0.46
2:N:25:ILE:HD11	2:N:653:VAL:O	2.16	0.46
2:N:26:THR:O	2:N:29:ASP:HB2	2.16	0.46
2:N:35:SER:HA	2:N:811:TYR:CE2	2.42	0.46
2:N:758:PHE:CE1	2:N:1027:ILE:HG22	2.50	0.46
2:N:871:THR:O	2:N:917:PRO:HG3	2.15	0.46
3:O:104:PHE:HD2	3:O:105:GLY:N	2.14	0.46
4:P:154:PHE:HZ	4:P:214:LEU:CD1	2.27	0.46
9:U:75:CYS:SG	9:U:78:CYS:SG	3.13	0.46
1:A:623:GLY:C	1:A:625:SER:H	2.24	0.46
1:A:868:TYR:CZ	1:A:1366:ARG:HD3	2.50	0.46
2:B:129:PHE:HD2	2:B:166:PHE:HA	1.79	0.46
2:B:1095:LEU:H	2:B:1095:LEU:CD1	2.05	0.46
4:D:208:GLU:HA	4:D:211:LEU:HD12	1.97	0.46
5:E:164:LEU:HD21	5:E:211:TYR:CD1	2.51	0.46
7:G:35:GLU:HG3	7:G:48:VAL:HG23	1.96	0.46
10:J:2:ILE:HG12	10:J:57:ILE:HD13	1.98	0.46
11:K:113:THR:O	11:K:114:LEU:CB	2.64	0.46
12:L:65:VAL:HG23	12:L:67:PHE:HE1	1.80	0.46
1:M:43:GLU:CG	1:M:46:THR:HB	2.39	0.46
1:M:694:THR:O	1:M:698:GLN:HG3	2.15	0.46
2:N:189:LEU:O	2:N:192:LEU:HB2	2.16	0.46
2:N:222:ILE:N	2:N:240:ILE:HD12	2.31	0.46
2:N:497:ARG:NH2	2:N:775:LYS:NZ	2.64	0.46
2:N:616:ILE:HD12	2:N:625:LYS:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:622:LYS:CE	9:U:59:VAL:HG13	2.45	0.46
2:N:642:ASP:HB3	2:N:649:LYS:CG	2.45	0.46
2:N:664:THR:CG2	2:N:678:GLU:N	2.78	0.46
2:N:744:HIS:CD2	2:N:745:PRO:CD	2.86	0.46
2:N:850:LEU:HD12	2:N:851:PHE:H	1.80	0.46
2:N:861:ASP:OD1	2:N:862:GLN:N	2.49	0.46
2:N:871:THR:HG22	2:N:872:GLU:N	2.30	0.46
3:O:65:HIS:O	3:O:69:LEU:CD1	2.63	0.46
3:O:238:ILE:HD11	3:O:246:ARG:CZ	2.45	0.46
5:Q:65:THR:O	5:Q:69:ILE:CD1	2.63	0.46
5:Q:100:ILE:CG2	5:Q:105:PHE:HB2	2.44	0.46
7:S:1:MET:SD	7:S:79:PHE:CD1	3.09	0.46
7:S:88:ASP:OD2	7:S:88:ASP:C	2.59	0.46
7:S:126:ASN:HA	7:S:127:PRO:C	2.40	0.46
1:A:2:VAL:HG22	1:A:3:GLY:H	1.81	0.46
1:A:218:ASP:O	1:A:219:PHE:C	2.59	0.46
1:A:316:GLN:O	1:A:317:LYS:C	2.59	0.46
1:A:322:VAL:CG1	1:A:322:VAL:O	2.63	0.46
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.29	0.46
1:A:1365:TYR:C	1:A:1365:TYR:CD2	2.94	0.46
1:A:1395:GLY:HA3	1:A:1419:ASP:OD2	2.16	0.46
2:B:39:ARG:CZ	2:B:665:GLU:HG2	2.45	0.46
2:B:303:TYR:CD2	2:B:303:TYR:N	2.83	0.46
2:B:558:LEU:O	2:B:559:SER:C	2.58	0.46
2:B:1208:MET:O	2:B:1211:ASN:N	2.43	0.46
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.98	0.46
3:C:88:CYS:SG	3:C:91:HIS:HA	2.55	0.46
7:G:7:LEU:CD1	7:G:45:ILE:HD11	2.45	0.46
9:I:14:LEU:HD22	9:I:28:GLU:C	2.40	0.46
1:M:338:GLY:HA2	2:N:1129:ARG:HH22	1.81	0.46
1:M:1111:MET:HE2	1:M:1114:PRO:HA	1.97	0.46
2:N:679:TYR:CE1	2:N:683:SER:HB2	2.51	0.46
2:N:732:SER:HB2	2:N:734:HIS:CE1	2.51	0.46
2:N:865:LYS:NZ	2:N:869:SER:HA	2.31	0.46
2:N:877:PRO:C	2:N:878:GLN:HG3	2.40	0.46
2:N:1027:ILE:C	2:N:1029:CYS:N	2.73	0.46
4:P:7:THR:HB	7:S:42:PHE:HE2	1.79	0.46
5:Q:29:PHE:HA	5:Q:65:THR:HG22	1.98	0.46
5:Q:158:SER:O	5:Q:162:ARG:HD3	2.16	0.46
6:R:90:ARG:HD3	6:R:155:LEU:CD1	2.40	0.46
7:S:96:GLN:H	7:S:96:GLN:HG2	1.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:47:PHE:HB3	8:T:95:TYR:HD1	1.80	0.46
13:4:15:DG:H2"	13:4:16:DT:H71	1.97	0.46
1:A:92:HIS:O	1:A:93:VAL:C	2.57	0.46
1:A:245:PRO:O	1:A:248:PRO:HD3	2.16	0.46
1:A:427:GLN:HB2	1:A:430:TRP:CD2	2.50	0.46
1:A:915:SER:O	1:A:919:ILE:HB	2.16	0.46
2:B:114:PRO:O	2:B:115:GLN:C	2.57	0.46
2:B:497:ARG:HH21	2:B:775:LYS:HZ1	1.64	0.46
2:B:637:LEU:HD22	2:B:742:GLU:HA	1.96	0.46
7:G:21:ARG:HD2	7:G:24:GLN:HB3	1.96	0.46
1:M:134:ARG:CD	1:M:221:SER:O	2.62	0.46
1:M:600:PRO:HA	8:T:25:ARG:NH1	2.31	0.46
1:M:670:ILE:HD13	1:M:670:ILE:N	2.31	0.46
1:M:690:VAL:HG21	1:M:718:VAL:HG13	1.97	0.46
1:M:740:LEU:HD12	1:M:740:LEU:C	2.40	0.46
1:M:828:ALA:C	1:M:831:THR:HG22	2.40	0.46
2:N:240:ILE:HG23	2:N:240:ILE:O	2.16	0.46
2:N:619:ILE:HD12	9:U:65:ASP:HB2	1.98	0.46
2:N:758:PHE:CE2	2:N:1044:ALA:CA	2.93	0.46
2:N:1183:LYS:CE	2:N:1183:LYS:H	2.28	0.46
4:P:16:LYS:O	4:P:18:VAL:N	2.41	0.46
4:P:191:ALA:O	4:P:193:THR:N	2.49	0.46
4:P:195:ILE:HB	4:P:198:LEU:HD11	1.97	0.46
10:V:36:LEU:HD11	10:V:51:LEU:HB2	1.98	0.46
1:A:230:ARG:HG3	1:A:233:TRP:CE3	2.51	0.46
1:A:365:GLY:HA3	1:A:463:ILE:HD13	1.97	0.46
1:A:920:LEU:HD23	1:A:920:LEU:C	2.41	0.46
1:A:1394:THR:CG2	1:A:1398:MET:SD	3.04	0.46
2:B:90:ILE:HD11	2:B:432:MET:SD	2.55	0.46
2:B:246:LYS:HA	2:B:249:ARG:CZ	2.46	0.46
2:B:552:MET:C	2:B:554:ILE:N	2.74	0.46
2:B:658:ILE:HG22	2:B:662:MET:HE2	1.96	0.46
3:C:239:PRO:O	3:C:242:GLN:N	2.45	0.46
5:E:100:ILE:HG23	5:E:105:PHE:CD1	2.51	0.46
5:E:147:HIS:CD2	5:E:149:LEU:H	2.27	0.46
6:F:93:ILE:CD1	6:F:134:ILE:HD11	2.37	0.46
9:I:15:TYR:N	9:I:15:TYR:HD1	2.13	0.46
11:K:50:LEU:HD11	11:K:75:ILE:HD11	1.97	0.46
1:M:697:ALA:CB	1:M:702:LEU:HD11	2.45	0.46
1:M:807:GLY:HA2	2:N:760:ASP:O	2.15	0.46
1:M:825:ILE:O	1:M:829:VAL:HG23	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:946:VAL:CG2	5:Q:201:LYS:HD2	2.45	0.46
2:N:311:LEU:O	2:N:312:GLU:C	2.57	0.46
2:N:521:LEU:HD22	2:N:633:VAL:CG1	2.26	0.46
3:O:3:GLU:OE1	3:O:4:GLU:HB2	2.16	0.46
3:O:16:ASP:OD1	3:O:16:ASP:N	2.49	0.46
3:O:73:GLN:HE21	3:O:75:MET:HB2	1.78	0.46
4:P:156:ASP:CB	4:P:159:THR:HG23	2.36	0.46
4:P:185:CYS:SG	4:P:191:ALA:CA	3.04	0.46
4:P:189:ASP:OD2	7:S:167:TYR:CE1	2.69	0.46
6:R:100:GLN:HE22	7:S:61:ILE:HD13	1.81	0.46
12:X:60:ARG:HG2	12:X:61:THR:N	2.31	0.46
1:A:35:ILE:HA	1:A:52:GLY:O	2.16	0.46
1:A:130:ASP:O	1:A:131:SER:C	2.59	0.46
1:A:181:LEU:HA	1:A:181:LEU:HD23	1.80	0.46
1:A:255:SER:OG	2:B:918:ILE:HD13	2.15	0.46
1:A:878:ILE:HG21	1:A:955:PRO:HB2	1.98	0.46
1:A:929:LEU:HD21	1:A:983:ILE:HG21	1.98	0.46
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.30	0.46
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.46	0.46
1:A:1450:LEU:O	1:A:1450:LEU:HG	2.15	0.46
2:B:331:LEU:HD21	2:B:353:LYS:HG2	1.97	0.46
2:B:331:LEU:O	2:B:334:ILE:HB	2.16	0.46
2:B:558:LEU:CD2	2:B:596:LEU:HD11	2.46	0.46
2:B:620:ARG:CZ	9:I:68:LEU:HD21	2.45	0.46
2:B:857:ARG:HH21	2:B:942:ARG:NH2	2.14	0.46
2:B:1115:THR:HG21	2:B:1117:GLN:HB2	1.98	0.46
2:B:1170:THR:O	2:B:1171:VAL:C	2.59	0.46
3:C:44:LEU:CD2	3:C:159:ALA:HB1	2.46	0.46
4:D:35:LEU:HD12	4:D:35:LEU:N	2.28	0.46
5:E:164:LEU:HD21	5:E:211:TYR:CG	2.50	0.46
8:H:77:ARG:HG2	8:H:78:SER:H	1.81	0.46
1:M:75:ASN:O	1:M:76:GLU:CB	2.62	0.46
1:M:208:LEU:HA	1:M:235:ILE:HD12	1.97	0.46
1:M:225:ASN:ND2	1:M:225:ASN:C	2.73	0.46
1:M:367:PRO:HB3	1:M:465:TYR:O	2.16	0.46
1:M:834:THR:CG2	1:M:835:GLY:N	2.79	0.46
2:N:51:PHE:O	2:N:54:PHE:HB3	2.16	0.46
2:N:247:GLY:C	2:N:249:ARG:N	2.71	0.46
2:N:277:LYS:HG2	2:N:336:ARG:CB	2.46	0.46
2:N:298:LEU:N	2:N:298:LEU:CD2	2.79	0.46
2:N:552:MET:C	2:N:554:ILE:N	2.74	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:1169:MET:CE	2:N:1204:PHE:HB2	2.46	0.46
3:O:177:GLU:HG3	3:O:231:ASN:HD22	1.81	0.46
4:P:35:LEU:CD1	4:P:35:LEU:H	2.28	0.46
4:P:67:ARG:HB2	4:P:133:THR:CG2	2.45	0.46
4:P:134:THR:CG2	4:P:135:GLY:N	2.79	0.46
4:P:194:LEU:CB	7:S:86:VAL:HG21	2.46	0.46
7:S:111:THR:O	7:S:112:LYS:C	2.59	0.46
8:T:95:TYR:C	8:T:95:TYR:CD2	2.94	0.46
1:A:575:LYS:HZ1	1:A:602:ASP:CG	2.24	0.45
1:A:829:VAL:HG11	2:B:508:LEU:HD22	1.98	0.45
1:A:960:ILE:HA	1:A:963:ILE:CG2	2.46	0.45
1:A:1036:ARG:NH1	1:A:1036:ARG:CG	2.74	0.45
2:B:121:ASN:HA	2:B:207:GLY:CA	2.46	0.45
2:B:233:PRO:HG2	2:B:234:ILE:HD13	1.97	0.45
2:B:613:VAL:HG22	2:B:628:THR:HA	1.98	0.45
2:B:860:MET:HB2	2:B:965:LYS:HG2	1.98	0.45
2:B:877:PRO:C	2:B:878:GLN:HG3	2.40	0.45
2:B:1008:PRO:HB3	2:B:1087:PHE:HE2	1.82	0.45
4:D:6:SER:HB3	7:G:8:SER:OG	2.16	0.45
4:D:220:LEU:CG	4:D:221:TYR:H	2.29	0.45
8:H:40:LEU:HD12	8:H:123:MET:CG	2.46	0.45
8:H:56:THR:HB	8:H:145:ARG:HG2	1.97	0.45
12:L:43:THR:HG22	12:L:43:THR:O	2.16	0.45
1:M:53:LEU:CD2	1:M:54:ASN:N	2.51	0.45
1:M:61:ILE:O	1:M:63:ARG:N	2.49	0.45
1:M:1109:LYS:C	1:M:1110:ASN:HD22	2.24	0.45
2:N:427:ASP:HA	2:N:430:ARG:HG3	1.97	0.45
2:N:1102:LYS:O	2:N:1103:ILE:C	2.58	0.45
3:O:80:LEU:HD11	3:O:95:CYS:CA	2.46	0.45
3:O:166:GLU:HG3	11:W:10:PHE:CZ	2.43	0.45
4:P:153:ARG:HB3	4:P:154:PHE:CE2	2.51	0.45
4:P:212:LYS:O	4:P:215:SER:OG	2.33	0.45
9:U:10:CYS:O	9:U:11:ASN:C	2.59	0.45
10:V:7:CYS:CB	10:V:49:MET:HE3	2.46	0.45
11:W:40:HIS:O	11:W:41:THR:C	2.59	0.45
11:W:47:ARG:HD2	11:W:47:ARG:O	2.16	0.45
1:A:185:TRP:CH2	1:A:200:ARG:HG2	2.51	0.45
1:A:1048:ASN:HD22	1:A:1048:ASN:N	2.14	0.45
1:A:1158:PRO:C	1:A:1159:ARG:HG3	2.41	0.45
2:B:619:ILE:HG22	2:B:620:ARG:N	2.30	0.45
2:B:806:THR:HG22	2:B:808:ALA:CB	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1109:GLY:O	2:B:1110:PRO:C	2.59	0.45
4:D:162:ALA:HA	4:D:165:GLN:HE21	1.80	0.45
11:K:12:LEU:HD12	11:K:37:LYS:HG3	1.98	0.45
11:K:13:GLY:O	11:K:14:GLU:C	2.59	0.45
1:M:315:LEU:HD23	1:M:315:LEU:N	2.31	0.45
1:M:321:PRO:O	1:M:322:VAL:CG1	2.60	0.45
1:M:899:VAL:CB	1:M:929:LEU:HD12	2.43	0.45
1:M:1127:ASP:CG	1:M:1130:GLN:CB	2.89	0.45
1:M:1148:ILE:HG12	1:M:1198:ASP:HB2	1.98	0.45
1:M:1208:THR:O	1:M:1209:MET:C	2.58	0.45
1:M:1323:ASP:C	1:M:1325:THR:H	2.24	0.45
1:M:1445:ILE:HD12	1:M:1445:ILE:N	2.30	0.45
2:N:167:ILE:HG21	2:N:424:LEU:HD21	1.99	0.45
3:O:43:THR:HG22	3:O:44:LEU:N	2.31	0.45
3:O:193:TYR:C	3:O:193:TYR:HD1	2.24	0.45
5:Q:134:THR:O	5:Q:135:PHE:CD1	2.69	0.45
1:A:133:LYS:O	1:A:136:ALA:HB3	2.16	0.45
1:A:167:CYS:HB2	1:A:169:ASN:ND2	2.32	0.45
2:B:167:ILE:HA	2:B:450:ALA:HB1	1.95	0.45
2:B:387:LEU:HD12	2:B:387:LEU:N	2.31	0.45
2:B:448:ILE:O	2:B:450:ALA:N	2.49	0.45
2:B:582:VAL:CG2	2:B:626:ILE:HB	2.43	0.45
3:C:183:TRP:O	3:C:185:LYS:HG3	2.16	0.45
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.98	0.45
5:E:190:LEU:C	5:E:191:LYS:HG2	2.42	0.45
6:F:109:VAL:CG1	6:F:110:ASP:N	2.73	0.45
8:H:27:GLU:HA	8:H:38:LEU:O	2.17	0.45
8:H:87:ARG:O	8:H:89:LEU:HD23	2.16	0.45
8:H:95:TYR:CE2	8:H:97:MET:CG	2.99	0.45
13:1:15:DG:H2''	13:1:16:DT:H71	1.98	0.45
1:M:920:LEU:HD23	1:M:920:LEU:C	2.41	0.45
1:M:1400:CYS:O	1:M:1405:THR:HG23	2.16	0.45
2:N:69:LEU:HD13	2:N:429:PHE:HD1	1.82	0.45
2:N:470:LYS:O	2:N:472:ALA:N	2.49	0.45
2:N:641:GLU:C	2:N:643:ASP:H	2.24	0.45
3:O:67:LEU:HD11	3:O:155:LEU:CD1	2.46	0.45
4:P:193:THR:CG2	4:P:194:LEU:HD23	2.46	0.45
9:U:73:ARG:NH1	9:U:112:SER:HB3	2.29	0.45
11:W:7:PHE:CD1	11:W:7:PHE:C	2.95	0.45
12:X:68:GLU:CD	12:X:68:GLU:H	2.11	0.45
15:6:5:C:O2'	15:6:6:A:H5'	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.82	0.45
1:A:566:ILE:O	1:A:567:LYS:O	2.34	0.45
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.17	0.45
1:A:898:ARG:HD3	1:A:933:TYR:CD1	2.51	0.45
1:A:1029:ARG:CG	1:A:1029:ARG:NH1	2.79	0.45
2:B:95:ILE:CB	2:B:130:VAL:HG22	2.47	0.45
2:B:100:PRO:HA	2:B:125:SER:O	2.16	0.45
2:B:222:ILE:N	2:B:240:ILE:CD1	2.79	0.45
2:B:227:LYS:HG3	2:B:395:GLN:OE1	2.17	0.45
2:B:347:LYS:HG3	2:B:348:ARG:H	1.80	0.45
2:B:803:LEU:HD13	2:B:1032:SER:HB3	1.97	0.45
2:B:990:ILE:HG22	2:B:991:GLY:N	2.30	0.45
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.16	0.45
2:B:1204:PHE:O	2:B:1208:MET:HG3	2.15	0.45
2:B:1220:ARG:HB3	2:B:1220:ARG:HH11	1.82	0.45
3:C:186:LEU:O	3:C:187:LYS:HB2	2.17	0.45
3:C:258:ILE:HG23	11:K:19:LEU:HD11	1.99	0.45
4:D:134:THR:CG2	4:D:135:GLY:H	2.28	0.45
4:D:216:ASN:O	4:D:218:GLU:N	2.50	0.45
5:E:89:GLY:C	5:E:91:LYS:N	2.74	0.45
5:E:106:GLN:HE22	5:E:129:PRO:HB2	1.82	0.45
8:H:83:GLN:C	8:H:85:GLY:H	2.23	0.45
8:H:133:ASN:O	8:H:135:LEU:N	2.48	0.45
1:M:130:ASP:O	1:M:131:SER:C	2.59	0.45
1:M:251:SER:HA	1:M:257:ARG:O	2.17	0.45
1:M:381:THR:HG21	1:M:383:TYR:CD1	2.52	0.45
1:M:590:ARG:O	1:M:591:PHE:CB	2.59	0.45
1:M:857:ARG:NH2	6:R:139:PRO:HG3	2.30	0.45
1:M:1095:THR:CG2	1:M:1112:LYS:HD2	2.46	0.45
1:M:1198:ASP:O	1:M:1202:MET:HG2	2.16	0.45
1:M:1227:ILE:HG22	1:M:1228:TRP:N	2.30	0.45
1:M:1313:LEU:HD23	1:M:1338:VAL:CG2	2.47	0.45
1:M:1396:ALA:HA	1:M:1399:ARG:NH2	2.31	0.45
1:M:1410:PHE:HA	2:N:1212:ILE:HD11	1.97	0.45
2:N:376:PHE:CZ	2:N:569:TYR:HB3	2.52	0.45
2:N:557:PHE:CE1	2:N:603:LEU:HD11	2.51	0.45
2:N:936:ASP:CG	2:N:937:ALA:N	2.74	0.45
2:N:1064:TYR:O	2:N:1065:GLN:C	2.59	0.45
3:O:144:ILE:HG22	3:O:145:CYS:HB3	1.98	0.45
3:O:239:PRO:O	3:O:242:GLN:N	2.47	0.45
3:O:243:VAL:O	3:O:243:VAL:CG1	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:142:ARG:CB	7:S:171:ILE:HD11	2.47	0.45
9:U:100:PHE:N	9:U:100:PHE:CD1	2.84	0.45
1:A:262:LEU:HD12	1:A:328:ARG:NH2	2.31	0.45
1:A:1291:VAL:CG2	1:A:1292:PRO:HD2	2.47	0.45
2:B:185:THR:O	2:B:188:ASP:N	2.50	0.45
2:B:230:ALA:HB3	2:B:231:PRO:HD3	1.97	0.45
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.82	0.45
2:B:637:LEU:HD22	2:B:741:CYS:O	2.17	0.45
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.58	0.45
2:B:847:ASP:CG	3:C:167:HIS:HD2	2.24	0.45
2:B:871:THR:O	2:B:917:PRO:HG3	2.15	0.45
2:B:1064:TYR:O	2:B:1065:GLN:C	2.59	0.45
2:B:1084:GLN:H	2:B:1084:GLN:HE21	1.64	0.45
2:B:1106:ARG:HH12	2:B:1110:PRO:HG2	1.81	0.45
3:C:208:GLU:O	3:C:210:GLU:N	2.49	0.45
4:D:130:LEU:C	4:D:132:GLN:N	2.75	0.45
4:D:190:GLU:O	4:D:194:LEU:HG	2.16	0.45
7:G:55:ASP:HB3	7:G:73:LYS:HB2	1.98	0.45
1:M:61:ILE:CG2	1:M:62:ASP:H	2.28	0.45
1:M:1217:LYS:O	1:M:1221:LYS:HA	2.15	0.45
2:N:552:MET:HE1	2:N:555:ILE:HG21	1.99	0.45
2:N:558:LEU:O	2:N:559:SER:C	2.59	0.45
2:N:1006:ILE:H	2:N:1006:ILE:HG13	1.33	0.45
2:N:1096:ARG:HB2	2:N:1096:ARG:HH11	1.81	0.45
2:N:1200:ALA:O	2:N:1201:LYS:C	2.60	0.45
3:O:29:MET:HE1	11:W:97:LYS:HD2	1.99	0.45
4:P:23:ASN:HA	4:P:28:GLN:O	2.15	0.45
4:P:195:ILE:N	4:P:196:PRO:CD	2.79	0.45
4:P:202:ILE:HD11	4:P:207:LEU:HA	1.98	0.45
5:Q:179:GLN:HB2	5:Q:182:ASP:HB2	1.99	0.45
9:U:74:GLU:HA	9:U:80:SER:O	2.17	0.45
12:X:40:LEU:HD13	12:X:44:ASP:CB	2.32	0.45
15:6:3:A:H2'	15:6:4:C:C6	2.51	0.45
1:A:44:THR:O	1:A:45:GLN:CB	2.64	0.45
1:A:56:PRO:O	1:A:57:ARG:CZ	2.65	0.45
1:A:66:LYS:O	1:A:67:CYS:CB	2.64	0.45
1:A:697:ALA:HA	1:A:702:LEU:HG	1.97	0.45
1:A:977:LYS:HB3	1:A:978:PRO:CD	2.44	0.45
1:A:1116:LEU:HB3	1:A:1308:THR:CG2	2.46	0.45
1:A:1152:ILE:HG23	1:A:1260:LEU:HD23	1.98	0.45
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:807:ARG:HB3	2:B:807:ARG:HH11	1.82	0.45
8:H:57:VAL:HG12	8:H:58:THR:N	2.32	0.45
10:J:14:VAL:O	10:J:14:VAL:CG1	2.63	0.45
1:M:107:CYS:SG	1:M:108:MET:O	2.75	0.45
1:M:683:ILE:HD13	1:M:801:GLU:HG3	1.99	0.45
1:M:878:ILE:HG21	1:M:955:PRO:HB2	1.98	0.45
1:M:1313:LEU:HB3	1:M:1338:VAL:HG21	1.98	0.45
1:M:1438:THR:CG2	6:R:92:ARG:HD2	2.47	0.45
2:N:112:LEU:HD12	2:N:113:TYR:H	1.81	0.45
2:N:223:VAL:HG21	2:N:380:TYR:HE2	1.82	0.45
2:N:435:THR:C	2:N:437:GLU:H	2.23	0.45
2:N:744:HIS:HD2	2:N:745:PRO:CG	2.30	0.45
2:N:1031:LEU:O	2:N:1031:LEU:HD12	2.16	0.45
3:O:133:ILE:CD1	3:O:236:GLY:C	2.89	0.45
4:P:35:LEU:HD11	4:P:173:HIS:NE2	2.32	0.45
4:P:134:THR:HG22	4:P:135:GLY:H	1.79	0.45
6:R:119:ARG:CG	6:R:119:ARG:NH1	2.80	0.45
10:V:42:LYS:HG2	10:V:43:ARG:N	2.32	0.45
1:A:66:LYS:NZ	1:A:68:GLN:H	2.14	0.45
1:A:72:GLU:HB3	1:A:76:GLU:CG	2.47	0.45
1:A:196:GLU:CG	1:A:197:PRO:HD2	2.46	0.45
1:A:472:LEU:HD11	2:B:835:GLN:NE2	2.32	0.45
1:A:837:ILE:HG12	1:A:840:ARG:NH1	2.31	0.45
1:A:855:THR:HG23	1:A:857:ARG:CG	2.39	0.45
1:A:879:GLU:O	1:A:955:PRO:HA	2.17	0.45
1:A:1447:GLU:OE2	7:G:23:LYS:HB2	2.17	0.45
2:B:174:LEU:HD22	2:B:202:TYR:CE1	2.52	0.45
2:B:975:GLN:HG2	2:B:976:ILE:H	1.82	0.45
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.53	0.45
2:B:1110:PRO:C	2:B:1119:VAL:HG13	2.42	0.45
3:C:114:TYR:CD2	3:C:140:ASN:CB	2.99	0.45
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.99	0.45
4:D:40:HIS:C	4:D:42:GLY:H	2.24	0.45
5:E:21:GLU:O	5:E:24:LYS:HG2	2.17	0.45
6:F:101:ILE:HD11	6:F:124:GLU:OE1	2.17	0.45
7:G:139:ILE:HD13	7:G:140:LYS:HE3	1.98	0.45
8:H:30:SER:HB3	8:H:36:CYS:HB3	1.99	0.45
8:H:123:MET:HE1	8:H:142:LEU:HD13	1.98	0.45
10:J:56:LEU:O	10:J:57:ILE:C	2.60	0.45
1:M:106:VAL:CG1	1:M:111:GLY:HA2	2.47	0.45
1:M:256:GLN:O	1:M:257:ARG:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1438:THR:HG23	6:R:92:ARG:HD2	1.98	0.45
2:N:555:ILE:HG22	2:N:556:THR:N	2.32	0.45
2:N:777:ALA:HA	2:N:1095:LEU:HA	1.98	0.45
2:N:796:LEU:HD12	2:N:852:ARG:O	2.17	0.45
3:O:233:GLU:OE1	10:V:12:LYS:HE2	2.16	0.45
