



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:25 pm BST

PDB ID : 1Y1V
Title : Refined RNA Polymerase II-TFIIS complex
Authors : Kettenberger, H.; Armache, K.-J.; Cramer, P.
Deposited on : 2004-11-19
Resolution : 3.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

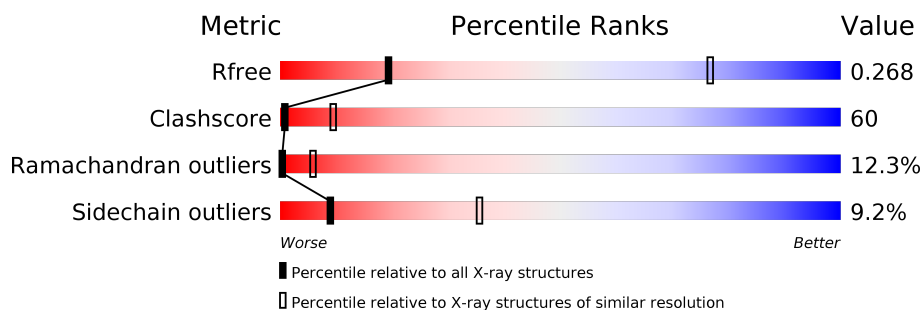
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1733	21% 47% 13% • 18%
2	B	1224	24% 52% 13% • 9%
3	C	318	22% 48% 12% • 16%
4	D	221	33% 40% 6% 20%
5	E	215	34% 55% 11%
6	F	155	15% 30% 8% 46%
7	G	171	33% 59% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	S	179	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 31803 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 largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1426	Total	C	N	O	S	0	0	0
			11214	7069	1959	2124	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1112	Total	C	N	O	S	58	0	0
			8837	5594	1548	1640	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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

- Molecule 4 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	177	Total	C	N	O	S	0	0	0
			1356	840	241	273	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

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

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	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 14.5 kDa polypeptide.

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

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

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

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

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

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

- Molecule 13 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	S	174	Total	C	N	O	S	0	0	104
			666	454	99	108	5			

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	J	1	Total	Zn	0	0
			1	1		
14	B	1	Total	Zn	0	0
			1	1		
14	I	2	Total	Zn	0	0
			2	2		
14	C	1	Total	Zn	0	0
			1	1		
14	A	2	Total	Zn	0	0
			2	2		
14	L	1	Total	Zn	0	0
			1	1		
14	S	1	Total	Zn	0	0
			1	1		

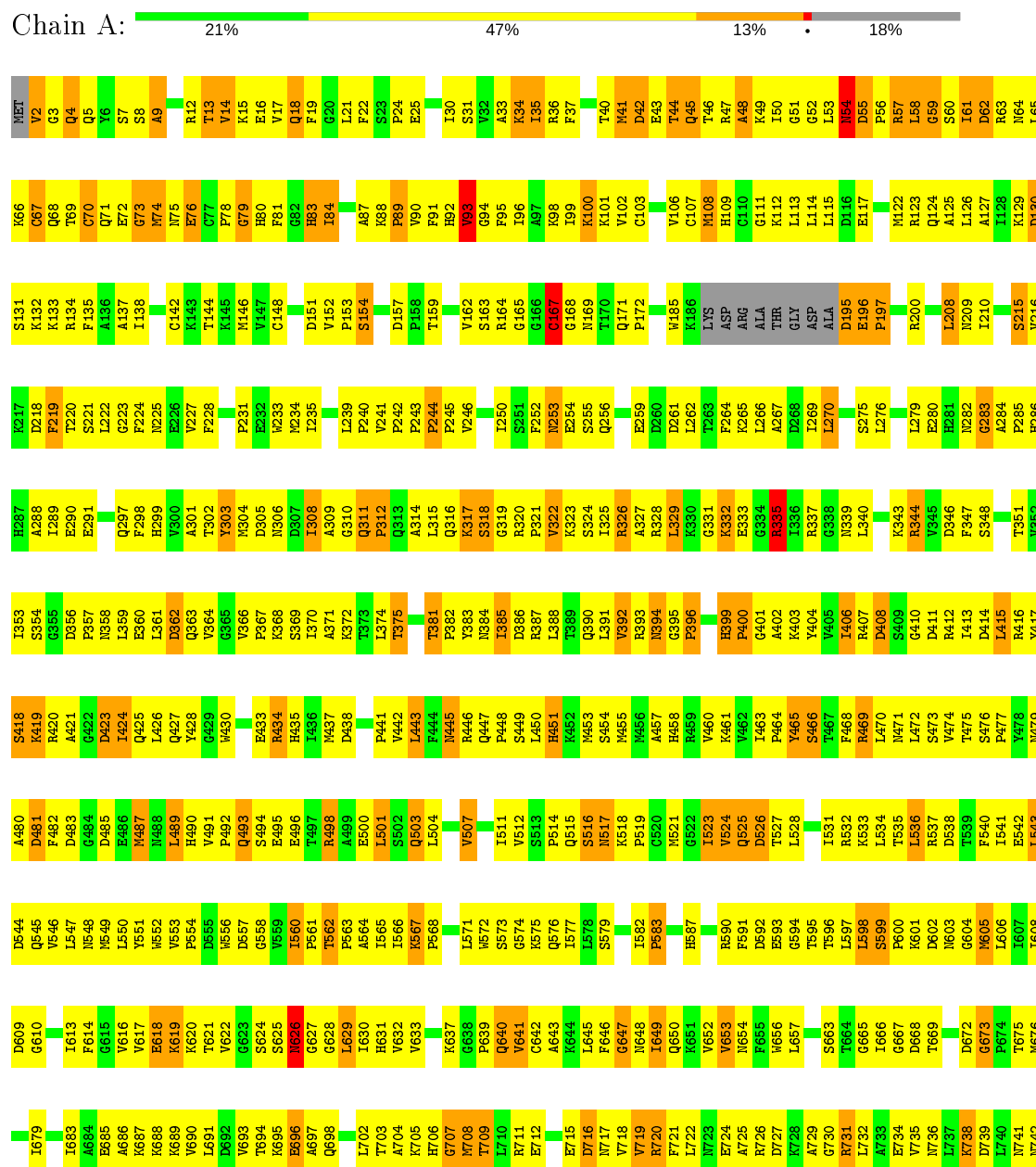
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	S	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

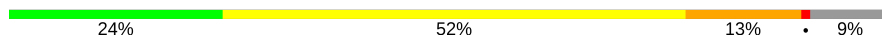
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

- Molecule 1: DNA-directed RNA polymerase II largest subunit

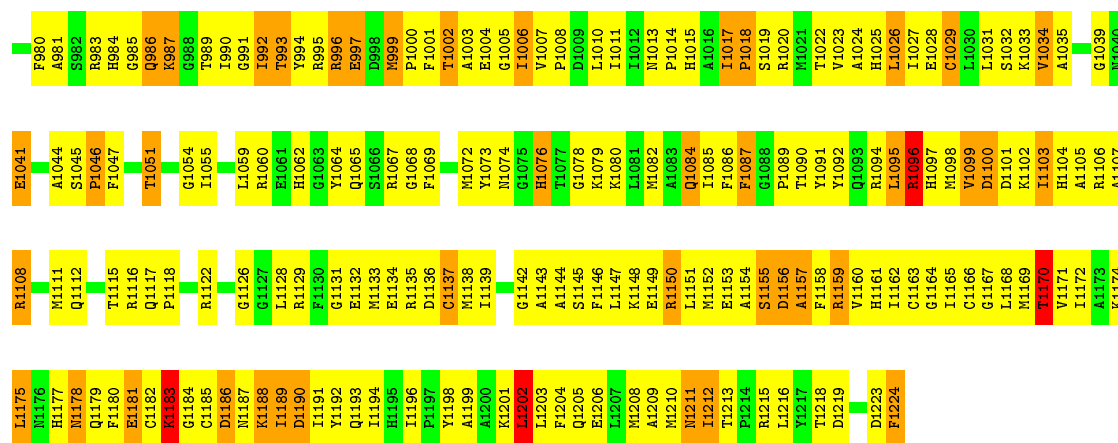


- Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide

Chain B:

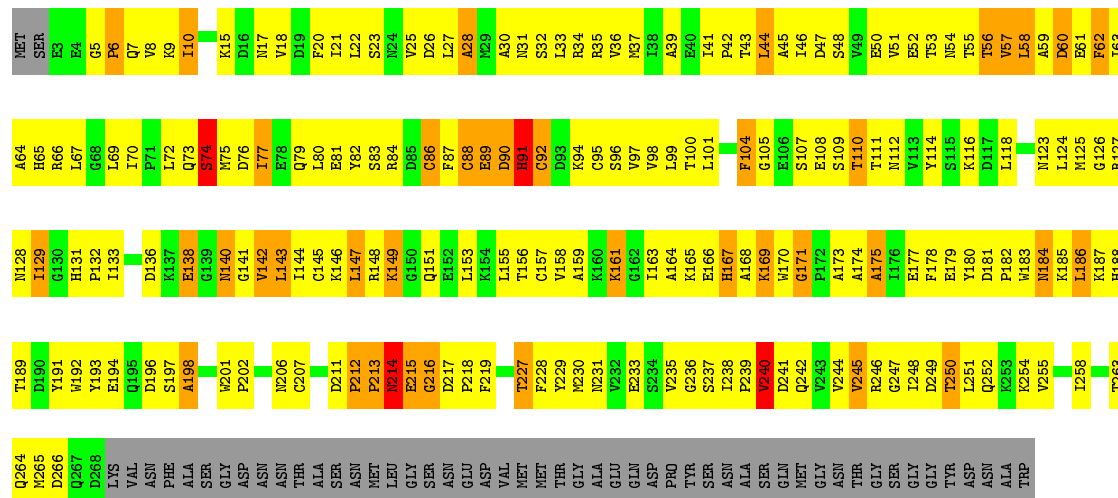


HET	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223	224	225	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240	241	242	243	244	245	246	247	248	249	250	251	252	253	254	255	256	257	258	259	260	261	262	263	264	265	266	267	268	269	270	271	272	273	274	275	276	277	278	279	280	281	282	283	284	285	286	287	288	289	290	291	292	293	294	295	296	297	298	299	300	301	302	303	304	305	306	307	308	309	310	311	312	313	314	315	316	317	318	319	320	321	322	323	324	325	326	327	328	329	330	331	332	333	334	335	336	337	338	339	340	341	342	343	344	345	346	347	348	349	350	351	352	353	354	355	356	357	358	359	360	361	362	363	364	365	366	367	368	369	370	371	372	373	374	375	376	377	378	379	380	381	382	383	384	385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406	407	408	409	410	411	412	413	414	415	416	417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442	443	444	445	446	447	448	449	450	451	452	453	454	455	456	457	458	459	460	461	462	463	464	465	466	467	468	469	470	471	472	473	474	475	476	477	478	479	480	481	482	483	484	485	486	487	488	489	490	491	492	493	494	495	496	497	498	499	500	501	502	503	504	505	506	507	508	509	510	511	512	513	514	515	516	517	518	519	520	521	522	523	524	525	526	527	528	529	530	531	532	533	534	535	536	537	538	539	540	541	542	543	544	545	546	547	548	549	550	551	552	553	554	555	556	557	558	559	560	561	562	563	564	565	566	567	568	569	570	571	572	573	574	575	576	577	578	579	580	581	582	583	584	585	586	587	588	589	590	591	592	593	594	595	596	597	598	599	600	601	602	603	604	605	606	607	608	609	610	611	612	613	614	615	616	617	618	619	620	621	622	623	624	625	626	627	628	629	630	631	632	633	634	635	636	637	638	639	640	641	642	643	644	645	646	647	648	649	650	651	652	653	654	655	656	657	658	659	660	661	662	663	664	665	666	667	668	669	670	671	672	673	674	675	676	677	678	679	680	681	682	683	684	685	686	687	688	689	690	691	692	693	694	695	696	697	698	699	700	701	702	703	704	705	706	707	708	709	710	711	712	713	714	715	716	717	718	719	720	721	722	723	724	725	726	727	728	729	730	731	732	733	734	735	736	737	738	739	740	741	742	743	744	745	746	747	748	749	750	751	752	753	754	755	756	757	758	759	760	761	762	763	764	765	766	767	768	769	770	771	772	773	774	775	776	777	778	779	780	781	782	783	784	785	786	787	788	789	790	791	792	793	794	795	796	797	798	799	800	801	802	803	804	805	806	807	808	809	810	811	812	813	814	815	816	817	818	819	820	821	822	823	824	825	826	827	828	829	830	831	832	833	834	835	836	837	838	839	840	841	842	843	844	845	846	847	848	849	850	851	852	853	854	855	856	857	858	859	860	861	862	863	864	865	866	867	868	869	870	871	872	873	874	875	876	877	878	879	880	881	882	883	884	885	886	887	888	889	890	891	892	893	894	895	896	897	898	899	900	901	902	903	904	905	906	907	908	909	910	911	912	913	914	915	916	917	918	919	920	921	922	923	924	925	926	927	928	929	930	931	932	933	934	935	936	937	938	939	940	941	942	943	944	945	946	947	948	949	950	951	952	953	954	955	956	957	958	959	960	961	962	963	964	965	966	967	968	969	970	971	972	973	974	975	976	977	978	979	980	981	982	983	984	985	986	987	988	989	990	991	992	993	994	995	996	997	998	999	1000	1001	1002	1003	1004	1005	1006	1007	1008	1009	1010	1011	1012	1013	1014	1015	1016	1017	1018	1019	1020	1021	1022	1023	1024	1025	1026	1027	1028	1029	1030	1031	1032	1033	1034	1035	1036	1037	1038	1039	1040	1041	1042	1043	1044	1045	1046	1047	1048	1049	1050	1051	1052	1053	1054	1055	1056	1057	1058	1059	1060	1061	1062	1063	1064	1065	1066	1067	1068	1069	1070	1071	1072	1073	1074	1075	1076	1077	1078	1079	1080	1081	1082	1083	1084	1085	1086	1087	1088	1089	1090	1091	1092	1093	1094	1095	1096	1097	1098	1099	1100	1101	1102	1103	1104	1105	1106	1107	1108	1109	1110	1111	1112	1113	1114	1115	1116	1117	1118	1119	1120	1121	1122	1123	1124	1125	1126	1127	1128	1129	1130	1131	1132	1133	1134	1135	1136	1137	1138	1139	1140	1141	1142	1143	1144	1145	1146	1147	1148	1149	1150	1151	1152	1153	1154	1155	1156	1157	1158	1159	1160	1161	1162	1163	1164	1165	1166	1167	1168	1169	1170	1171	1172	1173	1174	1175	1176	1177	1178	1179	1180	1181	1182	1183	1184	1185	1186	1187	1188	1189	1190	1191	1192	1193	1194	1195	1196	1197	1198	1199	1200	1201	1202	1203	1204	1205	1206	1207	1208	1209	1210	1211	1212	1213	1214	1215	1216	1217	1218	1219	1220	1221	1222	1223	1224	1225	1226	1227	1228	1229	1230	1231	1232	1233	1234	1235	1236	1237	1238	1239	1240	1241	1242	1243	1244	1245	1246	1247	1248	1249	1250	1251	1252	1253	1254	1255	1256	1257	1258	1259	1260	1261	1262	1263	1264	1265	1266	1267	1268	1269	1270	1271	1272	1273	1274	1275	1276	1277	1278	1279	1280	1281	1282	1283	1284	1285	1286	1287	1288	1289	1290	1291	1292	1293	1294	1295	1296	1297	1298	1299	1300	1301	1302	1303	1304	1305	1306	1307	1308	1309	1310	1311	1312	1313	1314	1315	1316	1317	1318	1319	1320	1321	1322	1323	1324	1325	1326	1327	1328	1329	1330	1331	1332	1333	1334	1335	1336	1337	1338	1339	1340	1341	1342	1343	1344	1345	1346	1347	1348	1349	1350	1351	1352	1353	1354	1355	1356	1357	1358	1359	1360	1361	1362	1363	1364	1365	1366	1367	1368	1369	1370	1371	1372	1373	1374	1375	1376	1377	1378	1379	1380	1381	1382	1383	1384	1385	1386	1387	1388	1389	1390	1391	1392	1393	1394	1395	1396	1397	1398	1399	1400	1401	1402	1403	1404	1405	1406	1407	1408	1409	1410	1411	1412	1413	1414	1415	1416	1417	1418	1419	1420	1421	1422	1423	1424	1425	1426	1427	1428	1429	1430	1431	1432	1433	1434	1435	1436	1437	1438	1439	1440	1441	1442	1443	1444	1445	1446	1447	1448	1449	1450	1451	1452	1453	1454	1455	1456	1457	1458	1459	1460	1461	1462	1463	1464	1465	1466	1467	1468	1469	1470	1471	1472	1473	1474	1475	1476	1477	1478	1479	1480	1481	1482	1483	1484	1485	1486	1487	1488	1489	1490	1491	1492	1493	1494	1495	1496	1497	1498	1499	1500	1501	1502	1503	1504	1505	1506	1507	1508	1509	1510	1511	1512	1513	1514	1515	1516	1517	1518	1519	1520	1521	1522	1523	1524	1525	1526	1527	1528	1529	1530	1531	1532	1533	1534	1535	1536	1537	1538	1539	1540	1541	1542	1543	1544	1545	1546	1547	1548	1549	1550	1551	1552	1553	1554	1555	1556	1557	1558	1559	1560	1561	1562	1563	1564	1565	1566	1567	1568	1569	1570	1571	1572	1573	1574	1575	1576	1577	1578	1579	1580	1581	1582	1583	1584	1585	1586	1587	1588	1589	1590	1591	1592	1593	1594	1595	1596	1597	1598	1599	1600	1601	16
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	----



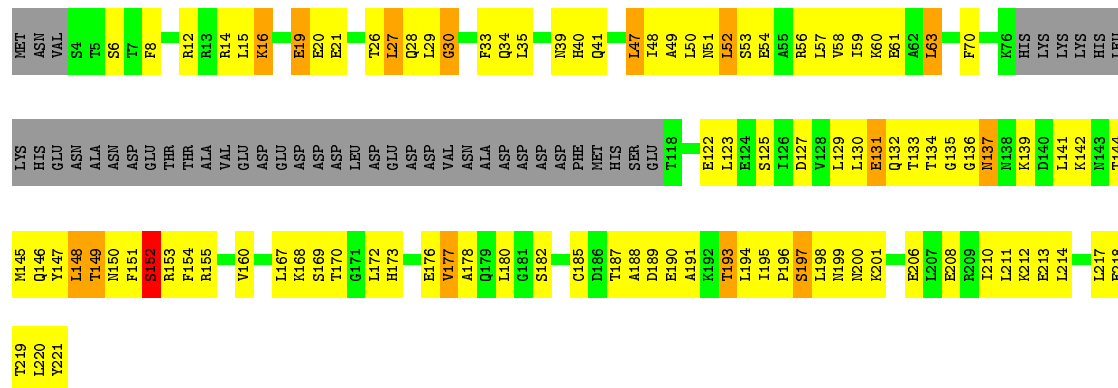
• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C: 22% 48% 12% 16%



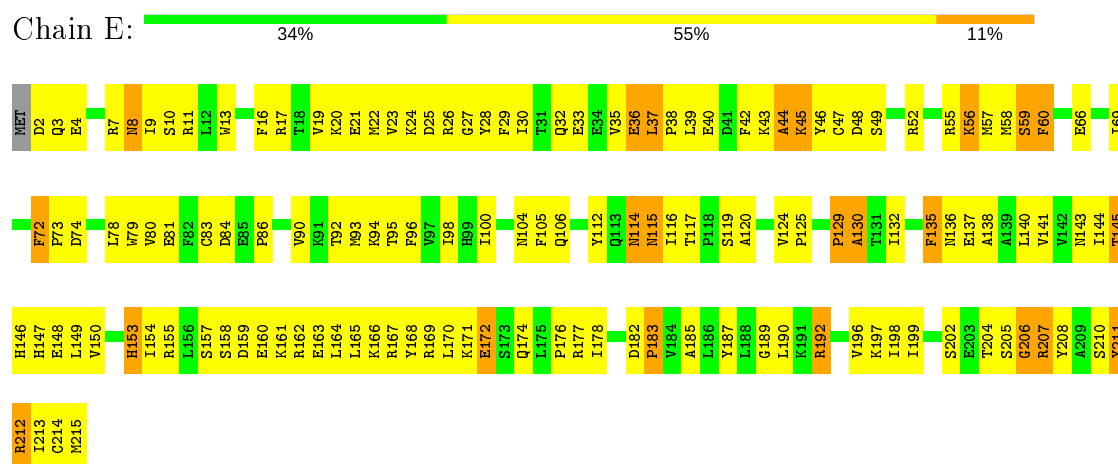
• Molecule 4: DNA-directed RNA polymerase II 32 kDa polypeptide

Chain D: 33% 40% 6% 20%



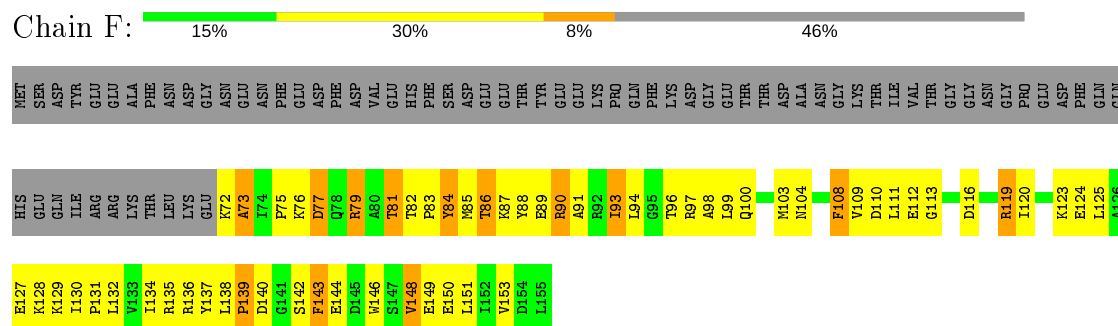
• Molecule 5: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E:



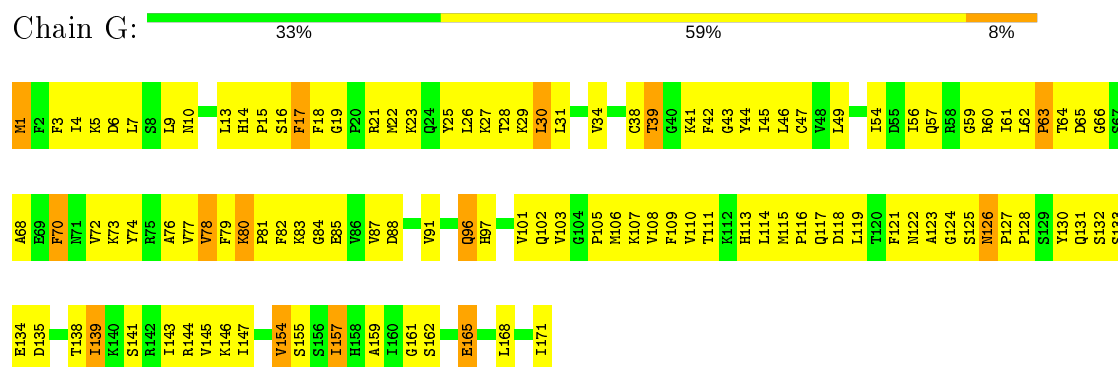
- Molecule 6: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

Chain F:



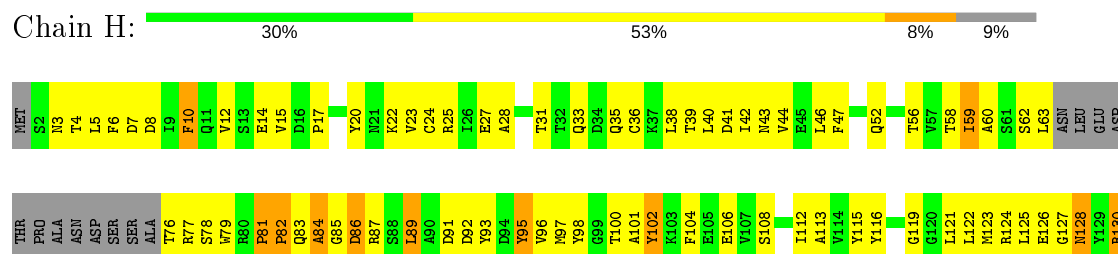
- Molecule 7: DNA-directed RNA polymerase II 19 kDa polypeptide

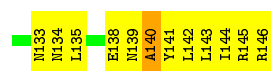
Chain G:



- Molecule 8: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

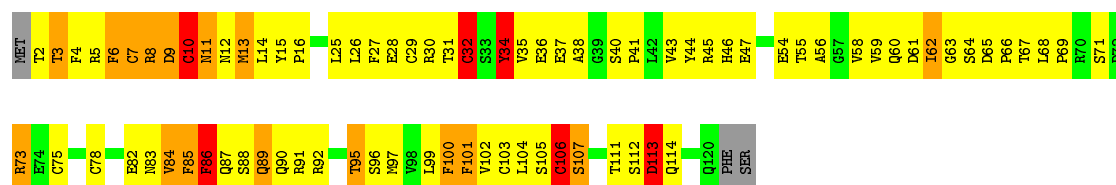
Chain H:





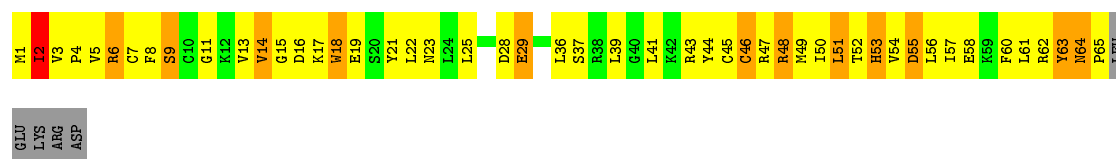
• Molecule 9: DNA-directed RNA polymerase II subunit 9

Chain I: 31% 48% 13% 5%



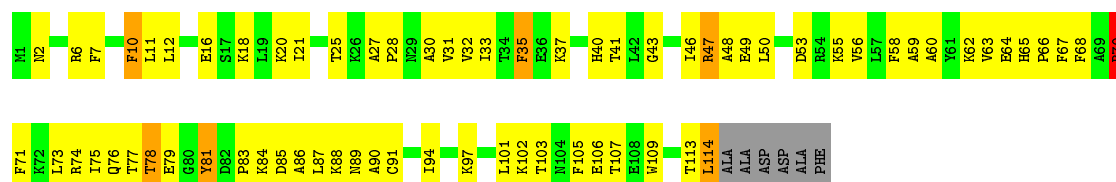
• Molecule 10: DNA-directed RNA polymerases I/II/III subunit 10

Chain J: 23% 51% 17% 7%



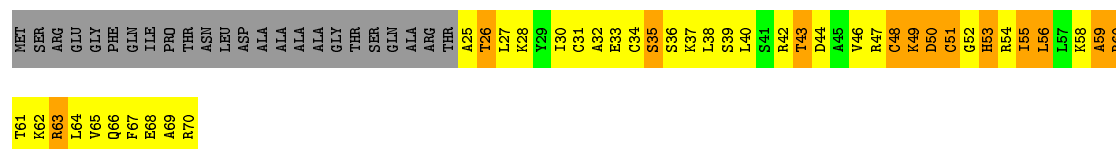
• Molecule 11: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K: 37% 53% 5% 5%



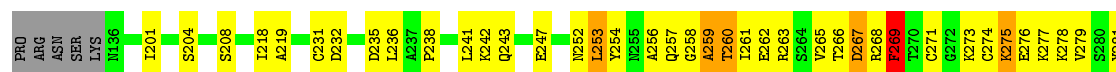
• Molecule 12: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide

Chain L: 6% 41% 19% 34%



• Molecule 13: Transcription elongation factor S-II

Chain S: 62% 28%



Y282	Q283	L284	Q285	T286	R287	S288	A289	D290	E291	P292	L293	T294	T295	F296	C297	T298	C299	E300	A301	C302	G303	N304	R305	W306	K307	F308	S309
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	218.90Å 395.30Å 281.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 49.41 – 3.74	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.80) 86.6 (49.41-3.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.52 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.282 , 0.294 0.257 , 0.268	Depositor DCC
R_{free} test set	2439 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	0.199 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.206 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	31803	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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, MG

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	0.50	2/11417 (0.0%)	0.78	4/15442 (0.0%)
2	B	0.51	4/9009 (0.0%)	0.76	8/12146 (0.1%)
3	C	0.48	0/2133	0.77	1/2891 (0.0%)
4	D	0.41	0/1365	0.64	0/1837
5	E	0.43	0/1788	0.66	0/2406
6	F	0.52	0/691	0.77	0/933
7	G	0.49	0/1368	0.72	0/1844
8	H	0.38	0/1086	0.65	1/1470 (0.1%)
9	I	0.46	0/989	0.77	1/1331 (0.1%)
10	J	0.48	0/541	0.75	0/727
11	K	0.45	0/937	0.67	0/1265
12	L	0.54	0/366	0.79	0/485
13	S	1.31	4/571 (0.7%)	1.64	7/765 (0.9%)
All	All	0.51	10/32261 (0.0%)	0.77	22/43542 (0.1%)

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	3
13	S	0	2
All	All	0	5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	S	269	PHE	C-N	-16.91	0.95	1.34
2	B	467	GLY	C-O	-11.91	1.04	1.23
13	S	260	THR	CA-CB	10.48	1.80	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	468	GLU	CB-CG	8.39	1.68	1.52
13	S	268	ARG	CG-CD	6.05	1.67	1.51
13	S	267	ASP	C-O	6.03	1.34	1.23
2	B	510	LYS	CB-CG	5.59	1.67	1.52
1	A	195	ASP	N-CA	5.47	1.57	1.46
2	B	468	GLU	CG-CD	5.18	1.59	1.51
1	A	196	GLU	CB-CG	5.13	1.61	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	S	269	PHE	O-C-N	-19.02	92.27	122.70
13	S	269	PHE	C-N-CA	16.73	163.51	121.70
13	S	269	PHE	CA-C-N	16.08	152.57	117.20
1	A	195	ASP	N-CA-C	9.35	136.25	111.00
2	B	510	LYS	CB-CA-C	-7.63	95.14	110.40
2	B	510	LYS	C-N-CD	-7.44	104.24	120.60
3	C	92	CYS	CA-CB-SG	-6.79	101.77	114.00
13	S	253	LEU	CA-CB-CG	-6.79	99.67	115.30
1	A	1310	GLY	N-CA-C	-6.49	96.88	113.10
9	I	10	CYS	CA-CB-SG	6.20	125.16	114.00
2	B	468	GLU	N-CA-C	5.96	127.09	111.00
13	S	292	PRO	N-CA-C	5.96	127.59	112.10
2	B	467	GLY	CA-C-N	5.86	130.10	117.20
2	B	511	PRO	CA-N-CD	-5.81	103.37	111.50
2	B	508	LEU	C-N-CA	-5.71	107.43	121.70
1	A	344	ARG	N-CA-C	-5.58	95.93	111.00
2	B	510	LYS	C-N-CA	5.55	145.30	122.00
8	H	89	LEU	CA-CB-CG	5.42	127.76	115.30
1	A	865	GLN	N-CA-C	-5.39	96.45	111.00
2	B	296	GLU	N-CA-C	-5.26	96.79	111.00
13	S	302	CYS	CA-CB-SG	5.18	123.32	114.00
13	S	303	GLY	N-CA-C	5.10	125.85	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	510	LYS	Mainchain
2	B	785	TYR	Sidechain
2	B	833	TYR	Sidechain
13	S	269	PHE	Sidechain,Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11214	0	11281	1514	0
2	B	8837	0	8871	1206	0
3	C	2095	0	2052	260	0
4	D	1356	0	1319	101	0
5	E	1752	0	1776	200	0
6	F	679	0	701	82	0
7	G	1340	0	1357	159	0
8	H	1068	0	1040	115	0
9	I	971	0	929	110	0
10	J	532	0	542	103	0
11	K	919	0	929	96	0
12	L	364	0	387	68	0
13	S	666	0	553	105	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
14	S	1	0	0	0	0
15	S	1	0	0	0	0
All	All	31803	0	31737	3774	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 60.

All (3774) 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)
13:S:260:THR:CA	13:S:260:THR:CB	1.80	1.53
13:S:269:PHE:CZ	13:S:297:CYS:SG	2.04	1.50
13:S:269:PHE:CE2	13:S:297:CYS:SG	2.14	1.39
1:A:1230:GLU:OE2	13:S:201:ILE:CA	1.75	1.32
1:A:1283:VAL:CG1	13:S:256:ALA:O	1.78	1.31
1:A:1172:LEU:CD1	13:S:204:SER:CA	2.12	1.27

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1232:ASN:HD21	13:S:238:PRO:CA	1.48	1.25
13:S:235:ASP:CA	13:S:242:LYS:HE2	1.72	1.18
1:A:1283:VAL:HG13	13:S:256:ALA:O	1.41	1.15
7:G:138:THR:HG22	7:G:139:ILE:H	1.11	1.15
1:A:1017:LEU:HB2	5:E:206:GLY:H	1.11	1.14
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.31	1.12
4:D:40:HIS:HB3	7:G:73:LYS:HZ3	1.09	1.12
1:A:794:PRO:HG2	1:A:795:GLU:OE2	1.49	1.11
1:A:225:ASN:ND2	1:A:228:PHE:H	1.47	1.11
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.14	1.09
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.88	1.09
1:A:590:ARG:NH2	1:A:620:LYS:HB3	1.66	1.09
1:A:913:LEU:HD12	1:A:914:GLU:H	1.15	1.09
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.02	1.09
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.33	1.08
1:A:855:THR:HG21	1:A:857:ARG:HE	1.10	1.08
2:B:1095:LEU:HD12	2:B:1095:LEU:H	1.11	1.08
7:G:14:HIS:HD2	7:G:16:SER:HB2	1.15	1.08
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.15	1.07
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.28	1.07
6:F:82:THR:HG22	6:F:84:TYR:H	1.15	1.07
1:A:1172:LEU:HD13	13:S:204:SER:CA	1.81	1.06
4:D:40:HIS:HB3	7:G:73:LYS:NZ	1.69	1.06
10:J:64:ASN:HB3	10:J:65:PRO:CD	1.86	1.05
2:B:112:LEU:HD12	2:B:113:TYR:H	1.19	1.05
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.20	1.05
1:A:47:ARG:HH12	1:A:254:GLU:HB3	1.21	1.05
13:S:235:ASP:CA	13:S:242:LYS:CE	2.34	1.05
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.19	1.04
2:B:839:MET:CG	2:B:1010:LEU:HD11	1.88	1.04
3:C:133:ILE:HD11	3:C:237:SER:HA	1.39	1.04
7:G:111:THR:HG22	7:G:113:HIS:H	1.19	1.04
1:A:834:THR:HG21	1:A:1077:THR:HG23	1.39	1.04
1:A:1135:ARG:NH1	13:S:256:ALA:HB2	1.72	1.03
1:A:901:LEU:H	1:A:926:GLN:NE2	1.54	1.03
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.39	1.02
13:S:291:GLU:N	13:S:292:PRO:HD2	1.72	1.02
2:B:508:LEU:CB	2:B:510:LYS:H	1.70	1.02
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.58	1.02
1:A:1172:LEU:HD11	13:S:204:SER:CA	1.85	1.02
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.42	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1199:ARG:HH22	13:S:241:LEU:HD13	1.21	1.01
2:B:589:VAL:HG12	2:B:590:HIS:H	1.24	1.00
1:A:164:ARG:HG3	1:A:165:GLY:H	1.26	1.00
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.43	1.00
2:B:918:ILE:HD12	2:B:935:ARG:HD2	1.43	1.00
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.44	1.00
1:A:53:LEU:HD23	1:A:54:ASN:N	1.76	1.00
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.44	0.99
1:A:1283:VAL:HG12	13:S:256:ALA:O	1.57	0.99
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.26	0.99
11:K:65:HIS:CD2	11:K:67:PHE:H	1.81	0.99
1:A:63:ARG:HA	1:A:74:MET:SD	2.01	0.99
2:B:510:LYS:HD2	2:B:510:LYS:O	1.60	0.99
1:A:853:ASP:OD1	1:A:855:THR:HB	1.62	0.99
1:A:1199:ARG:NH2	13:S:241:LEU:HD13	1.78	0.98
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.45	0.98
1:A:490:HIS:HB3	2:B:1150:ARG:NH1	1.79	0.98
2:B:295:GLY:H	2:B:298:LEU:HD23	1.27	0.98
2:B:65:GLU:HG3	2:B:66:ASP:H	1.27	0.98
3:C:56:THR:HG21	3:C:145:CYS:SG	2.03	0.98
2:B:839:MET:HG3	2:B:1010:LEU:HD11	1.01	0.97
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.45	0.97
1:A:225:ASN:HD22	1:A:228:PHE:H	1.03	0.97
2:B:863:GLU:OE2	2:B:873:THR:HA	1.64	0.97
1:A:913:LEU:HD12	1:A:914:GLU:N	1.81	0.96
1:A:1081:LEU:HD12	1:A:1082:ASN:OD1	1.66	0.96
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	1.78	0.96
2:B:882:THR:HG22	2:B:884:ARG:H	1.29	0.95
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.00	0.95
1:A:1172:LEU:CD2	13:S:204:SER:CA	2.44	0.95
2:B:211:VAL:O	2:B:480:SER:HA	1.65	0.95
2:B:824:ILE:HG12	10:J:48:ARG:HH12	1.31	0.95
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.66	0.95
2:B:583:ASN:HD21	2:B:628:THR:HB	1.29	0.95
2:B:987:LYS:HZ2	13:S:290:ASP:HB3	1.32	0.95
3:C:73:GLN:HE21	3:C:75:MET:H	1.03	0.95
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.45	0.94
1:A:1232:ASN:ND2	13:S:238:PRO:CA	2.29	0.94
2:B:1002:THR:HG21	2:B:1006:ILE:HD12	1.49	0.93
1:A:337:ARG:CZ	1:A:839:ARG:HH12	1.81	0.93
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.49	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:85:PHE:HD2	9:I:85:PHE:H	0.93	0.93
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.48	0.93
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.67	0.93
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.04	0.93
1:A:70:CYS:O	1:A:72:GLU:HG2	1.68	0.93
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.48	0.92
6:F:76:LYS:O	6:F:79:ARG:HD3	1.70	0.92
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.48	0.92
13:S:279:VAL:HG22	13:S:299:CYS:HA	1.50	0.92
1:A:49:LYS:NZ	1:A:61:ILE:HG13	1.84	0.92
2:B:1183:LYS:HE3	2:B:1183:LYS:N	1.85	0.92
5:E:153:HIS:O	5:E:154:ILE:HG13	1.69	0.92
1:A:1341:ILE:HG23	1:A:1342:GLU:H	1.32	0.92
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.27	0.92
7:G:14:HIS:CD2	7:G:16:SER:HB2	2.04	0.92
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.05	0.91
3:C:167:HIS:HD2	3:C:169:LYS:H	1.17	0.91
2:B:168:GLY:H	2:B:450:ALA:HB1	1.34	0.91
3:C:63:ILE:HA	3:C:66:ARG:HG3	1.50	0.91
1:A:1362:TYR:HD1	1:A:1363:VAL:H	1.18	0.91
2:B:549:THR:HG22	2:B:550:ASP:H	1.35	0.91
1:A:1329:THR:HG22	1:A:1331:SER:H	1.36	0.91
1:A:864:ILE:O	1:A:865:GLN:HG3	1.72	0.90
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.51	0.90
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.36	0.90
1:A:490:HIS:HB3	2:B:1150:ARG:HH11	1.36	0.90
11:K:65:HIS:HD2	11:K:67:PHE:H	1.10	0.90
9:I:111:THR:HG22	9:I:112:SER:H	1.37	0.90
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.52	0.89
1:A:1329:THR:N	1:A:1335:ILE:HD11	1.87	0.89
1:A:560:ILE:HG13	8:H:78:SER:HB2	1.51	0.89
1:A:666:ILE:HD12	1:A:667:GLY:H	1.35	0.89
1:A:1118:VAL:O	1:A:1305:VAL:HG13	1.71	0.89
2:B:35:SER:HA	2:B:811:TYR:HE2	1.36	0.89
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.52	0.89
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	1.88	0.89
11:K:56:VAL:HA	11:K:77:THR:HG22	1.55	0.89
1:A:708:MET:HE2	1:A:1089:VAL:HG13	1.55	0.88
1:A:524:VAL:HG12	1:A:525:GLN:H	1.38	0.88
2:B:1095:LEU:HD12	2:B:1095:LEU:N	1.88	0.88
10:J:6:ARG:HG2	10:J:13:VAL:HA	1.55	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:835:GLN:HA	2:B:1013:ASN:HD22	1.35	0.88
5:E:197:LYS:HE2	5:E:199:ILE:HD11	1.55	0.88
5:E:22:MET:HE3	5:E:26:ARG:NE	1.89	0.88
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.54	0.88
2:B:365:THR:HG23	2:B:367:LEU:HG	1.55	0.88
1:A:1029:ARG:HG3	1:A:1029:ARG:HH11	1.38	0.88
1:A:55:ASP:C	1:A:57:ARG:H	1.73	0.88
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.55	0.88
7:G:23:LYS:HG3	7:G:56:ILE:HD11	1.55	0.88
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.55	0.88
1:A:567:LYS:HB3	8:H:96:VAL:H	1.39	0.88
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.39	0.88
5:E:117:THR:HG22	5:E:119:SER:H	1.39	0.88
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.56	0.88
7:G:1:MET:HG3	7:G:85:GLU:CD	1.93	0.88
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.53	0.88
1:A:466:SER:O	2:B:1103:ILE:HD11	1.74	0.87
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.55	0.87
1:A:901:LEU:H	1:A:926:GLN:HE21	1.22	0.87
5:E:22:MET:HE3	5:E:26:ARG:HE	1.37	0.87
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.57	0.87
2:B:579:ARG:HB2	2:B:586:TRP:NE1	1.90	0.87
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.09	0.87
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.57	0.87
1:A:443:LEU:HG	2:B:1146:PHE:HE2	1.38	0.87
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.57	0.87
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.40	0.87
2:B:582:VAL:HG23	2:B:626:ILE:HB	1.57	0.87
1:A:855:THR:HG21	1:A:857:ARG:NE	1.89	0.86
2:B:113:TYR:HB3	2:B:114:PRO:HD2	1.55	0.86
1:A:587:HIS:CD2	1:A:969:GLN:HG2	2.11	0.86
7:G:1:MET:HG3	7:G:85:GLU:OE2	1.75	0.86
2:B:466:TRP:O	2:B:468:GLU:N	2.08	0.86
3:C:213:PRO:O	3:C:214:ASN:HB2	1.74	0.86
2:B:467:GLY:O	2:B:468:GLU:HB2	1.73	0.86
9:I:29:CYS:SG	9:I:32:CYS:N	2.48	0.86
2:B:39:ARG:NH2	2:B:665:GLU:HG2	1.89	0.86
1:A:1341:ILE:HG23	1:A:1342:GLU:N	1.89	0.85
13:S:265:VAL:CG1	13:S:278:LYS:HA	2.06	0.85
2:B:37:PHE:HE2	2:B:542:MET:HA	1.40	0.85
2:B:880:THR:HB	2:B:934:LYS:HD2	1.56	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:43:ARG:HG3	10:J:45:CYS:SG	2.16	0.85
2:B:493:SER:HA	2:B:751:VAL:HG21	1.57	0.85
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.12	0.85
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.44	0.85
1:A:665:GLY:HA2	2:B:1026:LEU:HD21	1.58	0.85
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.58	0.85
2:B:839:MET:HG3	2:B:1010:LEU:CD1	1.98	0.85
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	1.76	0.85
2:B:955:THR:HG23	12:L:54:ARG:O	1.77	0.85
1:A:1116:LEU:N	1:A:1308:THR:HG22	1.92	0.85
1:A:963:ILE:HD13	1:A:1049:ILE:HG13	1.58	0.85
7:G:138:THR:HG22	7:G:139:ILE:N	1.91	0.85
9:I:85:PHE:N	9:I:85:PHE:CD2	2.45	0.84
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.05	0.84
1:A:49:LYS:HZ3	1:A:61:ILE:HG13	1.39	0.84
5:E:153:HIS:HB3	5:E:196:VAL:HG11	1.58	0.84
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.41	0.84
2:B:781:PHE:O	2:B:782:LEU:HG	1.78	0.84
2:B:843:GLN:HB2	2:B:993:THR:HB	1.58	0.84
2:B:766:ARG:NH2	2:B:1020:ARG:HG2	1.92	0.84
2:B:1065:GLN:HE21	2:B:1067:ARG:H	0.86	0.84
2:B:1107:ALA:O	2:B:1108:ARG:HG2	1.77	0.84
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.60	0.84
1:A:537:ARG:HD2	8:H:20:TYR:HE1	1.40	0.84
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.11	0.84
3:C:244:VAL:O	3:C:248:ILE:HG13	1.76	0.84
1:A:540:PHE:HB3	1:A:571:LEU:HD23	1.59	0.84
1:A:472:LEU:HD11	2:B:835:GLN:NE2	1.93	0.84
5:E:153:HIS:HB3	5:E:196:VAL:CG1	2.08	0.84
1:A:503:GLN:HE21	6:F:90:ARG:HH21	1.25	0.83
3:C:92:CYS:SG	3:C:95:CYS:SG	2.75	0.83
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.59	0.83
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.59	0.83
8:H:100:THR:HG23	8:H:138:GLU:HA	1.58	0.83
1:A:1116:LEU:HD23	1:A:1311:VAL:HG22	1.60	0.83
1:A:353:ILE:HD12	1:A:470:LEU:HD21	1.61	0.83
10:J:9:SER:OG	10:J:45:CYS:HB2	1.79	0.83
1:A:743:VAL:O	1:A:747:VAL:HG23	1.79	0.83
2:B:510:LYS:O	2:B:510:LYS:CD	2.25	0.82
2:B:510:LYS:HG2	2:B:512:ARG:H	1.43	0.82
13:S:291:GLU:H	13:S:292:PRO:HD2	1.42	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:16:ASP:OD1	10:J:17:LYS:HD2	1.80	0.82
13:S:288:SER:O	13:S:292:PRO:HD3	1.80	0.82
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.09	0.82
2:B:1020:ARG:HG2	2:B:1020:ARG:HH11	1.44	0.82
2:B:502:ILE:HG22	2:B:502:ILE:O	1.79	0.82
9:I:111:THR:HG22	9:I:113:ASP:H	1.43	0.82
1:A:14:VAL:HG23	1:A:1432:GLN:NE2	1.95	0.82
1:A:1239:ARG:HH22	1:A:1241:ARG:HH22	1.25	0.82
2:B:295:GLY:N	2:B:298:LEU:HD23	1.94	0.81
1:A:649:ILE:O	1:A:653:VAL:HG23	1.80	0.81
6:F:86:THR:OG1	6:F:89:GLU:HG3	1.80	0.81
1:A:1237:ILE:HG22	1:A:1238:ILE:N	1.96	0.81
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.63	0.81
7:G:111:THR:HG22	7:G:113:HIS:N	1.95	0.81
2:B:816:GLU:O	2:B:817:LEU:HD23	1.80	0.81
1:A:628:GLY:O	1:A:632:VAL:HG23	1.81	0.81
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.10	0.81
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.44	0.81
1:A:669:THR:O	1:A:762:SER:HB3	1.81	0.81
9:I:56:ALA:HB2	9:I:89:GLN:CG	2.10	0.81
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.63	0.81
1:A:1372:VAL:O	1:A:1376:THR:HG22	1.81	0.81
1:A:78:PRO:HA	2:B:1201:LYS:NZ	1.96	0.81
2:B:1169:MET:CE	2:B:1201:LYS:HA	2.11	0.81
13:S:235:ASP:CA	13:S:242:LYS:CG	2.58	0.81
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.63	0.81
1:A:1317:MET:O	1:A:1322:ILE:HD11	1.80	0.81
1:A:795:GLU:CD	1:A:795:GLU:H	1.83	0.81
7:G:1:MET:HE3	7:G:80:LYS:C	2.00	0.81
9:I:6:PHE:HB3	9:I:12:ASN:O	1.80	0.81
1:A:666:ILE:HD12	1:A:667:GLY:N	1.95	0.80
2:B:510:LYS:HD2	2:B:510:LYS:C	1.98	0.80
1:A:471:ASN:O	1:A:474:VAL:HG12	1.81	0.80
2:B:862:GLN:HG2	2:B:963:PHE:HD1	1.45	0.80
1:A:399:HIS:O	1:A:401:GLY:N	2.14	0.80
2:B:1204:PHE:O	2:B:1208:MET:HG3	1.82	0.80
9:I:58:VAL:HG12	9:I:60:GLN:H	1.47	0.80
1:A:1017:LEU:HB2	5:E:206:GLY:N	1.93	0.80
2:B:1099:VAL:HG13	2:B:1100:ASP:H	1.44	0.80
6:F:82:THR:HG22	6:F:84:TYR:N	1.97	0.80
11:K:65:HIS:HD2	11:K:67:PHE:N	1.79	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.47	0.80
1:A:335:ARG:HE	1:A:339:ASN:ND2	1.79	0.79
1:A:56:PRO:O	1:A:57:ARG:HG3	1.82	0.79
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.62	0.79
2:B:508:LEU:C	2:B:510:LYS:N	2.30	0.79
2:B:589:VAL:HG12	2:B:590:HIS:N	1.95	0.79
9:I:58:VAL:HG22	9:I:62:ILE:HD12	1.63	0.79
3:C:73:GLN:NE2	3:C:75:MET:H	1.79	0.79
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.62	0.79
1:A:825:ILE:HG21	2:B:510:LYS:HE3	1.64	0.79
9:I:55:THR:HG23	9:I:100:PHE:HD2	1.48	0.79
2:B:359:GLU:O	2:B:362:PRO:HD3	1.82	0.79
2:B:509:ALA:O	2:B:510:LYS:HD2	1.81	0.79
2:B:508:LEU:C	2:B:510:LYS:H	1.81	0.79
9:I:85:PHE:HD2	9:I:85:PHE:N	1.78	0.79
3:C:133:ILE:CD1	3:C:237:SER:HA	2.12	0.79
13:S:265:VAL:HG13	13:S:278:LYS:HA	1.65	0.79
1:A:1435:PRO:HA	1:A:1439:GLY:O	1.82	0.79
1:A:299:HIS:HA	1:A:302:THR:HG22	1.65	0.79
1:A:494:SER:O	1:A:498:ARG:HG2	1.82	0.79
13:S:269:PHE:HZ	13:S:297:CYS:SG	1.97	0.79
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.65	0.79
3:C:98:VAL:C	3:C:99:LEU:HD23	2.04	0.79
2:B:806:THR:HG22	2:B:808:ALA:H	1.48	0.79
7:G:9:LEU:HD12	7:G:10:ASN:H	1.48	0.79
2:B:613:VAL:HG13	2:B:627:PHE:O	1.84	0.78
1:A:1444:MET:HG2	7:G:60:ARG:HA	1.65	0.78
1:A:1135:ARG:NH1	13:S:256:ALA:CB	2.46	0.78
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.65	0.78
2:B:593:PRO:HG2	2:B:617:ARG:NH2	1.99	0.78
1:A:537:ARG:HD2	8:H:20:TYR:CE1	2.18	0.78
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.48	0.78
3:C:167:HIS:CD2	3:C:169:LYS:H	2.02	0.78
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.64	0.78
5:E:124:VAL:HG13	5:E:132:ILE:HD12	1.64	0.78
5:E:154:ILE:H	5:E:196:VAL:HG13	1.49	0.78
13:S:271:CYS:SG	13:S:304:ASN:ND2	2.57	0.78
1:A:587:HIS:HD2	1:A:969:GLN:HG2	1.48	0.78
1:A:849:MET:HE1	1:A:1061:GLY:HA2	1.64	0.78
2:B:112:LEU:HD12	2:B:113:TYR:N	1.96	0.78
2:B:510:LYS:HG2	2:B:512:ARG:HG3	1.64	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:882:THR:HG22	2:B:884:ARG:N	1.99	0.78
4:D:40:HIS:CB	7:G:73:LYS:HZ3	1.94	0.78
2:B:987:LYS:NZ	13:S:290:ASP:HB3	1.98	0.78
1:A:1283:VAL:HG13	13:S:256:ALA:C	2.04	0.78
4:D:48:ILE:HG21	7:G:4:ILE:HD12	1.66	0.77
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.18	0.77
1:A:765:VAL:HG23	1:A:802:ASN:O	1.84	0.77
1:A:1127:ASP:HB3	1:A:1130:GLN:CB	2.14	0.77
1:A:866:PHE:O	1:A:867:ILE:HD12	1.85	0.77
1:A:1017:LEU:HB3	5:E:205:SER:HA	1.64	0.77
1:A:1090:ALA:HA	1:A:1093:LYS:HE3	1.66	0.77
1:A:164:ARG:HG3	1:A:165:GLY:N	1.98	0.77
1:A:515:GLN:O	1:A:516:SER:HB3	1.85	0.77
2:B:1206:GLU:O	2:B:1209:ALA:HB3	1.83	0.77
2:B:508:LEU:HB3	2:B:510:LYS:H	1.48	0.77
2:B:615:MET:HB3	2:B:626:ILE:HG12	1.66	0.77
10:J:45:CYS:O	10:J:48:ARG:HG3	1.85	0.77
2:B:1106:ARG:HG3	2:B:1107:ALA:N	1.96	0.77
3:C:47:ASP:HA	12:L:69:ALA:CB	2.15	0.77
4:D:35:LEU:H	4:D:35:LEU:HD12	1.48	0.77
7:G:87:VAL:HB	7:G:103:VAL:HG11	1.67	0.77
12:L:30:ILE:HD11	12:L:59:ALA:HB2	1.64	0.77
1:A:908:LEU:HD12	1:A:983:ILE:HD11	1.67	0.77
3:C:73:GLN:HE21	3:C:75:MET:N	1.82	0.76
9:I:62:ILE:HG22	9:I:62:ILE:O	1.84	0.76
7:G:121:PHE:HB2	7:G:130:TYR:CE2	2.20	0.76
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.67	0.76
1:A:830:LYS:HB2	1:A:1081:LEU:HD23	1.67	0.76
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.20	0.76
1:A:590:ARG:HD3	1:A:604:GLY:HA2	1.67	0.76
1:A:767:GLN:OE1	1:A:799:PHE:HB2	1.83	0.76
2:B:583:ASN:ND2	2:B:628:THR:HB	2.00	0.76
8:H:4:THR:HA	8:H:60:ALA:HB2	1.66	0.76
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.00	0.76
1:A:1224:LEU:HD12	1:A:1241:ARG:O	1.84	0.76
4:D:185:CYS:HA	4:D:190:GLU:OE1	1.85	0.76
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.68	0.76
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.68	0.76
1:A:963:ILE:HD11	1:A:1048:ASN:HB2	1.68	0.76
2:B:1165:ILE:HG22	2:B:1166:CYS:N	1.99	0.76
9:I:34:TYR:CD2	9:I:35:VAL:N	2.54	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:LEU:HD12	1:A:490:HIS:N	1.99	0.76
2:B:467:GLY:O	2:B:468:GLU:CB	2.29	0.76
1:A:106:VAL:HG13	1:A:112:LYS:O	1.86	0.76
1:A:1132:LYS:HE2	13:S:253:LEU:HD21	1.68	0.76
1:A:107:CYS:H	1:A:114:LEU:HD21	1.51	0.76
2:B:1084:GLN:HE21	2:B:1084:GLN:N	1.84	0.76
13:S:235:ASP:CA	13:S:242:LYS:HG2	2.16	0.76
2:B:1187:ASN:O	2:B:1188:LYS:HB2	1.84	0.76
5:E:7:ARG:HG3	5:E:8:ASN:N	2.00	0.76
11:K:113:THR:O	11:K:114:LEU:HB2	1.84	0.76
1:A:567:LYS:HB3	8:H:96:VAL:N	2.01	0.75
2:B:745:PRO:O	2:B:748:ILE:HG12	1.86	0.75