3:O:253:LYS:O	3:O:256:ALA:HB3	2.17	0.45
8:T:81:PRO:HB2	8:T:82:PRO:HD2	1.97	0.45
8:T:133:ASN:O	8:T:135:LEU:N	2.49	0.45
1:A:42:ASP:HB3	1:A:45:GLN:CA	2.47	0.45
1:A:182:VAL:HG23	1:A:201:VAL:HA	1.98	0.45
1:A:524:VAL:CG1	1:A:525:GLN:H	2.11	0.45
1:A:568:PRO:HB3	3:C:221:TYR:OH	2.17	0.45
1:A:1222:ASN:O	1:A:1223:ASP:HB3	2.16	0.45
1:A:1268:LEU:HD13	9:I:48:LEU:HD11	1.98	0.45
1:A:1297:GLU:N	1:A:1297:GLU:OE1	2.50	0.45
2:B:48:LEU:HD23	2:B:173:MET:SD	2.57	0.45
2:B:93:GLY:O	2:B:130:VAL:HG13	2.16	0.45
2:B:189:LEU:O	2:B:192:LEU:HB2	2.17	0.45
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.65	0.45
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.98	0.45
2:B:842:ASN:HD21	2:B:844:SER:HB2	1.82	0.45
2:B:908:GLU:O	2:B:909:ASP:C	2.59	0.45
4:D:146:GLN:HA	4:D:149:THR:CG2	2.44	0.45
5:E:55:ARG:C	5:E:57:MET:N	2.71	0.45
5:E:96:PHE:O	5:E:99:HIS:HB3	2.16	0.45
6:F:148:VAL:O	6:F:149:GLU:C	2.60	0.45
7:G:1:MET:HE2	7:G:1:MET:O	2.17	0.45
8:H:63:LEU:HD23	8:H:90:ALA:HB3	1.99	0.45
10:J:53:HIS:HD2	10:J:54:VAL:H	1.63	0.45
1:M:84:ILE:HG22	1:M:86:LEU:HD23	1.99	0.45
1:M:536:LEU:H	1:M:536:LEU:HG	1.54	0.45
1:M:670:ILE:HD13	1:M:670:ILE:H	1.80	0.45
1:M:878:ILE:CG2	1:M:955:PRO:HB2	2.47	0.45
1:M:1115:SER:OG	1:M:1116:LEU:N	2.50	0.45
1:M:1453:TYR:O	1:M:1454:MET:HB3	2.17	0.45
2:N:169:ARG:HB2	2:N:454:THR:HG23	1.99	0.45
3:O:46:ILE:HG13	3:O:72:LEU:HD11	1.98	0.45
4:P:12:ARG:HH12	4:P:14:ARG:HA	1.82	0.45
5:Q:55:ARG:C	5:Q:57:MET:N	2.71	0.45
6:R:69:LEU:HB3	6:R:71:GLU:CG	2.47	0.45
7:S:123:ALA:C	7:S:125:SER:H	2.25	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:83:GLN:C	8:T:85:GLY:H	2.24	0.45
9:U:77:LYS:C	9:U:79:HIS:H	2.24	0.45
14:5:3:DT:C2	14:5:4:DA:N7	2.85	0.45
1:A:61:ILE:O	1:A:63:ARG:N	2.50	0.45
1:A:164:ARG:HG3	1:A:165:GLY:H	1.82	0.45
1:A:225:ASN:ND2	1:A:227:VAL:N	2.63	0.45
1:A:259:GLU:OE1	1:A:259:GLU:HA	2.17	0.45
1:A:316:GLN:HG2	1:A:317:LYS:H	1.81	0.45
1:A:560:ILE:HD11	11:K:58:PHE:HD1	1.82	0.45
1:A:1107:VAL:O	1:A:1107:VAL:CG1	2.59	0.45
1:A:1111:MET:HG3	1:A:1114:PRO:HB3	1.97	0.45
2:B:24:PRO:O	2:B:25:ILE:HG23	2.17	0.45
2:B:69:LEU:HD13	2:B:429:PHE:HD1	1.81	0.45
2:B:205:ILE:HG12	2:B:461:LEU:HB3	1.99	0.45
2:B:311:LEU:O	2:B:312:GLU:C	2.58	0.45
2:B:582:VAL:O	2:B:582:VAL:HG12	2.16	0.45
2:B:591:ARG:O	2:B:592:ASN:C	2.59	0.45
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.99	0.45
2:B:899:ILE:HG22	2:B:900:ALA:O	2.16	0.45
4:D:138:ASN:C	4:D:140:ASP:N	2.71	0.45
4:D:167:LEU:C	4:D:169:SER:H	2.25	0.45
9:I:17:ARG:HG3	9:I:28:GLU:OE1	2.16	0.45
9:I:98:VAL:CG1	9:I:111:THR:HG23	2.46	0.45
9:I:100:PHE:N	9:I:100:PHE:CD1	2.85	0.45
1:M:295:LEU:O	1:M:298:PHE:HB3	2.17	0.45
1:M:511:ILE:HA	1:M:521:MET:HE3	1.99	0.45
1:M:524:VAL:O	1:M:525:GLN:C	2.60	0.45
1:M:767:GLN:HA	1:M:799:PHE:HA	1.99	0.45
1:M:1081:LEU:HD11	1:M:1098:VAL:H	1.82	0.45
1:M:1169:ILE:H	1:M:1169:ILE:HG13	1.55	0.45
2:N:345:LYS:HA	2:N:348:ARG:HG2	1.99	0.45
2:N:482:VAL:O	2:N:483:LEU:C	2.59	0.45
2:N:642:ASP:C	2:N:644:GLU:H	2.20	0.45
2:N:651:LEU:HD21	2:N:741:CYS:HB3	1.98	0.45
2:N:891:ASP:C	2:N:893:LEU:H	2.24	0.45
4:P:40:HIS:CE1	7:S:74:TYR:O	2.70	0.45
4:P:215:SER:HA	4:P:218:GLU:OE2	2.16	0.45
6:R:69:LEU:C	6:R:71:GLU:HG3	2.41	0.45
6:R:69:LEU:HD22	6:R:71:GLU:OE1	2.16	0.45
1:A:150:THR:HG22	1:A:150:THR:O	2.16	0.45
1:A:153:PRO:HB3	1:A:161:LEU:CD2	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:HIS:ND1	2:B:1074:ASN:ND2	2.65	0.45
1:A:688:LYS:HA	1:A:691:LEU:HB3	1.99	0.45
1:A:868:TYR:CE1	1:A:1064:VAL:HG13	2.51	0.45
1:A:1066:VAL:O	1:A:1070:GLN:HG3	2.16	0.45
2:B:26:THR:O	2:B:29:ASP:HB2	2.17	0.45
2:B:203:PHE:HB3	2:B:205:ILE:CD1	2.47	0.45
2:B:281:PRO:HG2	2:B:284:ILE:HD12	1.99	0.45
2:B:314:LEU:O	2:B:318:VAL:HG23	2.17	0.45
2:B:467:GLY:CA	2:B:475:SER:HB3	2.47	0.45
2:B:482:VAL:O	2:B:483:LEU:C	2.59	0.45
2:B:604:ARG:CB	2:B:609:ILE:HG13	2.46	0.45
2:B:976:ILE:HD13	2:B:992:ILE:HA	1.99	0.45
2:B:984:HIS:CD2	2:B:1025:HIS:HA	2.52	0.45
3:C:24:ASN:CG	3:C:24:ASN:O	2.59	0.45
3:C:82:TYR:O	3:C:83:SER:C	2.60	0.45
4:D:67:ARG:O	4:D:67:ARG:HG2	2.17	0.45
5:E:61:GLN:HB2	5:E:79:TRP:HE3	1.82	0.45
9:I:82:GLU:CB	9:I:104:LEU:HD12	2.47	0.45
11:K:7:PHE:CD1	11:K:7:PHE:C	2.95	0.45
1:M:62:ASP:O	1:M:62:ASP:OD1	2.34	0.45
1:M:392:VAL:HG13	1:M:415:LEU:CD1	2.47	0.45
1:M:720:ARG:O	1:M:724:GLU:CB	2.65	0.45
1:M:744:LYS:CG	1:M:748:MET:HE2	2.47	0.45
1:M:1011:GLN:NE2	1:M:1015:VAL:HG23	2.31	0.45
1:M:1329:THR:HG23	1:M:1331:SER:N	2.31	0.45
2:N:497:ARG:NH2	2:N:775:LYS:HZ2	2.15	0.45
2:N:710:LEU:HA	2:N:733:HIS:CB	2.24	0.45
2:N:787:VAL:O	2:N:787:VAL:HG12	2.17	0.45
2:N:865:LYS:C	2:N:866:TYR:HD1	2.25	0.45
2:N:941:LEU:HD11	2:N:968:VAL:HG21	1.98	0.45
2:N:970:THR:HG22	2:N:971:THR:N	2.31	0.45
2:N:1004:GLU:HG3	10:V:42:LYS:HZ3	1.82	0.45
3:O:189:THR:CG2	3:O:190:ASP:N	2.80	0.45
5:Q:128:PRO:HA	5:Q:129:PRO:O	2.17	0.45
8:T:56:THR:O	8:T:144:ILE:HA	2.17	0.45
1:A:162:VAL:HG12	1:A:163:SER:N	2.32	0.44
1:A:311:GLN:O	1:A:312:PRO:C	2.58	0.44
1:A:567:LYS:CG	1:A:568:PRO:CD	2.93	0.44
1:A:1100:ARG:O	1:A:1103:GLU:HB3	2.18	0.44
1:A:1454:MET:O	1:A:1454:MET:HG3	2.17	0.44
2:B:29:ASP:OD1	2:B:658:ILE:HG21	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:GLY:C	2:B:249:ARG:N	2.72	0.44
2:B:542:MET:HE3	2:B:747:MET:HG3	1.98	0.44
2:B:891:ASP:C	2:B:893:LEU:H	2.25	0.44
2:B:941:LEU:CD1	2:B:968:VAL:HG21	2.46	0.44
2:B:997:GLU:HG2	3:C:39:ALA:HB2	2.00	0.44
3:C:138:GLU:OE1	3:C:138:GLU:N	2.50	0.44
7:G:1:MET:SD	7:G:79:PHE:CE1	3.09	0.44
8:H:62:SER:OG	8:H:63:LEU:N	2.50	0.44
1:M:72:GLU:HB3	1:M:76:GLU:CG	2.47	0.44
1:M:547:LEU:HD21	1:M:560:ILE:HD13	1.98	0.44
1:M:1120:LEU:C	1:M:1120:LEU:HD12	2.41	0.44
2:N:361:LEU:HD11	2:N:381:MET:HE1	1.98	0.44
2:N:508:LEU:N	2:N:512:ARG:HE	2.15	0.44
2:N:552:MET:HA	2:N:552:MET:CE	2.45	0.44
2:N:773:MET:C	2:N:775:LYS:H	2.25	0.44
2:N:983:ARG:HD2	2:N:1091:TYR:HD2	1.81	0.44
4:P:188:ALA:CB	4:P:204:ASP:OD1	2.57	0.44
5:Q:4:GLU:HB3	5:Q:7:ARG:NE	2.31	0.44
7:S:98:GLY:HA3	7:S:110:VAL:O	2.16	0.44
8:T:27:GLU:HA	8:T:38:LEU:O	2.18	0.44
8:T:37:LYS:HD2	8:T:126:GLU:OE2	2.17	0.44
9:U:34:TYR:O	9:U:35:VAL:HG23	2.17	0.44
9:U:56:ALA:O	9:U:57:GLY:O	2.35	0.44
9:U:99:LEU:C	9:U:100:PHE:HD1	2.25	0.44
10:V:13:VAL:O	10:V:14:VAL:HG23	2.17	0.44
1:A:325:ILE:CG2	2:B:1210:MET:HE2	2.48	0.44
1:A:545:GLN:O	1:A:546:VAL:C	2.58	0.44
1:A:853:ASP:O	1:A:854:ASN:HB2	2.17	0.44
1:A:1255:GLU:CG	1:A:1258:HIS:CD2	3.00	0.44
2:B:916:THR:HB	2:B:935:ARG:CD	2.46	0.44
3:C:180:TYR:HB3	3:C:228:PHE:HD2	1.82	0.44
5:E:129:PRO:O	5:E:130:ALA:O	2.35	0.44
10:J:1:MET:HG3	10:J:1:MET:O	2.17	0.44
12:L:61:THR:HG22	12:L:62:LYS:N	2.33	0.44
1:M:153:PRO:HB3	1:M:161:LEU:CD2	2.47	0.44
1:M:635:ARG:HA	1:M:635:ARG:HH11	1.82	0.44
1:M:688:LYS:HA	1:M:691:LEU:HB3	1.99	0.44
1:M:902:LEU:HD21	1:M:923:LEU:HD23	1.99	0.44
1:M:904:THR:O	1:M:904:THR:CG2	2.66	0.44
1:M:914:GLU:C	1:M:916:GLY:H	2.26	0.44
1:M:1030:ARG:HG2	1:M:1034:GLU:OE2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1277:GLU:C	1:M:1279:ILE:N	2.74	0.44
1:M:1325:THR:CG2	1:M:1326:ARG:HG3	2.47	0.44
1:M:1370:LEU:O	1:M:1374:VAL:HG23	2.17	0.44
2:N:299:GLU:OE2	2:N:571:PRO:HG2	2.17	0.44
2:N:399:ASP:OD2	2:N:510:LYS:HB2	2.16	0.44
2:N:908:GLU:O	2:N:909:ASP:C	2.60	0.44
2:N:1197:PRO:O	2:N:1198:TYR:C	2.57	0.44
4:P:56:ARG:HG2	4:P:56:ARG:NH1	2.32	0.44
4:P:123:LEU:CD1	4:P:149:THR:HG21	2.47	0.44
4:P:130:LEU:C	4:P:132:GLN:N	2.75	0.44
4:P:155:ARG:HE	4:P:221:TYR:HE1	1.55	0.44
4:P:167:LEU:C	4:P:169:SER:H	2.25	0.44
4:P:220:LEU:CG	4:P:221:TYR:H	2.30	0.44
5:Q:157:SER:N	5:Q:160:GLU:OE1	2.47	0.44
8:T:91:ASP:O	8:T:93:TYR:N	2.46	0.44
10:V:48:ARG:NH1	10:V:48:ARG:CG	2.75	0.44
1:A:107:CYS:HB2	1:A:114:LEU:CD2	2.47	0.44
1:A:115:LEU:HD12	1:A:142:CYS:HB3	1.98	0.44
1:A:447:GLN:OE1	13:1:20:DG:H4'	2.17	0.44
1:A:1095:THR:CG2	1:A:1112:LYS:HD2	2.44	0.44
1:A:1445:ILE:HD12	7:G:59:GLY:O	2.17	0.44
2:B:128:LEU:HB2	2:B:168:GLY:O	2.17	0.44
2:B:773:MET:C	2:B:775:LYS:H	2.25	0.44
2:B:1113:VAL:CG2	15:3:1:C:H4'	2.48	0.44
3:C:214:ASN:O	3:C:217:ASP:OD2	2.36	0.44
4:D:15:LEU:O	4:D:17:LYS:HG3	2.18	0.44
4:D:156:ASP:C	4:D:158:GLU:N	2.74	0.44
4:D:218:GLU:O	4:D:219:THR:C	2.60	0.44
7:G:81:PRO:HG3	7:G:106:MET:SD	2.57	0.44
11:K:55:LYS:CB	11:K:81:TYR:CD1	3.00	0.44
11:K:88:LYS:O	11:K:91:CYS:HB2	2.18	0.44
15:3:3:A:H2'	15:3:4:C:C6	2.52	0.44
1:M:71:GLN:C	1:M:73:GLY:N	2.71	0.44
1:M:549:MET:SD	1:M:577:ILE:HD12	2.57	0.44
1:M:562:THR:HB	8:T:98:TYR:CD2	2.52	0.44
1:M:595:THR:C	1:M:596:THR:HG23	2.42	0.44
1:M:963:ILE:HD13	1:M:1049:ILE:CG1	2.48	0.44
1:M:1102:LYS:O	1:M:1106:ASN:ND2	2.50	0.44
1:M:1277:GLU:O	1:M:1279:ILE:HG12	2.18	0.44
1:M:1376:THR:O	1:M:1377:THR:C	2.59	0.44
2:N:46:GLN:NE2	2:N:539:LEU:HD12	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:469:GLN:HB3	2:N:470:LYS:H	1.44	0.44
2:N:593:PRO:O	2:N:594:ALA:C	2.60	0.44
2:N:644:GLU:HG3	2:N:646:LEU:C	2.43	0.44
3:O:123:ASN:HD21	3:O:125:MET:HG2	1.74	0.44
4:P:138:ASN:O	4:P:139:LYS:C	2.60	0.44
5:Q:17:ARG:O	5:Q:21:GLU:HG3	2.17	0.44
5:Q:22:MET:CE	5:Q:26:ARG:NH2	2.81	0.44
5:Q:155:ARG:NH1	5:Q:194:GLU:OE2	2.47	0.44
10:V:9:SER:CB	10:V:45:CYS:HB2	2.47	0.44
12:X:30:ILE:CD1	12:X:59:ALA:HB2	2.44	0.44
1:A:35:ILE:HD13	1:A:241:VAL:HG11	1.99	0.44
1:A:61:ILE:O	1:A:62:ASP:C	2.60	0.44
1:A:481:ASP:OD1	1:A:481:ASP:N	2.51	0.44
1:A:714:PHE:CG	9:I:97:MET:HE1	2.52	0.44
1:A:800:VAL:HG22	1:A:812:GLU:HB3	1.98	0.44
1:A:982:THR:N	1:A:985:ASP:HB2	2.32	0.44
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.98	0.44
2:B:51:PHE:O	2:B:54:PHE:HB3	2.17	0.44
3:C:258:ILE:HD12	3:C:258:ILE:N	2.31	0.44
6:F:83:PRO:HD2	6:F:84:TYR:HD1	1.83	0.44
6:F:110:ASP:O	6:F:123:LYS:CE	2.66	0.44
8:H:40:LEU:CD1	8:H:123:MET:HG3	2.47	0.44
11:K:18:LYS:NZ	11:K:37:LYS:O	2.50	0.44
12:L:47:ARG:CD	12:L:52:GLY:HA2	2.47	0.44
1:M:321:PRO:O	1:M:322:VAL:CB	2.65	0.44
1:M:458:HIS:CE1	1:M:507:VAL:HG21	2.52	0.44
1:M:461:LYS:O	1:M:463:ILE:HG23	2.18	0.44
1:M:1267:MET:HA	1:M:1271:ILE:HD12	2.00	0.44
1:M:1398:MET:HE3	1:M:1425:SER:HB2	1.99	0.44
1:M:1445:ILE:H	1:M:1445:ILE:CD1	2.27	0.44
2:N:558:LEU:HD21	2:N:600:LEU:HD11	1.98	0.44
2:N:591:ARG:O	2:N:592:ASN:C	2.59	0.44
2:N:617:ARG:NE	2:N:619:ILE:HG12	2.26	0.44
2:N:707:PRO:HG2	2:N:708:GLU:N	2.31	0.44
2:N:789:MET:HE3	2:N:965:LYS:CB	2.47	0.44
2:N:806:THR:HG22	2:N:808:ALA:CB	2.47	0.44
2:N:1039:GLY:HA2	10:V:51:LEU:CD2	2.48	0.44
2:N:1182:CYS:O	2:N:1182:CYS:SG	2.75	0.44
6:R:74:ILE:HD12	6:R:144:GLU:HG2	1.99	0.44
1:A:69:THR:HG21	2:B:1174:LYS:NZ	2.32	0.44
1:A:251:SER:HA	1:A:257:ARG:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.53	0.44
1:A:817:ALA:O	1:A:818:MET:C	2.60	0.44
1:A:905:ASP:C	1:A:906:HIS:ND1	2.76	0.44
1:A:914:GLU:C	1:A:916:GLY:H	2.26	0.44
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.98	0.44
1:A:997:LEU:HD13	1:A:1018:PHE:CE2	2.52	0.44
1:A:1116:LEU:N	1:A:1308:THR:CG2	2.67	0.44
1:A:1148:ILE:HG12	9:I:49:ILE:HD12	1.98	0.44
2:B:244:LEU:O	2:B:246:LYS:N	2.51	0.44
2:B:955:THR:HG23	2:B:956:THR:H	1.83	0.44
3:C:23:SER:O	3:C:24:ASN:HB3	2.18	0.44
7:G:9:LEU:HD12	7:G:10:ASN:H	1.83	0.44
1:M:311:GLN:O	1:M:312:PRO:C	2.59	0.44
1:M:316:GLN:HG2	1:M:317:LYS:CG	2.47	0.44
1:M:889:SER:OG	1:M:891:ALA:HB3	2.18	0.44
1:M:946:VAL:HG12	1:M:947:PHE:CD2	2.51	0.44
2:N:93:GLY:O	2:N:130:VAL:HG13	2.17	0.44
2:N:185:THR:O	2:N:188:ASP:N	2.51	0.44
2:N:203:PHE:CD1	2:N:203:PHE:N	2.86	0.44
2:N:293:PRO:C	2:N:294:ASP:O	2.59	0.44
2:N:347:LYS:HG3	2:N:348:ARG:N	2.33	0.44
2:N:461:LEU:CD1	2:N:461:LEU:H	2.31	0.44
2:N:1138:MET:HE2	2:N:1146:PHE:HD2	1.81	0.44
4:P:60:LYS:HE2	4:P:126:ILE:HG12	1.99	0.44
5:Q:37:LEU:O	5:Q:37:LEU:HG	2.18	0.44
6:R:118:LEU:O	6:R:122:MET:HG3	2.16	0.44
7:S:41:LYS:HD3	7:S:42:PHE:CE1	2.52	0.44
8:T:142:LEU:C	8:T:143:LEU:HD12	2.42	0.44
10:V:27:GLU:C	10:V:29:GLU:N	2.75	0.44
1:A:593:GLU:O	1:A:595:THR:N	2.45	0.44
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.35	0.44
1:A:1081:LEU:HD11	1:A:1097:GLY:HA3	1.99	0.44
1:A:1121:GLU:HG3	1:A:1122:PRO:HD2	1.95	0.44
1:A:1223:ASP:HA	1:A:1243:VAL:HG21	1.96	0.44
1:A:1265:ASN:C	1:A:1267:MET:N	2.73	0.44
2:B:25:ILE:HD13	2:B:653:VAL:HG12	1.99	0.44
2:B:530:GLY:O	2:B:531:GLN:C	2.61	0.44
3:C:11:ARG:NH1	3:C:205:LYS:NZ	2.63	0.44
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.99	0.44
3:C:134:ILE:HG21	3:C:139:GLY:HA2	1.99	0.44
3:C:167:HIS:CE1	12:L:70:ARG:HA	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:90:THR:HG22	7:G:91:VAL:N	2.32	0.44
9:I:16:PRO:HB3	9:I:27:PHE:HE2	1.82	0.44
10:J:31:ASP:O	10:J:32:GLU:C	2.60	0.44
1:M:69:THR:O	1:M:71:GLN:HG2	2.18	0.44
1:M:282:ASN:O	1:M:284:ALA:N	2.51	0.44
1:M:821:ARG:O	1:M:821:ARG:HG3	2.17	0.44
1:M:904:THR:O	1:M:904:THR:HG22	2.17	0.44
1:M:982:THR:N	1:M:985:ASP:HB2	2.33	0.44
2:N:431:TYR:CG	2:N:447:ALA:CB	3.01	0.44
2:N:613:VAL:HG13	2:N:627:PHE:C	2.41	0.44
2:N:847:ASP:CG	3:O:167:HIS:HD2	2.25	0.44
3:O:80:LEU:HD12	3:O:81:GLU:H	1.82	0.44
3:O:249:ASP:O	3:O:250:THR:C	2.61	0.44
4:P:153:ARG:NH2	4:P:184:ALA:HA	2.32	0.44
5:Q:127:ILE:HG13	5:Q:127:ILE:O	2.17	0.44
6:R:97:ARG:NH2	6:R:108:PHE:CE1	2.86	0.44
11:W:111:LEU:HD23	11:W:111:LEU:N	2.33	0.44
14:5:4:DA:C4	14:5:5:DC:C5	3.06	0.44
1:A:102:VAL:CG1	1:A:211:PHE:HE1	2.31	0.44
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.82	0.44
1:A:365:GLY:CA	1:A:463:ILE:HD13	2.48	0.44
1:A:659:HIS:O	2:B:1081:LEU:HD23	2.18	0.44
1:A:1116:LEU:C	1:A:1116:LEU:HD12	2.43	0.44
1:A:1257:ASP:HA	1:A:1260:LEU:HB3	2.00	0.44
2:B:35:SER:O	2:B:39:ARG:HG3	2.17	0.44
2:B:134:LYS:NZ	2:B:164:LYS:HE2	2.32	0.44
2:B:552:MET:O	2:B:554:ILE:N	2.51	0.44
2:B:640:VAL:O	2:B:640:VAL:CG1	2.66	0.44
2:B:840:ILE:CG2	2:B:994:TYR:HD1	2.29	0.44
3:C:66:ARG:NH1	10:J:2:ILE:CG2	2.78	0.44
5:E:112:TYR:OH	5:E:136:ASN:HB2	2.18	0.44
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.83	0.44
1:M:40:THR:HG22	1:M:41:MET:CG	2.46	0.44
1:M:92:HIS:HD2	1:M:236:LEU:HD21	1.82	0.44
1:M:225:ASN:HD22	1:M:225:ASN:C	2.25	0.44
1:M:343:LYS:HB2	2:N:1117:GLN:OE1	2.18	0.44
1:M:817:ALA:O	1:M:818:MET:C	2.60	0.44
1:M:855:THR:HG23	1:M:857:ARG:CG	2.43	0.44
1:M:1101:LEU:HB2	1:M:1355:VAL:HG11	1.99	0.44
1:M:1152:ILE:HG23	1:M:1260:LEU:CD2	2.48	0.44
2:N:125:SER:O	2:N:126:SER:HB3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:879:ARG:CZ	2:N:879:ARG:N	2.70	0.44
2:N:1103:ILE:HG23	2:N:1103:ILE:O	2.17	0.44
3:O:23:SER:O	3:O:24:ASN:HB3	2.18	0.44
3:O:113:VAL:HG23	3:O:147:LEU:HD21	1.99	0.44
4:P:208:GLU:HA	4:P:211:LEU:HD12	1.99	0.44
5:Q:43:LYS:O	5:Q:45:LYS:N	2.50	0.44
6:R:109:VAL:HG11	6:R:123:LYS:HG2	1.98	0.44
12:X:38:LEU:C	12:X:38:LEU:HD12	2.42	0.44
1:A:444:PHE:CE2	1:A:487:MET:CE	3.01	0.44
1:A:841:LEU:HD23	1:A:841:LEU:HA	1.84	0.44
1:A:868:TYR:OH	1:A:1366:ARG:HD3	2.17	0.44
1:A:893:PHE:CE1	1:A:940:ARG:HD2	2.52	0.44
4:D:156:ASP:HB2	4:D:159:THR:HG23	1.99	0.44
5:E:63:ASN:HB3	5:E:64:PRO:HD2	1.99	0.44
5:E:147:HIS:HD2	5:E:149:LEU:N	2.11	0.44
5:E:164:LEU:HD11	5:E:211:TYR:CD1	2.53	0.44
5:E:197:LYS:HE2	5:E:199:ILE:CD1	2.27	0.44
7:G:122:ASN:HB2	7:G:131:GLN:HG3	2.00	0.44
1:M:93:VAL:HG21	1:M:301:ALA:O	2.18	0.44
1:M:599:SER:HA	1:M:600:PRO:HD2	1.80	0.44
1:M:599:SER:HB2	1:M:603:ASN:H	1.82	0.44
1:M:709:THR:CG2	1:M:710:LEU:H	2.29	0.44
1:M:942:PHE:CZ	5:Q:207:ARG:HG3	2.53	0.44
1:M:1213:GLY:O	1:M:1214:GLU:C	2.60	0.44
2:N:118:ARG:HH11	2:N:204:ILE:CD1	2.30	0.44
2:N:362:PRO:C	2:N:363:HIS:O	2.57	0.44
2:N:816:GLU:O	2:N:817:LEU:HD23	2.18	0.44
2:N:916:THR:HB	2:N:935:ARG:HD2	2.00	0.44
3:O:70:ILE:HD11	3:O:144:ILE:HG12	2.00	0.44
3:O:132:PRO:O	3:O:134:ILE:HG13	2.17	0.44
3:O:147:LEU:HB2	3:O:151:GLN:CB	2.41	0.44
4:P:118:THR:HB	4:P:121:LYS:CG	2.48	0.44
5:Q:21:GLU:O	5:Q:24:LYS:HG2	2.18	0.44
5:Q:89:GLY:C	5:Q:91:LYS:N	2.76	0.44
5:Q:116:ILE:HG22	5:Q:117:THR:N	2.33	0.44
13:4:16:DT:H2''	13:4:17:DT:O5'	2.18	0.44
1:A:463:ILE:HD12	1:A:469:ARG:HD2	1.99	0.44