1:A:225:ASN:HD22	1:A:228:PHE:N	1.80	0.75
1:A:820:GLY:O	1:A:822:GLU:N	2.20	0.75
2:B:98:THR:O	2:B:126:SER:HB2	1.86	0.75
1:A:1027:ALA:HB3	1:A:1030:ARG:HB2	1.68	0.75
1:A:95:PHE:CD1	1:A:234:MET:HG2	2.20	0.75
1:A:826:ASP:O	1:A:830:LYS:HB3	1.85	0.75
2:B:515:HIS:CD2	2:B:517:THR:H	2.02	0.75
2:B:918:ILE:HD12	2:B:935:ARG:CD	2.15	0.75
2:B:1224:PHE:HE2	5:E:171:LYS:HG3	1.52	0.75
8:H:59:ILE:HG22	8:H:60:ALA:N	2.01	0.75
1:A:754:SER:H	1:A:757:ASN:HD22	1.35	0.75
2:B:705:MET:HA	2:B:705:MET:CE	2.17	0.75
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.67	0.75
1:A:1204:ASP:HA	13:S:252:ASN:HB3	1.65	0.75
2:B:39:ARG:HH21	2:B:665:GLU:HG2	1.46	0.75
3:C:90:ASP:O	3:C:91:HIS:CD2	2.39	0.75
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.68	0.75
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.17	0.75
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.67	0.75
1:A:95:PHE:O	1:A:99:ILE:HG13	1.87	0.75
2:B:510:LYS:HG2	2:B:512:ARG:CG	2.17	0.75
1:A:1107:VAL:HG12	1:A:1107:VAL:O	1.87	0.75
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.68	0.75
10:J:7:CYS:SG	10:J:49:MET:HE3	2.26	0.75
1:A:1079:MET:HE2	1:A:1101:LEU:HD23	1.67	0.74
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.51	0.74
4:D:145:MET:O	4:D:149:THR:HB	1.87	0.74
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.02	0.74
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.21	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.69	0.74
9:I:101:PHE:N	9:I:101:PHE:CD1	2.55	0.74
1:A:1406:VAL:HG12	1:A:1410:PHE:CE1	2.21	0.74
1:A:899:VAL:CB	1:A:929:LEU:HD11	2.16	0.74
2:B:1084:GLN:NE2	2:B:1084:GLN:N	2.35	0.74
1:A:1135:ARG:HH12	13:S:256:ALA:HB2	1.49	0.74
3:C:50:GLU:HG2	12:L:64:LEU:HD13	1.69	0.74
1:A:31:SER:HA	1:A:81:PHE:O	1.87	0.74
2:B:563:MET:HE1	2:B:580:VAL:HB	1.69	0.74
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.70	0.74
1:A:1172:LEU:HD22	13:S:204:SER:CA	2.16	0.74
1:A:853:ASP:OD1	1:A:855:THR:N	2.21	0.74
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.02	0.74
1:A:1239:ARG:HH22	1:A:1241:ARG:NH2	1.85	0.74
1:A:741:ASN:HD22	1:A:744:LYS:H	1.35	0.74
1:A:68:GLN:HE22	1:A:80:HIS:CD2	2.06	0.74
2:B:508:LEU:CB	2:B:510:LYS:N	2.50	0.74
2:B:508:LEU:HB2	2:B:510:LYS:H	1.52	0.74
9:I:111:THR:HG22	9:I:112:SER:N	2.03	0.74
1:A:337:ARG:CZ	1:A:839:ARG:NH1	2.50	0.74
1:A:897:TYR:HD1	1:A:897:TYR:N	1.85	0.74
2:B:515:HIS:HD2	2:B:517:THR:H	1.35	0.74
4:D:170:THR:CG2	4:D:172:LEU:HG	2.16	0.74
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.52	0.74
1:A:1170:ILE:HG23	1:A:1174:PHE:CE1	2.22	0.74
1:A:858:ASN:HD22	1:A:858:ASN:C	1.90	0.74
2:B:1142:GLY:HA3	6:F:88:TYR:HE2	1.52	0.74
2:B:769:TYR:CE2	2:B:987:LYS:NZ	2.55	0.74
2:B:1180:PHE:HB3	2:B:1191:ILE:HD12	1.69	0.73
2:B:541:LEU:HB2	2:B:747:MET:HE3	1.68	0.73
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.69	0.73
7:G:145:VAL:HG12	7:G:146:LYS:N	2.03	0.73
1:A:1445:ILE:HD12	1:A:1445:ILE:H	1.53	0.73
1:A:364:VAL:HG12	1:A:458:HIS:HB3	1.71	0.73
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.53	0.73
3:C:104:PHE:HD2	3:C:105:GLY:N	1.86	0.73
7:G:91:VAL:HG23	7:G:141:SER:O	1.88	0.73
9:I:101:PHE:H	9:I:101:PHE:HD1	1.34	0.73
1:A:1444:MET:CE	6:F:135:ARG:HB2	2.18	0.73
8:H:36:CYS:HA	8:H:126:GLU:O	1.88	0.73
1:A:335:ARG:NH1	2:B:1206:GLU:OE2	2.22	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLN:C	1:A:73:GLY:H	1.91	0.73
1:A:256:GLN:HE21	2:B:918:ILE:HD11	1.54	0.73
1:A:265:LYS:HE2	1:A:322:VAL:CG1	2.19	0.73
1:A:903:ASN:HD22	1:A:904:THR:N	1.87	0.73
3:C:6:PRO:HB3	3:C:25:VAL:HG12	1.69	0.73
4:D:144:THR:O	4:D:148:LEU:HB2	1.89	0.73
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.69	0.73
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.53	0.73
2:B:1002:THR:CG2	2:B:1006:ILE:HD12	2.19	0.72
7:G:115:MET:HB2	7:G:116:PRO:HD2	1.70	0.72
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.71	0.72
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.71	0.72
1:A:1341:ILE:CG2	1:A:1342:GLU:H	2.03	0.72
1:A:648:ASN:O	1:A:652:VAL:HG23	1.88	0.72
1:A:979:SER:OG	1:A:980:ASP:N	2.22	0.72
2:B:801:LYS:O	10:J:52:THR:HG23	1.89	0.72
1:A:1057:VAL:HG12	1:A:1058:VAL:H	1.54	0.72
1:A:1402:PHE:CE1	1:A:1403:GLU:HG3	2.24	0.72
1:A:288:ALA:HA	1:A:291:GLU:OE2	1.89	0.72
1:A:40:THR:HG21	1:A:259:GLU:OE2	1.89	0.72
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.53	0.72
2:B:172:ILE:HD13	2:B:178:ASN:CB	2.19	0.72
2:B:873:THR:O	2:B:914:LYS:HA	1.88	0.72
5:E:213:ILE:HG12	5:E:214:CYS:H	1.54	0.72
6:F:111:LEU:HD12	6:F:111:LEU:H	1.54	0.72
7:G:80:LYS:HG2	7:G:80:LYS:O	1.87	0.72
9:I:59:VAL:O	9:I:60:GLN:HB2	1.88	0.72
1:A:310:GLY:O	1:A:312:PRO:HD2	1.89	0.72
3:C:45:ALA:CA	3:C:72:LEU:HD12	2.16	0.72
1:A:1385:THR:O	1:A:1388:GLY:N	2.21	0.72
10:J:41:LEU:HD11	10:J:50:ILE:HG13	1.70	0.72
1:A:370:ILE:HG23	2:B:1105:ALA:HB2	1.72	0.72
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.52	0.72
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.71	0.72
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.25	0.72
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.25	0.72
9:I:34:TYR:CE2	9:I:36:GLU:HB3	2.25	0.72
1:A:1086:PHE:HE2	13:S:261:ILE:HD11	1.54	0.72
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.72	0.72
2:B:953:LEU:O	2:B:953:LEU:HD23	1.89	0.72
2:B:1031:LEU:HA	2:B:1055:ILE:HD13	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:43:GLY:HA3	7:G:80:LYS:HB3	1.70	0.71
8:H:44:VAL:HG12	8:H:44:VAL:O	1.89	0.71
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.30	0.71
1:A:215:SER:HB3	1:A:218:ASP:OD2	1.89	0.71
2:B:114:PRO:HG2	2:B:115:GLN:H	1.54	0.71
6:F:86:THR:HG23	6:F:89:GLU:CD	2.10	0.71
2:B:957:ASN:O	2:B:959:ASP:N	2.22	0.71
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.70	0.71
1:A:666:ILE:HD11	2:B:1067:ARG:O	1.90	0.71
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.70	0.71
3:C:32:SER:O	3:C:36:VAL:HG23	1.89	0.71
9:I:71:SER:OG	9:I:83:ASN:HB2	1.90	0.71
13:S:271:CYS:SG	13:S:302:CYS:SG	2.89	0.71
1:A:375:THR:OG1	1:A:433:GLU:HB3	1.91	0.71
2:B:123:THR:O	2:B:125:SER:N	2.22	0.71
1:A:1325:THR:O	5:E:148:GLU:HB2	1.90	0.71
1:A:1172:LEU:HD21	13:S:204:SER:CA	2.21	0.71
1:A:13:THR:O	2:B:1218:THR:HG22	1.90	0.71
2:B:1166:CYS:O	2:B:1168:LEU:N	2.22	0.71
2:B:363:HIS:O	2:B:364:ILE:HB	1.91	0.71
2:B:976:ILE:HD11	2:B:992:ILE:HA	1.71	0.71
4:D:54:GLU:O	4:D:58:VAL:HG23	1.89	0.71
9:I:56:ALA:HB2	9:I:89:GLN:HG3	1.72	0.71
1:A:225:ASN:ND2	1:A:228:PHE:N	2.32	0.71
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.72	0.71
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.73	0.71
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.00	0.71
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.05	0.71
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.30	0.71
1:A:90:VAL:HG12	1:A:91:PHE:N	2.03	0.71
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.72	0.71
2:B:604:ARG:NH2	2:B:613:VAL:O	2.23	0.71
3:C:73:GLN:NE2	3:C:74:SER:H	1.89	0.71
12:L:32:ALA:HB3	12:L:55:ILE:CD1	2.21	0.71
1:A:1334:ASP:C	1:A:1336:MET:H	1.94	0.70
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.06	0.70
2:B:261:ARG:O	2:B:267:ARG:HD3	1.90	0.70
1:A:315:LEU:HD23	1:A:321:PRO:HA	1.73	0.70
2:B:510:LYS:HB2	2:B:511:PRO:CD	2.21	0.70
2:B:563:MET:CE	2:B:580:VAL:HB	2.21	0.70
1:A:1147:THR:HG22	1:A:1149:ALA:H	1.56	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:THR:HB	2:B:1103:ILE:HD12	1.72	0.70
1:A:384:ASN:OD1	1:A:388:LEU:HD12	1.92	0.70
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.73	0.70
1:A:370:ILE:HG22	1:A:374:LEU:CD1	2.21	0.70
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.07	0.70
1:A:897:TYR:CD1	1:A:897:TYR:N	2.56	0.70
1:A:95:PHE:HD1	1:A:234:MET:HG2	1.57	0.70
8:H:102:TYR:N	8:H:102:TYR:CD2	2.58	0.70
1:A:1435:PRO:O	1:A:1436:ILE:HG13	1.91	0.70
1:A:888:GLY:O	1:A:940:ARG:NH2	2.25	0.70
2:B:496:ARG:HH11	2:B:496:ARG:HB3	1.56	0.70
1:A:1279:ILE:HD11	1:A:1316:VAL:HG21	1.72	0.70
1:A:1116:LEU:N	1:A:1308:THR:CG2	2.54	0.70
1:A:414:ASP:OD1	1:A:416:ARG:HG3	1.91	0.70
1:A:339:ASN:HB3	2:B:1117:GLN:NE2	2.05	0.70
2:B:794:ASN:C	2:B:795:ILE:HD12	2.11	0.70
2:B:857:ARG:HG2	2:B:858:SER:H	1.55	0.70
5:E:135:PHE:CD2	5:E:140:LEU:HD21	2.26	0.70
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.06	0.70
1:A:608:ILE:HG23	1:A:969:GLN:OE1	1.91	0.70
5:E:202:SER:OG	5:E:204:THR:HG22	1.91	0.70
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.27	0.70
1:A:698:GLN:HA	9:I:97:MET:O	1.90	0.70
1:A:1280:GLU:O	1:A:1281:ARG:O	2.10	0.70
2:B:292:ILE:HD13	2:B:326:ASP:HA	1.73	0.70
1:A:852:TYR:CD1	6:F:136:ARG:HB3	2.27	0.70
10:J:2:ILE:HG12	10:J:57:ILE:HD12	1.74	0.70
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.56	0.70
2:B:857:ARG:HH21	2:B:942:ARG:CZ	2.04	0.70
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.74	0.70
3:C:191:TYR:HD2	3:C:201:TRP:CD1	2.09	0.70
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.73	0.69
1:A:78:PRO:HA	2:B:1201:LYS:HZ2	1.57	0.69
2:B:510:LYS:HB2	2:B:511:PRO:HD2	1.74	0.69
2:B:637:LEU:O	2:B:690:VAL:HG13	1.90	0.69
2:B:831:SER:OG	2:B:840:ILE:HD11	1.92	0.69
3:C:105:GLY:HA3	3:C:149:LYS:O	1.92	0.69
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.73	0.69
2:B:546:SER:OG	2:B:631:GLY:N	2.22	0.69
5:E:2:ASP:O	5:E:3:GLN:HG2	1.92	0.69
13:S:291:GLU:N	13:S:292:PRO:CD	2.53	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:CG2	1:A:857:ARG:HE	1.99	0.69
3:C:147:LEU:HD12	3:C:151:GLN:O	1.91	0.69
1:A:1334:ASP:O	1:A:1336:MET:N	2.25	0.69
1:A:289:ILE:C	1:A:291:GLU:H	1.95	0.69
1:A:347:PHE:H	2:B:1107:ALA:HA	1.57	0.69
2:B:1023:VAL:O	2:B:1027:ILE:HG13	1.93	0.69
2:B:510:LYS:CD	2:B:510:LYS:C	2.61	0.69
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.22	0.69
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.73	0.69
13:S:271:CYS:SG	13:S:274:CYS:SG	2.90	0.69
1:A:265:LYS:HD2	1:A:265:LYS:N	2.06	0.69
1:A:367:PRO:HB3	1:A:465:TYR:O	1.91	0.69
1:A:69:THR:O	1:A:71:GLN:N	2.25	0.69
2:B:862:GLN:HG2	2:B:963:PHE:CD1	2.28	0.69
1:A:1283:VAL:HG12	1:A:1284:MET:H	1.58	0.69
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.27	0.69
1:A:92:HIS:O	1:A:94:GLY:N	2.25	0.69
9:I:56:ALA:HB2	9:I:89:GLN:HG2	1.72	0.69
11:K:12:LEU:H	11:K:12:LEU:HD12	1.58	0.69
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.74	0.69
2:B:510:LYS:CB	2:B:511:PRO:HD2	2.21	0.69
2:B:606:LYS:HD2	2:B:608:ASP:OD2	1.92	0.69
1:A:1261:LYS:HA	1:A:1264:GLU:HB3	1.73	0.69
1:A:1443:VAL:O	1:A:1444:MET:HG3	1.91	0.69
1:A:889:SER:HB3	1:A:1297:GLU:HG2	1.75	0.69
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.28	0.69
2:B:294:ASP:OD2	2:B:294:ASP:N	2.24	0.69
6:F:111:LEU:C	6:F:113:GLY:H	1.96	0.69
1:A:606:LEU:HG	1:A:613:ILE:HD12	1.74	0.69
12:L:38:LEU:O	12:L:39:SER:HB3	1.91	0.69
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.74	0.69
1:A:367:PRO:HG2	1:A:370:ILE:HG13	1.74	0.69
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.08	0.69
2:B:871:THR:HG22	2:B:872:GLU:O	1.93	0.69
7:G:123:ALA:C	7:G:125:SER:H	1.96	0.69
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.23	0.69
1:A:535:THR:HG21	1:A:616:VAL:HA	1.73	0.69
2:B:112:LEU:CD1	2:B:113:TYR:H	2.03	0.69
2:B:281:PRO:HG2	2:B:284:ILE:HG13	1.74	0.69
2:B:282:ILE:CD1	2:B:382:ILE:HD13	2.23	0.69
2:B:552:MET:HA	2:B:555:ILE:HB	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:983:ARG:NH1	2:B:1028:GLU:OE1	2.26	0.69
3:C:242:GLN:HA	3:C:245:VAL:HG23	1.73	0.69
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.74	0.69
1:A:1135:ARG:HH11	13:S:256:ALA:HB2	1.57	0.69
2:B:839:MET:CE	2:B:1010:LEU:HD21	2.23	0.68
2:B:948:ILE:HG22	2:B:949:VAL:O	1.93	0.68
7:G:96:GLN:HA	7:G:121:PHE:CE2	2.28	0.68
1:A:1079:MET:CE	1:A:1101:LEU:HD23	2.23	0.68
7:G:106:MET:HG3	7:G:157:ILE:O	1.93	0.68
8:H:81:PRO:HB2	8:H:82:PRO:HD2	1.74	0.68
2:B:1165:ILE:HG22	2:B:1166:CYS:H	1.59	0.68
1:A:390:GLN:HE21	1:A:394:ASN:ND2	1.91	0.68
3:C:6:PRO:HB3	3:C:25:VAL:CG1	2.24	0.68
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.57	0.68
1:A:858:ASN:ND2	1:A:860:LEU:H	1.92	0.68
2:B:986:GLN:OE1	2:B:986:GLN:HA	1.92	0.68
5:E:164:LEU:HD13	5:E:211:TYR:CE2	2.27	0.68
1:A:1237:ILE:HG22	1:A:1238:ILE:H	1.55	0.68
2:B:821:GLN:HE22	2:B:851:PHE:H	1.42	0.68
1:A:134:ARG:HG2	1:A:134:ARG:O	1.94	0.68
1:A:332:LYS:HG3	1:A:333:GLU:HG2	1.75	0.68
1:A:337:ARG:NH2	1:A:839:ARG:HH12	1.90	0.68
2:B:1146:PHE:CD1	2:B:1146:PHE:O	2.47	0.68
2:B:773:MET:C	2:B:775:LYS:H	1.95	0.68
4:D:130:LEU:C	4:D:132:GLN:H	1.97	0.68
5:E:207:ARG:HH11	5:E:207:ARG:HB3	1.58	0.68
1:A:709:THR:HG22	1:A:712:GLU:H	1.59	0.68
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.24	0.68
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.74	0.68
6:F:97:ARG:NH2	6:F:108:PHE:HE1	1.92	0.68
1:A:901:LEU:N	1:A:926:GLN:NE2	2.36	0.68
2:B:758:PHE:HE1	2:B:1027:ILE:HG22	1.56	0.68
1:A:1081:LEU:HD21	1:A:1098:VAL:HG21	1.74	0.68
1:A:837:ILE:HA	1:A:840:ARG:HD3	1.76	0.68
10:J:7:CYS:SG	10:J:46:CYS:HA	2.34	0.68
1:A:1089:VAL:O	1:A:1089:VAL:HG12	1.95	0.67
1:A:1364:ASN:OD1	1:A:1366:ARG:HD2	1.94	0.67
2:B:1115:THR:O	2:B:1116:ARG:HB2	1.92	0.67
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.23	0.67
5:E:143:ASN:HD22	5:E:146:HIS:CE1	2.12	0.67
1:A:1192:LEU:HG	1:A:1193:LEU:N	2.09	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.09	0.67
1:A:519:PRO:HG2	1:A:624:SER:O	1.94	0.67
2:B:1169:MET:HE1	2:B:1201:LYS:CA	2.24	0.67
1:A:1410:PHE:HA	2:B:1212:ILE:HD11	1.75	0.67
2:B:378:LEU:HD12	2:B:378:LEU:O	1.94	0.67
7:G:127:PRO:HG2	7:G:138:THR:HG21	1.74	0.67
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.24	0.67
1:A:1376:THR:OG1	1:A:1377:THR:N	2.23	0.67
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.09	0.67
1:A:115:LEU:HB2	1:A:122:MET:HE1	1.75	0.67
1:A:49:LYS:NZ	1:A:60:SER:HA	2.09	0.67
2:B:205:ILE:N	2:B:205:ILE:HD12	2.10	0.67
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.29	0.67
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.07	0.67
1:A:135:PHE:C	1:A:137:ALA:H	1.97	0.67
2:B:1010:LEU:HD12	2:B:1011:ILE:H	1.60	0.67
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.21	0.67
2:B:880:THR:O	2:B:881:ASN:HB2	1.94	0.67
5:E:210:SER:C	5:E:211:TYR:CD1	2.68	0.67
1:A:53:LEU:HD23	1:A:54:ASN:H	1.54	0.67
1:A:55:ASP:CG	1:A:55:ASP:O	2.31	0.67
2:B:854:LEU:HB3	2:B:856:PHE:HE1	1.60	0.67
3:C:73:GLN:HB3	3:C:131:HIS:H	1.60	0.67
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.30	0.67
7:G:13:LEU:HD23	7:G:14:HIS:N	2.10	0.67
1:A:1083:THR:HG21	1:A:1085:HIS:CE1	2.30	0.67
1:A:1447:GLU:OE2	7:G:23:LYS:HB2	1.94	0.67
1:A:709:THR:HB	1:A:712:GLU:HB2	1.76	0.67
7:G:91:VAL:HB	7:G:139:ILE:O	1.95	0.67
1:A:1118:VAL:HG12	1:A:1327:ILE:HG13	1.77	0.67
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	1.95	0.67
1:A:41:MET:O	1:A:50:ILE:HG13	1.94	0.67
3:C:86:CYS:O	3:C:88:CYS:N	2.27	0.67
12:L:58:LYS:O	12:L:59:ALA:O	2.13	0.67
1:A:829:VAL:HG13	2:B:507:LYS:HG2	1.76	0.67
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.76	0.67
1:A:886:ILE:CD1	1:A:943:LEU:HB3	2.22	0.67
1:A:982:THR:O	1:A:985:ASP:HB2	1.94	0.67
2:B:1159:ARG:HB3	2:B:1159:ARG:NH1	2.09	0.67
2:B:1198:TYR:CE1	2:B:1201:LYS:HD2	2.30	0.67
2:B:654:ARG:H	2:B:657:HIS:HD2	1.41	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:VAL:HG12	2:B:178:ASN:ND2	2.09	0.67
9:I:34:TYR:HE2	9:I:36:GLU:HB3	1.60	0.67
1:A:1104:ILE:O	1:A:1107:VAL:N	2.23	0.66
1:A:1161:THR:OG1	1:A:1170:ILE:HD11	1.95	0.66
2:B:240:ILE:HG22	2:B:254:LEU:HB3	1.77	0.66
2:B:622:LYS:HE3	9:I:59:VAL:HG22	1.76	0.66
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.77	0.66
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.76	0.66
13:S:265:VAL:HG11	13:S:278:LYS:HA	1.76	0.66
13:S:302:CYS:SG	13:S:304:ASN:ND2	2.68	0.66
1:A:75:ASN:O	1:A:76:GLU:HB3	1.95	0.66
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.75	0.66
7:G:73:LYS:HE2	7:G:74:TYR:O	1.95	0.66
1:A:1329:THR:H	1:A:1335:ILE:CD1	1.95	0.66
1:A:265:LYS:HD2	1:A:265:LYS:H	1.60	0.66
2:B:172:ILE:HD13	2:B:178:ASN:HB2	1.76	0.66
2:B:546:SER:OG	2:B:630:ALA:HA	1.95	0.66
2:B:898:LEU:HB2	12:L:58:LYS:NZ	2.10	0.66
1:A:1331:SER:OG	1:A:1333:ILE:HG22	1.94	0.66
1:A:90:VAL:HG13	1:A:297:GLN:OE1	1.96	0.66
1:A:997:LEU:HD13	1:A:1018:PHE:HE2	1.60	0.66
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.10	0.66
2:B:900:ALA:O	2:B:903:VAL:HG23	1.95	0.66
1:A:254:GLU:HB2	2:B:935:ARG:HH22	1.60	0.66
1:A:825:ILE:C	1:A:827:THR:H	1.96	0.66
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.77	0.66
2:B:1065:GLN:HB2	3:C:201:TRP:CZ3	2.31	0.66
3:C:43:THR:HG22	3:C:44:LEU:N	2.10	0.66
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.25	0.66
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.11	0.66