1:A:568:PRO:HG3	8:H:46:LEU:O	2.17	0.44
1:A:601:LYS:HB2	1:A:603:ASN:HD21	1.79	0.44
1:A:610:GLY:O	1:A:611:GLN:NE2	2.51	0.44
1:A:774:ARG:H	1:A:774:ARG:HG2	1.38	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.52	0.44
1:A:1120:LEU:H	1:A:1120:LEU:HG	1.57	0.44
1:A:1148:ILE:O	1:A:1148:ILE:HG22	2.18	0.44
1:A:1293:SER:HB3	1:A:1297:GLU:OE1	2.18	0.44
2:B:114:PRO:CG	2:B:181:LEU:HD11	2.33	0.44
2:B:322:PHE:CD2	2:B:322:PHE:C	2.95	0.44
2:B:707:PRO:CG	2:B:708:GLU:N	2.81	0.44
2:B:773:MET:O	2:B:775:LYS:N	2.50	0.44
2:B:866:TYR:CD2	2:B:870:ILE:HB	2.52	0.44
2:B:942:ARG:HB2	2:B:945:GLU:HB2	1.99	0.44
3:C:240:VAL:HG23	3:C:241:ASP:N	2.33	0.44
4:D:123:LEU:CD1	4:D:149:THR:HG21	2.48	0.44
4:D:173:HIS:ND1	4:D:174:PRO:HD2	2.33	0.44
5:E:52:ARG:HA	5:E:53:PRO:HD2	1.85	0.44
9:I:77:LYS:C	9:I:79:HIS:H	2.25	0.44
1:M:78:PRO:CA	2:N:1201:LYS:HZ1	2.29	0.44
1:M:219:PHE:HE1	1:M:230:ARG:HH21	1.64	0.44
1:M:893:PHE:CE1	1:M:940:ARG:HD2	2.52	0.44
2:N:281:PRO:HB3	2:N:320:ASP:OD2	2.18	0.44
2:N:310:MET:HB2	2:N:310:MET:HE3	1.93	0.44
3:O:13:ALA:O	11:W:114:LEU:HD13	2.18	0.44
3:O:133:ILE:HD11	3:O:237:SER:HA	2.00	0.44
3:O:166:GLU:CG	11:W:10:PHE:HZ	2.26	0.44
3:O:235:VAL:HG21	10:V:6:ARG:NH2	2.33	0.44
4:P:146:GLN:C	4:P:149:THR:HG22	2.41	0.44
4:P:186:ASP:OD1	4:P:186:ASP:N	2.51	0.44
5:Q:201:LYS:HD3	5:Q:201:LYS:HA	1.82	0.44
6:R:97:ARG:NH2	6:R:108:PHE:HE1	2.16	0.44
12:X:47:ARG:CG	12:X:52:GLY:HA2	2.48	0.44
1:A:528:LEU:O	1:A:531:ILE:HG22	2.18	0.43
1:A:595:THR:C	1:A:596:THR:HG23	2.42	0.43
1:A:920:LEU:C	1:A:920:LEU:CD2	2.90	0.43
1:A:971:PHE:CE2	1:A:1040:GLN:HG2	2.52	0.43
1:A:1167:GLU:O	1:A:1170:ILE:CD1	2.66	0.43
1:A:1207:LEU:HD11	1:A:1273:LEU:HD23	1.99	0.43
1:A:1209:MET:CE	1:A:1236:LEU:HB3	2.48	0.43
1:A:1215:ARG:O	1:A:1219:THR:N	2.47	0.43
1:A:1259:MET:HA	1:A:1262:LYS:CD	2.47	0.43
2:B:280:ILE:CD1	2:B:334:ILE:HG12	2.47	0.43
2:B:399:ASP:OD2	2:B:510:LYS:HB2	2.18	0.43
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:ASP:O	3:C:47:ASP:CG	2.61	0.43
3:C:248:ILE:HD11	11:K:101:LEU:HD22	2.00	0.43
4:D:52:LEU:HD12	4:D:182:SER:HB2	2.00	0.43
5:E:102:GLU:C	5:E:104:ASN:N	2.73	0.43
8:H:76:THR:HG22	8:H:141:TYR:OH	2.18	0.43
10:J:36:LEU:HB2	10:J:47:ARG:NH1	2.33	0.43
12:L:27:LEU:HD13	12:L:37:LYS:CD	2.47	0.43
15:3:5:C:O2'	15:3:6:A:H5'	2.18	0.43
1:M:929:LEU:HD21	1:M:983:ILE:HD13	1.99	0.43
2:N:429:PHE:O	2:N:433:GLN:HG3	2.18	0.43
2:N:594:ALA:CA	2:N:617:ARG:NH1	2.81	0.43
2:N:757:PRO:HG2	2:N:984:HIS:HE1	1.83	0.43
2:N:1050:ILE:HG22	2:N:1051:THR:N	2.32	0.43
2:N:1214:PRO:HG2	2:N:1214:PRO:O	2.18	0.43
3:O:101:LEU:C	3:O:102:GLN:CG	2.90	0.43
4:P:47:LEU:CD1	4:P:47:LEU:C	2.91	0.43
5:Q:63:ASN:HB3	5:Q:64:PRO:HD2	1.99	0.43
7:S:138:THR:CG2	7:S:139:ILE:H	2.29	0.43
9:U:34:TYR:CE2	9:U:36:GLU:HB3	2.53	0.43
12:X:33:GLU:CD	12:X:33:GLU:N	2.75	0.43
1:A:140:THR:HA	1:A:143:LYS:HE2	2.00	0.43
1:A:185:TRP:CE3	1:A:185:TRP:N	2.83	0.43
1:A:590:ARG:HG2	1:A:590:ARG:HH11	1.83	0.43
1:A:663:SER:OG	1:A:664:THR:N	2.45	0.43
1:A:718:VAL:O	1:A:721:PHE:HB2	2.18	0.43
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.36	0.43
2:B:797:TYR:HE1	2:B:854:LEU:HD23	1.82	0.43
2:B:847:ASP:O	2:B:849:GLY:N	2.51	0.43
2:B:999:MET:HB3	2:B:1007:VAL:CG2	2.47	0.43
3:C:69:LEU:O	10:J:6:ARG:HD2	2.17	0.43
4:D:138:ASN:O	4:D:139:LYS:C	2.61	0.43
5:E:135:PHE:HD2	5:E:140:LEU:CD2	2.30	0.43
8:H:145:ARG:O	8:H:146:ARG:CB	2.66	0.43
9:I:56:ALA:O	9:I:57:GLY:O	2.36	0.43
10:J:53:HIS:HE1	10:J:55:ASP:OD1	2.01	0.43
12:L:26:THR:HG23	12:L:62:LYS:HZ1	1.82	0.43
1:M:54:ASN:HB3	1:M:247:ARG:NH1	2.20	0.43
1:M:54:ASN:CB	1:M:247:ARG:HH12	2.22	0.43
2:N:291:ILE:HG22	2:N:297:ILE:HG12	1.99	0.43
2:N:461:LEU:N	2:N:461:LEU:CD1	2.80	0.43
2:N:679:TYR:HE1	2:N:687:GLU:OE2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:1004:GLU:OE1	10:V:42:LYS:HE2	2.18	0.43
2:N:1116:ARG:HG3	2:N:1198:TYR:CD2	2.53	0.43
2:N:1197:PRO:HG2	2:N:1200:ALA:HB2	2.00	0.43
3:O:73:GLN:NE2	3:O:75:MET:H	2.04	0.43
3:O:241:ASP:HB3	11:W:109:TRP:CE2	2.52	0.43
4:P:218:GLU:O	4:P:219:THR:C	2.61	0.43
5:Q:2:ASP:C	5:Q:3:GLN:HG2	2.43	0.43
5:Q:98:ILE:HA	5:Q:101:GLN:HB3	2.00	0.43
9:U:7:CYS:C	9:U:8:ARG:O	2.60	0.43
11:W:102:LYS:O	11:W:106:GLU:HG3	2.17	0.43
1:A:853:ASP:OD1	1:A:853:ASP:C	2.60	0.43
1:A:856:THR:HG21	1:A:1370:LEU:HD21	2.00	0.43
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.17	0.43
2:B:629:ASP:HB3	2:B:632:ARG:CD	2.49	0.43
2:B:769:TYR:C	2:B:771:SER:N	2.73	0.43
2:B:916:THR:HB	2:B:935:ARG:HG3	1.99	0.43
2:B:918:ILE:HD12	2:B:935:ARG:CZ	2.48	0.43
2:B:957:ASN:O	2:B:960:GLY:N	2.52	0.43
2:B:1033:LYS:NZ	2:B:1070:GLU:OE1	2.43	0.43
3:C:233:GLU:OE1	10:J:12:LYS:HE2	2.18	0.43
5:E:11:ARG:C	5:E:13:TRP:N	2.74	0.43
6:F:76:LYS:O	6:F:79:ARG:HD3	2.18	0.43
8:H:84:ALA:CA	8:H:87:ARG:HD2	2.47	0.43
10:J:37:SER:OG	10:J:47:ARG:NH2	2.51	0.43
12:L:47:ARG:CG	12:L:52:GLY:HA2	2.48	0.43
1:M:80:HIS:H	1:M:243:PRO:HB3	1.83	0.43
1:M:268:ASP:HB3	1:M:299:HIS:ND1	2.32	0.43
1:M:360:GLU:O	1:M:361:LEU:C	2.61	0.43
1:M:645:LEU:HG	1:M:649:ILE:HD12	1.99	0.43
1:M:718:VAL:O	1:M:721:PHE:HB2	2.17	0.43
1:M:1218:GLN:O	1:M:1221:LYS:HG3	2.18	0.43
1:M:1278:ASN:O	1:M:1310:GLY:HA3	2.18	0.43
2:N:100:PRO:HD2	2:N:180:TYR:CE1	2.53	0.43
2:N:229:ALA:HB1	2:N:231:PRO:HD2	2.00	0.43
2:N:387:LEU:HD12	2:N:387:LEU:H	1.84	0.43
2:N:942:ARG:HB2	2:N:945:GLU:HB2	2.00	0.43
5:Q:55:ARG:HD2	5:Q:113:GLN:HE21	1.83	0.43
5:Q:78:LEU:HD21	5:Q:80:VAL:HG23	1.99	0.43
7:S:127:PRO:HA	7:S:128:PRO:HD3	1.94	0.43
9:U:34:TYR:CD2	9:U:34:TYR:C	2.96	0.43
10:V:27:GLU:O	10:V:29:GLU:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASN:O	1:A:76:GLU:CB	2.65	0.43
1:A:832:ALA:O	13:1:18:DA:H5'	2.17	0.43
1:A:1021:LEU:O	1:A:1024:SER:HB3	2.19	0.43
1:A:1112:LYS:O	1:A:1114:PRO:CD	2.63	0.43
1:A:1427:ASN:O	1:A:1428:VAL:C	2.62	0.43
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.53	0.43
2:B:593:PRO:O	2:B:594:ALA:C	2.61	0.43
3:C:31:ASN:O	3:C:35:ARG:HG3	2.17	0.43
3:C:236:GLY:C	3:C:238:ILE:N	2.75	0.43
5:E:65:THR:O	5:E:66:GLU:C	2.62	0.43
6:F:123:LYS:NZ	6:F:127:GLU:OE2	2.52	0.43
7:G:18:PHE:HA	7:G:22:MET:CE	2.41	0.43
8:H:58:THR:O	8:H:142:LEU:HD12	2.18	0.43
9:I:34:TYR:CD2	9:I:34:TYR:C	2.96	0.43
11:K:18:LYS:HA	11:K:18:LYS:HD3	1.83	0.43
1:M:571:LEU:HD22	8:T:46:LEU:HD11	2.00	0.43
1:M:709:THR:HB	1:M:712:GLU:H	1.83	0.43
1:M:774:ARG:H	1:M:774:ARG:HG2	1.31	0.43
1:M:1164:PRO:HG2	1:M:1165:GLU:H	1.83	0.43
2:N:351:TYR:CD1	2:N:355:ILE:HD11	2.54	0.43
2:N:871:THR:HG22	2:N:872:GLU:O	2.18	0.43
2:N:941:LEU:O	2:N:942:ARG:C	2.61	0.43
2:N:1109:GLY:O	2:N:1110:PRO:C	2.61	0.43
3:O:62:PHE:C	3:O:62:PHE:CD2	2.97	0.43
4:P:40:HIS:C	4:P:42:GLY:H	2.26	0.43
4:P:40:HIS:HE1	7:S:74:TYR:O	2.00	0.43
8:T:77:ARG:HG2	8:T:78:SER:H	1.82	0.43
8:T:108:SER:O	8:T:109:LYS:HB3	2.18	0.43
9:U:58:VAL:HG13	9:U:62:ILE:CD1	2.48	0.43
1:A:65:LEU:HB3	1:A:71:GLN:CD	2.43	0.43
1:A:115:LEU:CG	1:A:142:CYS:HB3	2.47	0.43
1:A:173:THR:O	1:A:173:THR:HG22	2.19	0.43
1:A:791:ASP:OD1	1:A:791:ASP:C	2.62	0.43
1:A:821:ARG:O	1:A:825:ILE:HG13	2.17	0.43
1:A:839:ARG:NH1	1:A:1402:PHE:HD1	2.17	0.43
1:A:1169:ILE:H	1:A:1169:ILE:HG13	1.49	0.43
1:A:1235:LYS:O	1:A:1237:ILE:HD12	2.18	0.43
2:B:67:SER:HB3	2:B:92:PHE:HD1	1.83	0.43
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.48	0.43
2:B:798:TYR:HD2	2:B:798:TYR:N	2.16	0.43
2:B:941:LEU:O	2:B:942:ARG:C	2.62	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:LEU:HB2	3:C:230:MET:HE3	2.00	0.43
3:C:265:MET:HE3	3:C:265:MET:HB2	1.82	0.43
4:D:12:ARG:NH1	4:D:14:ARG:N	2.66	0.43
5:E:17:ARG:O	5:E:20:LYS:HB2	2.18	0.43
9:I:75:CYS:SG	9:I:78:CYS:SG	3.17	0.43
1:M:40:THR:CG2	1:M:41:MET:HG3	2.47	0.43
1:M:245:PRO:O	1:M:248:PRO:HD3	2.19	0.43
1:M:374:LEU:O	1:M:436:ILE:HG12	2.17	0.43
1:M:532:ARG:O	1:M:535:THR:HB	2.18	0.43
1:M:667:GLY:C	3:O:192:TRP:CZ2	2.97	0.43
1:M:738:LYS:HG3	1:M:740:LEU:HG	1.99	0.43
1:M:856:THR:HG21	1:M:1370:LEU:HD21	2.00	0.43
1:M:1193:LEU:HD12	1:M:1193:LEU:C	2.43	0.43
1:M:1242:VAL:CG1	1:M:1243:VAL:H	2.29	0.43
1:M:1402:PHE:CE1	1:M:1403:GLU:HG2	2.54	0.43
2:N:662:MET:HA	2:N:665:GLU:CG	2.46	0.43
2:N:785:TYR:CD1	2:N:785:TYR:C	2.96	0.43
2:N:864:LYS:HG3	2:N:872:GLU:OE1	2.19	0.43
3:O:101:LEU:C	3:O:102:GLN:HG2	2.43	0.43
3:O:260:LEU:O	3:O:263:THR:HB	2.18	0.43
4:P:145:MET:O	4:P:149:THR:HB	2.19	0.43
4:P:193:THR:HG22	4:P:194:LEU:HG	2.00	0.43
5:Q:108:GLY:O	5:Q:132:ILE:HG23	2.19	0.43
6:R:102:SER:C	6:R:104:ASN:H	2.26	0.43
7:S:1:MET:O	7:S:3:PHE:CZ	2.71	0.43
8:T:57:VAL:HG12	8:T:58:THR:N	2.33	0.43
12:X:29:TYR:C	12:X:30:ILE:HG13	2.43	0.43
1:A:253:ASN:ND2	2:B:935:ARG:HB2	2.34	0.43
1:A:295:LEU:O	1:A:298:PHE:HB3	2.19	0.43
1:A:532:ARG:HH22	1:A:745:GLN:HG2	1.84	0.43
1:A:535:THR:HG21	1:A:616:VAL:CA	2.46	0.43
1:A:913:LEU:HD13	1:A:981:LEU:O	2.19	0.43
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.49	0.43
1:A:1409:LEU:CD1	2:B:1207:LEU:HD21	2.49	0.43
2:B:129:PHE:HE2	2:B:166:PHE:CD1	2.37	0.43
2:B:231:PRO:O	2:B:231:PRO:HG2	2.19	0.43
2:B:287:ARG:HG2	2:B:292:ILE:HG12	2.00	0.43
2:B:314:LEU:O	2:B:317:CYS:HB2	2.19	0.43
2:B:570:VAL:CG2	2:B:573:GLN:HB3	2.48	0.43
2:B:664:THR:CG2	2:B:678:GLU:N	2.81	0.43
2:B:821:GLN:OE1	2:B:850:LEU:HD12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1102:LYS:O	2:B:1103:ILE:C	2.61	0.43
2:B:1115:THR:HG22	2:B:1117:GLN:CG	2.49	0.43
3:C:65:HIS:CE1	3:C:69:LEU:HD11	2.54	0.43
3:C:123:ASN:HD21	3:C:125:MET:HA	1.82	0.43
3:C:138:GLU:N	3:C:138:GLU:CD	2.77	0.43
5:E:90:VAL:HB	5:E:117:THR:HG21	2.00	0.43
7:G:151:ILE:HG12	7:S:114:LEU:CD1	2.48	0.43
8:H:91:ASP:O	8:H:93:TYR:N	2.47	0.43
11:K:12:LEU:HD12	11:K:12:LEU:HA	1.80	0.43
1:M:1127:ASP:O	1:M:1128:GLN:C	2.61	0.43
1:M:1299:VAL:HG12	1:M:1300:LYS:H	1.84	0.43
1:M:1308:THR:HG23	1:M:1309:ASP:H	1.82	0.43
1:M:1441:PHE:C	1:M:1441:PHE:CD1	2.97	0.43
2:N:110:HIS:HB2	12:X:54:ARG:NH2	2.34	0.43
2:N:830:TYR:CE2	2:N:1000:PRO:HD3	2.52	0.43
2:N:860:MET:SD	2:N:861:ASP:N	2.91	0.43
2:N:916:THR:HB	2:N:935:ARG:CG	2.47	0.43
2:N:1084:GLN:OE1	3:O:189:THR:CG2	2.67	0.43
3:O:258:ILE:O	3:O:262:LEU:HG	2.18	0.43
5:Q:79:TRP:NE1	5:Q:81:GLU:HB2	2.33	0.43
7:S:80:LYS:O	7:S:82:PHE:CE1	2.71	0.43
9:U:50:THR:CG2	9:U:51:ASN:N	2.67	0.43
9:U:100:PHE:N	9:U:100:PHE:HD1	2.16	0.43
12:X:44:ASP:O	12:X:45:ALA:HB3	2.18	0.43
13:4:12:DG:H1'	13:4:13:DT:O5'	2.19	0.43
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.65	0.43
1:A:1030:ARG:HG2	1:A:1034:GLU:OE2	2.19	0.43
1:A:1349:TYR:O	1:A:1350:LYS:C	2.61	0.43
1:A:1418:LEU:HD23	2:B:1222:ARG:HD2	1.99	0.43
2:B:112:LEU:HD12	2:B:113:TYR:H	1.82	0.43
2:B:254:LEU:HD12	2:B:272:THR:O	2.18	0.43
2:B:567:GLU:OE1	2:B:567:GLU:HA	2.19	0.43
2:B:589:VAL:CG1	2:B:590:HIS:N	2.79	0.43
3:C:56:THR:HG22	3:C:57:VAL:N	2.25	0.43
6:F:97:ARG:O	6:F:101:ILE:HG13	2.18	0.43
7:G:132:SER:HB3	7:G:135:ASP:H	1.83	0.43
10:J:32:GLU:OE2	10:J:32:GLU:N	2.32	0.43
1:M:351:THR:HG21	2:N:1103:ILE:CG1	2.49	0.43
1:M:593:GLU:O	1:M:595:THR:N	2.45	0.43
1:M:722:LEU:HB3	1:M:799:PHE:CD1	2.53	0.43
1:M:1146:VAL:HG12	1:M:1201:ALA:HB1	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1349:TYR:O	1:M:1350:LYS:C	2.61	0.43
2:N:102:VAL:CG2	2:N:112:LEU:HD22	2.49	0.43
2:N:108:VAL:HG23	2:N:109:THR:H	1.82	0.43
2:N:291:ILE:CD1	2:N:300:HIS:NE2	2.82	0.43
2:N:311:LEU:O	2:N:314:LEU:N	2.51	0.43
2:N:558:LEU:C	2:N:560:GLU:N	2.77	0.43
2:N:604:ARG:C	2:N:606:LYS:N	2.76	0.43
2:N:657:HIS:O	2:N:660:LYS:HB3	2.18	0.43
2:N:878:GLN:HB2	2:N:879:ARG:HH11	1.82	0.43
2:N:999:MET:HB3	2:N:1007:VAL:HG21	2.01	0.43
2:N:1001:PHE:CE2	3:O:34:ARG:CZ	3.01	0.43
3:O:62:PHE:C	3:O:62:PHE:HD2	2.27	0.43
4:P:207:LEU:HD11	4:P:211:LEU:HD11	2.00	0.43
4:P:219:THR:CG2	4:P:220:LEU:N	2.82	0.43
5:Q:11:ARG:C	5:Q:13:TRP:N	2.75	0.43
5:Q:102:GLU:C	5:Q:104:ASN:H	2.26	0.43
5:Q:154:ILE:HG22	5:Q:155:ARG:O	2.19	0.43
6:R:109:VAL:CG1	6:R:110:ASP:H	2.31	0.43
8:T:84:ALA:HA	8:T:87:ARG:HG3	2.00	0.43
10:V:17:LYS:HG2	10:V:39:LEU:HB3	2.01	0.43
10:V:56:LEU:O	10:V:57:ILE:C	2.62	0.43
1:A:49:LYS:HD3	1:A:55:ASP:HB3	1.99	0.43
1:A:67:CYS:O	1:A:67:CYS:SG	2.77	0.43
1:A:220:THR:O	1:A:221:SER:C	2.59	0.43
1:A:353:ILE:HD11	1:A:480:ALA:HB1	2.00	0.43
1:A:504:LEU:HD11	6:F:91:ALA:HB2	2.01	0.43
1:A:662:PHE:HD2	2:B:1014:PRO:HG3	1.84	0.43
1:A:1127:ASP:O	1:A:1128:GLN:C	2.61	0.43
1:A:1157:ASP:C	1:A:1159:ARG:H	2.27	0.43
2:B:1166:CYS:O	2:B:1168:LEU:N	2.47	0.43
2:B:1200:ALA:O	2:B:1201:LYS:C	2.62	0.43
5:E:12:LEU:HD22	5:E:55:ARG:CZ	2.49	0.43
5:E:22:MET:HE3	5:E:26:ARG:NH2	2.34	0.43
7:G:92:VAL:HG21	7:G:102:GLN:HB2	2.01	0.43
8:H:106:GLU:C	8:H:108:SER:N	2.76	0.43
9:I:86:PHE:HE1	9:I:100:PHE:HB2	1.83	0.43
10:J:36:LEU:HD12	10:J:47:ARG:HH11	1.80	0.43
10:J:53:HIS:NE2	10:J:55:ASP:HA	2.34	0.43
12:L:44:ASP:O	12:L:45:ALA:HB3	2.19	0.43
1:M:22:PHE:HE2	1:M:26:GLU:HG2	1.83	0.43
1:M:61:ILE:O	1:M:62:ASP:C	2.62	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:185:TRP:CE3	1:M:185:TRP:N	2.84	0.43
1:M:698:GLN:NE2	9:U:99:LEU:HD21	2.33	0.43
1:M:825:ILE:HD12	2:N:513:GLN:HG2	2.00	0.43
1:M:1116:LEU:HB3	1:M:1308:THR:CG2	2.47	0.43
2:N:121:ASN:HA	2:N:207:GLY:CA	2.48	0.43
2:N:230:ALA:HB3	2:N:231:PRO:HD3	1.99	0.43
2:N:281:PRO:O	2:N:283:VAL:N	2.52	0.43
2:N:522:VAL:HG12	2:N:523:CYS:N	2.34	0.43
2:N:542:MET:HE2	2:N:747:MET:HE2	2.00	0.43
3:O:67:LEU:HA	3:O:70:ILE:HD12	2.01	0.43
3:O:209:TYR:CD1	3:O:209:TYR:N	2.86	0.43
4:P:138:ASN:O	4:P:140:ASP:N	2.52	0.43
5:Q:96:PHE:CZ	5:Q:100:ILE:HD11	2.54	0.43
5:Q:129:PRO:O	5:Q:130:ALA:O	2.37	0.43
6:R:152:ILE:HG22	6:R:153:VAL:N	2.33	0.43
7:S:21:ARG:HD3	7:S:21:ARG:HA	1.78	0.43
8:T:95:TYR:C	8:T:95:TYR:HD2	2.26	0.43
9:U:55:THR:CG2	9:U:100:PHE:HD2	2.26	0.43
1:A:40:THR:CG2	1:A:41:MET:HG3	2.42	0.43
1:A:282:ASN:O	1:A:284:ALA:N	2.52	0.43
1:A:993:LEU:CD2	1:A:1022:LEU:HD21	2.49	0.43
2:B:175:ARG:HD2	2:B:175:ARG:HA	1.87	0.43
2:B:282:ILE:CD1	2:B:382:ILE:HD13	2.48	0.43
2:B:363:HIS:O	2:B:364:ILE:CB	2.63	0.43
2:B:378:LEU:O	2:B:378:LEU:HD12	2.18	0.43
2:B:390:LEU:O	2:B:392:ARG:N	2.52	0.43
2:B:431:TYR:CG	2:B:447:ALA:CB	3.02	0.43
2:B:603:LEU:HD12	2:B:609:ILE:HG12	2.01	0.43
2:B:861:ASP:OD1	2:B:862:GLN:N	2.52	0.43
2:B:935:ARG:HG3	2:B:935:ARG:O	2.19	0.43
6:F:69:LEU:C	6:F:71:GLU:H	2.26	0.43
6:F:89:GLU:CG	6:F:134:ILE:HD13	2.46	0.43
7:G:1:MET:HE2	7:G:3:PHE:CE1	2.53	0.43
7:G:127:PRO:HA	7:G:128:PRO:HD3	1.94	0.43
10:J:24:LEU:HA	10:J:28:ASP:HB2	2.01	0.43
1:M:139:TRP:O	1:M:140:THR:C	2.60	0.43
1:M:826:ASP:HA	1:M:829:VAL:HG23	1.99	0.43
2:N:90:ILE:HD12	2:N:432:MET:CE	2.49	0.43
2:N:294:ASP:N	2:N:294:ASP:OD2	2.51	0.43
2:N:423:LYS:HD2	2:N:470:LYS:HZ1	1.84	0.43
2:N:618:ASP:OD2	2:N:621:GLU:HB3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:769:TYR:C	2:N:771:SER:N	2.73	0.43
2:N:866:TYR:HB2	2:N:870:ILE:HB	2.01	0.43
2:N:1165:ILE:HG21	4:P:17:LYS:HG3	2.00	0.43
3:O:16:ASP:O	3:O:240:VAL:HG11	2.19	0.43
3:O:189:THR:HG22	3:O:190:ASP:H	1.79	0.43
3:O:267:GLN:N	3:O:267:GLN:CD	2.77	0.43
4:P:15:LEU:O	4:P:17:LYS:N	2.44	0.43
4:P:32:GLU:C	7:S:5:LYS:HZ3	2.21	0.43
4:P:57:LEU:HD23	4:P:57:LEU:HA	1.75	0.43
4:P:123:LEU:HD13	4:P:149:THR:HG21	2.01	0.43
5:Q:90:VAL:HA	5:Q:120:ALA:HB2	1.99	0.43
5:Q:103:LYS:HB3	5:Q:105:PHE:CE2	2.54	0.43
6:R:97:ARG:HA	6:R:97:ARG:HD2	1.86	0.43
7:S:138:THR:CG2	7:S:139:ILE:HG22	2.39	0.43
8:T:50:ALA:O	8:T:53:ASP:OD2	2.37	0.43
1:A:350:ARG:CB	2:B:1128:LEU:HD11	2.46	0.43
1:A:374:LEU:O	1:A:436:ILE:HG12	2.18	0.43
1:A:417:TYR:O	1:A:418:SER:C	2.62	0.43
1:A:770:VAL:HA	1:A:822:GLU:OE1	2.19	0.43
1:A:1239:ARG:HH11	1:A:1239:ARG:HB3	1.84	0.43
1:A:1293:SER:HB2	1:A:1299:VAL:CG2	2.49	0.43
1:A:1375:MET:HE3	1:A:1384:VAL:HG23	2.00	0.43
2:B:246:LYS:HA	2:B:249:ARG:NH2	2.34	0.43
2:B:257:LYS:HB3	2:B:258:LEU:H	1.55	0.43
2:B:324:ILE:O	2:B:324:ILE:HG22	2.19	0.43
2:B:405:ARG:HA	2:B:631:GLY:O	2.19	0.43
2:B:544:CYS:C	2:B:545:ILE:HG13	2.44	0.43
2:B:558:LEU:C	2:B:560:GLU:N	2.77	0.43
2:B:616:ILE:CG2	2:B:700:SER:OG	2.67	0.43
2:B:700:SER:C	2:B:701:ILE:CG2	2.92	0.43
2:B:1221:SER:C	2:B:1223:ASP:H	2.27	0.43
3:C:147:LEU:HB2	3:C:151:GLN:CB	2.41	0.43
3:C:209:TYR:H	3:C:209:TYR:HD1	1.63	0.43
3:C:254:LYS:HB3	11:K:42:LEU:HD11	2.01	0.43
9:I:4:PHE:HD1	9:I:5:ARG:N	2.16	0.43
9:I:99:LEU:C	9:I:100:PHE:HD1	2.27	0.43
1:M:330:LYS:O	1:M:334:GLY:HA3	2.19	0.43
1:M:701:LEU:HD21	9:U:114:GLN:HB2	2.01	0.43
1:M:1280:GLU:HB3	1:M:1281:ARG:H	1.60	0.43
1:M:1402:PHE:CZ	1:M:1403:GLU:HG2	2.54	0.43
1:M:1410:PHE:HA	2:N:1212:ILE:CD1	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1445:ILE:HD13	7:S:70:PHE:CE2	2.54	0.43
2:N:307:ASP:OD2	2:N:310:MET:HE3	2.18	0.43
2:N:363:HIS:O	2:N:364:ILE:HB	2.18	0.43
2:N:447:ALA:O	2:N:449:ASN:N	2.52	0.43
2:N:487:THR:CG2	2:N:488:TYR:N	2.82	0.43
2:N:594:ALA:HA	2:N:617:ARG:NH1	2.34	0.43
2:N:727:LYS:HE2	2:N:1049:ASP:OD1	2.19	0.43
2:N:840:ILE:HG21	2:N:994:TYR:HD1	1.83	0.43
2:N:957:ASN:O	2:N:960:GLY:N	2.52	0.43
2:N:1017:ILE:H	2:N:1018:PRO:HD2	1.84	0.43
3:O:239:PRO:O	3:O:240:VAL:C	2.62	0.43
4:P:8:PHE:CD2	7:S:6:ASP:O	2.71	0.43
4:P:60:LYS:HE2	4:P:126:ILE:CG1	2.48	0.43
5:Q:82:PHE:O	5:Q:83:CYS:HB2	2.18	0.43
5:Q:104:ASN:HD22	5:Q:104:ASN:HA	1.52	0.43
5:Q:124:VAL:HB	5:Q:125:PRO:CD	2.49	0.43
6:R:69:LEU:C	6:R:71:GLU:H	2.26	0.43
7:S:110:VAL:HG12	7:S:161:GLY:O	2.18	0.43
7:S:115:MET:HE1	7:S:130:TYR:CD2	2.53	0.43
7:S:129:SER:C	7:S:130:TYR:HD1	2.26	0.43
8:T:62:SER:OG	8:T:64:ASN:ND2	2.51	0.43
8:T:135:LEU:HB2	8:T:137:GLN:HE21	1.83	0.43
9:U:82:GLU:HB3	9:U:104:LEU:HD12	1.99	0.43
10:V:24:LEU:HA	10:V:28:ASP:HB2	1.99	0.43
1:A:33:ALA:HB1	1:A:56:PRO:HB2	2.00	0.42
1:A:219:PHE:CE1	1:A:230:ARG:HB3	2.54	0.42
1:A:500:GLU:O	1:A:504:LEU:HB2	2.19	0.42
1:A:1100:ARG:NH2	1:A:1351:GLU:CG	2.82	0.42
1:A:1148:ILE:HD11	1:A:1198:ASP:CA	2.46	0.42
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.54	0.42
1:A:1444:MET:CG	7:G:59:GLY:O	2.67	0.42
2:B:51:PHE:CD2	2:B:173:MET:HB3	2.54	0.42
2:B:203:PHE:N	2:B:203:PHE:HD1	2.16	0.42
2:B:521:LEU:HB3	2:B:633:VAL:CG1	2.47	0.42
2:B:557:PHE:HZ	2:B:603:LEU:HD21	1.83	0.42
2:B:654:ARG:HG3	2:B:654:ARG:NH1	2.33	0.42
2:B:910:VAL:HG13	2:B:938:SER:HB3	2.01	0.42
2:B:970:THR:HG22	2:B:971:THR:N	2.33	0.42
2:B:1017:ILE:H	2:B:1018:PRO:HD2	1.84	0.42
4:D:166:LEU:HD23	4:D:214:LEU:CD2	2.49	0.42
8:H:26:ILE:O	8:H:27:GLU:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:51:ALA:O	8:H:52:GLN:CB	2.67	0.42
12:L:29:TYR:O	12:L:30:ILE:CG1	2.66	0.42
1:M:426:LEU:C	1:M:427:GLN:HG2	2.44	0.42
1:M:846:GLU:HB2	1:M:847:ASP:H	1.67	0.42
2:N:384:ARG:HH12	2:N:393:LYS:CD	2.31	0.42
2:N:483:LEU:HD11	2:N:491:THR:HG22	1.99	0.42
2:N:731:VAL:HG12	2:N:734:HIS:NE2	2.34	0.42
3:O:101:LEU:CD1	3:O:118:LEU:HD23	2.49	0.42
3:O:104:PHE:HE2	3:O:150:GLY:HA2	1.84	0.42
3:O:168:ALA:O	3:O:169:LYS:C	2.62	0.42
4:P:5:THR:HG23	7:S:42:PHE:CE1	2.53	0.42
4:P:156:ASP:C	4:P:158:GLU:N	2.77	0.42
4:P:185:CYS:O	4:P:211:LEU:HD22	2.19	0.42
4:P:209:ARG:HA	4:P:212:LYS:HD2	1.99	0.42
8:T:58:THR:O	8:T:59:ILE:HG13	2.19	0.42
9:U:17:ARG:HG3	9:U:28:GLU:CD	2.44	0.42
11:W:21:ILE:HD13	11:W:84:LYS:HE3	2.00	0.42
11:W:59:ALA:HA	11:W:74:ARG:O	2.19	0.42
1:A:65:LEU:HD13	1:A:71:GLN:OE1	2.19	0.42
1:A:98:LYS:O	1:A:102:VAL:HG23	2.19	0.42
1:A:523:ILE:CG2	1:A:527:THR:HG22	2.49	0.42
1:A:648:ASN:O	1:A:649:ILE:C	2.62	0.42
1:A:883:LEU:HD21	1:A:1021:LEU:HB2	2.00	0.42
1:A:1311:VAL:HG21	1:A:1329:THR:CG2	2.49	0.42
2:B:125:SER:O	2:B:126:SER:HB3	2.19	0.42
3:C:239:PRO:O	3:C:240:VAL:C	2.62	0.42
4:D:138:ASN:O	4:D:140:ASP:N	2.52	0.42
5:E:43:LYS:O	5:E:45:LYS:N	2.52	0.42
8:H:56:THR:O	8:H:144:ILE:HA	2.19	0.42
8:H:128:ASN:C	8:H:128:ASN:HD22	2.26	0.42
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.84	0.42
1:M:69:THR:HB	2:N:1174:LYS:HE2	2.01	0.42
1:M:92:HIS:O	1:M:93:VAL:C	2.60	0.42
1:M:109:HIS:H	1:M:210:ILE:HD11	1.84	0.42
1:M:122:MET:HE3	1:M:126:LEU:CG	2.49	0.42
1:M:469:ARG:NH2	2:N:991:GLY:O	2.52	0.42
1:M:598:LEU:CD2	8:T:25:ARG:NH1	2.82	0.42
1:M:674:PRO:C	1:M:676:MET:N	2.77	0.42
1:M:785:PRO:C	1:M:786:HIS:HD2	2.27	0.42
1:M:1081:LEU:HD11	1:M:1097:GLY:CA	2.45	0.42
1:M:1156:PRO:HA	1:M:1190:PRO:CB	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1215:ARG:O	1:M:1219:THR:N	2.48	0.42
1:M:1265:ASN:C	1:M:1267:MET:N	2.75	0.42
1:M:1368:MET:HE3	1:M:1368:MET:HB2	1.75	0.42
2:N:334:ILE:O	2:N:334:ILE:CG2	2.66	0.42
2:N:604:ARG:NH2	2:N:615:MET:HE2	2.33	0.42
2:N:864:LYS:HG3	2:N:872:GLU:CD	2.45	0.42
2:N:899:ILE:CD1	2:N:911:ILE:HA	2.47	0.42
2:N:1106:ARG:HG3	2:N:1107:ALA:N	2.34	0.42
2:N:1165:ILE:O	2:N:1217:TYR:OH	2.34	0.42
3:O:179:GLU:O	3:O:180:TYR:HB3	2.20	0.42
4:P:52:LEU:H	4:P:182:SER:HB3	1.84	0.42
4:P:183:LEU:HA	4:P:183:LEU:HD23	1.46	0.42
5:Q:42:PHE:O	5:Q:43:LYS:C	2.61	0.42
5:Q:182:ASP:HB3	5:Q:185:ALA:CB	2.48	0.42
8:T:61:SER:O	8:T:62:SER:HB2	2.19	0.42
10:V:44:TYR:CD2	10:V:44:TYR:N	2.78	0.42
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.76	0.42
1:A:599:SER:HA	1:A:600:PRO:HD2	1.81	0.42
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.49	0.42
1:A:645:LEU:HD11	1:A:649:ILE:HD11	2.00	0.42
1:A:971:PHE:O	1:A:972:HIS:C	2.63	0.42
1:A:1127:ASP:CG	1:A:1130:GLN:HB2	2.45	0.42
1:A:1150:SER:HB3	1:A:1195:LEU:CD2	2.48	0.42
1:A:1239:ARG:HH12	1:A:1241:ARG:NH1	2.18	0.42
1:A:1378:GLN:HG2	5:E:177:ARG:NH1	2.35	0.42
2:B:364:ILE:HG13	2:B:585:VAL:HG22	2.00	0.42
2:B:447:ALA:O	2:B:449:ASN:N	2.53	0.42
2:B:508:LEU:O	2:B:509:ALA:CB	2.66	0.42
2:B:604:ARG:CA	2:B:609:ILE:HG13	2.49	0.42
2:B:744:HIS:CD2	2:B:745:PRO:CD	2.80	0.42
2:B:773:MET:SD	2:B:987:LYS:HD2	2.58	0.42
2:B:832:GLY:O	2:B:835:GLN:NE2	2.52	0.42
3:C:259:LEU:HD21	11:K:91:CYS:HB3	2.01	0.42
5:E:14:ARG:NH2	5:E:141:VAL:HG12	2.28	0.42
5:E:124:VAL:N	5:E:125:PRO:HD2	2.33	0.42
7:G:91:VAL:HG23	7:G:141:SER:O	2.19	0.42
8:H:100:THR:HG22	8:H:101:ALA:N	2.34	0.42
8:H:113:ALA:HB1	8:H:124:ARG:HE	1.84	0.42
9:I:62:ILE:O	9:I:62:ILE:HG12	2.19	0.42
9:I:100:PHE:N	9:I:100:PHE:HD1	2.17	0.42
9:I:101:PHE:N	9:I:101:PHE:HD1	2.15	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:219:PHE:CZ	1:M:230:ARG:HB3	2.55	0.42
1:M:320:ARG:NE	1:M:323:LYS:HZ1	2.18	0.42
1:M:353:ILE:HD11	1:M:480:ALA:HB1	2.01	0.42
1:M:417:TYR:O	1:M:418:SER:C	2.62	0.42
1:M:648:ASN:O	1:M:649:ILE:C	2.62	0.42
1:M:666:ILE:HD11	2:N:1067:ARG:O	2.19	0.42
1:M:874:ASP:OD1	1:M:876:ALA:N	2.40	0.42
1:M:908:LEU:CD1	1:M:983:ILE:HD11	2.49	0.42
1:M:942:PHE:HZ	5:Q:207:ARG:HG3	1.83	0.42
1:M:1111:MET:HE2	1:M:1113:THR:O	2.18	0.42
1:M:1206:ASP:O	1:M:1274:ARG:NH1	2.51	0.42
1:M:1312:ASN:O	1:M:1316:VAL:HG23	2.18	0.42
2:N:274:PRO:O	2:N:275:TYR:HB2	2.19	0.42
2:N:821:GLN:HE22	2:N:851:PHE:HA	1.84	0.42
2:N:980:PHE:CE2	2:N:1094:ARG:HG3	2.54	0.42
2:N:1166:CYS:O	2:N:1168:LEU:N	2.48	0.42
2:N:1221:SER:C	2:N:1223:ASP:H	2.27	0.42
3:O:77:ILE:HG23	3:O:161:LYS:HE3	2.02	0.42
4:P:190:GLU:HA	7:S:167:TYR:HD1	1.77	0.42
4:P:203:SER:OG	4:P:206:GLU:HB2	2.20	0.42
5:Q:65:THR:O	5:Q:66:GLU:C	2.63	0.42
5:Q:65:THR:O	5:Q:69:ILE:HD12	2.19	0.42
5:Q:124:VAL:N	5:Q:125:PRO:HD2	2.34	0.42
7:S:111:THR:O	7:S:114:LEU:N	2.47	0.42
8:T:129:TYR:C	8:T:131:ASN:H	2.27	0.42
1:A:41:MET:HB2	1:A:49:LYS:HA	1.94	0.42
1:A:211:PHE:HA	1:A:214:ILE:HG13	2.01	0.42
1:A:532:ARG:O	1:A:535:THR:HB	2.19	0.42
1:A:567:LYS:HE3	8:H:46:LEU:HB2	2.01	0.42
2:B:189:LEU:O	2:B:190:TYR:C	2.62	0.42
2:B:427:ASP:HA	2:B:430:ARG:CG	2.49	0.42
2:B:468:GLU:OE1	2:B:470:LYS:HE3	2.19	0.42
2:B:796:LEU:HB3	2:B:799:PRO:HG3	2.02	0.42
2:B:835:GLN:HE21	2:B:835:GLN:HB2	1.43	0.42
2:B:879:ARG:HB2	2:B:880:THR:H	1.41	0.42
3:C:62:PHE:C	3:C:62:PHE:CD2	2.98	0.42
3:C:166:GLU:HG2	11:K:10:PHE:HZ	1.84	0.42
4:D:53:SER:OG	4:D:54:GLU:N	2.52	0.42
5:E:102:GLU:C	5:E:104:ASN:H	2.27	0.42
6:F:76:LYS:HE3	6:F:150:GLU:OE2	2.18	0.42
6:F:100:GLN:HA	6:F:103:MET:HG3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:22:MET:O	7:G:23:LYS:C	2.63	0.42
8:H:26:ILE:CD1	8:H:49:VAL:CG1	2.98	0.42
12:L:46:VAL:O	12:L:46:VAL:HG12	2.20	0.42
13:1:16:DT:H2''	13:1:17:DT:O5'	2.19	0.42
13:1:19:DT:H2'	13:1:20:DG:H8	1.84	0.42
1:M:276:LEU:HD21	1:M:293:GLU:HG3	2.01	0.42
1:M:381:THR:C	1:M:383:TYR:N	2.75	0.42
1:M:655:PHE:O	1:M:658:LEU:HB3	2.19	0.42
1:M:711:ARG:NH2	9:U:87:GLN:OE1	2.52	0.42
1:M:722:LEU:HD23	1:M:799:PHE:CD1	2.55	0.42
1:M:820:GLY:O	1:M:821:ARG:C	2.62	0.42
1:M:897:TYR:CB	1:M:936:LEU:HD12	2.46	0.42
1:M:1033:GLN:O	1:M:1036:ARG:NH1	2.51	0.42
2:N:70:ILE:H	2:N:429:PHE:HE1	1.67	0.42
2:N:363:HIS:O	2:N:364:ILE:CB	2.67	0.42
2:N:640:VAL:O	2:N:640:VAL:CG1	2.67	0.42
2:N:644:GLU:C	2:N:646:LEU:H	2.27	0.42
2:N:773:MET:O	2:N:775:LYS:N	2.51	0.42
2:N:957:ASN:O	2:N:958:GLN:C	2.62	0.42
2:N:1132:GLU:O	2:N:1135:ARG:HB3	2.19	0.42
3:O:249:ASP:O	3:O:252:GLN:HB3	2.19	0.42
5:Q:78:LEU:HD11	5:Q:109:ILE:HD12	2.00	0.42
7:S:4:ILE:HA	7:S:76:ALA:O	2.19	0.42
7:S:146:LYS:HB2	7:S:168:LEU:HD11	2.00	0.42
9:U:59:VAL:C	9:U:61:ASP:N	2.75	0.42
10:V:1:MET:H1	10:V:56:LEU:CA	2.31	0.42
10:V:3:VAL:CG2	10:V:18:TRP:CG	3.02	0.42
10:V:31:ASP:O	10:V:32:GLU:C	2.62	0.42
11:W:31:VAL:HG23	11:W:83:PRO:HG3	2.02	0.42
1:A:173:THR:O	1:A:173:THR:CG2	2.65	0.42
1:A:203:SER:O	1:A:206:GLU:HB3	2.19	0.42
1:A:390:GLN:HE21	1:A:394:ASN:ND2	2.09	0.42
1:A:452:LYS:HB3	2:B:1141:HIS:CE1	2.55	0.42
1:A:672:ASP:OD2	1:A:674:PRO:HG2	2.18	0.42
1:A:836:TYR:O	1:A:840:ARG:HD3	2.19	0.42
1:A:1030:ARG:NH1	1:A:1035:TYR:OH	2.53	0.42
1:A:1147:THR:HB	9:I:48:LEU:CD1	2.45	0.42
1:A:1165:GLU:H	1:A:1165:GLU:HG2	1.61	0.42
1:A:1418:LEU:HD23	2:B:1222:ARG:CD	2.49	0.42
2:B:865:LYS:C	2:B:866:TYR:HD1	2.26	0.42
2:B:889:THR:HG23	2:B:891:ASP:H	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:156:ASP:HB2	4:D:159:THR:CG2	2.50	0.42
5:E:37:LEU:C	5:E:37:LEU:HD12	2.45	0.42
5:E:81:GLU:HG2	5:E:82:PHE:O	2.19	0.42
5:E:134:THR:O	5:E:135:PHE:CD1	2.73	0.42
6:F:105:ALA:HB1	6:F:106:PRO:CD	2.49	0.42
7:G:62:LEU:HD13	7:G:62:LEU:HA	1.83	0.42
10:J:12:LYS:O	10:J:14:VAL:HG23	2.20	0.42
11:K:33:ILE:HD13	11:K:87:LEU:HD22	2.00	0.42
12:L:29:TYR:C	12:L:30:ILE:HG13	2.45	0.42
1:M:224:PHE:CE2	1:M:234:MET:HE2	2.55	0.42
1:M:353:ILE:HD13	1:M:487:MET:CG	2.50	0.42
1:M:626:ASN:C	1:M:628:GLY:H	2.26	0.42
1:M:1152:ILE:HG12	1:M:1260:LEU:HD23	2.01	0.42
1:M:1157:ASP:C	1:M:1159:ARG:H	2.27	0.42
1:M:1166:ASP:OD2	1:M:1239:ARG:NE	2.52	0.42
2:N:100:PRO:HA	2:N:125:SER:O	2.19	0.42
2:N:257:LYS:HB3	2:N:258:LEU:H	1.57	0.42
2:N:331:LEU:HD21	2:N:353:LYS:HG2	2.01	0.42
2:N:390:LEU:O	2:N:392:ARG:N	2.52	0.42
2:N:571:PRO:O	2:N:574:SER:O	2.37	0.42
2:N:769:TYR:O	2:N:772:ALA:N	2.50	0.42
2:N:884:ARG:O	2:N:936:ASP:CB	2.67	0.42
2:N:948:ILE:O	2:N:949:VAL:C	2.60	0.42
2:N:1182:CYS:SG	2:N:1185:CYS:HB2	2.60	0.42
2:N:1208:MET:O	2:N:1211:ASN:N	2.47	0.42
3:O:77:ILE:HD13	3:O:77:ILE:HA	1.86	0.42
3:O:186:LEU:O	3:O:187:LYS:HB2	2.19	0.42
4:P:14:ARG:HH12	4:P:16:LYS:NZ	2.18	0.42
4:P:190:GLU:HG3	7:S:167:TYR:CD1	2.54	0.42
5:Q:88:VAL:HG21	5:Q:110:PHE:CE1	2.55	0.42
5:Q:147:HIS:CD2	5:Q:149:LEU:H	2.37	0.42
7:S:9:LEU:HD23	7:S:30:LEU:HD12	2.01	0.42
7:S:115:MET:CB	7:S:116:PRO:HD2	2.41	0.42
7:S:139:ILE:HG23	7:S:140:LYS:H	1.83	0.42
7:S:139:ILE:CG1	7:S:140:LYS:HG3	2.46	0.42
8:T:106:GLU:C	8:T:108:SER:N	2.77	0.42
8:T:135:LEU:HB2	8:T:137:GLN:NE2	2.35	0.42
1:A:34:LYS:HG3	1:A:36:ARG:HH22	1.83	0.42
1:A:973:ILE:O	1:A:973:ILE:HG22	2.19	0.42
1:A:1072:ILE:O	1:A:1075:PRO:HG2	2.19	0.42
1:A:1205:LYS:O	1:A:1207:LEU:HG	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:ALA:HB1	2:B:231:PRO:HD2	2.02	0.42
2:B:399:ASP:O	2:B:515:HIS:CD2	2.73	0.42
2:B:603:LEU:HB3	2:B:609:ILE:CD1	2.50	0.42
2:B:1079:LYS:CA	3:C:27:LEU:HD21	2.50	0.42
2:B:1084:GLN:OE1	3:C:189:THR:CG2	2.67	0.42
2:B:1181:GLU:HB2	2:B:1188:LYS:HG2	2.02	0.42
2:B:1221:SER:O	2:B:1223:ASP:N	2.53	0.42
3:C:133:ILE:CD1	3:C:237:SER:HA	2.49	0.42
3:C:236:GLY:O	3:C:237:SER:C	2.63	0.42
4:D:7:THR:HG21	4:D:32:GLU:OE1	2.20	0.42
4:D:134:THR:HG22	4:D:136:GLY:H	1.84	0.42
5:E:42:PHE:O	5:E:43:LYS:C	2.62	0.42
7:G:111:THR:O	7:G:112:LYS:C	2.62	0.42
1:M:270:LEU:HA	1:M:270:LEU:HD12	1.71	0.42
1:M:582:ILE:HA	1:M:583:PRO:HD2	1.88	0.42
1:M:787:PHE:CE1	1:M:796:SER:HA	2.54	0.42
1:M:1100:ARG:NH2	1:M:1351:GLU:CG	2.81	0.42
1:M:1161:THR:OG1	1:M:1239:ARG:NH2	2.53	0.42
2:N:189:LEU:O	2:N:190:TYR:C	2.62	0.42
2:N:299:GLU:CD	2:N:571:PRO:HG2	2.44	0.42
2:N:408:LEU:HD11	2:N:545:ILE:HD13	2.02	0.42
3:O:148:ARG:HB3	3:O:149:LYS:H	1.50	0.42
4:P:71:LYS:CA	4:P:74:GLN:HB2	2.45	0.42
4:P:128:VAL:O	4:P:129:LEU:C	2.63	0.42
4:P:146:GLN:CA	4:P:149:THR:HG22	2.50	0.42
4:P:195:ILE:HB	4:P:198:LEU:CD1	2.49	0.42
4:P:209:ARG:HH11	4:P:209:ARG:CG	2.33	0.42
5:Q:111:VAL:CG1	5:Q:137:GLU:HG2	2.50	0.42
6:R:110:ASP:O	6:R:123:LYS:HE3	2.19	0.42
7:S:34:VAL:HG13	7:S:45:ILE:CD1	2.49	0.42
7:S:48:VAL:HG13	7:S:74:TYR:HD1	1.84	0.42
9:U:109:ILE:O	9:U:109:ILE:HG22	2.19	0.42
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.55	0.42
1:A:344:ARG:C	1:A:345:VAL:CG1	2.93	0.42
1:A:415:LEU:HD23	1:A:415:LEU:HA	1.78	0.42
1:A:500:GLU:OE2	2:B:1145:SER:CB	2.66	0.42
1:A:525:GLN:O	1:A:526:ASP:C	2.61	0.42
1:A:590:ARG:O	1:A:591:PHE:CB	2.63	0.42
1:A:598:LEU:HD12	8:H:115:TYR:CD2	2.54	0.42
1:A:608:ILE:HD12	1:A:613:ILE:HD11	2.02	0.42
1:A:767:GLN:HA	1:A:799:PHE:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:LYS:O	1:A:1004:ASN:HB3	2.20	0.42
2:B:189:LEU:CD1	2:B:196:PRO:HA	2.49	0.42
2:B:488:TYR:CE2	2:B:813:LYS:HB2	2.54	0.42
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.35	0.42
3:C:116:LYS:HG3	3:C:117:ASP:OD1	2.19	0.42
4:D:32:GLU:HG3	7:G:5:LYS:HE2	2.01	0.42
4:D:61:GLU:O	4:D:64:VAL:HB	2.20	0.42
5:E:90:VAL:HA	5:E:120:ALA:HB2	2.01	0.42
7:G:14:HIS:HD2	7:G:16:SER:CB	2.32	0.42
14:2:4:DA:C4	14:2:5:DC:C5	3.08	0.42
1:M:49:LYS:NZ	1:M:60:SER:HA	2.33	0.42
1:M:65:LEU:HD13	1:M:71:GLN:OE1	2.20	0.42
1:M:456:MET:HE1	1:M:474:VAL:HG22	2.02	0.42
1:M:783:THR:HG21	1:M:815:PHE:CZ	2.55	0.42
1:M:1003:LYS:O	1:M:1004:ASN:HB3	2.19	0.42
1:M:1312:ASN:ND2	1:M:1315:GLU:HG3	2.35	0.42
2:N:434:ARG:O	2:N:436:VAL:N	2.52	0.42
2:N:603:LEU:HD12	2:N:609:ILE:HG12	2.02	0.42
2:N:634:TYR:CE1	2:N:692:TYR:CD1	3.07	0.42
4:P:29:LEU:HD12	7:S:82:PHE:CE1	2.54	0.42
5:Q:52:ARG:HA	5:Q:53:PRO:HD2	1.86	0.42
5:Q:191:LYS:HG3	5:Q:194:GLU:OE1	2.19	0.42
7:S:34:VAL:O	7:S:37:SER:OG	2.36	0.42
7:S:163:ILE:HG21	7:S:163:ILE:HD13	1.79	0.42
8:T:30:SER:HB3	8:T:36:CYS:HB3	2.01	0.42
11:W:52:ASN:O	11:W:54:ARG:N	2.53	0.42
1:A:93:VAL:HG21	1:A:301:ALA:O	2.19	0.42
1:A:351:THR:HG21	2:B:1103:ILE:CG1	2.47	0.42
1:A:460:VAL:CG1	1:A:461:LYS:N	2.83	0.42
1:A:468:PHE:CE2	1:A:489:LEU:HD23	2.55	0.42
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.52	0.42
1:A:722:LEU:HD23	1:A:799:PHE:CG	2.55	0.42
1:A:961:ARG:O	1:A:965:GLN:HG3	2.20	0.42
1:A:1402:PHE:CE2	1:A:1403:GLU:HG2	2.55	0.42
2:B:134:LYS:NZ	2:B:164:LYS:NZ	2.68	0.42
2:B:711:GLU:HB2	2:B:712:PRO:CD	2.50	0.42
2:B:745:PRO:O	2:B:747:MET:N	2.52	0.42
3:C:66:ARG:CZ	10:J:2:ILE:CG2	2.98	0.42
3:C:249:ASP:O	3:C:250:THR:C	2.63	0.42
10:J:27:GLU:C	10:J:29:GLU:N	2.77	0.42
10:J:61:LEU:C	10:J:63:TYR:H	2.27	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:69:THR:HG21	2:N:1174:LYS:HZ3	1.85	0.42
1:M:108:MET:O	1:M:109:HIS:HB3	2.20	0.42
1:M:316:GLN:HG2	1:M:317:LYS:HG2	2.01	0.42
1:M:415:LEU:HD23	1:M:415:LEU:HA	1.70	0.42
1:M:541:ILE:HD13	1:M:549:MET:HE3	1.96	0.42
1:M:567:LYS:HE3	8:T:46:LEU:HD12	2.00	0.42
1:M:714:PHE:CB	9:U:97:MET:HE1	2.43	0.42
1:M:809:THR:H	1:M:812:GLU:HB2	1.85	0.42
1:M:820:GLY:C	1:M:822:GLU:N	2.76	0.42
1:M:1011:GLN:NE2	1:M:1015:VAL:HG21	2.29	0.42
1:M:1057:VAL:HG12	1:M:1058:VAL:N	2.34	0.42
1:M:1120:LEU:HD23	1:M:1304:TRP:O	2.19	0.42
1:M:1207:LEU:HA	1:M:1211:GLN:OE1	2.20	0.42
2:N:63:ILE:HD12	2:N:63:ILE:HA	1.79	0.42
2:N:219:ALA:HB2	2:N:405:ARG:NH1	2.34	0.42
2:N:425:THR:HG22	2:N:426:LYS:N	2.35	0.42
2:N:486:TYR:N	2:N:486:TYR:HD2	2.16	0.42