1:A:1283:VAL:O	1:A:1306:LEU:HA	1.96	0.66
1:A:1445:ILE:HD12	1:A:1445:ILE:N	2.11	0.66
1:A:908:LEU:CD1	1:A:983:ILE:HD11	2.25	0.66
2:B:1065:GLN:HB3	2:B:1069:PHE:O	1.95	0.66
2:B:1102:LYS:O	2:B:1103:ILE:C	2.34	0.66
2:B:705:MET:H	2:B:710:LEU:CD1	2.09	0.66
9:I:58:VAL:HG13	9:I:62:ILE:CG1	2.25	0.66
13:S:218:ILE:CA	13:S:219:ALA:CA	2.73	0.66
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.25	0.66
1:A:1437:GLY:HA3	6:F:88:TYR:CD2	2.30	0.66
1:A:63:ARG:HG2	1:A:74:MET:SD	2.36	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:770:GLN:HG2	2:B:983:ARG:O	1.96	0.66
2:B:910:VAL:HG12	2:B:911:ILE:N	2.11	0.66
2:B:991:GLY:O	2:B:992:ILE:HB	1.94	0.66
3:C:263:THR:C	3:C:265:MET:H	1.99	0.66
12:L:28:LYS:HB2	12:L:39:SER:HB2	1.78	0.66
1:A:903:ASN:HD22	1:A:903:ASN:C	1.99	0.66
2:B:705:MET:H	2:B:710:LEU:HD12	1.61	0.66
1:A:275:SER:O	1:A:279:LEU:HG	1.96	0.66
1:A:34:LYS:HB2	1:A:36:ARG:HH21	1.60	0.66
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.25	0.66
2:B:1159:ARG:NE	2:B:1193:GLN:HE21	1.94	0.66
2:B:589:VAL:CG1	2:B:590:HIS:H	2.06	0.66
2:B:616:ILE:HD12	2:B:616:ILE:N	2.11	0.66
2:B:882:THR:CG2	2:B:884:ARG:HB2	2.25	0.66
2:B:899:ILE:CG2	2:B:903:VAL:HG21	2.25	0.66
5:E:182:ASP:O	5:E:185:ALA:N	2.28	0.66
8:H:41:ASP:O	8:H:42:ILE:HG13	1.96	0.66
13:S:235:ASP:CA	13:S:242:LYS:HE3	2.26	0.66
1:A:264:PHE:O	1:A:267:ALA:HB3	1.96	0.65
1:A:886:ILE:HG22	1:A:887:GLY:N	2.11	0.65
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.61	0.65
5:E:157:SER:OG	5:E:160:GLU:HG3	1.95	0.65
1:A:591:PHE:HA	1:A:595:THR:HG21	1.77	0.65
2:B:579:ARG:HD2	2:B:586:TRP:CZ2	2.30	0.65
2:B:65:GLU:HG3	2:B:66:ASP:N	2.07	0.65
2:B:322:PHE:HZ	9:I:30:ARG:HB3	1.61	0.65
2:B:953:LEU:CD2	2:B:965:LYS:HB2	2.26	0.65
3:C:63:ILE:CA	3:C:66:ARG:HG3	2.26	0.65
11:K:67:PHE:C	11:K:68:PHE:HD2	1.98	0.65
1:A:1291:VAL:HG13	1:A:1292:PRO:CD	2.25	0.65
2:B:23:ALA:HB1	2:B:24:PRO:CD	2.23	0.65
2:B:411:PRO:O	2:B:414:ALA:HB3	1.95	0.65
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.79	0.65
3:C:241:ASP:O	3:C:245:VAL:HG23	1.96	0.65
4:D:137:ASN:HD22	4:D:137:ASN:C	2.00	0.65
5:E:78:LEU:HD23	5:E:79:TRP:N	2.11	0.65
12:L:61:THR:HG21	12:L:63:ARG:HG2	1.78	0.65
1:A:107:CYS:N	1:A:114:LEU:HD21	2.11	0.65
2:B:856:PHE:N	2:B:856:PHE:CD1	2.64	0.65
3:C:174:ALA:O	3:C:175:ALA:HB2	1.95	0.65
3:C:50:GLU:HG2	12:L:64:LEU:CD1	2.25	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:ASP:O	2:B:296:GLU:N	2.30	0.65
2:B:687:GLU:O	2:B:689:LEU:HG	1.96	0.65
2:B:773:MET:C	2:B:775:LYS:N	2.48	0.65
1:A:55:ASP:N	1:A:56:PRO:HD3	2.11	0.65
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.29	0.65
2:B:594:ALA:HA	2:B:617:ARG:HH12	1.60	0.65
2:B:794:ASN:O	2:B:795:ILE:HD12	1.96	0.65
3:C:5:GLY:O	3:C:7:GLN:HG3	1.96	0.65
3:C:92:CYS:SG	3:C:94:LYS:HB3	2.36	0.65
4:D:211:LEU:HD23	4:D:214:LEU:HD12	1.79	0.65
1:A:1080:THR:HG21	13:S:284:LEU:HD13	1.77	0.65
2:B:365:THR:HG23	2:B:367:LEU:H	1.61	0.65
1:A:538:ASP:OD2	8:H:22:LYS:HB2	1.96	0.65
1:A:689:LYS:HE2	1:A:721:PHE:CE2	2.32	0.65
2:B:322:PHE:CZ	9:I:30:ARG:HB3	2.32	0.65
12:L:60:ARG:HG2	12:L:61:THR:H	1.60	0.65
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.77	0.65
1:A:550:LEU:HD22	1:A:556:TRP:CE2	2.31	0.65
2:B:820:GLY:N	2:B:1091:TYR:OH	2.29	0.65
7:G:14:HIS:HD2	7:G:16:SER:CB	2.03	0.65
9:I:101:PHE:N	9:I:101:PHE:HD1	1.91	0.65
1:A:47:ARG:NH2	1:A:255:SER:H	1.95	0.64
1:A:593:GLU:O	1:A:595:THR:N	2.30	0.64
2:B:1223:ASP:O	2:B:1224:PHE:HB2	1.96	0.64
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.10	0.64
2:B:54:PHE:CE2	2:B:59:LEU:HD13	2.32	0.64
2:B:825:VAL:HG22	2:B:1010:LEU:HB3	1.79	0.64
7:G:143:ILE:HG22	7:G:144:ARG:N	2.11	0.64
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.88	0.64
1:A:243:PRO:O	1:A:246:VAL:HG23	1.98	0.64
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.78	0.64
2:B:1184:GLY:C	2:B:1186:ASP:H	1.96	0.64
2:B:237:VAL:HG22	2:B:257:LYS:HA	1.78	0.64
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.32	0.64
2:B:37:PHE:HD2	2:B:542:MET:SD	2.21	0.64
2:B:39:ARG:HH21	2:B:665:GLU:CG	2.10	0.64
2:B:835:GLN:HA	2:B:1013:ASN:ND2	2.10	0.64
4:D:47:LEU:HD13	4:D:48:ILE:H	1.63	0.64
1:A:1409:LEU:O	1:A:1412:ALA:HB3	1.98	0.64
1:A:370:ILE:HG22	1:A:374:LEU:HD11	1.80	0.64
1:A:550:LEU:HD22	1:A:556:TRP:NE1	2.11	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.32	0.64
2:B:227:LYS:HB2	2:B:395:GLN:OE1	1.97	0.64
2:B:952:VAL:HG12	2:B:953:LEU:N	2.11	0.64
2:B:975:GLN:NE2	2:B:1100:ASP:OD2	2.30	0.64
7:G:138:THR:CG2	7:G:139:ILE:H	1.95	0.64
13:S:269:PHE:HE2	13:S:297:CYS:SG	2.14	0.64
1:A:1029:ARG:HH11	1:A:1029:ARG:CG	2.09	0.64
1:A:1199:ARG:HH22	13:S:241:LEU:CD1	2.02	0.64
1:A:1423:GLY:O	1:A:1426:GLU:N	2.31	0.64
1:A:535:THR:HG21	1:A:617:VAL:H	1.63	0.64
2:B:1060:ARG:HH11	2:B:1060:ARG:HG2	1.61	0.64
2:B:54:PHE:HE1	2:B:414:ALA:HA	1.62	0.64
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.80	0.64
1:A:1148:ILE:O	1:A:1148:ILE:HG22	1.98	0.64
1:A:67:CYS:O	1:A:70:CYS:HB3	1.96	0.64
2:B:955:THR:HG22	2:B:956:THR:N	2.12	0.64
8:H:102:TYR:N	8:H:102:TYR:HD2	1.96	0.64
1:A:1035:TYR:O	1:A:1037:LEU:N	2.25	0.64
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.80	0.64
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.33	0.64
2:B:315:LYS:N	2:B:316:PRO:HD2	2.11	0.64
3:C:179:GLU:HG2	3:C:180:TYR:N	2.12	0.64
6:F:86:THR:HG23	6:F:89:GLU:OE1	1.97	0.64
7:G:111:THR:CG2	7:G:113:HIS:H	2.04	0.64
1:A:1072:ILE:O	1:A:1075:PRO:HG2	1.98	0.64
2:B:1156:ASP:O	2:B:1157:ALA:O	2.15	0.64
2:B:261:ARG:HB3	2:B:261:ARG:NH1	2.11	0.64
4:D:35:LEU:N	4:D:35:LEU:HD12	2.12	0.64
2:B:1224:PHE:CE2	5:E:171:LYS:HG3	2.32	0.64
13:S:282:TYR:CE2	13:S:296:PHE:HB2	2.33	0.64
13:S:279:VAL:HG13	13:S:298:THR:O	1.98	0.64
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.13	0.64
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.28	0.64
1:A:768:GLN:CG	1:A:816:HIS:HA	2.22	0.64
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.79	0.64
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.33	0.64
3:C:235:VAL:HG13	10:J:13:VAL:HG23	1.79	0.64
1:A:1206:ASP:O	1:A:1274:ARG:NH1	2.31	0.64
1:A:1120:LEU:O	1:A:1323:ASP:HB2	1.98	0.64
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.78	0.64
1:A:642:CYS:O	1:A:645:LEU:N	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:ASP:OD1	1:A:855:THR:CB	2.40	0.64
1:A:996:ASN:C	1:A:998:LEU:HD12	2.18	0.64
2:B:446:LEU:O	2:B:447:ALA:HB3	1.97	0.64
2:B:508:LEU:HB2	2:B:510:LYS:N	2.10	0.64
2:B:859:TYR:HD1	2:B:859:TYR:H	1.44	0.64
5:E:177:ARG:C	5:E:212:ARG:HD3	2.18	0.64
1:A:1283:VAL:CG1	13:S:256:ALA:C	2.62	0.63
1:A:17:VAL:HG23	1:A:1421:CYS:SG	2.38	0.63
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.80	0.63
2:B:390:LEU:O	2:B:392:ARG:HG3	1.97	0.63
2:B:737:THR:HG21	9:I:66:PRO:HA	1.79	0.63
3:C:143:LEU:HD12	3:C:145:CYS:H	1.64	0.63
9:I:113:ASP:O	9:I:114:GLN:HG3	1.98	0.63
11:K:12:LEU:HD21	11:K:18:LYS:HG2	1.80	0.63
1:A:845:LEU:HB3	1:A:848:ILE:HD12	1.80	0.63
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.28	0.63
2:B:117:ALA:HA	2:B:122:LEU:HD12	1.78	0.63
12:L:28:LYS:HB2	12:L:39:SER:CB	2.28	0.63
1:A:1080:THR:O	1:A:1081:LEU:HD22	1.97	0.63
2:B:294:ASP:C	2:B:296:GLU:H	2.01	0.63
2:B:37:PHE:CE2	2:B:542:MET:HA	2.27	0.63
5:E:197:LYS:HG2	5:E:197:LYS:O	1.97	0.63
7:G:14:HIS:ND1	7:G:15:PRO:HD2	2.12	0.63
8:H:81:PRO:CB	8:H:82:PRO:CD	2.77	0.63
3:C:35:ARG:NH1	11:K:41:THR:N	2.47	0.63
1:A:637:LYS:HB3	1:A:641:VAL:HG21	1.81	0.63
1:A:706:HIS:CE1	13:S:257:GLN:OE1	2.51	0.63
2:B:1051:THR:HB	2:B:1054:GLY:H	1.64	0.63
2:B:204:ILE:C	2:B:205:ILE:HD12	2.19	0.63
3:C:35:ARG:NH1	11:K:41:THR:H	1.96	0.63
8:H:93:TYR:HB3	8:H:144:ILE:O	1.98	0.63
7:G:14:HIS:CE1	7:G:15:PRO:HD2	2.34	0.63
7:G:6:ASP:O	7:G:7:LEU:HD23	1.98	0.63
1:A:704:ALA:O	1:A:705:LYS:HB2	1.97	0.63
2:B:508:LEU:HB2	2:B:510:LYS:CA	2.28	0.63
8:H:42:ILE:HG23	8:H:95:TYR:CE1	2.34	0.63
1:A:367:PRO:HA	1:A:463:ILE:O	1.99	0.63
1:A:922:ASP:OD1	1:A:924:LYS:N	2.32	0.63
2:B:604:ARG:NH2	2:B:614:SER:HA	2.14	0.63
3:C:235:VAL:HG21	10:J:6:ARG:NH2	2.14	0.63
1:A:534:LEU:O	1:A:574:GLY:HA3	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:279:VAL:HG13	13:S:298:THR:C	2.19	0.63
2:B:1149:GLU:O	2:B:1151:LEU:N	2.32	0.63
2:B:604:ARG:HH22	2:B:614:SER:HA	1.62	0.63
1:A:1230:GLU:O	1:A:1232:ASN:N	2.32	0.62
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.80	0.62
1:A:61:ILE:O	1:A:63:ARG:N	2.32	0.62
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.81	0.62
2:B:292:ILE:HD11	2:B:327:ARG:H	1.64	0.62
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.81	0.62
8:H:89:LEU:HB3	8:H:91:ASP:OD1	1.98	0.62
1:A:283:GLY:O	1:A:285:PRO:HD3	1.99	0.62
2:B:1020:ARG:CG	2:B:1020:ARG:HH11	2.09	0.62
2:B:1099:VAL:HG22	2:B:1103:ILE:HD13	1.80	0.62
2:B:284:ILE:HD13	2:B:333:PHE:HD2	1.64	0.62
3:C:147:LEU:HB2	3:C:151:GLN:CB	2.29	0.62
5:E:192:ARG:HG3	5:E:192:ARG:HH11	1.64	0.62
7:G:126:ASN:HD22	7:G:127:PRO:HA	1.63	0.62
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.80	0.62
8:H:123:MET:HE3	8:H:142:LEU:CD2	2.29	0.62
8:H:123:MET:HE3	8:H:142:LEU:HD22	1.80	0.62
2:B:526:GLU:OE2	2:B:752:ALA:HB2	1.98	0.62
5:E:86:PRO:O	5:E:114:ASN:HB2	1.99	0.62
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.80	0.62
11:K:47:ARG:NH1	11:K:47:ARG:HB3	2.12	0.62
1:A:1402:PHE:O	1:A:1404:GLU:N	2.32	0.62
1:A:265:LYS:HE2	1:A:322:VAL:HG13	1.81	0.62
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.80	0.62
2:B:129:PHE:HA	2:B:165:VAL:O	1.99	0.62
8:H:40:LEU:CD1	8:H:123:MET:HB2	2.27	0.62
9:I:87:GLN:O	9:I:89:GLN:OE1	2.18	0.62
13:S:274:CYS:O	13:S:276:GLU:N	2.32	0.62
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.33	0.62
2:B:952:VAL:HG12	2:B:953:LEU:H	1.64	0.62
1:A:1342:GLU:CD	5:E:198:ILE:HG21	2.18	0.62
6:F:97:ARG:NH2	6:F:108:PHE:CE1	2.68	0.62
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.80	0.62
1:A:1172:LEU:CG	13:S:204:SER:CA	2.77	0.62
1:A:1279:ILE:HD11	1:A:1316:VAL:CG2	2.29	0.62
1:A:708:MET:O	1:A:709:THR:O	2.17	0.62
2:B:705:MET:HA	2:B:705:MET:HE2	1.81	0.62
2:B:780:VAL:HG12	2:B:782:LEU:O	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:LEU:HA	3:C:70:ILE:CD1	2.30	0.62
6:F:103:MET:HE2	7:G:65:ASP:HB2	1.81	0.62
1:A:1213:GLY:HA2	1:A:1216:ILE:HD12	1.81	0.62
1:A:21:LEU:HG	1:A:1413:GLY:O	2.00	0.62
1:A:44:THR:O	1:A:45:GLN:HB2	1.99	0.62
1:A:546:VAL:HG21	1:A:572:TRP:CE3	2.34	0.62
1:A:590:ARG:HG3	1:A:590:ARG:NH1	2.15	0.62
1:A:605:MET:SD	1:A:621:THR:HG21	2.40	0.62
1:A:998:LEU:HD12	1:A:998:LEU:H	1.65	0.62
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.35	0.62
2:B:859:TYR:CD1	2:B:859:TYR:N	2.67	0.62
5:E:168:TYR:HB3	5:E:170:LEU:HG	1.81	0.62
1:A:515:GLN:OE1	1:A:1071:SER:HA	1.99	0.62
1:A:818:MET:HG2	2:B:514:LEU:HG	1.81	0.62
2:B:762:ASN:HD21	2:B:1024:ALA:HB3	1.64	0.62
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.34	0.62
1:A:1017:LEU:CB	5:E:205:SER:HA	2.29	0.62
11:K:91:CYS:O	11:K:94:ILE:HB	1.99	0.62
2:B:763:GLN:NE2	13:S:293:LEU:HG	2.15	0.62
1:A:90:VAL:CG1	1:A:91:PHE:N	2.63	0.62
1:A:886:ILE:HG13	1:A:943:LEU:CD1	2.30	0.62
2:B:1033:LYS:HD2	2:B:1087:PHE:O	2.00	0.62
2:B:37:PHE:CD1	2:B:41:LYS:HG3	2.35	0.62
6:F:97:ARG:HH22	6:F:108:PHE:HE1	1.45	0.62
7:G:114:LEU:HD23	7:G:161:GLY:O	2.00	0.62
1:A:289:ILE:O	1:A:291:GLU:N	2.33	0.62
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.65	0.62
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.35	0.62
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.35	0.62
2:B:601:ARG:O	2:B:605:ARG:HG3	2.00	0.62
2:B:69:LEU:HD22	2:B:429:PHE:CE1	2.35	0.62
7:G:80:LYS:HE2	7:G:82:PHE:CZ	2.34	0.62
1:A:1001:ARG:O	1:A:1002:GLY:O	2.18	0.61
1:A:1019:CYS:O	1:A:1022:LEU:HB3	1.99	0.61
1:A:455:MET:HE3	2:B:1134:GLU:HG3	1.82	0.61
1:A:590:ARG:HH21	1:A:620:LYS:CB	2.08	0.61
1:A:858:ASN:ND2	1:A:858:ASN:C	2.53	0.61
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	2.00	0.61
2:B:750:GLY:O	2:B:751:VAL:C	2.39	0.61
12:L:31:CYS:HB3	12:L:34:CYS:C	2.21	0.61
1:A:756:ILE:HG21	13:S:283:GLN:NE2	2.14	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:GLN:NE2	2:B:918:ILE:HD11	2.14	0.61
7:G:80:LYS:HE2	7:G:82:PHE:HZ	1.64	0.61
1:A:705:LYS:HA	13:S:254:TYR:OH	2.00	0.61
1:A:691:LEU:O	1:A:694:THR:HB	1.99	0.61
1:A:866:PHE:C	1:A:867:ILE:HD12	2.21	0.61
2:B:1106:ARG:HG3	2:B:1107:ALA:H	1.65	0.61
2:B:510:LYS:CG	2:B:512:ARG:H	2.11	0.61
2:B:773:MET:O	2:B:776:GLN:N	2.28	0.61
3:C:46:ILE:HD13	3:C:157:CYS:SG	2.41	0.61
1:A:1206:ASP:O	1:A:1207:LEU:HG	2.00	0.61
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.63	0.61
1:A:442:VAL:O	1:A:457:ALA:HA	2.00	0.61
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.35	0.61
2:B:292:ILE:CD1	2:B:326:ASP:HA	2.30	0.61
2:B:541:LEU:HD12	2:B:747:MET:HE1	1.83	0.61
3:C:58:LEU:CD2	3:C:58:LEU:H	2.14	0.61
5:E:157:SER:C	5:E:159:ASP:H	2.04	0.61
5:E:78:LEU:HD21	5:E:80:VAL:HG23	1.81	0.61
6:F:79:ARG:HG3	6:F:144:GLU:OE1	2.00	0.61
1:A:489:LEU:HD12	1:A:489:LEU:C	2.21	0.61
1:A:50:ILE:C	1:A:52:GLY:H	2.03	0.61
1:A:412:ARG:NH2	2:B:1108:ARG:NH1	2.48	0.61
3:C:248:ILE:HD13	11:K:101:LEU:HD22	1.82	0.61
4:D:40:HIS:CE1	4:D:41:GLN:HG3	2.35	0.61
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.36	0.61
1:A:1081:LEU:HD11	1:A:1098:VAL:HB	1.81	0.61
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.64	0.61
1:A:244:PRO:HG2	1:A:245:PRO:HD3	1.81	0.61
1:A:91:PHE:HD2	1:A:96:ILE:HG12	1.66	0.61
9:I:8:ARG:O	9:I:10:CYS:N	2.33	0.61
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.66	0.61
1:A:133:LYS:C	1:A:135:PHE:H	2.02	0.61
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.31	0.61
1:A:335:ARG:HE	1:A:339:ASN:HD22	1.45	0.61
1:A:629:LEU:O	1:A:633:VAL:HG23	2.01	0.61
1:A:857:ARG:HD3	1:A:861:GLY:O	2.00	0.61
2:B:562:GLY:HA3	2:B:590:HIS:HE1	1.65	0.61
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.30	0.61
7:G:108:VAL:HG22	7:G:159:ALA:HB3	1.81	0.61
10:J:57:ILE:HG23	10:J:58:GLU:N	2.16	0.61
1:A:1081:LEU:CD1	1:A:1098:VAL:HB	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:LEU:O	1:A:531:ILE:HG22	2.01	0.61
2:B:35:SER:HA	2:B:811:TYR:CE2	2.27	0.61
2:B:508:LEU:HB2	2:B:510:LYS:HB3	1.83	0.61
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.36	0.61
1:A:694:THR:O	1:A:698:GLN:HG3	1.99	0.61
1:A:804:TYR:OH	2:B:763:GLN:HA	2.01	0.61
3:C:212:PRO:CB	3:C:213:PRO:HD2	2.31	0.61
8:H:23:VAL:HG13	8:H:42:ILE:O	2.00	0.61
9:I:106:CYS:O	9:I:107:SER:HB2	1.99	0.61
1:A:869:GLY:O	5:E:204:THR:HG21	2.01	0.61
2:B:496:ARG:NH1	2:B:539:LEU:HB2	2.16	0.61
4:D:134:THR:HG22	4:D:135:GLY:N	2.16	0.61
1:A:902:LEU:O	1:A:903:ASN:HB2	2.01	0.60
2:B:533:CYS:O	2:B:535:LEU:N	2.34	0.60
5:E:198:ILE:CD1	5:E:212:ARG:HH11	2.14	0.60
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.31	0.60
2:B:487:THR:HG22	2:B:488:TYR:N	2.15	0.60
4:D:51:ASN:O	4:D:54:GLU:HB3	2.01	0.60
9:I:55:THR:HG23	9:I:100:PHE:CD2	2.33	0.60
1:A:1161:THR:C	1:A:1163:ILE:H	2.04	0.60
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.31	0.60
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.83	0.60
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.83	0.60
7:G:146:LYS:HB2	7:G:168:LEU:HD11	1.82	0.60
8:H:56:THR:O	8:H:144:ILE:HA	2.01	0.60
10:J:57:ILE:HG23	10:J:58:GLU:H	1.66	0.60
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.37	0.60
1:A:606:LEU:HB2	1:A:614:PHE:CE2	2.37	0.60
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.00	0.60
2:B:510:LYS:HG2	2:B:512:ARG:CB	2.30	0.60
2:B:545:ILE:HG22	2:B:546:SER:O	2.01	0.60
3:C:142:VAL:H	10:J:16:ASP:HB3	1.66	0.60
5:E:55:ARG:C	5:E:57:MET:H	2.03	0.60
5:E:60:PHE:CE2	5:E:80:VAL:HB	2.36	0.60
13:S:291:GLU:H	13:S:292:PRO:CD	2.14	0.60
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.66	0.60
1:A:254:GLU:CB	2:B:935:ARG:HH22	2.14	0.60
1:A:49:LYS:HE2	1:A:61:ILE:CD1	2.29	0.60
1:A:786:HIS:CD2	1:A:786:HIS:N	2.69	0.60
2:B:605:ARG:CZ	2:B:639:ILE:HD13	2.31	0.60
8:H:113:ALA:HB2	8:H:126:GLU:HG3	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:298:THR:HG23	13:S:305:ARG:HG2	1.82	0.60
1:A:134:ARG:O	1:A:138:ILE:HG13	2.01	0.60
1:A:225:ASN:ND2	1:A:227:VAL:H	1.98	0.60
1:A:47:ARG:HH22	1:A:254:GLU:HA	1.65	0.60
1:A:761:MET:HA	1:A:804:TYR:HB2	1.83	0.60
2:B:189:LEU:HA	2:B:192:LEU:HD12	1.82	0.60
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.84	0.60
2:B:705:MET:N	2:B:710:LEU:HD12	2.16	0.60
2:B:830:TYR:HE2	2:B:1000:PRO:HD3	1.66	0.60
4:D:35:LEU:H	4:D:35:LEU:CD1	2.14	0.60
6:F:72:LYS:O	6:F:73:ALA:HB3	2.02	0.60
7:G:23:LYS:HG3	7:G:56:ILE:CD1	2.28	0.60
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.30	0.60
1:A:1116:LEU:HB3	1:A:1311:VAL:HG22	1.83	0.60
2:B:1159:ARG:HE	2:B:1193:GLN:HE21	1.50	0.60
3:C:107:SER:C	3:C:109:SER:H	2.04	0.60
4:D:33:PHE:CE2	7:G:80:LYS:NZ	2.70	0.60
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.31	0.60
13:S:287:ARG:HD3	13:S:291:GLU:OE1	2.01	0.60
1:A:144:THR:O	1:A:146:MET:HG3	2.01	0.60
1:A:820:GLY:C	1:A:822:GLU:H	2.05	0.60
2:B:880:THR:HG21	2:B:934:LYS:HE3	1.82	0.60
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.30	0.60
12:L:31:CYS:HB3	12:L:35:SER:HA	1.84	0.60
1:A:1134:ILE:O	1:A:1138:ILE:HG13	2.02	0.60
1:A:1164:PRO:HG2	1:A:1165:GLU:HG3	1.82	0.60
1:A:332:LYS:H	1:A:337:ARG:HB3	1.67	0.60
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.84	0.60
1:A:863:VAL:HG12	1:A:864:ILE:N	2.17	0.60
2:B:216:GLU:HA	2:B:406:LEU:HD23	1.84	0.60
2:B:578:THR:HG23	2:B:622:LYS:HA	1.84	0.60
4:D:210:ILE:O	4:D:214:LEU:HG	2.01	0.60
1:A:852:TYR:CE1	6:F:136:ARG:HG2	2.36	0.60
1:A:1261:LYS:O	1:A:1264:GLU:HB3	2.01	0.60
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.37	0.60
1:A:567:LYS:HD3	8:H:95:TYR:CD2	2.37	0.60
1:A:863:VAL:O	1:A:864:ILE:HG12	2.02	0.60
1:A:896:ARG:HB3	1:A:897:TYR:CD1	2.37	0.60
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.31	0.60
4:D:19:GLU:O	4:D:21:GLU:N	2.35	0.60
3:C:169:LYS:NZ	12:L:69:ALA:HB3	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1334:ASP:C	1:A:1336:MET:N	2.55	0.59
1:A:1372:VAL:CG1	1:A:1373:ASP:N	2.65	0.59
1:A:1423:GLY:O	1:A:1424:VAL:C	2.40	0.59
2:B:1159:ARG:HE	2:B:1193:GLN:NE2	2.00	0.59
2:B:429:PHE:HA	2:B:432:MET:HE2	1.84	0.59
2:B:789:MET:HE2	2:B:965:LYS:HB3	1.83	0.59
2:B:797:TYR:C	2:B:798:TYR:HD2	2.04	0.59
5:E:23:VAL:HG13	5:E:78:LEU:HD13	1.84	0.59
8:H:91:ASP:C	8:H:93:TYR:H	2.04	0.59
1:A:1104:ILE:O	1:A:1106:ASN:N	2.35	0.59
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.26	0.59
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.33	0.59
2:B:129:PHE:HE2	2:B:166:PHE:HD1	1.49	0.59
2:B:898:LEU:HB2	12:L:58:LYS:HZ3	1.67	0.59
1:A:1237:ILE:CG2	1:A:1238:ILE:H	2.15	0.59
1:A:469:ARG:HG2	1:A:469:ARG:HH11	1.67	0.59
1:A:821:ARG:O	1:A:825:ILE:HG13	2.01	0.59
2:B:1183:LYS:CE	2:B:1183:LYS:N	2.62	0.59
2:B:510:LYS:CB	2:B:511:PRO:CD	2.79	0.59
4:D:176:GLU:OE2	4:D:198:LEU:HD23	2.02	0.59
5:E:46:TYR:CE2	5:E:58:MET:HA	2.37	0.59
8:H:56:THR:HB	8:H:145:ARG:HG2	1.84	0.59
8:H:59:ILE:HG22	8:H:60:ALA:H	1.64	0.59
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.31	0.59
1:A:475:THR:HG23	1:A:476:SER:N	2.17	0.59
1:A:40:THR:HG23	1:A:54:ASN:HD21	1.67	0.59
1:A:343:LYS:HE2	2:B:1156:ASP:OD2	2.02	0.59
2:B:310:MET:O	2:B:313:MET:HB2	2.02	0.59
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.30	0.59
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.32	0.59
2:B:807:ARG:HH11	2:B:807:ARG:HB3	1.66	0.59
9:I:111:THR:CG2	9:I:112:SER:H	2.13	0.59
10:J:41:LEU:CD1	10:J:50:ILE:HG13	2.32	0.59
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.83	0.59
1:A:556:TRP:C	1:A:558:GLY:H	2.05	0.59
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.32	0.59
2:B:1166:CYS:HB2	2:B:1168:LEU:HD12	1.84	0.59
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.84	0.59
3:C:104:PHE:CD2	3:C:105:GLY:N	2.70	0.59
7:G:145:VAL:CG1	7:G:146:LYS:N	2.64	0.59
7:G:6:ASP:HB3	7:G:73:LYS:HZ1	1.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:58:VAL:HA	9:I:62:ILE:CD1	2.32	0.59
2:B:46:GLN:HG3	2:B:47:GLN:H	1.68	0.59
3:C:58:LEU:N	3:C:58:LEU:CD2	2.65	0.59
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.84	0.59
7:G:1:MET:SD	7:G:1:MET:O	2.61	0.59
1:A:834:THR:HG23	1:A:1077:THR:HA	1.85	0.59
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.84	0.59
1:A:391:LEU:O	1:A:394:ASN:N	2.35	0.59
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.85	0.59
2:B:899:ILE:HG22	2:B:900:ALA:N	2.17	0.59
1:A:72:GLU:O	1:A:73:GLY:O	2.20	0.59
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.77	0.59
2:B:1095:LEU:CD1	2:B:1095:LEU:H	1.87	0.59
2:B:240:ILE:O	2:B:240:ILE:HG23	2.02	0.59
2:B:546:SER:HG	2:B:630:ALA:HA	1.68	0.59
2:B:854:LEU:HB3	2:B:856:PHE:CE1	2.37	0.59
3:C:174:ALA:O	3:C:175:ALA:CB	2.51	0.59
4:D:170:THR:HG22	4:D:172:LEU:HG	1.82	0.59
1:A:1397:LEU:HA	1:A:1400:CYS:CB	2.32	0.59
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.83	0.59
1:A:808:LEU:HD21	1:A:816:HIS:HD2	1.68	0.59
2:B:1160:VAL:CG1	2:B:1161:HIS:N	2.66	0.59
3:C:35:ARG:HH11	11:K:41:THR:N	2.01	0.59
5:E:164:LEU:HD22	5:E:211:TYR:CD2	2.37	0.59
2:B:954:VAL:O	12:L:55:ILE:O	2.20	0.59
1:A:1151:GLU:HB3	1:A:1153:TYR:HE1	1.68	0.59
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.37	0.59
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.02	0.59
1:A:25:GLU:CD	1:A:25:GLU:H	2.06	0.59
2:B:113:TYR:HB3	2:B:114:PRO:CD	2.29	0.59
1:A:782:ARG:NH2	2:B:699:GLU:O	2.34	0.59
2:B:798:TYR:CE1	10:J:4:PRO:HB3	2.38	0.59
2:B:841:MET:O	2:B:993:THR:HG22	2.02	0.59
8:H:40:LEU:HD12	8:H:122:LEU:O	2.03	0.59
9:I:101:PHE:O	9:I:102:VAL:HG23	2.03	0.59
1:A:1116:LEU:HB3	1:A:1311:VAL:CG2	2.33	0.58
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.26	0.58
1:A:687:LYS:O	1:A:690:VAL:HB	2.03	0.58
1:A:697:ALA:HB2	1:A:702:LEU:HD12	1.85	0.58
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.03	0.58
2:B:879:ARG:O	2:B:880:THR:HB	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:295:THR:O	13:S:295:THR:HG22	2.02	0.58
1:A:1030:ARG:HG3	1:A:1034:GLU:OE2	2.03	0.58
1:A:1095:THR:OG1	1:A:1112:LYS:HB2	2.03	0.58
1:A:528:LEU:HD23	1:A:751:SER:HA	1.85	0.58
2:B:549:THR:HG22	2:B:550:ASP:N	2.12	0.58
1:A:667:GLY:HA3	3:C:192:TRP:CH2	2.38	0.58
5:E:114:ASN:O	5:E:115:ASN:HB3	2.03	0.58
8:H:24:CYS:SG	8:H:44:VAL:HG21	2.43	0.58
1:A:1342:GLU:CG	5:E:198:ILE:HD13	2.33	0.58
1:A:265:LYS:O	1:A:266:LEU:C	2.41	0.58
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.84	0.58
1:A:361:LEU:HG	1:A:507:VAL:HG11	1.85	0.58
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.17	0.58
2:B:1065:GLN:HG3	2:B:1068:GLY:H	1.69	0.58
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.03	0.58
1:A:1422:ARG:HH22	2:B:1224:PHE:C	2.06	0.58
2:B:189:LEU:O	2:B:192:LEU:N	2.31	0.58
2:B:511:PRO:C	2:B:513:GLN:N	2.51	0.58
3:C:66:ARG:NH2	10:J:5:VAL:HG23	2.18	0.58
6:F:111:LEU:N	6:F:111:LEU:HD12	2.18	0.58
10:J:19:GLU:O	10:J:23:ASN:HB2	2.03	0.58
11:K:31:VAL:HG12	11:K:32:VAL:N	2.18	0.58
1:A:321:PRO:O	1:A:322:VAL:HG23	2.03	0.58
1:A:535:THR:CG2	1:A:616:VAL:HA	2.33	0.58
1:A:847:ASP:HB2	1:A:859:SER:H	1.68	0.58
2:B:763:GLN:HE22	13:S:293:LEU:HG	1.67	0.58
2:B:807:ARG:NH1	2:B:807:ARG:HB3	2.19	0.58
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.34	0.58
3:C:59:ALA:O	3:C:62:PHE:HB3	2.03	0.58
4:D:48:ILE:HG21	7:G:4:ILE:HB	1.85	0.58
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.34	0.58
8:H:42:ILE:HG23	8:H:95:TYR:HE1	1.67	0.58
1:A:848:ILE:HB	1:A:1065:GLY:HA3	1.85	0.58
1:A:1127:ASP:O	1:A:1130:GLN:HB3	2.03	0.58
1:A:1222:ASN:O	1:A:1223:ASP:HB3	2.04	0.58
2:B:570:VAL:HG23	2:B:573:GLN:HB3	1.85	0.58
2:B:815:ARG:HD3	2:B:1041:GLU:OE2	2.03	0.58
2:B:918:ILE:CD1	2:B:935:ARG:HD2	2.27	0.58
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.19	0.58
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.03	0.58
1:A:785:PRO:HG2	1:A:786:HIS:HD2	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:SER:HB3	2:B:258:LEU:HG	1.86	0.58
2:B:404:LYS:HE2	2:B:404:LYS:HA	1.85	0.58
3:C:17:ASN:OD1	3:C:233:GLU:HG3	2.02	0.58
5:E:144:ILE:O	5:E:146:HIS:N	2.37	0.58
1:A:305:ASP:CG	1:A:326:ARG:HD2	2.24	0.58
1:A:666:ILE:CD1	1:A:667:GLY:N	2.66	0.58
2:B:483:LEU:HD12	2:B:484:ASN:H	1.67	0.58
2:B:519:TRP:C	2:B:519:TRP:CD1	2.77	0.58
2:B:380:TYR:OH	2:B:623:GLU:OE2	2.21	0.58
2:B:782:LEU:HD12	2:B:788:ARG:HH11	1.67	0.58
4:D:33:PHE:CE1	7:G:80:LYS:HE3	2.39	0.58
7:G:119:LEU:HD13	7:G:132:SER:HB2	1.86	0.58
7:G:9:LEU:HD12	7:G:10:ASN:N	2.16	0.58
9:I:2:THR:O	9:I:3:THR:C	2.41	0.58
2:B:824:ILE:CG1	10:J:48:ARG:HH12	2.11	0.58
2:B:785:TYR:HE2	10:J:60:PHE:CE1	2.22	0.58
13:S:300:GLU:HG3	13:S:300:GLU:O	2.04	0.58
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.04	0.58
1:A:567:LYS:CB	1:A:568:PRO:CD	2.81	0.58
1:A:69:THR:C	1:A:71:GLN:N	2.57	0.58
1:A:827:THR:O	1:A:831:THR:HB	2.04	0.58
3:C:124:LEU:O	3:C:127:ARG:HG2	2.04	0.58
5:E:13:TRP:O	5:E:16:PHE:HB3	2.03	0.58
7:G:117:GLN:O	7:G:119:LEU:N	2.37	0.58
1:A:446:ARG:HB2	1:A:487:MET:SD	2.43	0.58
1:A:55:ASP:C	1:A:57:ARG:N	2.46	0.58
1:A:744:LYS:HE2	1:A:748:MET:HE2	1.86	0.58
1:A:903:ASN:ND2	1:A:905:ASP:H	2.02	0.58
2:B:762:ASN:HD21	2:B:1024:ALA:CB	2.17	0.58
2:B:1147:LEU:HD23	2:B:1147:LEU:C	2.24	0.58
2:B:1186:ASP:OD1	2:B:1186:ASP:O	2.22	0.58
2:B:461:LEU:HD12	2:B:461:LEU:H	1.68	0.58
2:B:855:PHE:CD1	2:B:855:PHE:C	2.75	0.58
9:I:58:VAL:HG13	9:I:62:ILE:HG13	1.84	0.58
11:K:53:ASP:HB3	11:K:56:VAL:HG23	1.86	0.58
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.34	0.58
1:A:1316:VAL:O	1:A:1322:ILE:HD13	2.04	0.58
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.04	0.58
2:B:325:GLN:HG2	9:I:31:THR:CG2	2.34	0.58
2:B:708:GLU:O	2:B:710:LEU:N	2.37	0.58
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:162:ARG:HG2	5:E:162:ARG:HH11	1.68	0.58
6:F:85:MET:HE1	6:F:148:VAL:HG12	1.85	0.58
1:A:598:LEU:HD22	8:H:25:ARG:NH1	2.18	0.58
10:J:8:PHE:HD1	10:J:49:MET:HE1	1.69	0.58
1:A:115:LEU:HD12	1:A:142:CYS:SG	2.44	0.57
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.04	0.57
1:A:895:LYS:HG2	1:A:895:LYS:O	2.03	0.57
2:B:394:ASP:OD1	9:I:91:ARG:HB3	2.05	0.57
2:B:57:TYR:CD1	2:B:57:TYR:N	2.72	0.57
2:B:603:LEU:HB3	2:B:609:ILE:HD11	1.84	0.57
2:B:903:VAL:HG12	2:B:904:ARG:N	2.17	0.57
2:B:992:ILE:HD13	2:B:994:TYR:CE1	2.38	0.57
3:C:82:TYR:CE1	3:C:161:LYS:HD3	2.39	0.57
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.86	0.57
5:E:157:SER:O	5:E:159:ASP:N	2.37	0.57
7:G:117:GLN:C	7:G:119:LEU:H	2.07	0.57
8:H:84:ALA:C	8:H:86:ASP:H	2.06	0.57
9:I:88:SER:C	9:I:90:GLN:H	2.07	0.57
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.14	0.57
1:A:1421:CYS:HA	1:A:1426:GLU:HB3	1.87	0.57
1:A:168:GLY:O	1:A:169:ASN:C	2.43	0.57
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.86	0.57
2:B:773:MET:O	2:B:775:LYS:N	2.37	0.57
9:I:59:VAL:HG12	9:I:59:VAL:O	2.04	0.57
10:J:1:MET:H2	10:J:56:LEU:N	2.00	0.57
1:A:963:ILE:CD1	1:A:1049:ILE:HG13	2.30	0.57
1:A:443:LEU:HG	2:B:1146:PHE:CE2	2.28	0.57
1:A:642:CYS:O	1:A:645:LEU:HB3	2.04	0.57
1:A:808:LEU:N	1:A:808:LEU:HD12	2.20	0.57
1:A:818:MET:HA	2:B:514:LEU:HB3	1.87	0.57
3:C:69:LEU:H	3:C:69:LEU:HD12	1.69	0.57
8:H:100:THR:HG22	8:H:101:ALA:N	2.19	0.57
10:J:14:VAL:HG13	10:J:50:ILE:HD11	1.85	0.57
11:K:47:ARG:HD3	11:K:59:ALA:O	2.04	0.57
3:C:167:HIS:CE1	12:L:70:ARG:HA	2.39	0.57
13:S:236:LEU:CA	13:S:242:LYS:HE3	2.34	0.57
1:A:1353:TYR:CD2	1:A:1353:TYR:C	2.77	0.57
1:A:42:ASP:C	1:A:44:THR:H	2.07	0.57
1:A:57:ARG:O	1:A:58:LEU:O	2.21	0.57
2:B:1145:SER:C	2:B:1147:LEU:N	2.55	0.57
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1164:PRO:O	1:A:1166:ASP:N	2.36	0.57
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.25	0.57
1:A:984:LYS:O	1:A:988:LEU:HB2	2.03	0.57
2:B:192:LEU:O	2:B:193:LYS:HB2	2.04	0.57
2:B:640:VAL:O	2:B:641:GLU:C	2.41	0.57
2:B:694:ASP:O	2:B:698:GLU:HB2	2.05	0.57
3:C:114:TYR:HB3	3:C:140:ASN:O	2.04	0.57
5:E:153:HIS:O	5:E:154:ILE:CG1	2.49	0.57
7:G:80:LYS:CE	7:G:82:PHE:HZ	2.17	0.57
1:A:1289:ARG:NH1	1:A:1326:ARG:NH1	2.52	0.57
2:B:860:MET:HB2	2:B:965:LYS:HG2	1.87	0.57
3:C:196:ASP:OD1	3:C:198:ALA:HB3	2.05	0.57
5:E:204:THR:CG2	5:E:205:SER:N	2.67	0.57
6:F:77:ASP:C	6:F:79:ARG:H	2.08	0.57
7:G:109:PHE:CD1	7:G:110:VAL:N	2.71	0.57
10:J:8:PHE:CD1	10:J:49:MET:SD	2.98	0.57
1:A:1362:TYR:HD1	1:A:1363:VAL:N	1.85	0.57
2:B:296:GLU:O	2:B:299:GLU:HB2	2.04	0.57
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.87	0.57
1:A:469:ARG:NH2	2:B:991:GLY:O	2.37	0.57
1:A:1359:ASP:HB3	13:S:307:LYS:HE2	1.87	0.57
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.35	0.57
1:A:403:LYS:O	1:A:404:TYR:CG	2.58	0.57
1:A:560:ILE:HD12	8:H:79:TRP:O	2.05	0.57
1:A:92:HIS:O	1:A:95:PHE:N	2.37	0.57
2:B:557:PHE:C	2:B:557:PHE:CD2	2.77	0.57
5:E:84:ASP:O	5:E:86:PRO:HD3	2.05	0.57
9:I:58:VAL:HA	9:I:62:ILE:HD11	1.87	0.57
9:I:6:PHE:HA	9:I:14:LEU:HG	1.85	0.57
1:A:1335:ILE:O	1:A:1335:ILE:HG22	2.05	0.57
1:A:491:VAL:HG12	1:A:492:PRO:O	2.04	0.57
2:B:1085:ILE:HG22	2:B:1086:PHE:N	2.19	0.57
2:B:217:ARG:HE	2:B:405:ARG:CB	2.15	0.57
2:B:522:VAL:HG12	2:B:523:CYS:N	2.19	0.57
2:B:558:LEU:O	2:B:560:GLU:N	2.37	0.57
2:B:620:ARG:NH2	9:I:89:GLN:NE2	2.52	0.57
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.85	0.57
8:H:83:GLN:C	8:H:85:GLY:H	2.08	0.57
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.05	0.57
1:A:289:ILE:C	1:A:291:GLU:N	2.58	0.57
1:A:492:PRO:O	1:A:493:GLN:NE2	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:GLY:C	1:A:732:LEU:H	2.09	0.57
1:A:798:GLY:HA2	1:A:815:PHE:CD1	2.39	0.57
2:B:1182:CYS:C	2:B:1183:LYS:HE3	2.25	0.57
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.70	0.57
2:B:325:GLN:HG2	9:I:31:THR:HG23	1.86	0.57
3:C:181:ASP:OD1	3:C:186:LEU:HD13	2.05	0.57
6:F:75:PRO:O	6:F:77:ASP:O	2.23	0.57
12:L:43:THR:O	12:L:43:THR:HG22	2.04	0.57
1:A:1080:THR:HG22	1:A:1081:LEU:N	2.20	0.56
1:A:1090:ALA:CA	1:A:1093:LYS:HE3	2.34	0.56
1:A:1203:ASN:O	1:A:1204:ASP:C	2.44	0.56
1:A:18:GLN:HG3	1:A:228:PHE:CE1	2.40	0.56
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.40	0.56
1:A:495:GLU:O	1:A:498:ARG:HG3	2.04	0.56
1:A:666:ILE:H	2:B:1026:LEU:HD22	1.70	0.56
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.32	0.56
2:B:1172:ILE:O	2:B:1172:ILE:HG22	2.05	0.56
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.86	0.56
3:C:89:GLU:O	3:C:90:ASP:HB3	2.05	0.56
4:D:40:HIS:CB	7:G:73:LYS:NZ	2.58	0.56
1:A:730:GLY:O	1:A:732:LEU:N	2.38	0.56
2:B:603:LEU:HB3	2:B:609:ILE:CD1	2.35	0.56
3:C:167:HIS:HD2	3:C:169:LYS:N	1.97	0.56
3:C:82:TYR:O	3:C:84:ARG:N	2.38	0.56
7:G:1:MET:CE	7:G:80:LYS:H	2.18	0.56
1:A:1051:ALA:O	1:A:1053:PHE:N	2.39	0.56
1:A:685:GLU:HG3	1:A:686:ALA:N	2.20	0.56
1:A:84:ILE:HG23	1:A:239:LEU:HB3	1.86	0.56
1:A:899:VAL:CG2	1:A:908:LEU:HD21	2.35	0.56
2:B:1000:PRO:O	2:B:1007:VAL:HG23	2.05	0.56
2:B:278:GLN:HG2	2:B:279:ASP:H	1.68	0.56
4:D:51:ASN:ND2	4:D:54:GLU:OE2	2.38	0.56
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.41	0.56
1:A:1081:LEU:HD21	1:A:1098:VAL:CG2	2.35	0.56
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.19	0.56
1:A:306:ASN:ND2	1:A:322:VAL:HB	2.21	0.56
1:A:34:LYS:CB	1:A:36:ARG:HH21	2.18	0.56
1:A:775:ILE:HG13	1:A:798:GLY:HA3	1.86	0.56
1:A:996:ASN:O	1:A:998:LEU:HD12	2.04	0.56
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.88	0.56
5:E:35:VAL:C	5:E:37:LEU:H	2.08	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:65:HIS:CD2	11:K:67:PHE:N	2.60	0.56
12:L:62:LYS:H	12:L:62:LYS:HD2	1.70	0.56
1:A:130:ASP:O	1:A:132:LYS:N	2.39	0.56
1:A:532:ARG:HH22	1:A:745:GLN:HG2	1.69	0.56
2:B:247:GLY:H	2:B:418:LYS:HZ3	1.54	0.56
2:B:528:PRO:HG2	2:B:533:CYS:HA	1.88	0.56
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.35	0.56
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.34	0.56
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.86	0.56
3:C:143:LEU:C	3:C:143:LEU:HD12	2.25	0.56
1:A:1453:TYR:CZ	6:F:129:LYS:HA	2.40	0.56
9:I:111:THR:HG22	9:I:113:ASP:N	2.19	0.56
1:A:1438:THR:HB	2:B:1144:ALA:CB	2.36	0.56
1:A:78:PRO:CB	2:B:1201:LYS:HE3	2.36	0.56
2:B:286:PHE:HE2	2:B:375:ALA:HB1	1.70	0.56
2:B:511:PRO:C	2:B:513:GLN:H	2.08	0.56
2:B:766:ARG:NH2	2:B:1020:ARG:CG	2.67	0.56
2:B:784:ASN:O	2:B:788:ARG:HG3	2.06	0.56
10:J:57:ILE:O	10:J:60:PHE:N	2.39	0.56
1:A:928:LEU:O	1:A:930:ASP:N	2.39	0.56
2:B:1135:ARG:O	2:B:1139:ILE:HG13	2.06	0.56
2:B:1177:HIS:C	2:B:1179:GLN:H	2.08	0.56
2:B:47:GLN:O	2:B:173:MET:HE1	2.06	0.56
2:B:857:ARG:HH21	2:B:942:ARG:NH1	2.04	0.56
3:C:123:ASN:ND2	3:C:125:MET:SD	2.79	0.56
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.70	0.56
5:E:19:VAL:O	5:E:23:VAL:HG23	2.06	0.56
5:E:178:ILE:HG22	5:E:213:ILE:O	2.06	0.56
9:I:64:SER:O	9:I:66:PRO:HD3	2.05	0.56
10:J:13:VAL:HG12	10:J:14:VAL:N	2.21	0.56
13:S:241:LEU:O	13:S:242:LYS:C	2.43	0.56
1:A:98:LYS:O	1:A:102:VAL:HG23	2.05	0.56
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.86	0.56
1:A:4:GLN:O	1:A:5:GLN:HB2	2.05	0.56
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.40	0.56
2:B:1020:ARG:CG	2:B:1020:ARG:NH1	2.68	0.56
2:B:498:THR:O	2:B:536:VAL:HG13	2.05	0.56
2:B:642:ASP:O	2:B:644:GLU:N	2.30	0.56
3:C:163:ILE:O	3:C:166:GLU:N	2.36	0.56
5:E:56:LYS:HE3	5:E:84:ASP:HB2	1.87	0.56
1:A:874:ASP:CA	1:A:1058:VAL:HG23	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.06	0.56
1:A:663:SER:OG	2:B:1085:ILE:HG23	2.06	0.56
1:A:71:GLN:O	1:A:73:GLY:N	2.39	0.56
1:A:936:LEU:N	1:A:936:LEU:HD23	2.21	0.56
1:A:339:ASN:CB	2:B:1117:GLN:HE22	2.19	0.56
2:B:254:LEU:HD23	2:B:381:MET:CE	2.36	0.56