2:N:552:MET:O	2:N:554:ILE:N	2.53	0.42
2:N:640:VAL:HG12	2:N:649:LYS:HG2	2.01	0.42
2:N:698:GLU:O	2:N:701:ILE:HG12	2.20	0.42
2:N:893:LEU:HD22	2:N:897:GLY:C	2.45	0.42
2:N:976:ILE:O	2:N:990:ILE:HB	2.19	0.42
4:P:207:LEU:HG	4:P:211:LEU:HD12	2.02	0.42
5:Q:17:ARG:O	5:Q:20:LYS:HB2	2.20	0.42
11:W:70:ARG:O	11:W:70:ARG:HG3	2.18	0.42
1:A:425:GLN:N	1:A:425:GLN:CD	2.78	0.42
1:A:904:THR:O	1:A:904:THR:HG22	2.20	0.42
1:A:1011:GLN:HE22	1:A:1015:VAL:HG23	1.83	0.42
2:B:39:ARG:HH21	2:B:665:GLU:HG2	1.81	0.42
2:B:123:THR:CB	2:B:458:LYS:HE2	2.49	0.42
2:B:434:ARG:O	2:B:436:VAL:N	2.52	0.42
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.93	0.42
2:B:640:VAL:HG12	2:B:649:LYS:HG2	2.02	0.42
2:B:745:PRO:C	2:B:747:MET:N	2.78	0.42
2:B:842:ASN:HD22	2:B:845:SER:CB	2.33	0.42
2:B:905:VAL:HG23	2:B:941:LEU:HD22	2.02	0.42
2:B:1125:ASP:O	2:B:1125:ASP:CG	2.62	0.42
4:D:175:PHE:O	4:D:178:ALA:HB3	2.20	0.42
5:E:112:TYR:C	5:E:112:TYR:HD1	2.27	0.42
6:F:69:LEU:C	6:F:71:GLU:N	2.78	0.42
6:F:88:TYR:O	6:F:89:GLU:C	2.60	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:50:ASP:O	7:G:51:TYR:C	2.61	0.42
8:H:55:LEU:HD22	8:H:144:ILE:CG2	2.49	0.42
11:K:53:ASP:HB3	11:K:56:VAL:HG23	2.00	0.42
11:K:89:ASN:O	11:K:90:ALA:C	2.62	0.42
1:M:154:SER:HB3	1:M:162:VAL:CG2	2.50	0.42
1:M:172:PRO:HD3	1:M:185:TRP:NE1	2.34	0.42
1:M:385:ILE:CG2	1:M:386:ASP:N	2.81	0.42
1:M:426:LEU:O	1:M:427:GLN:HG2	2.19	0.42
1:M:577:ILE:HA	1:M:580:VAL:HG23	2.01	0.42
1:M:672:ASP:OD2	1:M:674:PRO:HG2	2.20	0.42
1:M:777:PHE:CD1	1:M:781:ASP:HA	2.55	0.42
1:M:848:ILE:HA	1:M:857:ARG:O	2.19	0.42
2:N:31:TRP:CE3	2:N:31:TRP:HA	2.54	0.42
2:N:31:TRP:O	2:N:32:ALA:C	2.63	0.42
2:N:225:VAL:HG11	2:N:385:LEU:HA	2.01	0.42
2:N:278:GLN:CG	2:N:279:ASP:H	2.33	0.42
2:N:508:LEU:O	2:N:509:ALA:CB	2.66	0.42
2:N:702:LEU:HG	2:N:738:PHE:HD2	1.85	0.42
2:N:838:SER:HA	2:N:989:THR:O	2.19	0.42
2:N:872:GLU:CD	2:N:914:LYS:HE2	2.44	0.42
2:N:1060:ARG:HD2	2:N:1060:ARG:HA	1.51	0.42
2:N:1094:ARG:HH21	2:N:1098:MET:HG2	1.85	0.42
3:O:8:VAL:CG1	3:O:9:LYS:N	2.80	0.42
3:O:105:GLY:O	3:O:149:LYS:O	2.37	0.42
3:O:236:GLY:O	3:O:237:SER:C	2.63	0.42
4:P:198:LEU:HB2	4:P:199:ASN:H	1.59	0.42
5:Q:121:MET:C	5:Q:123:LEU:N	2.77	0.42
5:Q:134:THR:C	5:Q:135:PHE:CD1	2.98	0.42
6:R:72:LYS:H	6:R:72:LYS:HG2	1.69	0.42
7:S:121:PHE:CD1	7:S:130:TYR:CE1	3.08	0.42
9:U:17:ARG:HG3	9:U:28:GLU:OE1	2.19	0.42
1:A:370:ILE:HG23	1:A:374:LEU:HD12	2.02	0.42
1:A:596:THR:C	1:A:598:LEU:N	2.63	0.42
1:A:622:VAL:HG22	1:A:622:VAL:O	2.20	0.42
1:A:1127:ASP:CG	1:A:1130:GLN:CB	2.93	0.42
1:A:1264:GLU:OE2	9:I:46:HIS:CD2	2.72	0.42
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.49	0.42
2:B:695:ALA:O	2:B:698:GLU:HB3	2.19	0.42
4:D:16:LYS:O	4:D:18:VAL:N	2.45	0.42
4:D:123:LEU:HD13	4:D:149:THR:HG21	2.01	0.42
5:E:82:PHE:O	5:E:83:CYS:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:61:LEU:O	10:J:63:TYR:N	2.51	0.42
11:K:65:HIS:NE2	11:K:67:PHE:CG	2.85	0.42
1:M:252:PHE:HB2	1:M:256:GLN:NE2	2.35	0.42
1:M:583:PRO:O	1:M:610:GLY:HA3	2.20	0.42
1:M:596:THR:C	1:M:598:LEU:N	2.62	0.42
1:M:709:THR:HG23	9:U:94:ASP:HA	2.01	0.42
1:M:973:ILE:HG12	1:M:1038:THR:HG23	2.02	0.42
1:M:1029:ARG:NH1	1:M:1029:ARG:CG	2.83	0.42
1:M:1407:GLU:N	1:M:1407:GLU:CD	2.78	0.42
1:M:1433:MET:HE2	2:N:1145:SER:OG	2.20	0.42
2:N:274:PRO:HG2	2:N:359:GLU:HB3	2.02	0.42
2:N:758:PHE:CE1	2:N:1027:ILE:CG2	3.02	0.42
2:N:840:ILE:HB	2:N:1011:ILE:HB	2.02	0.42
2:N:880:THR:CB	2:N:934:LYS:HD2	2.35	0.42
2:N:1160:VAL:HG11	2:N:1169:MET:SD	2.60	0.42
2:N:1185:CYS:HA	4:P:17:LYS:HE3	2.02	0.42
4:P:69:ALA:C	4:P:71:LYS:N	2.78	0.42
4:P:159:THR:HG21	4:P:219:THR:OG1	2.20	0.42
5:Q:61:GLN:HG2	5:Q:62:ALA:H	1.84	0.42
6:R:69:LEU:C	6:R:71:GLU:N	2.78	0.42
8:T:100:THR:HG22	8:T:101:ALA:N	2.35	0.42
1:A:100:LYS:O	1:A:104:GLU:HG3	2.20	0.41
1:A:254:GLU:HB3	1:A:255:SER:H	1.46	0.41
1:A:533:LYS:HE2	1:A:533:LYS:HB3	1.90	0.41
1:A:848:ILE:HA	1:A:857:ARG:O	2.20	0.41
1:A:900:ASP:HB3	1:A:906:HIS:HB2	2.02	0.41
1:A:929:LEU:N	1:A:929:LEU:HD22	2.35	0.41
1:A:1129:GLU:HG2	1:A:1132:LYS:NZ	2.35	0.41
1:A:1155:ASP:CG	1:A:1162:VAL:HG23	2.45	0.41
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	2.02	0.41
1:A:1239:ARG:HB3	1:A:1239:ARG:NH1	2.35	0.41
2:B:307:ASP:OD2	2:B:310:MET:HE3	2.20	0.41
2:B:360:PHE:CD2	2:B:361:LEU:HB2	2.55	0.41
2:B:522:VAL:CG1	2:B:537:LYS:HB3	2.50	0.41
2:B:531:GLN:HG2	2:B:532:ALA:N	2.35	0.41
2:B:604:ARG:C	2:B:606:LYS:N	2.77	0.41
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.52	0.41
2:B:785:TYR:CD1	2:B:785:TYR:C	2.98	0.41
2:B:1114:LEU:HG	2:B:1202:LEU:HD11	2.02	0.41
3:C:31:ASN:O	3:C:34:ARG:HB3	2.20	0.41
3:C:36:VAL:HG21	3:C:251:LEU:HD13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:76:ASP:OD2	3:C:128:ASN:N	2.52	0.41
4:D:63:LEU:O	4:D:133:THR:HG21	2.19	0.41
4:D:148:LEU:HD23	4:D:148:LEU:HA	1.92	0.41
5:E:157:SER:O	5:E:159:ASP:N	2.53	0.41
7:G:1:MET:HE3	7:G:80:LYS:H	1.84	0.41
1:M:120:GLU:C	1:M:122:MET:N	2.75	0.41
1:M:288:ALA:HA	1:M:291:GLU:CG	2.50	0.41
1:M:688:LYS:C	1:M:690:VAL:N	2.78	0.41
1:M:1074:GLU:HB3	1:M:1075:PRO:CD	2.50	0.41
1:M:1098:VAL:N	1:M:1099:PRO:HD2	2.35	0.41
2:N:241:ARG:CG	2:N:253:THR:HG22	2.39	0.41
2:N:292:ILE:HD13	2:N:326:ASP:HA	2.01	0.41
2:N:768:THR:O	2:N:771:SER:HB2	2.20	0.41
3:O:101:LEU:HD13	3:O:118:LEU:CD2	2.49	0.41
4:P:27:LEU:HA	4:P:27:LEU:HD23	1.69	0.41
4:P:180:LEU:HD23	4:P:180:LEU:HA	1.53	0.41
5:Q:50:MET:HG2	5:Q:52:ARG:HE	1.85	0.41
5:Q:61:GLN:HB2	5:Q:79:TRP:HE3	1.85	0.41
5:Q:177:ARG:O	5:Q:212:ARG:HD3	2.20	0.41
6:R:116:ASP:OD1	6:R:116:ASP:C	2.63	0.41
6:R:120:ILE:O	6:R:124:GLU:HG3	2.20	0.41
7:S:26:LEU:CD1	7:S:56:ILE:HD11	2.50	0.41
12:X:38:LEU:O	12:X:39:SER:CB	2.68	0.41
1:A:134:ARG:HG2	1:A:138:ILE:CD1	2.49	0.41
1:A:332:LYS:HB2	1:A:332:LYS:HE3	1.80	0.41
1:A:482:PHE:C	1:A:484:GLY:H	2.28	0.41
1:A:546:VAL:HG21	1:A:572:TRP:HB2	2.01	0.41
1:A:582:ILE:HA	1:A:583:PRO:HD2	1.91	0.41
1:A:722:LEU:H	1:A:722:LEU:CD1	2.26	0.41
1:A:828:ALA:HB2	2:B:530:GLY:HA2	2.02	0.41
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.85	0.41
1:A:1313:LEU:HB3	1:A:1338:VAL:HG21	2.02	0.41
2:B:27:ALA:C	2:B:29:ASP:N	2.78	0.41
2:B:56:ASP:HB3	2:B:57:TYR:CE1	2.54	0.41
2:B:879:ARG:H	2:B:879:ARG:CD	2.31	0.41
2:B:916:THR:CB	2:B:935:ARG:HD2	2.50	0.41
2:B:948:ILE:O	2:B:949:VAL:C	2.61	0.41
2:B:1029:CYS:O	2:B:1030:LEU:C	2.61	0.41
2:B:1069:PHE:CD1	2:B:1069:PHE:N	2.78	0.41
2:B:1197:PRO:O	2:B:1198:TYR:C	2.62	0.41
6:F:118:LEU:O	6:F:122:MET:HG3	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:31:LEU:CD2	7:G:48:VAL:HG21	2.50	0.41
12:L:33:GLU:CD	12:L:33:GLU:N	2.78	0.41
1:M:34:LYS:CG	1:M:36:ARG:NH2	2.82	0.41
1:M:66:LYS:HZ3	1:M:68:GLN:H	1.66	0.41
1:M:116:ASP:C	1:M:118:HIS:N	2.77	0.41
1:M:436:ILE:HD11	1:M:491:VAL:HG11	2.01	0.41
1:M:482:PHE:C	1:M:484:GLY:N	2.77	0.41
1:M:541:ILE:HG21	1:M:549:MET:HE3	2.02	0.41
1:M:847:ASP:N	1:M:847:ASP:OD1	2.51	0.41
1:M:905:ASP:C	1:M:906:HIS:ND1	2.72	0.41
2:N:33:VAL:O	2:N:36:ALA:HB3	2.20	0.41
2:N:459:TYR:CZ	2:N:469:GLN:HG3	2.55	0.41
2:N:893:LEU:HD22	2:N:897:GLY:HA2	2.02	0.41
2:N:1072:MET:HE3	2:N:1085:ILE:HD13	2.01	0.41
2:N:1107:ALA:O	2:N:1108:ARG:CB	2.67	0.41
2:N:1170:THR:O	2:N:1171:VAL:C	2.62	0.41
3:O:69:LEU:H	3:O:69:LEU:CD1	2.28	0.41
3:O:208:GLU:O	3:O:210:GLU:N	2.53	0.41
8:T:93:TYR:N	8:T:93:TYR:CD1	2.88	0.41
11:W:22:ASP:O	11:W:31:VAL:HG12	2.19	0.41
1:A:157:ASP:C	1:A:159:THR:N	2.77	0.41
1:A:230:ARG:HG3	1:A:233:TRP:CZ3	2.55	0.41
1:A:447:GLN:CD	13:1:20:DG:H4'	2.45	0.41
1:A:655:PHE:O	1:A:658:LEU:HB3	2.21	0.41
1:A:1277:GLU:C	1:A:1279:ILE:N	2.77	0.41
2:B:362:PRO:C	2:B:363:HIS:O	2.59	0.41
2:B:371:GLU:CD	2:B:371:GLU:H	2.29	0.41
2:B:853:SER:OG	2:B:1094:ARG:NH1	2.53	0.41
2:B:1060:ARG:C	2:B:1062:HIS:H	2.29	0.41
3:C:193:TYR:C	3:C:193:TYR:HD1	2.25	0.41
4:D:53:SER:C	4:D:55:ALA:N	2.77	0.41
4:D:63:LEU:O	4:D:129:LEU:HD11	2.20	0.41
4:D:151:PHE:CD1	4:D:151:PHE:N	2.87	0.41
5:E:43:LYS:H	5:E:43:LYS:HG3	1.67	0.41
5:E:117:THR:C	5:E:119:SER:H	2.28	0.41
8:H:93:TYR:N	8:H:93:TYR:CD1	2.89	0.41
9:I:8:ARG:HG3	9:I:8:ARG:H	1.67	0.41
10:J:57:ILE:O	10:J:60:PHE:HB2	2.20	0.41
12:L:65:VAL:HG23	12:L:67:PHE:CE1	2.55	0.41
1:M:208:LEU:O	1:M:208:LEU:HD23	2.21	0.41
1:M:278:THR:HG22	1:M:278:THR:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:365:GLY:O	1:M:468:PHE:HA	2.20	0.41
1:M:675:THR:O	1:M:675:THR:HG22	2.20	0.41
1:M:715:GLU:OE1	1:M:774:ARG:HD3	2.19	0.41
2:N:39:ARG:HH21	2:N:665:GLU:HG2	1.82	0.41
2:N:323:VAL:O	2:N:323:VAL:HG12	2.20	0.41
2:N:405:ARG:HA	2:N:631:GLY:O	2.20	0.41
2:N:637:LEU:HD12	2:N:693:ILE:CD1	2.50	0.41
2:N:700:SER:C	2:N:701:ILE:HG23	2.44	0.41
2:N:745:PRO:O	2:N:747:MET:N	2.53	0.41
2:N:759:PRO:C	2:N:761:HIS:H	2.28	0.41
3:O:98:VAL:C	3:O:99:LEU:HD22	2.45	0.41
3:O:162:GLY:HA3	3:O:170:TRP:CE2	2.56	0.41
3:O:217:ASP:HA	3:O:218:PRO:HD3	1.91	0.41
3:O:236:GLY:C	3:O:238:ILE:N	2.77	0.41
4:P:149:THR:HG23	4:P:150:ASN:N	2.35	0.41
8:T:77:ARG:CG	8:T:78:SER:H	2.33	0.41
8:T:143:LEU:C	8:T:144:ILE:HG13	2.44	0.41
9:U:11:ASN:C	9:U:11:ASN:OD1	2.63	0.41
9:U:70:ARG:HA	9:U:83:ASN:O	2.20	0.41
11:W:89:ASN:O	11:W:90:ALA:C	2.63	0.41
13:4:18:DA:H3'	13:4:18:DA:OP1	2.20	0.41
1:A:106:VAL:HG21	1:A:214:ILE:CD1	2.51	0.41
1:A:277:GLU:C	1:A:279:LEU:H	2.28	0.41
1:A:288:ALA:HA	1:A:291:GLU:HG3	2.00	0.41
2:B:97:VAL:O	2:B:97:VAL:CG1	2.66	0.41
2:B:175:ARG:HB2	2:B:200:GLY:HA3	2.02	0.41
2:B:641:GLU:OE1	2:B:641:GLU:HA	2.20	0.41
2:B:1183:LYS:N	2:B:1183:LYS:CE	2.80	0.41
3:C:66:ARG:O	3:C:67:LEU:C	2.62	0.41
4:D:70:PHE:O	4:D:74:GLN:HG2	2.20	0.41
5:E:55:ARG:HG3	5:E:55:ARG:NH1	2.34	0.41
5:E:67:GLU:O	5:E:70:SER:HB3	2.20	0.41
7:G:123:ALA:C	7:G:125:SER:H	2.27	0.41
7:G:155:SER:O	7:G:156:SER:HB3	2.20	0.41
1:M:5:GLN:O	2:N:1159:ARG:NH2	2.52	0.41
1:M:79:GLY:N	2:N:1201:LYS:HZ1	2.18	0.41
1:M:344:ARG:NE	2:N:1120:GLU:HB2	2.35	0.41
1:M:715:GLU:O	1:M:716:ASP:C	2.63	0.41
1:M:956:LEU:HD21	1:M:1017:LEU:HG	2.01	0.41
1:M:960:ILE:CA	1:M:963:ILE:HG22	2.50	0.41
1:M:1063:MET:SD	1:M:1436:ILE:HB	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:51:PHE:HB2	2:N:173:MET:CE	2.50	0.41
2:N:129:PHE:CE2	2:N:166:PHE:HD1	2.38	0.41
2:N:129:PHE:CD2	2:N:166:PHE:HA	2.49	0.41
2:N:227:LYS:HG3	2:N:395:GLN:OE1	2.20	0.41
2:N:244:LEU:O	2:N:246:LYS:N	2.53	0.41
2:N:245:GLU:O	2:N:245:GLU:HG2	2.20	0.41
2:N:280:ILE:HG23	2:N:281:PRO:HD2	2.01	0.41
2:N:757:PRO:HG2	2:N:984:HIS:CE1	2.55	0.41
2:N:856:PHE:N	2:N:856:PHE:CD1	2.88	0.41
2:N:910:VAL:CG1	2:N:938:SER:HB3	2.50	0.41
2:N:945:GLU:O	2:N:946:ASN:HB3	2.20	0.41
2:N:1207:LEU:HD23	2:N:1207:LEU:HA	1.81	0.41
3:O:174:ALA:O	3:O:175:ALA:CB	2.67	0.41
7:S:122:ASN:HB2	7:S:131:GLN:CG	2.51	0.41
13:4:19:DT:H2'	13:4:20:DG:H8	1.86	0.41
13:4:27:DC:H2''	13:4:28:DA:C8	2.55	0.41
1:A:12:ARG:O	2:B:1194:ILE:HG22	2.21	0.41
1:A:224:PHE:HB3	1:A:225:ASN:H	1.78	0.41
1:A:352:VAL:HG12	1:A:353:ILE:N	2.35	0.41
1:A:741:ASN:ND2	1:A:741:ASN:C	2.78	0.41
1:A:825:ILE:O	1:A:829:VAL:HG23	2.19	0.41
1:A:908:LEU:CD1	1:A:983:ILE:HD11	2.46	0.41
1:A:1213:GLY:O	1:A:1214:GLU:C	2.62	0.41
1:A:1312:ASN:CG	1:A:1315:GLU:HG3	2.46	0.41
1:A:1438:THR:HB	2:B:1144:ALA:CB	2.49	0.41
2:B:52:ASN:O	2:B:56:ASP:HB2	2.20	0.41
2:B:54:PHE:HE1	2:B:414:ALA:HA	1.85	0.41
2:B:64:CYS:HA	2:B:67:SER:HG	1.83	0.41
2:B:126:SER:O	2:B:169:ARG:HA	2.20	0.41
2:B:298:LEU:N	2:B:298:LEU:CD2	2.82	0.41
2:B:598:GLU:O	2:B:602:THR:OG1	2.39	0.41
2:B:644:GLU:C	2:B:646:LEU:H	2.27	0.41
2:B:769:TYR:O	2:B:772:ALA:N	2.51	0.41
2:B:842:ASN:ND2	2:B:845:SER:N	2.66	0.41
2:B:911:ILE:HG22	2:B:911:ILE:O	2.21	0.41
2:B:1130:PHE:HZ	2:B:1138:MET:HG2	1.84	0.41
4:D:50:LEU:HD21	7:G:4:ILE:HD12	2.02	0.41
5:E:83:CYS:SG	5:E:85:GLU:HB2	2.61	0.41
8:H:103:LYS:HG2	8:H:104:PHE:N	2.36	0.41
9:I:7:CYS:C	9:I:8:ARG:O	2.61	0.41
9:I:59:VAL:C	9:I:61:ASP:N	2.75	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:49:GLU:HG3	11:K:94:ILE:HG13	2.02	0.41
11:K:51:LEU:HD12	11:K:51:LEU:HA	1.86	0.41
1:M:150:THR:HA	1:M:165:GLY:O	2.19	0.41
1:M:219:PHE:O	1:M:222:LEU:HB2	2.21	0.41
1:M:437:MET:O	1:M:438:ASP:C	2.63	0.41
1:M:672:ASP:CG	1:M:674:PRO:HD2	2.45	0.41
1:M:844:ALA:O	1:M:845:LEU:HD23	2.21	0.41
1:M:1125:ALA:C	1:M:1127:ASP:H	2.28	0.41
1:M:1402:PHE:CZ	1:M:1403:GLU:CG	3.03	0.41
2:N:67:SER:HB3	2:N:92:PHE:HD1	1.86	0.41
2:N:113:TYR:CD2	2:N:192:LEU:HD22	2.55	0.41
2:N:308:TRP:HA	2:N:311:LEU:HD12	2.01	0.41
2:N:335:GLY:O	2:N:336:ARG:HB2	2.19	0.41
2:N:427:ASP:HA	2:N:430:ARG:CG	2.50	0.41
2:N:593:PRO:C	2:N:595:ARG:N	2.77	0.41
6:R:79:ARG:HG3	6:R:144:GLU:HB3	2.02	0.41
7:S:93:SER:OG	7:S:100:GLU:HB3	2.21	0.41
7:S:99:PHE:CE1	7:S:143:ILE:HD12	2.55	0.41
10:V:57:ILE:HA	10:V:60:PHE:CD2	2.37	0.41
13:4:15:DG:C8	13:4:16:DT:C7	3.04	0.41
1:A:6:TYR:CD1	1:A:7:SER:N	2.88	0.41
1:A:172:PRO:HD3	1:A:185:TRP:CD1	2.56	0.41
1:A:667:GLY:CA	1:A:670:ILE:HD11	2.40	0.41
1:A:896:ARG:HB3	1:A:897:TYR:CD1	2.56	0.41
1:A:929:LEU:N	1:A:929:LEU:CD2	2.84	0.41
1:A:1115:SER:OG	1:A:1116:LEU:N	2.54	0.41
1:A:1206:ASP:O	1:A:1274:ARG:CZ	2.68	0.41
2:B:31:TRP:O	2:B:32:ALA:C	2.64	0.41
2:B:436:VAL:O	2:B:436:VAL:HG12	2.20	0.41
2:B:846:ILE:HG23	2:B:974:PRO:CG	2.42	0.41
3:C:208:GLU:C	3:C:210:GLU:H	2.27	0.41
3:C:209:TYR:CD1	3:C:209:TYR:N	2.88	0.41
3:C:254:LYS:HE2	11:K:42:LEU:HD13	2.02	0.41
4:D:52:LEU:CD1	4:D:182:SER:HB2	2.50	0.41
4:D:156:ASP:O	4:D:158:GLU:N	2.53	0.41
5:E:55:ARG:HD2	5:E:84:ASP:HA	2.03	0.41
5:E:55:ARG:NE	5:E:113:GLN:NE2	2.68	0.41
6:F:69:LEU:HB2	6:F:72:LYS:HD2	2.01	0.41
7:G:1:MET:HE1	7:G:80:LYS:H	1.85	0.41
8:H:4:THR:HG22	8:H:5:LEU:H	1.86	0.41
8:H:38:LEU:HD12	8:H:124:ARG:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.38	0.41
13:1:12:DG:H1'	13:1:13:DT:O5'	2.21	0.41
1:M:102:VAL:CG1	1:M:211:PHE:CE1	3.03	0.41
1:M:418:SER:C	1:M:420:ARG:H	2.29	0.41
1:M:1155:ASP:O	1:M:1190:PRO:O	2.38	0.41
1:M:1205:LYS:O	1:M:1206:ASP:C	2.62	0.41
2:N:186:GLU:CG	10:V:62:ARG:NH2	2.84	0.41
2:N:259:TYR:CD1	2:N:259:TYR:N	2.89	0.41
2:N:653:VAL:HG22	2:N:689:LEU:HB3	1.99	0.41
2:N:705:MET:HB3	2:N:706:GLN:H	1.68	0.41
2:N:745:PRO:C	2:N:747:MET:N	2.79	0.41
2:N:797:TYR:CE1	2:N:854:LEU:CD2	3.04	0.41
2:N:886:LYS:HD2	2:N:887:HIS:NE2	2.36	0.41
2:N:898:LEU:HD13	2:N:952:VAL:CG1	2.50	0.41
2:N:1096:ARG:CG	2:N:1097:HIS:N	2.84	0.41
3:O:183:TRP:O	3:O:185:LYS:HG3	2.20	0.41
4:P:173:HIS:CE1	4:P:175:PHE:HB2	2.55	0.41
6:R:136:ARG:O	6:R:143:PHE:HA	2.21	0.41
7:S:34:VAL:HG13	7:S:45:ILE:HG21	2.02	0.41
1:A:55:ASP:OD1	1:A:57:ARG:CA	2.69	0.41
1:A:562:THR:HA	1:A:563:PRO:HD3	1.89	0.41
1:A:738:LYS:HG3	1:A:740:LEU:HG	2.01	0.41
1:A:765:VAL:HB	1:A:800:VAL:HG12	2.02	0.41
1:A:867:ILE:HG12	1:A:1000:LEU:HD11	2.02	0.41
1:A:1081:LEU:HD11	1:A:1098:VAL:N	2.31	0.41
1:A:1311:VAL:HG11	1:A:1334:ASP:OD2	2.21	0.41
2:B:31:TRP:CZ2	2:B:807:ARG:HB2	2.55	0.41
2:B:120:ARG:HH11	12:L:54:ARG:HH11	1.64	0.41
2:B:308:TRP:CZ3	9:I:45:ARG:HG2	2.54	0.41
2:B:553:PRO:C	2:B:554:ILE:HD12	2.46	0.41
2:B:791:THR:O	2:B:792:MET:HB2	2.20	0.41
2:B:884:ARG:O	2:B:936:ASP:CB	2.69	0.41
2:B:957:ASN:O	2:B:958:GLN:C	2.63	0.41
4:D:7:THR:HB	7:G:42:PHE:CE2	2.55	0.41
4:D:12:ARG:HH11	4:D:12:ARG:CG	2.34	0.41
4:D:32:GLU:C	7:G:5:LYS:HZ3	2.24	0.41
4:D:66:ARG:O	4:D:67:ARG:C	2.63	0.41
5:E:72:PHE:CD1	5:E:72:PHE:N	2.89	0.41
7:G:14:HIS:CD2	7:G:16:SER:HB3	2.56	0.41
9:I:73:ARG:NH1	9:I:112:SER:HB3	2.35	0.41
13:1:18:DA:H3'	13:1:18:DA:OP1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:244:PRO:HB2	1:M:245:PRO:CD	2.41	0.41
1:M:317:LYS:O	1:M:318:SER:HB3	2.18	0.41
1:M:401:GLY:H	1:M:435:HIS:HD2	1.68	0.41
1:M:780:VAL:O	1:M:782:ARG:HG2	2.20	0.41
1:M:947:PHE:O	1:M:948:VAL:C	2.64	0.41
1:M:1220:PHE:CD1	1:M:1224:LEU:HD23	2.55	0.41
2:N:203:PHE:HB3	2:N:205:ILE:HD11	2.03	0.41
2:N:234:ILE:HG12	2:N:257:LYS:HG2	2.03	0.41
2:N:238:ALA:HB3	2:N:256:VAL:HB	2.02	0.41
2:N:639:ILE:HG22	2:N:641:GLU:HG2	2.03	0.41