2:B:377:PHE:O	2:B:380:TYR:N	2.39	0.56
2:B:37:PHE:CD2	2:B:542:MET:SD	2.99	0.56
2:B:999:MET:HB3	2:B:1007:VAL:HG21	1.88	0.56
7:G:1:MET:O	7:G:1:MET:HE1	2.05	0.56
9:I:90:GLN:NE2	9:I:92:ARG:HD2	2.21	0.56
1:A:567:LYS:CB	8:H:95:TYR:HA	2.36	0.56
1:A:986:ILE:HD11	1:A:1032:LEU:HD11	1.87	0.56
2:B:766:ARG:HH21	2:B:1020:ARG:HG2	1.71	0.56
2:B:327:ARG:O	2:B:331:LEU:HD13	2.06	0.56
2:B:521:LEU:HB3	2:B:633:VAL:CG1	2.36	0.56
2:B:996:ARG:NH2	3:C:175:ALA:HA	2.20	0.56
3:C:242:GLN:O	3:C:246:ARG:N	2.37	0.56
3:C:82:TYR:CD1	3:C:161:LYS:HD3	2.41	0.56
5:E:176:PRO:O	5:E:212:ARG:HA	2.06	0.56
2:B:798:TYR:HE1	10:J:4:PRO:HB3	1.71	0.56
1:A:1044:TRP:O	1:A:1047:SER:N	2.38	0.56
1:A:306:ASN:HB2	1:A:324:SER:HB3	1.87	0.56
1:A:42:ASP:HB3	1:A:45:GLN:H	1.70	0.56
1:A:503:GLN:C	1:A:504:LEU:HD12	2.25	0.56
1:A:72:GLU:HB3	1:A:76:GLU:HG3	1.88	0.56
1:A:963:ILE:HD13	1:A:1049:ILE:CG1	2.32	0.56
1:A:78:PRO:HB3	2:B:1201:LYS:HE3	1.88	0.56
2:B:744:HIS:CG	2:B:745:PRO:HD2	2.41	0.56
2:B:945:GLU:O	2:B:946:ASN:HB3	2.06	0.56
7:G:114:LEU:HG	7:G:162:SER:CB	2.36	0.56
11:K:21:ILE:HG23	11:K:31:VAL:HG11	1.88	0.56
1:A:861:GLY:HA3	5:E:174:GLN:NE2	2.21	0.55
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	1.88	0.55
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.41	0.55
2:B:60:GLN:O	2:B:63:ILE:HG22	2.06	0.55
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.29	0.55
11:K:67:PHE:C	11:K:68:PHE:CD2	2.78	0.55
12:L:30:ILE:O	12:L:56:LEU:HA	2.06	0.55
1:A:1127:ASP:HB3	1:A:1130:GLN:HB2	1.89	0.55
3:C:133:ILE:CD1	3:C:237:SER:CA	2.82	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:1:MET:CE	7:G:1:MET:O	2.54	0.55
11:K:58:PHE:HE2	11:K:74:ARG:HE	1.53	0.55
1:A:414:ASP:OD1	1:A:416:ARG:CG	2.54	0.55
1:A:679:ILE:O	1:A:683:ILE:HG13	2.06	0.55
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.42	0.55
1:A:808:LEU:CD1	1:A:808:LEU:H	2.19	0.55
1:A:853:ASP:CG	1:A:855:THR:HB	2.25	0.55
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.41	0.55
2:B:582:VAL:HA	2:B:626:ILE:O	2.06	0.55
2:B:847:ASP:C	2:B:849:GLY:H	2.09	0.55
3:C:31:ASN:O	3:C:32:SER:C	2.45	0.55
4:D:39:ASN:ND2	4:D:41:GLN:HB2	2.21	0.55
8:H:5:LEU:HB2	8:H:60:ALA:H	1.71	0.55
9:I:105:SER:O	9:I:106:CYS:HB3	2.06	0.55
1:A:1373:ASP:O	1:A:1376:THR:HG23	2.06	0.55
1:A:1341:ILE:HD12	1:A:1379:GLY:O	2.05	0.55
1:A:265:LYS:HE2	1:A:322:VAL:HG11	1.89	0.55
1:A:708:MET:HE2	1:A:1089:VAL:CG1	2.33	0.55
1:A:71:GLN:C	1:A:73:GLY:N	2.60	0.55
1:A:823:GLY:C	1:A:825:ILE:H	2.08	0.55
2:B:1189:ILE:HG22	2:B:1190:ASP:N	2.22	0.55
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.72	0.55
4:D:27:LEU:HD11	4:D:197:SER:HB2	1.89	0.55
5:E:47:CYS:HA	5:E:52:ARG:O	2.06	0.55
12:L:30:ILE:HG22	12:L:31:CYS:N	2.20	0.55
12:L:49:LYS:O	12:L:50:ASP:HB2	2.05	0.55
1:A:1265:ASN:C	1:A:1267:MET:N	2.60	0.55
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.07	0.55
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.72	0.55
2:B:242:SER:OG	2:B:252:SER:O	2.23	0.55
2:B:502:ILE:CG2	2:B:502:ILE:O	2.52	0.55
2:B:54:PHE:HA	2:B:58:THR:HB	1.88	0.55
2:B:635:ARG:HB2	2:B:636:PRO:CD	2.36	0.55
1:A:1313:LEU:O	1:A:1315:GLU:N	2.39	0.55
1:A:18:GLN:HG3	1:A:228:PHE:HE1	1.72	0.55
1:A:78:PRO:O	1:A:79:GLY:O	2.25	0.55
1:A:896:ARG:HB3	1:A:897:TYR:HD1	1.70	0.55
1:A:896:ARG:O	1:A:1029:ARG:HB3	2.07	0.55
3:C:9:LYS:O	3:C:10:ILE:C	2.44	0.55
3:C:90:ASP:O	3:C:91:HIS:CG	2.60	0.55
5:E:211:TYR:CD1	5:E:211:TYR:N	2.74	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:100:GLN:O	6:F:103:MET:HB2	2.07	0.55
6:F:84:TYR:N	6:F:84:TYR:CD1	2.73	0.55
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.89	0.55
1:A:997:LEU:HD13	1:A:1018:PHE:CE2	2.42	0.55
1:A:730:GLY:C	1:A:732:LEU:N	2.59	0.55
1:A:668:ASP:CB	1:A:743:VAL:HG23	2.36	0.55
1:A:965:GLN:O	1:A:968:GLN:HB2	2.06	0.55
3:C:70:ILE:HD13	3:C:144:ILE:HD11	1.88	0.55
3:C:166:GLU:O	3:C:167:HIS:HB2	2.07	0.55
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.88	0.55
3:C:90:ASP:O	3:C:90:ASP:CG	2.43	0.55
5:E:124:VAL:HG13	5:E:132:ILE:CD1	2.36	0.55
5:E:213:ILE:HG12	5:E:214:CYS:N	2.21	0.55
7:G:13:LEU:HD23	7:G:14:HIS:H	1.70	0.55
4:D:47:LEU:HD11	7:G:3:PHE:HD2	1.72	0.55
10:J:21:TYR:HA	10:J:39:LEU:HD11	1.87	0.55
1:A:390:GLN:HE21	1:A:394:ASN:HD21	1.53	0.55
1:A:897:TYR:HB3	1:A:936:LEU:HD12	1.89	0.55
2:B:363:HIS:CD2	2:B:364:ILE:HG13	2.42	0.55
2:B:378:LEU:O	2:B:382:ILE:HG13	2.07	0.55
2:B:563:MET:HE2	2:B:587:HIS:C	2.28	0.55
2:B:873:THR:HG22	2:B:874:PHE:N	2.22	0.55
3:C:58:LEU:HD23	3:C:58:LEU:H	1.71	0.55
9:I:84:VAL:O	9:I:84:VAL:HG22	2.07	0.55
12:L:31:CYS:HB3	12:L:35:SER:N	2.21	0.55
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.88	0.55
1:A:1265:ASN:C	1:A:1267:MET:H	2.09	0.55
1:A:848:ILE:HB	1:A:1065:GLY:CA	2.37	0.55
1:A:901:LEU:N	1:A:926:GLN:HE21	1.98	0.55
2:B:1020:ARG:NH1	2:B:1020:ARG:HG2	2.20	0.55
2:B:488:TYR:CE2	2:B:813:LYS:HB2	2.42	0.55
2:B:533:CYS:C	2:B:535:LEU:H	2.09	0.55
2:B:363:HIS:CD2	2:B:585:VAL:HG22	2.42	0.55
2:B:597:MET:SD	2:B:624:LEU:HD11	2.47	0.55
8:H:7:ASP:O	8:H:8:ASP:HB2	2.06	0.55
9:I:25:LEU:HB3	9:I:38:ALA:HB2	1.89	0.55
12:L:47:ARG:HH11	12:L:47:ARG:HG3	1.72	0.55
1:A:1334:ASP:O	1:A:1337:GLU:N	2.40	0.55
1:A:356:ASP:HB3	1:A:359:LEU:HG	1.88	0.55
1:A:715:GLU:O	1:A:717:ASN:N	2.39	0.55
2:B:1084:GLN:HE21	2:B:1084:GLN:H	1.55	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:SER:O	2:B:266:ALA:HB3	2.07	0.55
2:B:25:ILE:HG23	2:B:29:ASP:HB3	1.89	0.55
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.88	0.55
2:B:781:PHE:O	2:B:782:LEU:CG	2.54	0.55
2:B:805:THR:HA	2:B:809:MET:HE1	1.89	0.55
3:C:27:LEU:HD12	3:C:228:PHE:HE2	1.70	0.55
8:H:127:GLY:HA3	8:H:130:ARG:NH2	2.22	0.55
2:B:800:GLN:CB	10:J:52:THR:HG21	2.33	0.55
1:A:1102:LYS:HG2	1:A:1106:ASN:ND2	2.22	0.54
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.07	0.54
1:A:15:LYS:HG3	2:B:1218:THR:O	2.06	0.54
1:A:820:GLY:C	1:A:822:GLU:N	2.60	0.54
1:A:919:ILE:O	1:A:921:GLY:N	2.40	0.54
1:A:982:THR:HG22	1:A:984:LYS:H	1.73	0.54
1:A:786:HIS:HE1	2:B:519:TRP:CZ2	2.25	0.54
2:B:542:MET:HG2	2:B:747:MET:HB3	1.89	0.54
2:B:711:GLU:H	2:B:712:PRO:HD2	1.72	0.54
1:A:1017:LEU:HD23	5:E:204:THR:C	2.27	0.54
13:S:243:GLN:O	13:S:247:GLU:HG3	2.07	0.54
1:A:1329:THR:HG22	1:A:1331:SER:N	2.15	0.54
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.42	0.54
1:A:381:THR:HG23	1:A:382:PRO:CD	2.37	0.54
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.42	0.54
2:B:1017:ILE:HG22	2:B:1018:PRO:N	2.21	0.54
2:B:382:ILE:O	2:B:385:LEU:HB3	2.08	0.54
3:C:67:LEU:HD23	3:C:70:ILE:HD11	1.89	0.54
5:E:124:VAL:CA	5:E:132:ILE:HD12	2.37	0.54
5:E:48:ASP:CG	5:E:49:SER:H	2.11	0.54
7:G:88:ASP:HA	7:G:144:ARG:HA	1.88	0.54
1:A:1397:LEU:O	1:A:1400:CYS:HB3	2.06	0.54
1:A:353:ILE:HG21	1:A:487:MET:CG	2.20	0.54
1:A:49:LYS:HZ1	1:A:61:ILE:N	2.05	0.54
1:A:775:ILE:CG1	1:A:798:GLY:HA3	2.38	0.54
2:B:356:LEU:HA	2:B:360:PHE:HB2	1.90	0.54
3:C:183:TRP:O	3:C:185:LYS:HG3	2.06	0.54
8:H:126:GLU:C	8:H:130:ARG:HH22	2.11	0.54
8:H:139:ASN:O	8:H:140:ALA:HB2	2.08	0.54
11:K:46:ILE:O	11:K:50:LEU:HB2	2.07	0.54
1:A:1396:ALA:O	1:A:1398:MET:N	2.41	0.54
1:A:41:MET:O	1:A:42:ASP:C	2.45	0.54
1:A:597:LEU:HD12	1:A:597:LEU:N	2.21	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:GLY:O	1:A:605:MET:HB2	2.07	0.54
1:A:855:THR:HG23	1:A:856:THR:N	2.23	0.54
1:A:867:ILE:CG2	1:A:872:GLY:N	2.71	0.54
1:A:905:ASP:C	1:A:906:HIS:HD1	2.10	0.54
1:A:996:ASN:HA	1:A:998:LEU:CD1	2.38	0.54
2:B:1165:ILE:CG2	2:B:1166:CYS:N	2.70	0.54
3:C:143:LEU:HD12	3:C:145:CYS:N	2.22	0.54
3:C:250:THR:O	3:C:254:LYS:HG3	2.07	0.54
5:E:90:VAL:O	5:E:90:VAL:HG22	2.07	0.54
7:G:18:PHE:HZ	7:G:68:ALA:HB2	1.71	0.54
9:I:34:TYR:HD2	9:I:35:VAL:N	2.05	0.54
13:S:293:LEU:HD23	13:S:293:LEU:N	2.23	0.54
1:A:1079:MET:HE2	1:A:1101:LEU:CD2	2.37	0.54
1:A:470:LEU:CD2	1:A:487:MET:CE	2.86	0.54
2:B:1219:ASP:O	2:B:1219:ASP:OD1	2.25	0.54
2:B:210:LYS:HA	2:B:481:GLN:O	2.07	0.54
2:B:693:ILE:HD11	2:B:740:HIS:CD2	2.43	0.54
2:B:861:ASP:OD1	2:B:862:GLN:N	2.41	0.54
5:E:39:LEU:O	5:E:42:PHE:HB3	2.08	0.54
10:J:23:ASN:C	10:J:25:LEU:H	2.09	0.54
1:A:1017:LEU:O	1:A:1017:LEU:HD12	2.07	0.54
1:A:1021:LEU:O	1:A:1025:ARG:HG2	2.08	0.54
1:A:877:HIS:CD2	1:A:1056:SER:HA	2.41	0.54
1:A:1125:ALA:C	1:A:1127:ASP:H	2.10	0.54
1:A:133:LYS:C	1:A:135:PHE:N	2.60	0.54
1:A:308:ILE:HG22	1:A:309:ALA:H	1.73	0.54
1:A:476:SER:OG	1:A:477:PRO:HD3	2.08	0.54
1:A:626:ASN:O	1:A:631:HIS:HB2	2.07	0.54
1:A:69:THR:C	1:A:71:GLN:H	2.10	0.54
2:B:1099:VAL:O	2:B:1102:LYS:N	2.36	0.54
2:B:1106:ARG:CG	2:B:1107:ALA:N	2.69	0.54
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.89	0.54
2:B:865:LYS:NZ	2:B:869:SER:HA	2.23	0.54
3:C:174:ALA:HB2	3:C:235:VAL:HG22	1.90	0.54
3:C:183:TRP:O	3:C:185:LYS:N	2.41	0.54
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.37	0.54
4:D:130:LEU:C	4:D:132:GLN:N	2.61	0.54
5:E:144:ILE:HG13	5:E:145:THR:H	1.72	0.54
5:E:60:PHE:HE2	5:E:80:VAL:HB	1.73	0.54
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.89	0.54
7:G:81:PRO:HG3	7:G:106:MET:SD	2.47	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:58:THR:HG22	8:H:59:ILE:H	1.73	0.54
9:I:62:ILE:CG2	9:I:62:ILE:O	2.55	0.54
11:K:83:PRO:O	11:K:86:ALA:N	2.41	0.54
1:A:703:THR:O	1:A:705:LYS:HG2	2.07	0.54
1:A:68:GLN:C	1:A:70:CYS:H	2.09	0.54
1:A:886:ILE:HG13	1:A:943:LEU:HD12	1.90	0.54
2:B:1072:MET:HE2	2:B:1085:ILE:HB	1.89	0.54
3:C:44:LEU:HD23	3:C:72:LEU:HB2	1.90	0.54
6:F:84:TYR:HD1	6:F:84:TYR:N	2.06	0.54
8:H:14:GLU:HG2	8:H:15:VAL:N	2.22	0.54
8:H:95:TYR:HE2	8:H:97:MET:HG2	1.72	0.54
9:I:88:SER:O	9:I:90:GLN:N	2.41	0.54
1:A:1305:VAL:HG12	1:A:1306:LEU:N	2.23	0.54
1:A:1313:LEU:CD1	1:A:1327:ILE:HD13	2.38	0.54
1:A:534:LEU:HD13	1:A:656:TRP:CG	2.43	0.54
1:A:75:ASN:O	1:A:76:GLU:CB	2.55	0.54
2:B:431:TYR:CE2	2:B:447:ALA:HB2	2.42	0.54
2:B:498:THR:HB	2:B:537:LYS:O	2.08	0.54
2:B:555:ILE:HG22	2:B:556:THR:N	2.21	0.54
2:B:955:THR:CG2	2:B:956:THR:N	2.71	0.54
4:D:213:GLU:O	4:D:217:LEU:HG	2.07	0.54
9:I:7:CYS:SG	9:I:8:ARG:O	2.66	0.54
1:A:1161:THR:C	1:A:1163:ILE:N	2.61	0.54
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.48	0.54
2:B:1165:ILE:CG2	2:B:1185:CYS:HB3	2.38	0.54
2:B:203:PHE:HB3	2:B:205:ILE:HD11	1.90	0.54
2:B:658:ILE:O	2:B:661:LEU:HB2	2.07	0.54
2:B:879:ARG:O	2:B:934:LYS:HD2	2.08	0.54
2:B:94:LYS:HG2	2:B:95:ILE:N	2.22	0.54
2:B:970:THR:HG22	2:B:971:THR:N	2.22	0.54
8:H:130:ARG:HA	8:H:133:ASN:HB2	1.90	0.54
11:K:65:HIS:CD2	11:K:66:PRO:CD	2.90	0.54
1:A:1116:LEU:CD2	1:A:1311:VAL:HG22	2.36	0.54
1:A:1376:THR:O	1:A:1377:THR:C	2.46	0.54
1:A:35:ILE:HA	1:A:52:GLY:O	2.07	0.54
1:A:688:LYS:C	1:A:690:VAL:H	2.12	0.54
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.72	0.54
2:B:1182:CYS:O	2:B:1182:CYS:SG	2.66	0.54
2:B:230:ALA:N	2:B:231:PRO:HD2	2.23	0.54
2:B:94:LYS:HG2	2:B:95:ILE:H	1.73	0.54
11:K:31:VAL:CG1	11:K:32:VAL:N	2.70	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1123:GLY:O	1:A:1125:ALA:N	2.41	0.53
1:A:1436:ILE:O	1:A:1437:GLY:C	2.46	0.53
2:B:197:PHE:HZ	2:B:816:GLU:HG2	1.73	0.53
2:B:205:ILE:N	2:B:205:ILE:CD1	2.72	0.53
2:B:487:THR:HG22	2:B:488:TYR:H	1.73	0.53
1:A:1441:PHE:HZ	6:F:89:GLU:HA	1.67	0.53
9:I:55:THR:CG2	9:I:100:PHE:HD2	2.17	0.53
11:K:47:ARG:HH11	11:K:48:ALA:N	2.06	0.53
11:K:58:PHE:HB3	11:K:76:GLN:HE21	1.72	0.53
1:A:1063:MET:CE	1:A:1436:ILE:HG12	2.39	0.53
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.43	0.53
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.48	0.53
2:B:203:PHE:HB3	2:B:205:ILE:CD1	2.37	0.53
2:B:224:GLN:O	2:B:238:ALA:HA	2.08	0.53
2:B:984:HIS:NE2	2:B:1025:HIS:HA	2.24	0.53
5:E:55:ARG:O	5:E:57:MET:N	2.41	0.53
6:F:77:ASP:C	6:F:79:ARG:N	2.61	0.53
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.90	0.53
1:A:1261:LYS:CA	1:A:1264:GLU:HB3	2.38	0.53
1:A:1305:VAL:CG1	1:A:1306:LEU:N	2.71	0.53
1:A:1454:MET:HG3	1:A:1454:MET:O	2.08	0.53
1:A:335:ARG:HH11	2:B:1206:GLU:CD	2.10	0.53
1:A:41:MET:HB3	1:A:48:ALA:O	2.08	0.53
1:A:423:ASP:OD1	1:A:424:ILE:N	2.42	0.53
1:A:468:PHE:CE2	1:A:489:LEU:HD23	2.43	0.53
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.43	0.53
2:B:827:ILE:CD1	2:B:1086:PHE:HD2	2.21	0.53
2:B:817:LEU:O	2:B:818:PRO:O	2.26	0.53
3:C:27:LEU:O	3:C:28:ALA:C	2.46	0.53
3:C:92:CYS:H	3:C:95:CYS:HG	1.57	0.53
6:F:116:ASP:O	6:F:120:ILE:HG13	2.09	0.53
1:A:1204:ASP:HA	13:S:252:ASN:CB	2.36	0.53
1:A:129:LYS:O	1:A:130:ASP:HB2	2.08	0.53
1:A:1343:ALA:O	1:A:1346:ALA:HB3	2.09	0.53
1:A:381:THR:HG22	1:A:383:TYR:H	1.73	0.53
1:A:392:VAL:HG21	1:A:426:LEU:HD11	1.91	0.53
3:C:97:VAL:HG12	3:C:98:VAL:N	2.23	0.53
4:D:123:LEU:HD23	4:D:149:THR:HG21	1.90	0.53
7:G:78:VAL:HG12	7:G:79:PHE:H	1.74	0.53
8:H:84:ALA:C	8:H:86:ASP:N	2.60	0.53
9:I:103:CYS:HB3	9:I:106:CYS:SG	2.48	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1079:MET:HE3	1:A:1098:VAL:HG22	1.90	0.53
1:A:1148:ILE:O	1:A:1149:ALA:HB2	2.09	0.53
1:A:1299:VAL:HG12	1:A:1300:LYS:H	1.74	0.53
1:A:135:PHE:C	1:A:137:ALA:N	2.60	0.53
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.38	0.53
1:A:708:MET:SD	1:A:1091:SER:OG	2.66	0.53
1:A:720:ARG:O	1:A:724:GLU:HB2	2.09	0.53
1:A:63:ARG:CA	1:A:74:MET:SD	2.89	0.53
2:B:1010:LEU:HD12	2:B:1011:ILE:N	2.23	0.53
2:B:1032:SER:C	2:B:1034:VAL:H	2.12	0.53
2:B:1187:ASN:O	2:B:1188:LYS:CB	2.56	0.53
3:C:88:CYS:SG	3:C:91:HIS:C	2.87	0.53
4:D:129:LEU:O	4:D:132:GLN:HB2	2.08	0.53
4:D:14:ARG:O	4:D:16:LYS:N	2.41	0.53
11:K:53:ASP:HB3	11:K:56:VAL:CG2	2.39	0.53
1:A:1396:ALA:O	1:A:1399:ARG:N	2.41	0.53
1:A:503:GLN:HE21	6:F:90:ARG:NH2	2.02	0.53
1:A:523:ILE:HG22	1:A:528:LEU:HB2	1.88	0.53
1:A:867:ILE:HG22	1:A:871:ASP:N	2.24	0.53
2:B:125:SER:HA	2:B:171:PRO:HA	1.89	0.53
2:B:214:ALA:HB3	2:B:498:THR:HA	1.90	0.53
3:C:112:ASN:HB3	3:C:114:TYR:CE1	2.44	0.53
3:C:144:ILE:O	3:C:145:CYS:HB2	2.08	0.53
9:I:61:ASP:C	9:I:63:GLY:H	2.12	0.53
1:A:1086:PHE:O	1:A:1087:ALA:C	2.47	0.53
1:A:1385:THR:O	1:A:1387:HIS:N	2.42	0.53
1:A:151:ASP:OD1	1:A:163:SER:HB3	2.09	0.53
1:A:303:TYR:CE1	1:A:325:ILE:HD11	2.43	0.53
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.24	0.53
2:B:31:TRP:O	2:B:34:ILE:N	2.42	0.53
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.73	0.53
2:B:551:PRO:C	2:B:553:PRO:HD2	2.29	0.53
3:C:33:LEU:HG	3:C:37:MET:CE	2.38	0.53
5:E:154:ILE:O	5:E:196:VAL:HA	2.09	0.53
7:G:128:PRO:O	7:G:138:THR:HG23	2.09	0.53
1:A:511:ILE:O	1:A:519:PRO:HA	2.08	0.53
1:A:587:HIS:HD2	1:A:969:GLN:CG	2.19	0.53
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.91	0.53
2:B:225:VAL:HA	2:B:237:VAL:O	2.08	0.53
2:B:37:PHE:HE2	2:B:542:MET:CA	2.17	0.53
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:196:PRO:C	4:D:198:LEU:H	2.11	0.53
7:G:123:ALA:C	7:G:125:SER:N	2.63	0.53
8:H:6:PHE:O	8:H:58:THR:HA	2.08	0.53
9:I:106:CYS:SG	9:I:107:SER:N	2.82	0.53
10:J:57:ILE:O	10:J:60:PHE:HB2	2.09	0.53
13:S:231:CYS:CA	13:S:232:ASP:CA	2.86	0.53
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.74	0.53
1:A:1097:GLY:O	1:A:1100:ARG:HB3	2.09	0.53
1:A:47:ARG:NH1	1:A:254:GLU:HB3	2.06	0.53
1:A:317:LYS:O	1:A:318:SER:CB	2.57	0.53
1:A:84:ILE:HG22	1:A:239:LEU:O	2.08	0.53
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.43	0.53
2:B:273:LEU:HD21	2:B:360:PHE:CE1	2.44	0.53
2:B:856:PHE:N	2:B:856:PHE:HD1	2.06	0.53
10:J:48:ARG:HE	10:J:49:MET:HE2	1.73	0.53
11:K:49:GLU:OE2	11:K:97:LYS:HE3	2.09	0.53
1:A:231:PRO:HA	1:A:234:MET:HE2	1.91	0.53
1:A:785:PRO:HG2	2:B:703:ILE:HD12	1.91	0.53
1:A:823:GLY:O	1:A:825:ILE:N	2.41	0.53
1:A:898:ARG:HD3	1:A:933:TYR:CD1	2.45	0.53
2:B:298:LEU:CD2	2:B:298:LEU:N	2.72	0.53
2:B:906:SER:O	2:B:941:LEU:HD23	2.09	0.53
3:C:35:ARG:HH11	11:K:41:THR:CA	2.22	0.53
4:D:49:ALA:HB1	4:D:178:ALA:HB2	1.91	0.53
5:E:161:LYS:C	5:E:163:GLU:N	2.61	0.53
13:S:258:GLY:O	13:S:259:ALA:C	2.46	0.53
1:A:106:VAL:HA	1:A:114:LEU:HD21	1.90	0.52
2:B:562:GLY:HA3	2:B:590:HIS:ND1	2.24	0.52
2:B:806:THR:HG22	2:B:808:ALA:N	2.22	0.52
3:C:133:ILE:HD11	3:C:237:SER:CA	2.24	0.52
5:E:7:ARG:O	5:E:9:ILE:N	2.42	0.52
7:G:25:TYR:O	7:G:28:THR:HB	2.09	0.52
10:J:1:MET:HE2	10:J:60:PHE:HE2	1.74	0.52
1:A:823:GLY:HA3	13:S:285:GLN:HB2	1.90	0.52
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.09	0.52
1:A:1397:LEU:HA	1:A:1400:CYS:HB3	1.90	0.52
1:A:262:LEU:HD22	1:A:303:TYR:HE1	1.73	0.52
1:A:49:LYS:HZ2	1:A:60:SER:HA	1.72	0.52
1:A:825:ILE:C	1:A:827:THR:N	2.61	0.52
1:A:964:ILE:O	1:A:968:GLN:HG2	2.09	0.52
2:B:1115:THR:HG22	2:B:1117:GLN:HG3	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.68	0.52
2:B:323:VAL:O	2:B:323:VAL:HG12	2.09	0.52
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.91	0.52
2:B:789:MET:HE2	2:B:965:LYS:O	2.09	0.52
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.92	0.52
6:F:111:LEU:C	6:F:113:GLY:N	2.62	0.52