2:N:642:ASP:N	2:N:649:LYS:HG3	2.35	0.41
2:N:762:ASN:OD1	2:N:1022:THR:HA	2.20	0.41
3:O:186:LEU:N	3:O:186:LEU:CD1	2.83	0.41
3:O:215:GLU:O	3:O:217:ASP:N	2.53	0.41
1:A:108:MET:O	1:A:109:HIS:HB3	2.21	0.41
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.51	0.41
1:A:273:ASN:O	1:A:274:ILE:C	2.64	0.41
1:A:416:ARG:NH1	1:A:417:TYR:CE1	2.89	0.41
1:A:482:PHE:C	1:A:484:GLY:N	2.78	0.41
1:A:709:THR:HG22	1:A:711:ARG:H	1.85	0.41
1:A:722:LEU:HD12	1:A:722:LEU:N	2.25	0.41
1:A:820:GLY:O	1:A:821:ARG:C	2.64	0.41
1:A:1155:ASP:O	1:A:1190:PRO:O	2.38	0.41
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.20	0.41
1:A:1265:ASN:O	1:A:1266:THR:C	2.62	0.41
2:B:188:ASP:O	2:B:192:LEU:HD12	2.21	0.41
2:B:280:ILE:HD11	2:B:334:ILE:HG12	2.03	0.41
2:B:281:PRO:O	2:B:283:VAL:N	2.54	0.41
2:B:508:LEU:HB3	14:2:1:DA:O3'	2.21	0.41
2:B:571:PRO:O	2:B:574:SER:O	2.38	0.41
2:B:770:GLN:HB2	2:B:985:GLY:H	1.85	0.41
2:B:847:ASP:O	3:C:65:HIS:HE1	2.03	0.41
2:B:859:TYR:CD1	2:B:859:TYR:N	2.89	0.41
2:B:887:HIS:CD2	2:B:887:HIS:H	2.37	0.41
2:B:958:GLN:C	2:B:960:GLY:H	2.29	0.41
3:C:196:ASP:OD1	3:C:198:ALA:N	2.54	0.41
4:D:32:GLU:O	4:D:33:PHE:CG	2.74	0.41
5:E:13:TRP:CE3	5:E:39:LEU:HD13	2.55	0.41
7:G:14:HIS:HD2	7:G:16:SER:HB3	1.85	0.41
8:H:116:TYR:HE2	8:H:140:ALA:CB	2.33	0.41
11:K:21:ILE:HG12	11:K:33:ILE:HG23	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:425:GLN:N	1:M:425:GLN:CD	2.79	0.41
1:M:591:PHE:HA	1:M:595:THR:CG2	2.39	0.41
1:M:1208:THR:HG22	1:M:1210:GLY:N	2.34	0.41
2:N:52:ASN:O	2:N:56:ASP:HB2	2.21	0.41
2:N:460:ALA:HB1	2:N:466:TRP:CE3	2.56	0.41
2:N:492:LEU:HB2	2:N:751:VAL:HG11	2.03	0.41
2:N:941:LEU:CD2	2:N:946:ASN:HA	2.50	0.41
3:O:208:GLU:C	3:O:210:GLU:H	2.27	0.41
5:Q:22:MET:HE3	5:Q:26:ARG:NH2	2.34	0.41
5:Q:63:ASN:HB3	5:Q:64:PRO:CD	2.51	0.41
7:S:59:GLY:HA3	7:S:70:PHE:CD2	2.56	0.41
7:S:132:SER:HB3	7:S:135:ASP:HB2	2.03	0.41
8:T:11:GLN:C	8:T:28:ALA:CB	2.94	0.41
11:W:65:HIS:NE2	11:W:67:PHE:CG	2.87	0.41
1:A:145:LYS:HE3	1:A:145:LYS:CA	2.51	0.41
1:A:360:GLU:O	1:A:361:LEU:C	2.63	0.41
1:A:381:THR:O	1:A:382:PRO:C	2.63	0.41
1:A:381:THR:C	1:A:383:TYR:N	2.76	0.41
1:A:628:GLY:C	1:A:630:ILE:N	2.77	0.41
1:A:696:GLU:O	1:A:696:GLU:HG2	2.21	0.41
1:A:715:GLU:O	1:A:716:ASP:C	2.63	0.41
1:A:947:PHE:O	1:A:948:VAL:C	2.64	0.41
1:A:1094:VAL:HG13	1:A:1113:THR:CB	2.50	0.41
1:A:1094:VAL:HG13	1:A:1113:THR:HB	2.03	0.41
2:B:38:PHE:O	2:B:39:ARG:C	2.64	0.41
2:B:63:ILE:HD12	2:B:63:ILE:HA	1.76	0.41
2:B:128:LEU:HD12	2:B:128:LEU:HA	1.93	0.41
2:B:222:ILE:O	2:B:240:ILE:HA	2.21	0.41
2:B:241:ARG:HG2	2:B:253:THR:HG21	2.01	0.41
2:B:244:LEU:C	2:B:246:LYS:N	2.79	0.41
2:B:360:PHE:CD2	2:B:360:PHE:C	2.99	0.41
2:B:360:PHE:HD2	2:B:374:LYS:HD3	1.85	0.41
2:B:466:TRP:O	2:B:468:GLU:N	2.53	0.41
2:B:579:ARG:NH1	2:B:579:ARG:CG	2.82	0.41
2:B:593:PRO:C	2:B:595:ARG:N	2.78	0.41
2:B:796:LEU:HD12	2:B:796:LEU:HA	1.88	0.41
2:B:936:ASP:CG	2:B:937:ALA:N	2.79	0.41
2:B:1085:ILE:N	2:B:1085:ILE:HD12	2.36	0.41
2:B:1110:PRO:HB2	2:B:1119:VAL:HG11	2.03	0.41
2:B:1159:ARG:O	2:B:1159:ARG:HD2	2.21	0.41
3:C:33:LEU:CG	3:C:37:MET:HE2	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:ARG:O	3:C:38:ILE:HG13	2.21	0.41
4:D:52:LEU:H	4:D:182:SER:HB3	1.86	0.41
4:D:166:LEU:HD23	4:D:214:LEU:HD22	2.03	0.41
5:E:65:THR:O	5:E:69:ILE:CD1	2.68	0.41
6:F:109:VAL:CG1	6:F:110:ASP:H	2.28	0.41
7:G:87:VAL:CG2	7:G:103:VAL:HG21	2.51	0.41
7:G:117:GLN:NE2	7:S:153:GLN:HG3	2.34	0.41
8:H:11:GLN:C	8:H:28:ALA:CB	2.94	0.41
8:H:97:MET:HE2	8:H:142:LEU:HD23	2.03	0.41
8:H:105:GLU:O	8:H:112:ILE:HD12	2.21	0.41
10:J:6:ARG:HA	10:J:12:LYS:O	2.21	0.41
11:K:56:VAL:HA	11:K:77:THR:HG22	2.02	0.41
12:L:27:LEU:HD13	12:L:37:LYS:CG	2.51	0.41
12:L:48:CYS:HB3	12:L:51:CYS:O	2.20	0.41
1:M:40:THR:HG21	1:M:259:GLU:OE2	2.21	0.41
1:M:355:GLY:N	1:M:482:PHE:CZ	2.89	0.41
1:M:444:PHE:CE2	1:M:487:MET:HE3	2.55	0.41
1:M:446:ARG:HD2	1:M:480:ALA:HB2	2.03	0.41
1:M:472:LEU:CD1	2:N:835:GLN:NE2	2.82	0.41
1:M:492:PRO:HB3	1:M:497:THR:HG22	2.02	0.41
1:M:532:ARG:NH2	1:M:745:GLN:HG2	2.36	0.41
1:M:553:VAL:HA	1:M:554:PRO:HD2	1.87	0.41
1:M:562:THR:HA	1:M:563:PRO:HD3	1.89	0.41
1:M:794:PRO:C	1:M:796:SER:N	2.78	0.41
1:M:1155:ASP:CG	1:M:1162:VAL:HG23	2.45	0.41
1:M:1161:THR:HG22	1:M:1163:ILE:HG13	2.03	0.41
1:M:1166:ASP:O	1:M:1167:GLU:C	2.64	0.41
1:M:1212:VAL:O	1:M:1215:ARG:HB2	2.21	0.41
1:M:1395:GLY:HA3	1:M:1419:ASP:OD2	2.21	0.41
2:N:101:MET:HB3	2:N:109:THR:HG22	2.03	0.41
2:N:228:LYS:HD3	2:N:228:LYS:HA	1.85	0.41
2:N:261:ARG:O	2:N:262:GLU:C	2.63	0.41
2:N:449:ASN:O	2:N:451:LYS:N	2.53	0.41
2:N:610:ASN:HA	2:N:611:PRO:HD3	1.97	0.41
2:N:637:LEU:HD21	2:N:742:GLU:HA	2.03	0.41
2:N:654:ARG:HG3	2:N:654:ARG:NH1	2.31	0.41
2:N:886:LYS:HB2	2:N:890:TYR:OH	2.21	0.41
2:N:990:ILE:HG22	2:N:991:GLY:N	2.35	0.41
2:N:1034:VAL:O	2:N:1037:LEU:N	2.53	0.41
2:N:1104:HIS:ND1	2:N:1105:ALA:N	2.68	0.41
2:N:1106:ARG:HH12	2:N:1110:PRO:HG2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:1106:ARG:HD3	2:N:1126:GLY:C	2.46	0.41
3:O:75:MET:O	3:O:246:ARG:NH2	2.53	0.41
4:P:150:ASN:HB2	4:P:151:PHE:CE1	2.56	0.41
4:P:155:ARG:HB2	4:P:155:ARG:CZ	2.50	0.41
4:P:155:ARG:HH11	4:P:155:ARG:HB3	1.83	0.41
5:Q:156:LEU:O	5:Q:157:SER:C	2.62	0.41
7:S:7:LEU:HD13	7:S:45:ILE:HD11	2.03	0.41
7:S:111:THR:HG22	7:S:114:LEU:CB	2.47	0.41
7:S:112:LYS:C	7:S:114:LEU:H	2.29	0.41
8:T:138:GLU:OE1	8:T:138:GLU:C	2.64	0.41
8:T:145:ARG:O	8:T:146:ARG:CB	2.69	0.41
9:U:6:PHE:CD2	9:U:12:ASN:O	2.73	0.41
9:U:22:ASN:O	9:U:23:ASN:HB2	2.21	0.41
11:W:13:GLY:O	11:W:14:GLU:C	2.64	0.41
12:X:37:LYS:HE3	12:X:37:LYS:HB2	1.81	0.41
1:A:68:GLN:O	1:A:70:CYS:N	2.51	0.41
1:A:543:LEU:O	1:A:544:ASP:C	2.64	0.41
1:A:550:LEU:HD23	1:A:550:LEU:HA	1.95	0.41
1:A:606:LEU:HG	1:A:613:ILE:HD12	2.02	0.41
1:A:1017:LEU:HB2	5:E:206:GLY:N	2.36	0.41
1:A:1035:TYR:O	1:A:1036:ARG:HB2	2.19	0.41
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.51	0.41
2:B:377:PHE:O	2:B:380:TYR:N	2.53	0.41
2:B:469:GLN:HB3	2:B:470:LYS:H	1.53	0.41
2:B:644:GLU:C	2:B:646:LEU:N	2.79	0.41
2:B:992:ILE:HD11	11:K:66:PRO:HB2	2.01	0.41
3:C:11:ARG:HE	3:C:21:ILE:HD11	1.86	0.41
3:C:217:ASP:HA	3:C:218:PRO:HD3	1.92	0.41
4:D:12:ARG:NH1	4:D:14:ARG:HG2	2.36	0.41
4:D:25:ALA:HB1	4:D:196:PRO:HG3	2.03	0.41
4:D:128:VAL:O	4:D:129:LEU:C	2.64	0.41
4:D:191:ALA:C	4:D:193:THR:N	2.79	0.41
5:E:90:VAL:HG23	5:E:120:ALA:HA	2.02	0.41
7:G:1:MET:SD	7:G:79:PHE:HD1	2.42	0.41
8:H:129:TYR:CD1	8:H:130:ARG:CD	3.03	0.41
9:I:55:THR:HG22	9:I:86:PHE:HZ	1.86	0.41
13:1:27:DC:H2"	13:1:28:DA:C8	2.56	0.41
1:M:34:LYS:HB2	1:M:36:ARG:NH2	2.36	0.41
1:M:84:ILE:CD1	1:M:270:LEU:HD13	2.51	0.41
1:M:95:PHE:O	1:M:98:LYS:N	2.54	0.41
1:M:113:LEU:HD23	1:M:113:LEU:HA	1.95	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:205:GLU:CD	1:M:205:GLU:H	2.28	0.41
1:M:344:ARG:C	1:M:345:VAL:HG13	2.46	0.41
1:M:826:ASP:OD1	1:M:827:THR:N	2.54	0.41
2:N:276:ILE:HD11	2:N:334:ILE:HG23	2.03	0.41
2:N:658:ILE:HG22	2:N:659:ALA:N	2.35	0.41
2:N:886:LYS:HB2	2:N:890:TYR:CE1	2.56	0.41
3:O:29:MET:HE3	3:O:29:MET:HB2	1.95	0.41
3:O:112:ASN:CB	3:O:114:TYR:CE1	3.03	0.41
4:P:118:THR:HG21	4:P:121:LYS:HD2	2.03	0.41
4:P:119:ARG:CG	4:P:221:TYR:CZ	3.03	0.41
5:Q:69:ILE:N	5:Q:69:ILE:CD1	2.82	0.41
5:Q:90:VAL:HG23	5:Q:120:ALA:HA	2.02	0.41
6:R:79:ARG:NH2	6:R:150:GLU:OE1	2.47	0.41
7:S:14:HIS:CE1	7:S:15:PRO:HD2	2.55	0.41
8:T:26:ILE:O	8:T:27:GLU:HG3	2.21	0.41
8:T:51:ALA:O	8:T:52:GLN:CB	2.69	0.41
11:W:53:ASP:OD2	11:W:81:TYR:OH	2.28	0.41
12:X:27:LEU:HD13	12:X:37:LYS:HG2	2.03	0.41
1:A:55:ASP:OD1	1:A:57:ARG:HA	2.21	0.40
1:A:179:LEU:HD23	1:A:179:LEU:N	2.36	0.40
1:A:335:ARG:NH1	2:B:1206:GLU:OE1	2.55	0.40
1:A:673:GLY:O	1:A:676:MET:HB2	2.21	0.40
1:A:878:ILE:CG2	1:A:955:PRO:HB2	2.51	0.40
1:A:1279:ILE:HG23	1:A:1308:THR:OG1	2.21	0.40
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.21	0.40
1:A:1444:MET:HE3	1:A:1444:MET:HB2	1.58	0.40
2:B:167:ILE:HD12	2:B:167:ILE:N	2.35	0.40
2:B:563:MET:HE1	2:B:580:VAL:CB	2.49	0.40
2:B:652:LYS:HD2	2:B:688:GLY:O	2.22	0.40
2:B:809:MET:O	2:B:810:GLU:C	2.64	0.40
2:B:910:VAL:CG1	2:B:938:SER:HB3	2.51	0.40
2:B:1160:VAL:CG1	2:B:1161:HIS:N	2.84	0.40
3:C:73:GLN:HB3	3:C:131:HIS:H	1.85	0.40
3:C:123:ASN:CG	3:C:125:MET:H	2.30	0.40
5:E:3:GLN:NE2	5:E:52:ARG:HH22	2.18	0.40
7:G:132:SER:HB3	7:G:135:ASP:HB2	2.03	0.40
8:H:35:GLN:HB3	8:H:111:LEU:HD21	2.03	0.40
9:I:58:VAL:CG1	9:I:62:ILE:HG21	2.51	0.40
12:L:38:LEU:CG	12:L:39:SER:H	2.27	0.40
1:M:16:GLU:CD	2:N:1220:ARG:HA	2.46	0.40
1:M:122:MET:HE3	1:M:126:LEU:HD21	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:225:ASN:HD22	1:M:227:VAL:N	2.19	0.40
1:M:535:THR:HG22	1:M:616:VAL:HA	2.00	0.40
1:M:541:ILE:CD1	1:M:549:MET:HE1	2.40	0.40
1:M:565:ILE:O	1:M:570:PRO:HA	2.21	0.40
1:M:996:ASN:C	1:M:998:LEU:HD12	2.46	0.40
1:M:1112:LYS:O	1:M:1114:PRO:CD	2.66	0.40
1:M:1383:SER:O	1:M:1385:THR:N	2.54	0.40
2:N:460:ALA:HB1	2:N:466:TRP:CZ3	2.55	0.40
2:N:570:VAL:CG2	2:N:573:GLN:HB3	2.51	0.40
2:N:593:PRO:O	2:N:595:ARG:N	2.53	0.40
2:N:766:ARG:HD3	2:N:766:ARG:HA	1.80	0.40
2:N:893:LEU:CD2	2:N:897:GLY:C	2.94	0.40
2:N:1031:LEU:HD12	2:N:1031:LEU:C	2.45	0.40
3:O:31:ASN:O	3:O:34:ARG:HB3	2.22	0.40
4:P:8:PHE:CD1	4:P:38:ILE:O	2.74	0.40
4:P:14:ARG:NH1	4:P:16:LYS:HG2	2.35	0.40
4:P:41:GLN:N	4:P:41:GLN:NE2	2.69	0.40
4:P:156:ASP:O	4:P:157:GLN:C	2.63	0.40
5:Q:13:TRP:O	5:Q:16:PHE:HB3	2.21	0.40
5:Q:136:ASN:OD1	5:Q:138:ALA:N	2.54	0.40
5:Q:157:SER:C	5:Q:159:ASP:H	2.29	0.40
9:U:80:SER:HB2	9:U:103:CYS:SG	2.61	0.40
11:W:6:ARG:O	11:W:9:LEU:HG	2.21	0.40
12:X:53:HIS:O	12:X:55:ILE:HD13	2.21	0.40
13:4:15:DG:C8	13:4:16:DT:H73	2.56	0.40
1:A:320:ARG:HA	1:A:321:PRO:HD3	1.91	0.40
1:A:598:LEU:HA	8:H:122:LEU:HD13	2.03	0.40
1:A:650:GLN:O	1:A:654:ASN:HB2	2.21	0.40
1:A:674:PRO:C	1:A:676:MET:N	2.79	0.40
1:A:996:ASN:HA	1:A:998:LEU:HD12	2.03	0.40
1:A:1081:LEU:CD1	1:A:1097:GLY:HA3	2.51	0.40
1:A:1242:VAL:C	1:A:1243:VAL:HG13	2.46	0.40
1:A:1264:GLU:OE2	9:I:46:HIS:HD2	2.05	0.40
2:B:59:LEU:HG	2:B:95:ILE:HD13	2.03	0.40
2:B:102:VAL:HG23	2:B:112:LEU:CB	2.25	0.40
2:B:313:MET:HE1	2:B:390:LEU:HG	2.04	0.40
3:C:215:GLU:O	3:C:217:ASP:N	2.54	0.40
4:D:64:VAL:C	4:D:66:ARG:N	2.78	0.40
5:E:207:ARG:HB3	5:E:207:ARG:NH1	2.31	0.40
8:H:129:TYR:C	8:H:131:ASN:H	2.29	0.40
9:I:88:SER:HB3	9:I:95:THR:HG21	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:320:ARG:HE	1:M:323:LYS:NZ	2.20	0.40
1:M:332:LYS:O	1:M:334:GLY:N	2.54	0.40
1:M:369:SER:HB3	11:W:2:ASN:HD21	1.86	0.40
1:M:381:THR:O	1:M:382:PRO:C	2.64	0.40
1:M:476:SER:O	1:M:477:PRO:C	2.63	0.40
1:M:871:ASP:OD1	1:M:1366:ARG:NH2	2.54	0.40
1:M:963:ILE:HD11	1:M:1049:ILE:N	2.36	0.40
1:M:1005:GLU:O	1:M:1009:ASN:ND2	2.54	0.40
1:M:1157:ASP:O	1:M:1159:ARG:N	2.49	0.40
1:M:1279:ILE:HG23	1:M:1308:THR:OG1	2.20	0.40
1:M:1402:PHE:CE2	1:M:1403:GLU:CG	3.04	0.40
2:N:38:PHE:O	2:N:39:ARG:C	2.64	0.40
2:N:449:ASN:C	2:N:451:LYS:N	2.80	0.40
2:N:466:TRP:O	2:N:468:GLU:N	2.53	0.40
2:N:617:ARG:HA	2:N:624:LEU:HD12	2.03	0.40
2:N:782:LEU:HB3	2:N:784:ASN:OD1	2.21	0.40
2:N:1001:PHE:CD1	2:N:1001:PHE:C	2.99	0.40
3:O:239:PRO:O	3:O:242:GLN:HB2	2.21	0.40
4:P:64:VAL:C	4:P:66:ARG:N	2.78	0.40
4:P:121:LYS:HA	4:P:124:GLU:OE2	2.20	0.40
4:P:151:PHE:N	4:P:151:PHE:HD1	2.04	0.40
7:S:102:GLN:HG3	7:S:106:MET:O	2.21	0.40
8:T:43:ASN:C	8:T:45:GLU:H	2.29	0.40
9:U:58:VAL:O	9:U:58:VAL:HG12	2.21	0.40
9:U:73:ARG:NH1	9:U:101:PHE:CZ	2.89	0.40
12:X:38:LEU:CG	12:X:39:SER:H	2.29	0.40
12:X:58:LYS:O	12:X:59:ALA:C	2.65	0.40
1:A:40:THR:C	1:A:41:MET:HG3	2.46	0.40
1:A:55:ASP:O	1:A:55:ASP:OD2	2.39	0.40
1:A:196:GLU:HG2	1:A:197:PRO:CD	2.52	0.40
1:A:347:PHE:H	2:B:1107:ALA:HA	1.87	0.40
1:A:385:ILE:O	1:A:389:THR:OG1	2.34	0.40
1:A:698:GLN:NE2	9:I:99:LEU:HD11	2.37	0.40
1:A:752:LYS:HD3	1:A:752:LYS:HA	1.93	0.40
1:A:818:MET:HE3	2:B:514:LEU:O	2.22	0.40
1:A:850:VAL:HG21	1:A:1058:VAL:HG11	2.04	0.40
1:A:925:LEU:C	1:A:927:VAL:N	2.79	0.40
1:A:1143:LEU:O	1:A:1146:VAL:HG22	2.21	0.40
1:A:1410:PHE:HD2	2:B:1212:ILE:CD1	2.33	0.40
2:B:129:PHE:CE2	2:B:166:PHE:CD1	3.10	0.40
2:B:211:VAL:HG21	2:B:483:LEU:HD13	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:722:ASP:HB3	2:B:723:VAL:H	1.58	0.40
2:B:780:VAL:HG21	10:J:56:LEU:CD1	2.47	0.40
2:B:838:SER:HA	2:B:989:THR:O	2.21	0.40
2:B:847:ASP:HB3	3:C:167:HIS:NE2	2.37	0.40
2:B:893:LEU:CD2	2:B:897:GLY:C	2.94	0.40
2:B:996:ARG:HH12	3:C:174:ALA:CA	2.24	0.40
2:B:1045:SER:O	2:B:1046:PRO:O	2.39	0.40
3:C:111:THR:O	3:C:147:LEU:HD23	2.20	0.40
3:C:128:ASN:O	3:C:129:ILE:HG13	2.21	0.40
4:D:66:ARG:C	4:D:68:ARG:N	2.79	0.40
4:D:187:THR:C	4:D:189:ASP:N	2.77	0.40
8:H:58:THR:C	8:H:59:ILE:HG13	2.46	0.40
1:M:316:GLN:HG2	1:M:317:LYS:H	1.85	0.40
1:M:843:LYS:HD3	1:M:843:LYS:HA	1.76	0.40
1:M:967:ALA:HB2	1:M:1045:VAL:HG22	2.03	0.40
1:M:1350:LYS:O	1:M:1354:ASN:ND2	2.54	0.40
2:N:222:ILE:N	2:N:240:ILE:CD1	2.85	0.40
2:N:624:LEU:HD12	2:N:624:LEU:HA	1.92	0.40
2:N:1190:ASP:C	2:N:1191:ILE:HG13	2.45	0.40
3:O:34:ARG:O	3:O:38:ILE:HG13	2.22	0.40
3:O:107:SER:C	3:O:109:SER:H	2.30	0.40
4:P:56:ARG:HB2	4:P:148:LEU:HD22	2.03	0.40
4:P:176:GLU:CD	4:P:197:SER:HB2	2.45	0.40
5:Q:90:VAL:HB	5:Q:117:THR:HG21	2.04	0.40
7:S:90:THR:CG2	7:S:91:VAL:N	2.84	0.40
1:A:49:LYS:HZ3	1:A:61:ILE:HG13	1.87	0.40
1:A:349:ALA:CB	1:A:374:LEU:HD11	2.52	0.40
1:A:436:ILE:HD11	1:A:491:VAL:HG11	2.03	0.40
1:A:444:PHE:HB2	1:A:458:HIS:HD2	1.86	0.40
1:A:675:THR:O	1:A:675:THR:HG22	2.22	0.40
1:A:730:GLY:C	1:A:732:LEU:N	2.75	0.40
1:A:823:GLY:O	1:A:824:LEU:C	2.63	0.40
1:A:996:ASN:HA	1:A:998:LEU:CD1	2.52	0.40
1:A:1125:ALA:C	1:A:1127:ASP:H	2.29	0.40
1:A:1291:VAL:HG22	1:A:1292:PRO:CD	2.51	0.40
1:A:1444:MET:HE1	6:F:135:ARG:HB2	2.02	0.40
2:B:90:ILE:HD12	2:B:432:MET:CE	2.51	0.40
2:B:189:LEU:HD13	2:B:196:PRO:HA	2.03	0.40
2:B:204:ILE:O	2:B:204:ILE:HG22	2.21	0.40
2:B:211:VAL:CG1	2:B:495:LEU:HD23	2.51	0.40
2:B:345:LYS:HE2	2:B:349:ILE:HD11	2.01	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:542:MET:CE	2:B:747:MET:HE2	2.49	0.40
2:B:654:ARG:O	2:B:657:HIS:HB2	2.22	0.40
2:B:813:LYS:HD2	2:B:816:GLU:OE1	2.21	0.40
2:B:847:ASP:OD2	3:C:167:HIS:HD2	2.03	0.40
2:B:1158:PHE:CE2	2:B:1160:VAL:HG22	2.56	0.40
3:C:98:VAL:C	3:C:99:LEU:HD22	2.46	0.40
4:D:54:GLU:OE1	4:D:164:ILE:HD11	2.21	0.40
5:E:127:ILE:N	5:E:128:PRO:CD	2.84	0.40
6:F:69:LEU:HB3	6:F:71:GLU:HG3	2.03	0.40
8:H:26:ILE:HD11	8:H:49:VAL:CG1	2.51	0.40
10:J:32:GLU:O	10:J:33:GLY:C	2.64	0.40
1:M:254:GLU:HB3	1:M:255:SER:H	1.49	0.40
1:M:347:PHE:H	2:N:1107:ALA:HA	1.86	0.40
1:M:500:GLU:O	1:M:504:LEU:HB2	2.21	0.40
1:M:566:ILE:O	1:M:567:LYS:O	2.40	0.40
1:M:870:GLU:HB2	5:Q:204:THR:HG21	2.03	0.40
1:M:1153:TYR:HB2	1:M:1192:LEU:HD23	2.03	0.40
1:M:1222:ASN:O	1:M:1223:ASP:HB3	2.21	0.40
1:M:1291:VAL:CG2	1:M:1292:PRO:CD	2.99	0.40
2:N:39:ARG:NH2	2:N:665:GLU:OE1	2.48	0.40
2:N:40:GLU:OE1	2:N:681:TRP:HB3	2.22	0.40
2:N:269:ILE:CG2	2:N:282:ILE:HD13	2.52	0.40
2:N:323:VAL:O	2:N:324:ILE:HG13	2.21	0.40
2:N:364:ILE:HG22	2:N:365:THR:N	2.37	0.40
2:N:905:VAL:HG23	2:N:941:LEU:HD22	2.04	0.40
2:N:958:GLN:C	2:N:960:GLY:H	2.30	0.40
2:N:979:LYS:HG2	2:N:1095:LEU:CD1	2.51	0.40
2:N:984:HIS:NE2	2:N:1025:HIS:HA	2.37	0.40
3:O:66:ARG:C	3:O:68:GLY:N	2.80	0.40
3:O:245:VAL:HG13	11:W:102:LYS:HG3	2.04	0.40
4:P:47:LEU:HD13	4:P:47:LEU:C	2.46	0.40
5:Q:7:ARG:O	5:Q:8:ASN:C	2.65	0.40
6:R:109:VAL:HG12	6:R:110:ASP:H	1.83	0.40
8:T:27:GLU:CG	8:T:39:THR:HG23	2.51	0.40
9:U:44:TYR:CD1	9:U:44:TYR:C	2.99	0.40
10:V:1:MET:H1	10:V:57:ILE:H	1.61	0.40
11:W:110:ASN:C	11:W:112:GLN:H	2.30	0.40
12:X:55:ILE:O	12:X:56:LEU:HB2	2.21	0.40
1:A:33:ALA:CA	1:A:57:ARG:HH12	2.23	0.40
1:A:116:ASP:C	1:A:118:HIS:N	2.79	0.40
1:A:367:PRO:HB3	1:A:465:TYR:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:783:THR:HG21	1:A:796:SER:O	2.20	0.40
1:A:820:GLY:C	1:A:822:GLU:N	2.78	0.40
1:A:905:ASP:O	1:A:906:HIS:ND1	2.55	0.40
1:A:1339:LEU:HD13	5:E:147:HIS:CG	2.56	0.40
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	2.02	0.40
2:B:273:LEU:HA	2:B:274:PRO:HD2	1.93	0.40
2:B:277:LYS:HG2	2:B:336:ARG:CB	2.44	0.40
2:B:321:GLY:O	2:B:322:PHE:C	2.65	0.40
2:B:601:ARG:HD3	2:B:605:ARG:NH2	2.36	0.40
2:B:700:SER:C	2:B:701:ILE:HG23	2.47	0.40
2:B:759:PRO:C	2:B:761:HIS:H	2.30	0.40
2:B:811:TYR:CD1	2:B:811:TYR:N	2.89	0.40
2:B:945:GLU:O	2:B:946:ASN:HB3	2.21	0.40
2:B:976:ILE:O	2:B:990:ILE:HB	2.21	0.40
3:C:46:ILE:HD12	3:C:67:LEU:O	2.22	0.40
3:C:252:GLN:CG	11:K:95:ILE:HG23	2.51	0.40
4:D:12:ARG:HH12	4:D:13:ARG:C	2.29	0.40
5:E:63:ASN:HB3	5:E:64:PRO:CD	2.52	0.40
5:E:110:PHE:C	5:E:110:PHE:CD1	2.99	0.40
6:F:81:THR:HG23	6:F:144:GLU:OE2	2.22	0.40
8:H:93:TYR:HB3	8:H:144:ILE:O	2.20	0.40
9:I:34:TYR:C	9:I:35:VAL:HG23	2.47	0.40
13:1:15:DG:C8	13:1:16:DT:C7	3.05	0.40
1:M:730:GLY:C	1:M:732:LEU:N	2.76	0.40
1:M:752:LYS:HD3	1:M:752:LYS:HA	1.86	0.40
1:M:831:THR:HG23	1:M:832:ALA:N	2.37	0.40
1:M:896:ARG:HB3	1:M:897:TYR:CD1	2.57	0.40
1:M:971:PHE:O	1:M:972:HIS:C	2.65	0.40
1:M:1048:ASN:N	1:M:1048:ASN:ND2	2.70	0.40
1:M:1241:ARG:O	1:M:1242:VAL:HG23	2.22	0.40
1:M:1436:ILE:HD13	1:M:1436:ILE:HG21	1.91	0.40
2:N:27:ALA:C	2:N:29:ASP:N	2.78	0.40
2:N:98:THR:O	2:N:126:SER:CB	2.69	0.40
2:N:212:LEU:HD21	2:N:466:TRP:CH2	2.56	0.40
2:N:377:PHE:O	2:N:380:TYR:N	2.54	0.40
2:N:629:ASP:HB3	2:N:632:ARG:CD	2.51	0.40
2:N:654:ARG:O	2:N:656:GLY:N	2.55	0.40
2:N:810:GLU:CA	2:N:815:ARG:HH22	2.35	0.40
2:N:826:ALA:HB2	2:N:1087:PHE:CE2	2.57	0.40
2:N:911:ILE:HG21	2:N:966:VAL:HG11	2.01	0.40
2:N:1221:SER:O	2:N:1223:ASP:N	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:184:ASN:OD1	3:O:187:LYS:CA	2.69	0.40
5:Q:48:ASP:OD1	5:Q:52:ARG:HB2	2.22	0.40
8:T:36:CYS:HA	8:T:126:GLU:O	2.22	0.40
11:W:37:LYS:O	11:W:38:GLU:HG2	2.21	0.40
11:W:47:ARG:HB3	11:W:47:ARG:NH1	2.28	0.40
12:X:33:GLU:CD	12:X:33:GLU:H	2.28	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1406/1733 (81%)	1075 (76%)	225 (16%)	106 (8%)	1	5
1	M	1406/1733 (81%)	1073 (76%)	228 (16%)	105 (8%)	1	5
2	B	1082/1224 (88%)	800 (74%)	186 (17%)	96 (9%)	0	3
2	N	1082/1224 (88%)	798 (74%)	186 (17%)	98 (9%)	0	3
3	C	264/318 (83%)	202 (76%)	41 (16%)	21 (8%)	1	4
3	O	264/318 (83%)	203 (77%)	42 (16%)	19 (7%)	1	6
4	D	174/221 (79%)	120 (69%)	37 (21%)	17 (10%)	0	2
4	P	174/221 (79%)	122 (70%)	34 (20%)	18 (10%)	0	2
5	E	212/215 (99%)	155 (73%)	41 (19%)	16 (8%)	1	5
5	Q	212/215 (99%)	159 (75%)	37 (18%)	16 (8%)	1	5
6	F	85/155 (55%)	72 (85%)	11 (13%)	2 (2%)	4	28
6	R	85/155 (55%)	72 (85%)	11 (13%)	2 (2%)	4	28
7	G	169/171 (99%)	141 (83%)	23 (14%)	5 (3%)	3	23
7	S	169/171 (99%)	139 (82%)	23 (14%)	7 (4%)	2	17
8	H	130/146 (89%)	85 (65%)	25 (19%)	20 (15%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	T	130/146 (89%)	85 (65%)	25 (19%)	20 (15%)	0	0
9	I	117/122 (96%)	77 (66%)	28 (24%)	12 (10%)	0	2
9	U	117/122 (96%)	78 (67%)	28 (24%)	11 (9%)	0	3
10	J	63/70 (90%)	43 (68%)	9 (14%)	11 (18%)	0	0
10	V	63/70 (90%)	42 (67%)	10 (16%)	11 (18%)	0	0
11	K	112/120 (93%)	89 (80%)	20 (18%)	3 (3%)	4	25
11	W	112/120 (93%)	89 (80%)	19 (17%)	4 (4%)	2	19
12	L	44/70 (63%)	19 (43%)	15 (34%)	10 (23%)	0	0
12	X	44/70 (63%)	19 (43%)	15 (34%)	10 (23%)	0	0
All	All	7716/9130 (84%)	5757 (75%)	1319 (17%)	640 (8%)	0	4

All (640) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	43	GLU
1	A	57	ARG
1	A	62	ASP
1	A	63	ARG
1	A	67	CYS
1	A	70	CYS
1	A	130	ASP
1	A	250	ILE
1	A	255	SER
1	A	257	ARG
1	A	286	HIS
1	A	311	GLN
1	A	318	SER
1	A	332	LYS
1	A	399	HIS
1	A	410	GLY
1	A	423	ASP
1	A	517	ASN
1	A	567	LYS
1	A	597	LEU
1	A	1112	LYS
1	A	1114	PRO
1	A	1120	LEU
1	A	1122	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1124	HIS
1	A	1223	ASP
1	A	1233	ASP
1	A	1242	VAL
1	A	1255	GLU
1	A	1281	ARG
1	A	1403	GLU
1	A	1438	THR
2	B	21	GLU
2	B	67	SER
2	B	68	THR
2	B	108	VAL
2	B	124	TYR
2	B	186	GLU
2	B	291	ILE
2	B	295	GLY
2	B	334	ILE
2	B	365	THR
2	B	367	LEU
2	B	391	ASP
2	B	435	THR
2	B	468	GLU
2	B	509	ALA
2	B	643	ASP
2	B	708	GLU
2	B	709	ASP
2	B	728	ARG
2	B	731	VAL
2	B	734	HIS
2	B	907	GLY
2	B	958	GLN
2	B	1046	PRO
2	B	1156	ASP
2	B	1175	LEU
3	C	110	THR
3	C	141	GLY
3	C	184	ASN
3	C	209	TYR
3	C	215	GLU
4	D	5	THR
4	D	8	PHE
4	D	17	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	19	GLU
4	D	52	LEU
4	D	218	GLU
5	E	45	LYS
5	E	115	ASN
5	E	129	PRO
5	E	130	ALA
7	G	139	ILE
8	H	77	ARG
8	H	82	PRO
8	H	128	ASN
8	H	140	ALA
9	I	11	ASN
9	I	78	CYS
10	J	2	ILE
10	J	55	ASP
10	J	64	ASN
12	L	27	LEU
12	L	50	ASP
12	L	53	HIS
12	L	59	ALA
12	L	60	ARG
1	M	4	GLN
1	M	43	GLU
1	M	57	ARG
1	M	62	ASP
1	M	63	ARG
1	M	67	CYS
1	M	70	CYS
1	M	130	ASP
1	M	250	ILE
1	M	255	SER
1	M	257	ARG
1	M	286	HIS
1	M	311	GLN
1	M	318	SER
1	M	332	LYS
1	M	399	HIS
1	M	410	GLY
1	M	423	ASP
1	M	453	MET
1	M	517	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	567	LYS
1	M	597	LEU
1	M	1112	LYS
1	M	1114	PRO
1	M	1120	LEU
1	M	1122	PRO
1	M	1124	HIS
1	M	1223	ASP
1	M	1233	ASP
1	M	1242	VAL
1	M	1255	GLU
1	M	1281	ARG
1	M	1403	GLU
1	M	1438	THR
2	N	21	GLU
2	N	67	SER
2	N	68	THR
2	N	108	VAL
2	N	124	TYR
2	N	186	GLU
2	N	258	LEU
2	N	334	ILE
2	N	365	THR
2	N	367	LEU
2	N	391	ASP
2	N	435	THR
2	N	468	GLU
2	N	509	ALA
2	N	643	ASP
2	N	708	GLU
2	N	709	ASP
2	N	728	ARG
2	N	731	VAL
2	N	734	HIS
2	N	907	GLY
2	N	958	GLN
2	N	1046	PRO
2	N	1069	PHE
2	N	1097	HIS
2	N	1156	ASP
2	N	1175	LEU
3	O	110	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	O	141	GLY
3	O	184	ASN
3	O	215	GLU
3	O	216	GLY
4	P	5	THR
4	P	8	PHE
4	P	17	LYS
4	P	19	GLU
4	P	218	GLU
5	Q	45	LYS
5	Q	115	ASN
5	Q	129	PRO
5	Q	130	ALA
7	S	139	ILE
8	T	77	ARG
8	T	82	PRO
8	T	107	VAL
8	T	128	ASN
8	T	140	ALA
9	U	11	ASN
9	U	78	CYS
9	U	106	CYS
10	V	2	ILE
10	V	55	ASP
10	V	64	ASN
12	X	27	LEU
12	X	50	ASP
12	X	59	ALA
12	X	60	ARG
1	A	41	MET
1	A	42	ASP
1	A	54	ASN
1	A	59	GLY
1	A	61	ILE
1	A	66	LYS
1	A	76	GLU
1	A	154	SER
1	A	167	CYS
1	A	253	ASN
1	A	314	ALA
1	A	322	VAL
1	A	331	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	424	ILE
1	A	453	MET
1	A	525	GLN
1	A	821	ARG
1	A	958	VAL
1	A	1002	GLY
1	A	1123	GLY
1	A	1139	GLU
1	A	1221	LYS
1	A	1308	THR
1	A	1314	SER
2	B	28	GLU
2	B	65	GLU
2	B	206	ASN
2	B	257	LYS
2	B	258	LEU
2	B	264	SER
2	B	294	ASP
2	B	369	GLY
2	B	448	ILE
2	B	450	ALA
2	B	466	TRP
2	B	467	GLY
2	B	531	GLN
2	B	591	ARG
2	B	619	ILE
2	B	641	GLU
2	B	642	ASP
2	B	751	VAL
2	B	777	ALA
2	B	848	ARG
2	B	869	SER
2	B	879	ARG
2	B	943	SER
2	B	992	ILE
2	B	1069	PHE
2	B	1097	HIS
2	B	1155	SER
2	B	1176	ASN
3	C	126	GLY
3	C	149	LYS
3	C	216	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	237	SER
4	D	14	ARG
4	D	119	ARG
4	D	131	GLU
4	D	198	LEU
4	D	199	ASN
5	E	36	GLU
5	E	74	ASP
5	E	106	GLN
6	F	112	GLU
7	G	154	VAL
8	H	12	VAL
8	H	17	PRO
8	H	32	THR
8	H	59	ILE
8	H	62	SER
8	H	92	ASP
8	H	107	VAL
8	H	108	SER
8	H	134	ASN
9	I	54	GLU
9	I	57	GLY
9	I	59	VAL
9	I	62	ILE
9	I	79	HIS
9	I	106	CYS
10	J	6	ARG
10	J	24	LEU
10	J	28	ASP
10	J	42	LYS
10	J	62	ARG
12	L	28	LYS
12	L	35	SER
1	M	41	MET
1	M	42	ASP
1	M	54	ASN
1	M	61	ILE
1	M	66	LYS
1	M	76	GLU
1	M	167	CYS
1	M	219	PHE
1	M	253	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	314	ALA
1	M	322	VAL
1	M	331	GLY
1	M	424	ILE
1	M	525	GLN
1	M	789	LYS
1	M	821	ARG
1	M	1002	GLY
1	M	1123	GLY
1	M	1169	ILE
1	M	1221	LYS
1	M	1308	THR
1	M	1314	SER
2	N	28	GLU
2	N	46	GLN
2	N	65	GLU
2	N	206	ASN
2	N	257	LYS
2	N	259	TYR
2	N	264	SER
2	N	291	ILE
2	N	294	ASP
2	N	295	GLY
2	N	369	GLY
2	N	448	ILE
2	N	449	ASN
2	N	450	ALA
2	N	466	TRP
2	N	467	GLY
2	N	531	GLN
2	N	591	ARG
2	N	619	ILE
2	N	641	GLU
2	N	642	ASP
2	N	655	LYS
2	N	751	VAL
2	N	777	ALA
2	N	869	SER
2	N	879	ARG
2	N	943	SER
2	N	992	ILE
2	N	1155	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	1176	ASN
3	O	126	GLY
3	O	149	LYS
3	O	209	TYR
3	O	237	SER
4	P	14	ARG
4	P	16	LYS
4	P	52	LEU
4	P	119	ARG
4	P	131	GLU
4	P	198	LEU
5	Q	36	GLU
5	Q	74	ASP
5	Q	106	GLN
7	S	154	VAL
8	T	17	PRO
8	T	32	THR
8	T	59	ILE
8	T	62	SER
8	T	92	ASP
8	T	108	SER
8	T	134	ASN
9	U	8	ARG
9	U	54	GLU
9	U	57	GLY
9	U	59	VAL
9	U	62	ILE
9	U	79	HIS
10	V	6	ARG
10	V	24	LEU
10	V	28	ASP
10	V	62	ARG
11	W	53	ASP
12	X	28	LYS
12	X	35	SER
12	X	53	HIS
1	A	48	ALA
1	A	65	LEU
1	A	69	THR
1	A	93	VAL
1	A	128	ILE
1	A	138	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	219	PHE
1	A	400	PRO
1	A	789	LYS
1	A	795	GLU
1	A	846	GLU
1	A	986	ILE
1	A	1140	HIS
1	A	1231	ASP
1	A	1309	ASP
1	A	1405	THR
1	A	1448	GLU
2	B	24	PRO
2	B	27	ALA
2	B	46	GLN
2	B	58	THR
2	B	245	GLU
2	B	259	TYR
2	B	433	GLN
2	B	449	ASN
2	B	559	SER
2	B	711	GLU
2	B	738	PHE
2	B	746	SER
2	B	906	SER
2	B	938	SER
2	B	1103	ILE
2	B	1222	ARG
3	C	90	ASP
3	C	132	PRO
3	C	148	ARG
3	C	213	PRO
4	D	15	LEU
4	D	16	LYS
4	D	21	GLU
4	D	168	LYS
5	E	44	ALA
5	E	92	THR
8	H	139	ASN
9	I	8	ARG
10	J	14	VAL
10	J	29	GLU
11	K	14	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	53	ASP
12	L	26	THR
1	M	48	ALA
1	M	58	LEU
1	M	59	GLY
1	M	65	LEU
1	M	93	VAL
1	M	154	SER
1	M	400	PRO
1	M	415	LEU
1	M	479	ASN
1	M	795	GLU
1	M	846	GLU
1	M	958	VAL
1	M	963	ILE
1	M	986	ILE
1	M	1115	SER
1	M	1139	GLU
1	M	1140	HIS
1	M	1231	ASP
1	M	1309	ASP
1	M	1405	THR
1	M	1448	GLU
2	N	24	PRO
2	N	27	ALA
2	N	58	THR
2	N	245	GLU
2	N	282	ILE
2	N	433	GLN
2	N	559	SER
2	N	711	GLU
2	N	738	PHE
2	N	746	SER
2	N	810	GLU
2	N	848	ARG
2	N	906	SER
2	N	938	SER
2	N	1103	ILE
2	N	1222	ARG
3	O	90	ASP
3	O	132	PRO
3	O	148	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	O	213	PRO
4	P	15	LEU
4	P	53	SER
4	P	168	LYS
4	P	199	ASN
5	Q	44	ALA
6	R	112	GLU
7	S	136	VAL
8	T	139	ASN
10	V	42	LYS
11	W	14	GLU
12	X	26	THR
1	A	256	GLN
1	A	312	PRO
1	A	415	LEU
1	A	479	ASN
1	A	591	PHE
1	A	1168	GLU
1	A	1169	ILE
1	A	1280	GLU
1	A	1316	VAL
2	B	45	SER
2	B	114	PRO
2	B	282	ILE
2	B	323	VAL
2	B	575	PRO
2	B	636	PRO
2	B	655	LYS
2	B	792	MET
2	B	810	GLU
2	B	818	PRO
2	B	1017	ILE
2	B	1108	ARG
2	B	1171	VAL
2	B	1181	GLU
3	C	12	GLU
3	C	142	VAL
5	E	192	ARG
6	F	128	LYS
8	H	52	GLN
8	H	81	PRO
8	H	90	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	91	ASP
9	I	9	ASP
12	L	40	LEU
1	M	69	THR
1	M	96	ILE
1	M	138	ILE
1	M	256	GLN
1	M	312	PRO
1	M	591	PHE
1	M	1168	GLU
1	M	1280	GLU
1	M	1316	VAL
2	N	114	PRO
2	N	323	VAL
2	N	575	PRO
2	N	636	PRO
2	N	705	MET
2	N	792	MET
2	N	946	ASN
2	N	1017	ILE
2	N	1181	GLU
3	O	142	VAL
4	P	21	GLU
4	P	192	LYS
5	Q	3	GLN
5	Q	92	THR
5	Q	192	ARG
8	T	12	VAL
8	T	52	GLN
8	T	81	PRO
8	T	90	ALA
8	T	91	ASP
8	T	95	TYR
9	U	9	ASP
9	U	56	ALA
10	V	14	VAL
10	V	17	LYS
10	V	29	GLU
12	X	40	LEU
1	A	58	LEU
1	A	72	GLU
1	A	96	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	556	TRP
1	A	780	VAL
1	A	884	ASP
1	A	963	ILE
1	A	1390	ASN
2	B	680	THR
2	B	1157	ALA
3	C	11	ARG
3	C	48	SER
3	C	172	PRO
3	C	214	ASN
4	D	53	SER
4	D	75	LYS
5	E	3	GLN
5	E	73	PRO
7	G	20	PRO
7	G	113	HIS
7	G	136	VAL
8	H	95	TYR
9	I	56	ALA
10	J	17	LYS
11	K	107	THR
1	M	128	ILE
1	M	145	LYS
1	M	556	TRP
1	M	1149	ALA
1	M	1390	ASN
2	N	45	SER
2	N	55	VAL
2	N	56	ASP
2	N	461	LEU
2	N	561	TRP
2	N	1157	ALA
2	N	1171	VAL
3	O	11	ARG
3	O	240	VAL
4	P	75	LYS
5	Q	154	ILE
6	R	128	LYS
7	S	112	LYS
7	S	113	HIS
11	W	64	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	W	107	THR
1	A	35	ILE
1	A	51	GLY
1	A	357	PRO
1	A	599	SER
1	A	972	HIS
1	A	1174	PHE
2	B	55	VAL
2	B	56	ASP
2	B	461	LEU
2	B	946	ASN
2	B	1214	PRO
5	E	40	GLU
5	E	154	ILE
9	I	3	THR
1	M	35	ILE
1	M	51	GLY
1	M	284	ALA
1	M	599	SER
1	M	972	HIS
1	M	1278	ASN
2	N	249	ARG
2	N	594	ALA
2	N	680	THR
2	N	1214	PRO
3	O	175	ALA
3	O	214	ASN
5	Q	73	PRO
7	S	20	PRO
7	S	128	PRO
2	B	1110	PRO
3	C	240	VAL
5	E	51	GLY
5	E	64	PRO
8	H	44	VAL
1	M	283	GLY
1	M	780	VAL
1	M	948	VAL
3	O	172	PRO
5	Q	51	GLY
8	T	44	VAL
1	A	283	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	284	ALA
1	A	308	ILE
1	A	948	VAL
2	B	1018	PRO
12	L	46	VAL
1	M	308	ILE
1	M	357	PRO
2	N	100	PRO
2	N	818	PRO
5	Q	64	PRO
12	X	46	VAL
1	A	231	PRO
2	B	613	VAL
3	C	176	ILE
1	M	364	VAL
2	N	1018	PRO
2	N	1110	PRO
5	Q	76	GLY
1	A	196	GLU
1	A	336	ILE
1	A	364	VAL
2	B	553	PRO
1	M	196	GLU
2	N	260	GLY
1	A	693	VAL
2	B	100	PRO
1	M	231	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1239/1520 (82%)	1102 (89%)	137 (11%)	6	25
1	M	1239/1520 (82%)	1105 (89%)	134 (11%)	6	27
2	B	958/1061 (90%)	847 (88%)	111 (12%)	5	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	958/1061 (90%)	840 (88%)	118 (12%)	4	22
3	C	234/274 (85%)	206 (88%)	28 (12%)	5	23
3	O	234/274 (85%)	204 (87%)	30 (13%)	4	20
4	D	160/200 (80%)	135 (84%)	25 (16%)	2	13
4	P	160/200 (80%)	122 (76%)	38 (24%)	1	4
5	E	196/197 (100%)	185 (94%)	11 (6%)	19	52
5	Q	196/197 (100%)	185 (94%)	11 (6%)	19	52
6	F	77/137 (56%)	70 (91%)	7 (9%)	9	34
6	R	77/137 (56%)	70 (91%)	7 (9%)	9	34
7	G	152/152 (100%)	140 (92%)	12 (8%)	11	40
7	S	152/152 (100%)	127 (84%)	25 (16%)	2	12
8	H	118/128 (92%)	107 (91%)	11 (9%)	8	33
8	T	118/128 (92%)	108 (92%)	10 (8%)	10	37
9	I	113/116 (97%)	101 (89%)	12 (11%)	6	27
9	U	113/116 (97%)	104 (92%)	9 (8%)	11	40
10	J	60/65 (92%)	51 (85%)	9 (15%)	3	15
10	V	60/65 (92%)	51 (85%)	9 (15%)	3	15
11	K	99/102 (97%)	90 (91%)	9 (9%)	9	34
11	W	99/102 (97%)	88 (89%)	11 (11%)	6	25
12	L	40/57 (70%)	34 (85%)	6 (15%)	3	15
12	X	40/57 (70%)	34 (85%)	6 (15%)	3	15
All	All	6892/8018 (86%)	6106 (89%)	786 (11%)	5	24

All (786) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	34	LYS
1	A	37	PHE
1	A	41	MET
1	A	53	LEU
1	A	68	GLN
1	A	70	CYS
1	A	93	VAL
1	A	121	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	131	SER
1	A	141	LEU
1	A	145	LYS
1	A	157	ASP
1	A	160	GLN
1	A	162	VAL
1	A	173	THR
1	A	182	VAL
1	A	185	TRP
1	A	200	ARG
1	A	207	ILE
1	A	208	LEU
1	A	219	PHE
1	A	221	SER
1	A	230	ARG
1	A	231	PRO
1	A	244	PRO
1	A	265	LYS
1	A	289	ILE
1	A	297	GLN
1	A	302	THR
1	A	315	LEU
1	A	320	ARG
1	A	322	VAL
1	A	324	SER
1	A	337	ARG
1	A	344	ARG
1	A	345	VAL
1	A	385	ILE
1	A	394	ASN
1	A	408	ASP
1	A	425	GLN
1	A	434	ARG
1	A	443	LEU
1	A	445	ASN
1	A	449	SER
1	A	451	HIS
1	A	461	LYS
1	A	469	ARG
1	A	470	LEU
1	A	475	THR
1	A	481	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	486	GLU
1	A	489	LEU
1	A	493	GLN
1	A	503	GLN
1	A	504	LEU
1	A	505	CYS
1	A	512	VAL
1	A	524	VAL
1	A	538	ASP
1	A	597	LEU
1	A	618	GLU
1	A	629	LEU
1	A	635	ARG
1	A	666	ILE
1	A	670	ILE
1	A	680	THR
1	A	685	GLU
1	A	690	VAL
1	A	691	LEU
1	A	710	LEU
1	A	738	LYS
1	A	741	ASN
1	A	762	SER
1	A	768	GLN
1	A	774	ARG
1	A	783	THR
1	A	805	LEU
1	A	821	ARG
1	A	827	THR
1	A	834	THR
1	A	849	MET
1	A	855	THR
1	A	858	ASN
1	A	874	ASP
1	A	903	ASN
1	A	907	THR
1	A	920	LEU
1	A	936	LEU
1	A	937	VAL
1	A	941	LYS
1	A	961	ARG
1	A	976	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	978	PRO
1	A	983	ILE
1	A	987	VAL
1	A	1005	GLU
1	A	1029	ARG
1	A	1033	GLN
1	A	1036	ARG
1	A	1047	SER
1	A	1049	ILE
1	A	1095	THR
1	A	1114	PRO
1	A	1116	LEU
1	A	1120	LEU
1	A	1122	PRO
1	A	1124	HIS
1	A	1129	GLU
1	A	1165	GLU
1	A	1170	ILE
1	A	1171	GLN
1	A	1193	LEU
1	A	1217	LYS
1	A	1257	ASP
1	A	1264	GLU
1	A	1270	ASN
1	A	1273	LEU
1	A	1276	VAL
1	A	1280	GLU
1	A	1288	ASP
1	A	1295	THR
1	A	1297	GLU
1	A	1299	VAL
1	A	1315	GLU
1	A	1325	THR
1	A	1333	ILE
1	A	1353	TYR
1	A	1370	LEU
1	A	1377	THR
1	A	1385	THR
1	A	1386	ARG
1	A	1394	THR
1	A	1426	GLU
1	A	1444	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1445	ILE
1	A	1451	VAL
2	B	20	ASP
2	B	21	GLU
2	B	25	ILE
2	B	30	SER
2	B	46	GLN
2	B	57	TYR
2	B	70	ILE
2	B	97	VAL
2	B	98	THR
2	B	119	LEU
2	B	128	LEU
2	B	194	GLU
2	B	203	PHE
2	B	217	ARG
2	B	225	VAL
2	B	249	ARG
2	B	258	LEU
2	B	261	ARG
2	B	265	SER
2	B	268	THR
2	B	272	THR
2	B	299	GLU
2	B	323	VAL
2	B	325	GLN
2	B	334	ILE
2	B	364	ILE
2	B	368	GLU
2	B	371	GLU
2	B	376	PHE
2	B	384	ARG
2	B	393	LYS
2	B	416	LEU
2	B	425	THR
2	B	427	ASP
2	B	430	ARG
2	B	452	THR
2	B	465	ASN
2	B	466	TRP
2	B	474	SER
2	B	479	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	491	THR
2	B	498	THR
2	B	502	ILE
2	B	516	ASN
2	B	552	MET
2	B	555	ILE
2	B	563	MET
2	B	580	VAL
2	B	582	VAL
2	B	597	MET
2	B	602	THR
2	B	609	ILE
2	B	615	MET
2	B	616	ILE
2	B	620	ARG
2	B	636	PRO
2	B	694	ASP
2	B	705	MET
2	B	714	GLU
2	B	722	ASP
2	B	730	ARG
2	B	732	SER
2	B	737	THR
2	B	743	ILE
2	B	748	ILE
2	B	786	ASN
2	B	790	ASP
2	B	797	TYR
2	B	805	THR
2	B	816	GLU
2	B	831	SER
2	B	835	GLN
2	B	839	MET
2	B	868	MET
2	B	878	GLN
2	B	879	ARG
2	B	887	HIS
2	B	889	THR
2	B	895	ASP
2	B	901	PRO
2	B	915	THR
2	B	939	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	944	THR
2	B	954	VAL
2	B	956	THR
2	B	959	ASP
2	B	976	ILE
2	B	987	LYS
2	B	997	GLU
2	B	999	MET
2	B	1006	ILE
2	B	1007	VAL
2	B	1049	ASP
2	B	1053	GLU
2	B	1069	PHE
2	B	1084	GLN
2	B	1087	PHE
2	B	1095	LEU
2	B	1098	MET
2	B	1119	VAL
2	B	1120	GLU
2	B	1147	LEU
2	B	1149	GLU
2	B	1151	LEU
2	B	1159	ARG
2	B	1175	LEU
2	B	1183	LYS
2	B	1185	CYS
2	B	1202	LEU
2	B	1212	ILE
2	B	1220	ARG
3	C	3	GLU
3	C	11	ARG
3	C	17	ASN
3	C	22	LEU
3	C	23	SER
3	C	26	ASP
3	C	43	THR
3	C	53	THR
3	C	57	VAL
3	C	66	ARG
3	C	77	ILE
3	C	78	GLU
3	C	89	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	91	HIS
3	C	99	LEU
3	C	102	GLN
3	C	106	GLU
3	C	124	LEU
3	C	129	ILE
3	C	138	GLU
3	C	145	CYS
3	C	147	LEU
3	C	166	GLU
3	C	176	ILE
3	C	177	GLU
3	C	194	GLU
3	C	238	ILE
3	C	259	LEU
4	D	4	SER
4	D	11	ARG
4	D	12	ARG
4	D	17	LYS
4	D	18	VAL
4	D	20	GLU
4	D	22	GLU
4	D	23	ASN
4	D	29	LEU
4	D	38	ILE
4	D	40	HIS
4	D	47	LEU
4	D	52	LEU
4	D	65	GLU
4	D	70	PHE
4	D	120	GLU
4	D	124	GLU
4	D	187	THR
4	D	200	ASN
4	D	206	GLU
4	D	214	LEU
4	D	217	LEU
4	D	219	THR
4	D	220	LEU
4	D	221	TYR
5	E	7	ARG
5	E	31	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	37	LEU
5	E	72	PHE
5	E	78	LEU
5	E	104	ASN
5	E	115	ASN
5	E	150	VAL
5	E	183	PRO
5	E	192	ARG
5	E	212	ARG
6	F	79	ARG
6	F	81	THR
6	F	90	ARG
6	F	93	ILE
6	F	111	LEU
6	F	112	GLU
6	F	119	ARG
7	G	1	MET
7	G	13	LEU
7	G	21	ARG
7	G	24	GLN
7	G	45	ILE
7	G	53	ASN
7	G	74	TYR
7	G	77	VAL
7	G	111	THR
7	G	113	HIS
7	G	120	THR
7	G	171	ILE
8	H	2	SER
8	H	26	ILE
8	H	33	GLN
8	H	61	SER
8	H	64	ASN
8	H	89	LEU
8	H	123	MET
8	H	129	TYR
8	H	130	ARG
8	H	138	GLU
8	H	143	LEU
9	I	6	PHE
9	I	8	ARG
9	I	12	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	15	TYR
9	I	55	THR
9	I	59	VAL
9	I	86	PHE
9	I	93	LYS
9	I	94	ASP
9	I	96	SER
9	I	101	PHE
9	I	111	THR
10	J	2	ILE
10	J	7	CYS
10	J	13	VAL
10	J	23	ASN
10	J	24	LEU
10	J	43	ARG
10	J	44	TYR
10	J	48	ARG
10	J	55	ASP
11	K	1	MET
11	K	12	LEU
11	K	34	THR
11	K	42	LEU
11	K	47	ARG
11	K	50	LEU
11	K	51	LEU
11	K	111	LEU
11	K	114	LEU
12	L	27	LEU
12	L	35	SER
12	L	38	LEU
12	L	54	ARG
12	L	55	ILE
12	L	68	GLU
1	M	11	LEU
1	M	18	GLN
1	M	34	LYS
1	M	37	PHE
1	M	41	MET
1	M	53	LEU
1	M	54	ASN
1	M	68	GLN
1	M	93	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	110	CYS
1	M	121	LEU
1	M	145	LYS
1	M	160	GLN
1	M	173	THR
1	M	182	VAL
1	M	185	TRP
1	M	200	ARG
1	M	203	SER
1	M	204	THR
1	M	208	LEU
1	M	219	PHE
1	M	221	SER
1	M	225	ASN
1	M	230	ARG
1	M	237	THR
1	M	244	PRO
1	M	265	LYS
1	M	289	ILE
1	M	297	GLN
1	M	302	THR
1	M	315	LEU
1	M	320	ARG
1	M	322	VAL
1	M	324	SER
1	M	337	ARG
1	M	344	ARG
1	M	385	ILE
1	M	394	ASN
1	M	408	ASP
1	M	425	GLN
1	M	443	LEU
1	M	445	ASN
1	M	451	HIS
1	M	454	SER
1	M	461	LYS
1	M	469	ARG
1	M	470	LEU
1	M	476	SER
1	M	481	ASP
1	M	489	LEU
1	M	493	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	504	LEU
1	M	505	CYS
1	M	512	VAL
1	M	516	SER
1	M	524	VAL
1	M	538	ASP
1	M	597	LEU
1	M	618	GLU
1	M	629	LEU
1	M	635	ARG
1	M	666	ILE
1	M	670	ILE
1	M	680	THR
1	M	685	GLU
1	M	690	VAL
1	M	691	LEU
1	M	710	LEU
1	M	738	LYS
1	M	740	LEU
1	M	741	ASN
1	M	756	ILE
1	M	762	SER
1	M	769	SER
1	M	774	ARG
1	M	783	THR
1	M	786	HIS
1	M	805	LEU
1	M	821	ARG
1	M	827	THR
1	M	829	VAL
1	M	834	THR
1	M	855	THR
1	M	858	ASN
1	M	874	ASP
1	M	907	THR
1	M	909	ASP
1	M	936	LEU
1	M	937	VAL
1	M	941	LYS
1	M	961	ARG
1	M	964	ILE
1	M	973	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	976	THR
1	M	978	PRO
1	M	983	ILE
1	M	1005	GLU
1	M	1029	ARG
1	M	1033	GLN
1	M	1110	ASN
1	M	1114	PRO
1	M	1116	LEU
1	M	1122	PRO
1	M	1124	HIS
1	M	1129	GLU
1	M	1165	GLU
1	M	1170	ILE
1	M	1171	GLN
1	M	1187	GLN
1	M	1193	LEU
1	M	1217	LYS
1	M	1257	ASP
1	M	1264	GLU
1	M	1270	ASN
1	M	1273	LEU
1	M	1280	GLU
1	M	1295	THR
1	M	1297	GLU
1	M	1325	THR
1	M	1329	THR
1	M	1333	ILE
1	M	1345	ARG
1	M	1353	TYR
1	M	1370	LEU
1	M	1385	THR
1	M	1386	ARG
1	M	1394	THR
1	M	1405	THR
1	M	1409	LEU
1	M	1426	GLU
1	M	1442	ASP
1	M	1444	MET
1	M	1445	ILE
1	M	1451	VAL
2	N	20	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	22	SER
2	N	25	ILE
2	N	30	SER
2	N	57	TYR
2	N	97	VAL
2	N	100	PRO
2	N	128	LEU
2	N	167	ILE
2	N	169	ARG
2	N	194	GLU
2	N	205	ILE
2	N	217	ARG
2	N	218	SER
2	N	222	ILE
2	N	235	SER
2	N	249	ARG
2	N	258	LEU
2	N	261	ARG
2	N	272	THR
2	N	294	ASP
2	N	298	LEU
2	N	299	GLU
2	N	319	GLU
2	N	323	VAL
2	N	325	GLN
2	N	336	ARG
2	N	364	ILE
2	N	368	GLU
2	N	371	GLU
2	N	376	PHE
2	N	393	LYS
2	N	401	PHE
2	N	416	LEU
2	N	419	THR
2	N	425	THR
2	N	427	ASP
2	N	429	PHE
2	N	430	ARG
2	N	465	ASN
2	N	466	TRP
2	N	475	SER
2	N	479	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	485	ARG
2	N	487	THR
2	N	490	SER
2	N	498	THR
2	N	502	ILE
2	N	516	ASN
2	N	547	VAL
2	N	552	MET
2	N	555	ILE
2	N	563	MET
2	N	570	VAL
2	N	582	VAL
2	N	597	MET
2	N	599	THR
2	N	615	MET
2	N	616	ILE
2	N	636	PRO
2	N	643	ASP
2	N	645	SER
2	N	680	THR
2	N	694	ASP
2	N	705	MET
2	N	714	GLU
2	N	722	ASP
2	N	730	ARG
2	N	732	SER
2	N	737	THR
2	N	748	ILE
2	N	786	ASN
2	N	787	VAL
2	N	790	ASP
2	N	805	THR
2	N	811	TYR
2	N	815	ARG
2	N	831	SER
2	N	835	GLN
2	N	837	ASP
2	N	839	MET
2	N	844	SER
2	N	868	MET
2	N	878	GLN
2	N	879	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	887	HIS
2	N	889	THR
2	N	895	ASP
2	N	901	PRO
2	N	909	ASP
2	N	915	THR
2	N	939	THR
2	N	944	THR
2	N	956	THR
2	N	959	ASP
2	N	962	LYS
2	N	976	ILE
2	N	997	GLU
2	N	999	MET
2	N	1006	ILE
2	N	1007	VAL
2	N	1022	THR
2	N	1049	ASP
2	N	1053	GLU
2	N	1060	ARG
2	N	1084	GLN
2	N	1095	LEU
2	N	1119	VAL
2	N	1147	LEU
2	N	1150	ARG
2	N	1151	LEU
2	N	1159	ARG
2	N	1175	LEU
2	N	1183	LYS
2	N	1185	CYS
2	N	1202	LEU
2	N	1214	PRO
2	N	1220	ARG
3	O	3	GLU
3	O	11	ARG
3	O	25	VAL
3	O	26	ASP
3	O	43	THR
3	O	52	GLU
3	O	54	ASN
3	O	57	VAL
3	O	58	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	O	62	PHE
3	O	66	ARG
3	O	69	LEU
3	O	77	ILE
3	O	78	GLU
3	O	89	GLU
3	O	91	HIS
3	O	99	LEU
3	O	124	LEU
3	O	129	ILE
3	O	138	GLU
3	O	145	CYS
3	O	147	LEU
3	O	166	GLU
3	O	177	GLU
3	O	197	SER
3	O	202	PRO
3	O	235	VAL
3	O	238	ILE
3	O	245	VAL
3	O	259	LEU
4	P	4	SER
4	P	10	THR
4	P	17	LYS
4	P	20	GLU
4	P	22	GLU
4	P	23	ASN
4	P	26	THR
4	P	29	LEU
4	P	38	ILE
4	P	40	HIS
4	P	47	LEU
4	P	52	LEU
4	P	59	ILE
4	P	65	GLU
4	P	70	PHE
4	P	74	GLN
4	P	120	GLU
4	P	124	GLU
4	P	140	ASP
4	P	151	PHE
4	P	152	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	P	158	GLU
4	P	167	LEU
4	P	185	CYS
4	P	187	THR
4	P	192	LYS
4	P	193	THR
4	P	197	SER
4	P	204	ASP
4	P	206	GLU
4	P	207	LEU
4	P	211	LEU
4	P	213	GLU
4	P	214	LEU
4	P	215	SER
4	P	216	ASN
4	P	219	THR
4	P	221	TYR
5	Q	31	THR
5	Q	37	LEU
5	Q	78	LEU
5	Q	104	ASN
5	Q	115	ASN
5	Q	134	THR
5	Q	140	LEU
5	Q	150	VAL
5	Q	183	PRO
5	Q	191	LYS
5	Q	212	ARG
6	R	79	ARG
6	R	90	ARG
6	R	93	ILE
6	R	111	LEU
6	R	112	GLU
6	R	119	ARG
6	R	144	GLU
7	S	1	MET
7	S	12	THR
7	S	13	LEU
7	S	21	ARG
7	S	45	ILE
7	S	53	ASN
7	S	74	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	S	75	ARG
7	S	77	VAL
7	S	78	VAL
7	S	87	VAL
7	S	95	SER
7	S	110	VAL
7	S	111	THR
7	S	113	HIS
7	S	114	LEU
7	S	120	THR
7	S	128	PRO
7	S	129	SER
7	S	131	GLN
7	S	139	ILE
7	S	141	SER
7	S	143	ILE
7	S	145	VAL
7	S	154	VAL
8	T	2	SER
8	T	42	ILE
8	T	64	ASN
8	T	89	LEU
8	T	95	TYR
8	T	123	MET
8	T	129	TYR
8	T	130	ARG
8	T	135	LEU
8	T	138	GLU
9	U	7	CYS
9	U	15	TYR
9	U	55	THR
9	U	59	VAL
9	U	86	PHE
9	U	93	LYS
9	U	94	ASP
9	U	101	PHE
9	U	106	CYS
10	V	7	CYS
10	V	13	VAL
10	V	23	ASN
10	V	26	GLN
10	V	30	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	V	43	ARG
10	V	44	TYR
10	V	48	ARG
10	V	59	LYS
11	W	12	LEU
11	W	17	SER
11	W	25	THR
11	W	31	VAL
11	W	34	THR
11	W	42	LEU
11	W	47	ARG
11	W	50	LEU
11	W	51	LEU
11	W	111	LEU
11	W	114	LEU
12	X	27	LEU
12	X	38	LEU
12	X	54	ARG
12	X	55	ILE
12	X	63	ARG
12	X	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (265) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	54	ASN
1	A	75	ASN
1	A	169	ASN
1	A	171	GLN
1	A	225	ASN
1	A	253	ASN
1	A	282	ASN
1	A	297	GLN
1	A	316	GLN
1	A	339	ASN
1	A	390	GLN
1	A	394	ASN
1	A	435	HIS
1	A	451	HIS
1	A	479	ASN
1	A	493	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	503	GLN
1	A	517	ASN
1	A	603	ASN
1	A	611	GLN
1	A	631	HIS
1	A	640	GLN
1	A	698	GLN
1	A	723	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	786	HIS
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	969	GLN
1	A	1011	GLN
1	A	1048	ASN
1	A	1052	GLN
1	A	1106	ASN
1	A	1140	HIS
1	A	1203	ASN
1	A	1258	HIS
1	A	1354	ASN
1	A	1387	HIS
1	A	1432	GLN
2	B	47	GLN
2	B	115	GLN
2	B	178	ASN
2	B	224	GLN
2	B	236	HIS
2	B	366	GLN
2	B	433	GLN
2	B	465	ASN
2	B	484	ASN
2	B	499	ASN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	686	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	706	GLN
2	B	744	HIS
2	B	842	ASN
2	B	862	GLN
2	B	946	ASN
2	B	951	GLN
2	B	957	ASN
2	B	958	GLN
2	B	975	GLN
2	B	986	GLN
2	B	1025	HIS
2	B	1065	GLN
2	B	1074	ASN
2	B	1161	HIS
2	B	1178	ASN
2	B	1179	GLN
2	B	1211	ASN
3	C	17	ASN
3	C	24	ASN
3	C	65	HIS
3	C	73	GLN
3	C	79	GLN
3	C	112	ASN
3	C	123	ASN
3	C	131	HIS
3	C	135	GLN
3	C	151	GLN
3	C	167	HIS
3	C	252	GLN
4	D	9	GLN
4	D	28	GLN
4	D	39	ASN
4	D	40	HIS
4	D	138	ASN
4	D	165	GLN
5	E	3	GLN
5	E	5	ASN
5	E	54	GLN
5	E	99	HIS
5	E	101	GLN
5	E	104	ASN
5	E	106	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	113	GLN
5	E	114	ASN
5	E	147	HIS
6	F	100	GLN
7	G	10	ASN
7	G	14	HIS
7	G	53	ASN
7	G	57	GLN
7	G	71	ASN
7	G	97	HIS
7	G	117	GLN
7	G	122	ASN
7	G	126	ASN
7	G	158	HIS
8	H	64	ASN
8	H	128	ASN
8	H	131	ASN
8	H	133	ASN
8	H	137	GLN
9	I	12	ASN
9	I	46	HIS
9	I	51	ASN
9	I	83	ASN
9	I	90	GLN
9	I	108	HIS
9	I	114	GLN
9	I	120	GLN
10	J	53	HIS
11	K	65	HIS
11	K	76	GLN
11	K	89	ASN
11	K	104	ASN
1	M	18	GLN
1	M	75	ASN
1	M	169	ASN
1	M	171	GLN
1	M	209	ASN
1	M	225	ASN
1	M	253	ASN
1	M	256	GLN
1	M	282	ASN
1	M	316	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	339	ASN
1	M	394	ASN
1	M	435	HIS
1	M	451	HIS
1	M	479	ASN
1	M	490	HIS
1	M	493	GLN
1	M	503	GLN
1	M	517	ASN
1	M	545	GLN
1	M	611	GLN
1	M	631	HIS
1	M	650	GLN
1	M	698	GLN
1	M	736	ASN
1	M	741	ASN
1	M	742	ASN
1	M	745	GLN
1	M	757	ASN
1	M	786	HIS
1	M	858	ASN
1	M	903	ASN
1	M	926	GLN
1	M	965	GLN
1	M	969	GLN
1	M	1011	GLN
1	M	1048	ASN
1	M	1106	ASN
1	M	1110	ASN
1	M	1203	ASN
1	M	1218	GLN
1	M	1258	HIS
1	M	1378	GLN
1	M	1432	GLN
2	N	115	GLN
2	N	121	ASN
2	N	178	ASN
2	N	224	GLN
2	N	236	HIS
2	N	363	HIS
2	N	366	GLN
2	N	383	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	465	ASN
2	N	499	ASN
2	N	513	GLN
2	N	515	HIS
2	N	516	ASN
2	N	518	HIS
2	N	531	GLN
2	N	538	ASN
2	N	592	ASN
2	N	744	HIS
2	N	762	ASN
2	N	794	ASN
2	N	835	GLN
2	N	842	ASN
2	N	862	GLN
2	N	951	GLN
2	N	975	GLN
2	N	984	HIS
2	N	1015	HIS
2	N	1025	HIS
2	N	1062	HIS
2	N	1065	GLN
2	N	1074	ASN
2	N	1076	HIS
2	N	1084	GLN
2	N	1161	HIS
2	N	1176	ASN
2	N	1179	GLN
2	N	1193	GLN
2	N	1211	ASN
3	O	17	ASN
3	O	65	HIS
3	O	73	GLN
3	O	79	GLN
3	O	102	GLN
3	O	112	ASN
3	O	123	ASN
3	O	131	HIS
3	O	151	GLN
3	O	167	HIS
3	O	195	GLN
3	O	252	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	P	28	GLN
4	P	40	HIS
4	P	51	ASN
4	P	74	GLN
5	Q	3	GLN
5	Q	5	ASN
5	Q	54	GLN
5	Q	99	HIS
5	Q	101	GLN
5	Q	104	ASN
5	Q	113	GLN
5	Q	114	ASN
5	Q	147	HIS
6	R	100	GLN
7	S	10	ASN
7	S	14	HIS
7	S	53	ASN
7	S	57	GLN
7	S	97	HIS
7	S	122	ASN
7	S	126	ASN
7	S	153	GLN
8	T	35	GLN
8	T	64	ASN
8	T	83	GLN
8	T	128	ASN
8	T	131	ASN
8	T	133	ASN
8	T	137	GLN
9	U	46	HIS
9	U	83	ASN
9	U	90	GLN
9	U	108	HIS
9	U	120	GLN
10	V	53	HIS
10	V	64	ASN
11	W	65	HIS
11	W	76	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	3	10/17 (58%)	0	0
15	6	10/17 (58%)	0	0
All	All	20/34 (58%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BRU	4	23	15,13	18,21,22	3.92	1 (5%)	25,30,33	0.99	1 (4%)
13	BRU	1	23	15,13	18,21,22	3.90	1 (5%)	25,30,33	0.99	1 (4%)

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
13	BRU	4	23	15,13	-	1/7/21/22	0/2/2/2
13	BRU	1	23	15,13	-	1/7/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	4	23	BRU	BR-C5	-16.55	1.50	1.88
13	1	23	BRU	BR-C5	-16.45	1.50	1.88

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	4	23	BRU	C6-C5-C4	-2.99	117.64	120.67
13	1	23	BRU	C6-C5-C4	-2.99	117.64	120.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	1	23	BRU	O4'-C4'-C5'-O5'
13	4	23	BRU	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	4	23	BRU	6	0
13	1	23	BRU	6	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1416/1733 (81%)	-1.70	0 100 100	12, 52, 93, 119	0
1	M	1416/1733 (81%)	-1.68	0 100 100	10, 53, 94, 123	0
2	B	1104/1224 (90%)	-1.61	0 100 100	12, 62, 103, 120	0
2	N	1104/1224 (90%)	-1.59	0 100 100	16, 65, 104, 121	0
3	C	266/318 (83%)	-1.72	0 100 100	24, 52, 83, 100	0
3	O	266/318 (83%)	-1.70	0 100 100	25, 54, 85, 106	0
4	D	178/221 (80%)	-1.57	0 100 100	36, 68, 100, 108	0
4	P	178/221 (80%)	-1.43	0 100 100	55, 85, 105, 113	0
5	E	214/215 (99%)	-1.53	0 100 100	35, 80, 106, 114	0
5	Q	214/215 (99%)	-1.49	0 100 100	35, 82, 107, 119	0
6	F	87/155 (56%)	-1.81	0 100 100	13, 34, 62, 78	0
6	R	87/155 (56%)	-1.83	0 100 100	15, 34, 63, 76	0
7	G	171/171 (100%)	-1.70	0 100 100	37, 55, 85, 99	0
7	S	171/171 (100%)	-1.55	0 100 100	37, 69, 110, 116	0
8	H	134/146 (91%)	-1.39	0 100 100	60, 88, 105, 114	0
8	T	134/146 (91%)	-1.38	0 100 100	66, 89, 104, 116	0
9	I	119/122 (97%)	-1.46	0 100 100	47, 81, 102, 117	0
9	U	119/122 (97%)	-1.45	0 100 100	45, 84, 102, 119	0
10	J	65/70 (92%)	-1.75	0 100 100	23, 52, 74, 91	0
10	V	65/70 (92%)	-1.73	0 100 100	28, 53, 78, 91	0
11	K	114/120 (95%)	-1.74	0 100 100	23, 54, 72, 83	0
11	W	114/120 (95%)	-1.75	0 100 100	21, 54, 74, 84	0
12	L	46/70 (65%)	-1.30	0 100 100	37, 89, 107, 107	0
12	X	46/70 (65%)	-1.31	0 100 100	42, 93, 107, 108	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9	
13	1	17/26 (65%)	-1.34	0	100100	47, 101, 140, 144	0
13	4	17/26 (65%)	-1.32	0	100100	50, 102, 139, 142	0
14	2	6/13 (46%)	-0.87	0	100100	114, 121, 127, 133	0
14	5	6/13 (46%)	-0.84	0	100100	114, 121, 129, 136	0
15	3	11/17 (64%)	-1.70	0	100100	88, 93, 131, 133	0
15	6	11/17 (64%)	-1.67	0	100100	88, 96, 130, 133	0
All	All	7896/9242 (85%)	-1.63	0	100100	10, 61, 102, 144	0

There are no RSRZ outliers to report.

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
13	BRU	1	23	20/21	0.99	0.04	85,89,94,97	0
13	BRU	4	23	20/21	0.99	0.04	83,89,95,98	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	ZN	A	9984	1/1	1.00	0.01	70,70,70,70	0
16	ZN	A	9985	1/1	1.00	0.00	40,40,40,40	0
16	ZN	B	9986	1/1	1.00	0.01	33,33,33,33	0
16	ZN	C	9987	1/1	1.00	0.00	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	ZN	I	9988	1/1	1.00	0.00	65,65,65,65	0
16	ZN	I	9989	1/1	1.00	0.02	117,117,117,117	0
16	ZN	J	9990	1/1	1.00	0.01	52,52,52,52	0
16	ZN	L	9991	1/1	1.00	0.01	90,90,90,90	0
16	ZN	M	9992	1/1	1.00	0.01	74,74,74,74	0
16	ZN	M	9993	1/1	1.00	0.00	37,37,37,37	0
16	ZN	N	9994	1/1	1.00	0.00	38,38,38,38	0
16	ZN	O	9995	1/1	1.00	0.00	43,43,43,43	0
16	ZN	U	9996	1/1	1.00	0.00	71,71,71,71	0
16	ZN	U	9997	1/1	1.00	0.02	119,119,119,119	0
16	ZN	V	9998	1/1	1.00	0.01	52,52,52,52	0
16	ZN	X	9999	1/1	1.00	0.01	103,103,103,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.