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.49	0.52
1:A:1114:PRO:O	1:A:1311:VAL:CG2	2.58	0.52
1:A:583:PRO:O	1:A:610:GLY:HA3	2.10	0.52
1:A:751:SER:O	1:A:752:LYS:HG2	2.09	0.52
1:A:808:LEU:H	1:A:808:LEU:HD12	1.74	0.52
2:B:347:LYS:HG3	2:B:348:ARG:H	1.74	0.52
2:B:257:LYS:O	2:B:385:LEU:HD21	2.08	0.52
2:B:401:PHE:HB2	2:B:517:THR:OG1	2.10	0.52
2:B:558:LEU:C	2:B:560:GLU:H	2.12	0.52
2:B:644:GLU:C	2:B:646:LEU:H	2.13	0.52
2:B:901:PRO:O	2:B:903:VAL:N	2.41	0.52
3:C:9:LYS:O	3:C:10:ILE:O	2.26	0.52
3:C:263:THR:C	3:C:265:MET:N	2.63	0.52
3:C:61:GLU:HA	3:C:64:ALA:HB3	1.91	0.52
5:E:147:HIS:CD2	5:E:149:LEU:H	2.27	0.52
5:E:78:LEU:HD23	5:E:78:LEU:C	2.30	0.52
5:E:7:ARG:HG3	5:E:8:ASN:H	1.73	0.52
7:G:17:PHE:N	7:G:17:PHE:CD2	2.76	0.52
11:K:31:VAL:O	11:K:74:ARG:HA	2.10	0.52
1:A:14:VAL:HG23	1:A:1432:GLN:HE22	1.75	0.52
1:A:326:ARG:HG2	1:A:327:ALA:N	2.24	0.52
1:A:477:PRO:CG	1:A:521:MET:HG2	2.39	0.52
1:A:53:LEU:HD23	1:A:54:ASN:HB3	1.91	0.52
1:A:808:LEU:HD21	1:A:816:HIS:CD2	2.44	0.52
1:A:853:ASP:O	1:A:854:ASN:HB2	2.09	0.52
1:A:864:ILE:O	1:A:865:GLN:CG	2.50	0.52
2:B:205:ILE:O	2:B:206:ASN:C	2.47	0.52
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.28	0.52
2:B:57:TYR:N	2:B:57:TYR:HD1	2.06	0.52
3:C:239:PRO:O	3:C:240:VAL:C	2.46	0.52
3:C:31:ASN:O	3:C:34:ARG:N	2.43	0.52
3:C:99:LEU:HD12	3:C:118:LEU:HD13	1.91	0.52
4:D:185:CYS:HB3	4:D:211:LEU:CD1	2.39	0.52
7:G:109:PHE:CG	7:G:110:VAL:N	2.78	0.52
7:G:146:LYS:NZ	7:G:165:GLU:OE2	2.38	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:18:PHE:CZ	7:G:68:ALA:HB2	2.44	0.52
9:I:68:LEU:HB3	9:I:84:VAL:HG23	1.90	0.52
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.43	0.52
1:A:1310:GLY:O	1:A:1311:VAL:HG23	2.08	0.52
1:A:514:PRO:O	1:A:875:ALA:HB1	2.08	0.52
1:A:877:HIS:O	1:A:878:ILE:HG12	2.09	0.52
2:B:212:LEU:HD21	2:B:466:TRP:HH2	1.74	0.52
2:B:210:LYS:HD2	2:B:481:GLN:O	2.09	0.52
2:B:782:LEU:CD1	2:B:788:ARG:HH11	2.23	0.52
4:D:198:LEU:O	4:D:200:ASN:N	2.42	0.52
5:E:212:ARG:HH11	5:E:212:ARG:HG3	1.75	0.52
1:A:1394:THR:O	1:A:1399:ARG:NE	2.38	0.52
1:A:1406:VAL:CG1	1:A:1410:PHE:CE1	2.90	0.52
1:A:316:GLN:O	1:A:317:LYS:C	2.47	0.52
1:A:688:LYS:C	1:A:690:VAL:N	2.61	0.52
1:A:695:LYS:C	1:A:697:ALA:H	2.11	0.52
1:A:744:LYS:HG2	1:A:748:MET:HE3	1.91	0.52
1:A:412:ARG:NH2	2:B:1108:ARG:HH12	2.07	0.52
2:B:225:VAL:HG22	2:B:396:ASP:OD2	2.10	0.52
2:B:360:PHE:O	2:B:361:LEU:C	2.47	0.52
2:B:522:VAL:CG1	2:B:523:CYS:N	2.71	0.52
3:C:215:GLU:O	3:C:217:ASP:N	2.43	0.52
3:C:99:LEU:HD23	3:C:99:LEU:N	2.23	0.52
1:A:866:PHE:CD2	5:E:168:TYR:CE1	2.98	0.52
9:I:100:PHE:CD1	9:I:100:PHE:N	2.78	0.52
1:A:1073:GLY:HA2	1:A:1076:ALA:HB3	1.91	0.52
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.75	0.52
2:B:431:TYR:CZ	2:B:447:ALA:HB2	2.44	0.52
7:G:143:ILE:CG2	7:G:144:ARG:N	2.73	0.52
8:H:59:ILE:O	8:H:60:ALA:HB3	2.10	0.52
1:A:1088:GLY:O	1:A:1089:VAL:HG23	2.09	0.52
1:A:1213:GLY:O	1:A:1216:ILE:N	2.42	0.52
2:B:457:LEU:O	2:B:461:LEU:HD12	2.10	0.52
2:B:49:ASP:HA	2:B:52:ASN:HD22	1.75	0.52
2:B:857:ARG:NH2	2:B:942:ARG:NH1	2.57	0.52
3:C:236:GLY:C	3:C:238:ILE:H	2.13	0.52
3:C:58:LEU:N	3:C:58:LEU:HD22	2.25	0.52
5:E:168:TYR:CB	5:E:170:LEU:HG	2.40	0.52
1:A:1444:MET:O	6:F:132:LEU:HA	2.10	0.52
1:A:553:VAL:HG22	1:A:652:VAL:HG22	1.92	0.52
2:B:1045:SER:O	2:B:1046:PRO:O	2.27	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:VAL:CG1	2:B:381:MET:HG2	2.40	0.52
1:A:785:PRO:CG	2:B:703:ILE:HD12	2.40	0.52
2:B:865:LYS:HE2	2:B:871:THR:OG1	2.10	0.52
2:B:870:ILE:CG2	2:B:917:PRO:HG2	2.40	0.52
3:C:31:ASN:OD1	3:C:34:ARG:HD3	2.10	0.52
5:E:55:ARG:C	5:E:57:MET:N	2.63	0.52
10:J:55:ASP:OD2	10:J:58:GLU:HG2	2.10	0.52
12:L:28:LYS:HB2	12:L:39:SER:HA	1.91	0.52
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.91	0.52
1:A:1377:THR:O	1:A:1379:GLY:N	2.42	0.52
1:A:1443:VAL:C	1:A:1444:MET:HG3	2.30	0.52
1:A:18:GLN:HB3	2:B:1215:ARG:HG3	1.92	0.52
1:A:55:ASP:N	1:A:56:PRO:CD	2.73	0.52
1:A:898:ARG:HD3	1:A:933:TYR:CE1	2.45	0.52
2:B:1147:LEU:O	2:B:1148:LYS:C	2.45	0.52
2:B:508:LEU:O	2:B:510:LYS:N	2.42	0.52
2:B:57:TYR:O	2:B:59:LEU:N	2.42	0.52
2:B:640:VAL:HG23	2:B:740:HIS:HA	1.92	0.52
8:H:89:LEU:C	8:H:91:ASP:H	2.12	0.52
1:A:321:PRO:O	1:A:322:VAL:CB	2.57	0.51
1:A:35:ILE:O	1:A:35:ILE:HG22	2.11	0.51
1:A:841:LEU:O	1:A:845:LEU:HG	2.10	0.51
1:A:351:THR:HG21	2:B:1103:ILE:HG13	1.91	0.51
5:E:161:LYS:C	5:E:163:GLU:H	2.14	0.51
5:E:92:THR:O	5:E:95:THR:HB	2.10	0.51
13:S:235:ASP:CA	13:S:242:LYS:HG3	2.38	0.51
1:A:675:THR:O	1:A:679:ILE:HG13	2.11	0.51
1:A:725:ALA:O	1:A:729:ALA:N	2.42	0.51
1:A:856:THR:HB	1:A:865:GLN:HB2	1.93	0.51
2:B:1032:SER:C	2:B:1034:VAL:N	2.64	0.51
2:B:1034:VAL:HG23	2:B:1059:LEU:CD1	2.40	0.51
2:B:1082:MET:O	3:C:189:THR:HG23	2.10	0.51
2:B:54:PHE:CE1	2:B:414:ALA:HA	2.42	0.51
2:B:508:LEU:HB2	2:B:510:LYS:CB	2.40	0.51
2:B:758:PHE:CE2	2:B:1044:ALA:CA	2.92	0.51
3:C:104:PHE:HD2	3:C:105:GLY:H	1.56	0.51
4:D:134:THR:HG22	4:D:136:GLY:H	1.75	0.51
9:I:54:GLU:O	9:I:100:PHE:CE2	2.63	0.51
12:L:36:SER:O	12:L:37:LYS:C	2.48	0.51
12:L:38:LEU:HG	12:L:39:SER:N	2.26	0.51
1:A:1029:ARG:NH1	1:A:1029:ARG:CG	2.70	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1148:ILE:O	1:A:1148:ILE:CG2	2.59	0.51
1:A:1325:THR:CG2	1:A:1326:ARG:HG3	2.40	0.51
1:A:348:SER:HB2	2:B:1128:LEU:HB2	1.90	0.51
1:A:50:ILE:C	1:A:52:GLY:N	2.62	0.51
1:A:648:ASN:O	1:A:649:ILE:C	2.47	0.51
2:B:758:PHE:CE1	2:B:1027:ILE:CG2	2.94	0.51
2:B:62:ILE:HG23	2:B:418:LYS:HG2	1.92	0.51
2:B:879:ARG:O	2:B:880:THR:CB	2.58	0.51
3:C:31:ASN:O	3:C:34:ARG:HB3	2.10	0.51
9:I:100:PHE:N	9:I:100:PHE:HD1	2.08	0.51
11:K:65:HIS:CD2	11:K:66:PRO:HD2	2.46	0.51
11:K:67:PHE:O	11:K:68:PHE:HD2	1.93	0.51
12:L:25:ALA:O	12:L:26:THR:HB	2.10	0.51
1:A:1005:GLU:O	1:A:1006:ILE:C	2.49	0.51
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.25	0.51
1:A:602:ASP:OD2	1:A:616:VAL:HG23	2.11	0.51
1:A:898:ARG:HB2	1:A:933:TYR:HE1	1.75	0.51
2:B:298:LEU:N	2:B:298:LEU:HD22	2.24	0.51
2:B:38:PHE:CD1	2:B:811:TYR:CD2	2.98	0.51
2:B:46:GLN:CG	2:B:47:GLN:H	2.22	0.51
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.92	0.51
3:C:80:LEU:CD1	3:C:95:CYS:HA	2.40	0.51
8:H:62:SER:O	8:H:63:LEU:C	2.48	0.51
9:I:95:THR:HG22	9:I:96:SER:N	2.25	0.51
11:K:87:LEU:O	11:K:87:LEU:HD12	2.09	0.51
1:A:1134:ILE:O	1:A:1135:ARG:C	2.49	0.51
1:A:56:PRO:O	1:A:57:ARG:CG	2.57	0.51
1:A:78:PRO:HA	2:B:1201:LYS:HZ1	1.75	0.51
2:B:525:ALA:O	2:B:768:THR:HG23	2.11	0.51
2:B:843:GLN:O	2:B:846:ILE:HB	2.11	0.51
3:C:51:VAL:HG22	3:C:155:LEU:HD21	1.93	0.51
5:E:124:VAL:HG13	5:E:132:ILE:CB	2.39	0.51
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.45	0.51
7:G:123:ALA:O	7:G:125:SER:N	2.43	0.51
8:H:143:LEU:N	8:H:143:LEU:HD12	2.25	0.51
11:K:35:PHE:CD1	11:K:35:PHE:N	2.79	0.51
1:A:1369:ALA:O	1:A:1372:VAL:HG12	2.11	0.51
1:A:516:SER:O	1:A:517:ASN:C	2.47	0.51
1:A:901:LEU:HD22	1:A:919:ILE:HG21	1.91	0.51
1:A:986:ILE:CD1	1:A:1032:LEU:HD11	2.40	0.51
2:B:97:VAL:HG12	2:B:178:ASN:HD21	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:424:LEU:HD22	2:B:453:ILE:HD11	1.92	0.51
2:B:446:LEU:HD23	2:B:446:LEU:N	2.26	0.51
2:B:44:VAL:O	2:B:45:SER:C	2.49	0.51
2:B:496:ARG:HH12	2:B:539:LEU:HB2	1.74	0.51
2:B:59:LEU:HD12	2:B:417:PHE:CE2	2.46	0.51
2:B:708:GLU:HG3	2:B:709:ASP:H	1.76	0.51
3:C:213:PRO:O	3:C:214:ASN:CB	2.55	0.51
5:E:144:ILE:HG13	5:E:145:THR:N	2.26	0.51
10:J:60:PHE:O	10:J:63:TYR:HD1	1.94	0.51
11:K:50:LEU:HD11	11:K:75:ILE:HD13	1.92	0.51
1:A:877:HIS:CG	1:A:1056:SER:HA	2.46	0.51
1:A:1090:ALA:O	1:A:1091:SER:OG	2.28	0.51
1:A:1323:ASP:C	1:A:1325:THR:H	2.14	0.51
1:A:311:GLN:O	1:A:312:PRO:C	2.49	0.51
1:A:470:LEU:CD2	1:A:487:MET:HE3	2.41	0.51
1:A:770:VAL:O	1:A:771:GLU:HB2	2.11	0.51
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.40	0.51
2:B:1065:GLN:NE2	2:B:1067:ARG:HG2	2.25	0.51
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.92	0.51
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.91	0.51
5:E:79:TRP:HE1	5:E:81:GLU:HB2	1.76	0.51
9:I:43:VAL:HG12	9:I:43:VAL:O	2.09	0.51
1:A:1191:TRP:HD1	1:A:1256:GLU:HB2	1.76	0.51
1:A:1349:TYR:CD2	1:A:1349:TYR:C	2.84	0.51
1:A:1372:VAL:HG12	1:A:1373:ASP:N	2.25	0.51
1:A:34:LYS:HG2	1:A:36:ARG:NH2	2.26	0.51
1:A:899:VAL:HG22	1:A:908:LEU:HD21	1.93	0.51
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.25	0.51
2:B:575:PRO:C	2:B:577:ALA:H	2.13	0.51
1:A:472:LEU:CD1	2:B:835:GLN:NE2	2.69	0.51
2:B:857:ARG:HG2	2:B:858:SER:N	2.24	0.51
3:C:60:ASP:OD2	12:L:60:ARG:NH2	2.44	0.51
7:G:6:ASP:HB3	7:G:73:LYS:NZ	2.25	0.51
8:H:40:LEU:HG	8:H:41:ASP:O	2.11	0.51
10:J:5:VAL:O	10:J:6:ARG:O	2.28	0.51
1:A:1030:ARG:CG	1:A:1034:GLU:OE2	2.59	0.51
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.89	0.51
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.46	0.51
1:A:391:LEU:O	1:A:392:VAL:C	2.49	0.51
1:A:525:GLN:HB3	2:B:1015:HIS:HD2	1.74	0.51
1:A:556:TRP:O	1:A:558:GLY:N	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:LYS:C	1:A:707:GLY:N	2.62	0.51
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.75	0.51
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.45	0.51
1:A:92:HIS:O	1:A:93:VAL:C	2.48	0.51
2:B:1202:LEU:O	2:B:1203:LEU:C	2.49	0.51
2:B:209:GLU:CD	2:B:485:ARG:HE	2.14	0.51
2:B:334:ILE:O	2:B:334:ILE:HG22	2.09	0.51
2:B:429:PHE:HA	2:B:432:MET:CE	2.40	0.51
2:B:69:LEU:HD22	2:B:429:PHE:HE1	1.74	0.51
5:E:100:ILE:CG2	5:E:105:PHE:HB2	2.40	0.51
7:G:114:LEU:HG	7:G:162:SER:HB3	1.93	0.51
12:L:49:LYS:O	12:L:50:ASP:CB	2.59	0.51
1:A:1230:GLU:C	1:A:1232:ASN:H	2.14	0.51
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.11	0.51
1:A:1290:LYS:O	1:A:1291:VAL:HG23	2.11	0.51
1:A:1364:ASN:O	1:A:1365:TYR:C	2.49	0.51
1:A:335:ARG:NE	1:A:339:ASN:HD22	2.09	0.51
1:A:384:ASN:O	1:A:385:ILE:C	2.49	0.51
1:A:474:VAL:HG22	1:A:474:VAL:O	2.10	0.51
2:B:1102:LYS:O	2:B:1103:ILE:O	2.29	0.51
2:B:798:TYR:CD1	10:J:4:PRO:HG3	2.45	0.51
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.93	0.51
2:B:936:ASP:OD1	2:B:938:SER:N	2.42	0.51
3:C:35:ARG:HD3	11:K:41:THR:HA	1.93	0.51
1:A:496:GLU:OE1	7:G:64:THR:HA	2.11	0.51
8:H:25:ARG:HA	8:H:41:ASP:HA	1.93	0.51
10:J:46:CYS:O	10:J:49:MET:N	2.44	0.51
10:J:7:CYS:CA	10:J:49:MET:HE3	2.40	0.51
1:A:1168:GLU:OE1	13:S:208:SER:CA	2.59	0.51
1:A:1167:GLU:O	1:A:1169:ILE:N	2.44	0.50
1:A:167:CYS:SG	1:A:167:CYS:O	2.69	0.50
1:A:42:ASP:C	1:A:44:THR:N	2.64	0.50
1:A:774:ARG:O	1:A:775:ILE:C	2.49	0.50
1:A:992:ASP:O	1:A:995:GLU:HB2	2.11	0.50
2:B:212:LEU:HD21	2:B:466:TRP:CH2	2.47	0.50
2:B:763:GLN:C	2:B:765:PRO:HD2	2.32	0.50
2:B:197:PHE:CZ	2:B:816:GLU:HG2	2.46	0.50
3:C:168:ALA:O	3:C:170:TRP:N	2.44	0.50
4:D:47:LEU:HD13	4:D:48:ILE:N	2.25	0.50
4:D:52:LEU:C	4:D:54:GLU:H	2.14	0.50
5:E:10:SER:O	5:E:13:TRP:HB3	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:49:LEU:N	7:G:49:LEU:HD23	2.25	0.50
9:I:58:VAL:HG12	9:I:60:GLN:N	2.20	0.50
12:L:30:ILE:HG22	12:L:31:CYS:O	2.10	0.50
1:A:115:LEU:HB2	1:A:122:MET:CE	2.40	0.50
1:A:1208:THR:O	1:A:1209:MET:C	2.48	0.50
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.26	0.50
1:A:996:ASN:HA	1:A:998:LEU:HD12	1.92	0.50
2:B:242:SER:HB2	2:B:362:PRO:HG2	1.93	0.50
2:B:546:SER:HA	2:B:612:GLU:OE2	2.11	0.50
2:B:488:TYR:HE2	2:B:813:LYS:HB2	1.75	0.50
4:D:51:ASN:O	4:D:52:LEU:C	2.48	0.50
2:B:377:PHE:O	2:B:378:LEU:C	2.50	0.50
2:B:240:ILE:HG21	2:B:381:MET:HE1	1.92	0.50
2:B:510:LYS:O	2:B:513:GLN:HB2	2.11	0.50
7:G:70:PHE:N	7:G:70:PHE:CD1	2.79	0.50
10:J:52:THR:O	10:J:53:HIS:O	2.30	0.50
11:K:68:PHE:N	11:K:68:PHE:CD2	2.77	0.50
1:A:1038:THR:O	1:A:1039:LYS:C	2.49	0.50
1:A:1199:ARG:HG3	1:A:1236:LEU:HD11	1.93	0.50
1:A:1424:VAL:CG2	1:A:1436:ILE:HD11	2.32	0.50
1:A:335:ARG:HA	1:A:339:ASN:ND2	2.26	0.50
1:A:406:ILE:HG22	1:A:411:ASP:O	2.11	0.50
1:A:519:PRO:HG3	1:A:625:SER:O	2.12	0.50
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.75	0.50
2:B:1145:SER:C	2:B:1147:LEU:H	2.14	0.50
2:B:269:ILE:HG22	2:B:282:ILE:HG23	1.94	0.50
2:B:303:TYR:N	2:B:303:TYR:CD2	2.80	0.50
2:B:996:ARG:HH22	3:C:175:ALA:HA	1.75	0.50
3:C:239:PRO:HB2	3:C:241:ASP:OD1	2.12	0.50
3:C:33:LEU:HG	3:C:37:MET:HE2	1.92	0.50
3:C:53:THR:O	3:C:153:LEU:HA	2.10	0.50
3:C:88:CYS:O	3:C:88:CYS:SG	2.70	0.50
5:E:42:PHE:O	5:E:43:LYS:C	2.50	0.50
6:F:119:ARG:HH11	6:F:119:ARG:CG	2.25	0.50
9:I:58:VAL:HG13	9:I:62:ILE:HD12	1.93	0.50
10:J:64:ASN:HB3	10:J:65:PRO:HD2	1.84	0.50
1:A:590:ARG:O	1:A:591:PHE:HB2	2.12	0.50
1:A:864:ILE:HG22	1:A:864:ILE:O	2.10	0.50
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.93	0.50
2:B:1029:CYS:SG	2:B:1086:PHE:CE2	3.05	0.50
2:B:1074:ASN:O	2:B:1078:GLY:N	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:LEU:O	2:B:51:PHE:N	2.44	0.50
2:B:681:TRP:C	2:B:683:SER:H	2.14	0.50
2:B:809:MET:O	2:B:812:LEU:N	2.37	0.50
1:A:472:LEU:CD1	2:B:835:GLN:CD	2.79	0.50
2:B:839:MET:N	2:B:989:THR:O	2.44	0.50
3:C:235:VAL:HG13	10:J:13:VAL:CG2	2.40	0.50
3:C:43:THR:CG2	3:C:44:LEU:N	2.74	0.50
10:J:1:MET:HE2	10:J:60:PHE:CE2	2.46	0.50
1:A:1308:THR:HG23	1:A:1309:ASP:N	2.26	0.50
1:A:1341:ILE:O	1:A:1344:GLY:N	2.45	0.50
1:A:1344:GLY:O	1:A:1345:ARG:C	2.50	0.50
1:A:148:CYS:O	1:A:168:GLY:HA2	2.12	0.50
1:A:50:ILE:O	1:A:52:GLY:N	2.39	0.50
2:B:758:PHE:HE2	2:B:1044:ALA:HA	1.73	0.50
2:B:1149:GLU:O	2:B:1150:ARG:C	2.47	0.50
4:D:26:THR:O	4:D:28:GLN:HG3	2.11	0.50
7:G:91:VAL:HA	7:G:101:VAL:HA	1.94	0.50
10:J:1:MET:HA	10:J:57:ILE:H	1.76	0.50
10:J:21:TYR:O	10:J:23:ASN:N	2.44	0.50
1:A:547:LEU:HD22	11:K:58:PHE:CE1	2.46	0.50
1:A:1114:PRO:O	1:A:1311:VAL:HG21	2.11	0.50
1:A:1398:MET:HB2	1:A:1426:GLU:OE2	2.11	0.50
1:A:265:LYS:NZ	1:A:322:VAL:HG22	2.27	0.50
1:A:719:VAL:O	1:A:721:PHE:N	2.45	0.50
1:A:744:LYS:HG2	1:A:748:MET:CE	2.41	0.50
2:B:851:PHE:CD2	2:B:1094:ARG:HB2	2.46	0.50
5:E:3:GLN:HG3	5:E:4:GLU:N	2.27	0.50
10:J:21:TYR:C	10:J:23:ASN:H	2.15	0.50
11:K:84:LYS:O	11:K:87:LEU:HB3	2.12	0.50
1:A:1053:PHE:O	1:A:1056:SER:N	2.44	0.50
1:A:1410:PHE:C	1:A:1412:ALA:H	2.15	0.50
1:A:208:LEU:HG	1:A:235:ILE:HG21	1.93	0.50
1:A:556:TRP:C	1:A:558:GLY:N	2.65	0.50
1:A:709:THR:CG2	1:A:712:GLU:H	2.23	0.50
2:B:1022:THR:HG23	2:B:1022:THR:O	2.12	0.50
2:B:1060:ARG:NH1	2:B:1060:ARG:HG2	2.27	0.50
1:A:22:PHE:CE1	2:B:1213:THR:HG22	2.47	0.50
2:B:196:PRO:HG2	2:B:197:PHE:H	1.77	0.50
2:B:376:PHE:HB3	2:B:586:TRP:CZ3	2.46	0.50
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.35	0.50
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:53:SER:HB3	4:D:152:SER:CB	2.42	0.50
5:E:7:ARG:C	5:E:9:ILE:N	2.65	0.50
6:F:127:GLU:O	6:F:129:LYS:HG3	2.12	0.50
1:A:1125:ALA:O	1:A:1127:ASP:N	2.45	0.50
1:A:1213:GLY:HA2	1:A:1216:ILE:CD1	2.42	0.50
1:A:12:ARG:CZ	2:B:1192:TYR:HE2	2.25	0.50
1:A:726:ARG:O	1:A:727:ASP:C	2.50	0.50
2:B:210:LYS:HE2	2:B:462:ALA:O	2.11	0.50
2:B:218:SER:O	2:B:219:ALA:O	2.29	0.50
2:B:578:THR:HA	2:B:622:LYS:HB3	1.94	0.50
2:B:806:THR:O	2:B:807:ARG:C	2.50	0.50
2:B:843:GLN:O	2:B:846:ILE:N	2.44	0.50
2:B:877:PRO:C	2:B:878:GLN:HG3	2.31	0.50
2:B:91:SER:OG	2:B:133:LYS:HB2	2.11	0.50
6:F:103:MET:O	6:F:104:ASN:HB2	2.11	0.50
8:H:81:PRO:HB3	8:H:82:PRO:HD2	1.92	0.50
12:L:28:LYS:HB2	12:L:39:SER:CA	2.42	0.50
12:L:60:ARG:HG2	12:L:61:THR:N	2.27	0.50
1:A:416:ARG:O	1:A:417:TYR:HD2	1.94	0.49
1:A:541:ILE:HD12	1:A:577:ILE:HD11	1.94	0.49
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.12	0.49
1:A:853:ASP:C	1:A:853:ASP:OD1	2.51	0.49
1:A:863:VAL:HG12	1:A:865:GLN:H	1.76	0.49
2:B:984:HIS:CD2	2:B:1025:HIS:HB2	2.47	0.49
1:A:347:PHE:N	2:B:1107:ALA:HA	2.26	0.49
2:B:1131:GLY:O	2:B:1132:GLU:C	2.50	0.49
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.94	0.49
2:B:763:GLN:HG2	2:B:765:PRO:CD	2.38	0.49
2:B:999:MET:HA	2:B:999:MET:CE	2.42	0.49
3:C:63:ILE:O	3:C:64:ALA:C	2.50	0.49
4:D:134:THR:CG2	4:D:135:GLY:N	2.75	0.49
6:F:93:ILE:O	6:F:94:LEU:C	2.49	0.49
7:G:96:GLN:HG3	7:G:97:HIS:HD2	1.76	0.49
8:H:93:TYR:N	8:H:93:TYR:CD1	2.80	0.49
3:C:84:ARG:NH2	11:K:11:LEU:HD21	2.27	0.49
1:A:1019:CYS:O	1:A:1022:LEU:N	2.45	0.49
1:A:1161:THR:O	1:A:1163:ILE:N	2.45	0.49
1:A:1364:ASN:HD22	1:A:1365:TYR:N	2.10	0.49
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.93	0.49
1:A:14:VAL:CG2	1:A:1430:LEU:HD13	2.42	0.49
1:A:254:GLU:HB2	2:B:935:ARG:NH2	2.25	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:PHE:HA	1:A:758:ILE:HG13	1.94	0.49
1:A:989:GLY:O	1:A:992:ASP:N	2.44	0.49
2:B:215:GLN:OE1	2:B:215:GLN:HA	2.12	0.49
2:B:25:ILE:HG23	2:B:29:ASP:CB	2.42	0.49
2:B:314:LEU:O	2:B:317:CYS:HB3	2.12	0.49
2:B:459:TYR:CD2	2:B:459:TYR:C	2.85	0.49
2:B:526:GLU:HG2	2:B:538:ASN:HD22	1.77	0.49
2:B:850:LEU:HD12	2:B:851:PHE:H	1.77	0.49
3:C:143:LEU:HD21	3:C:146:LYS:HE2	1.94	0.49
3:C:86:CYS:SG	3:C:95:CYS:HB3	2.52	0.49
4:D:144:THR:OG1	7:G:105:PRO:HD3	2.12	0.49
4:D:48:ILE:HG21	7:G:4:ILE:CD1	2.41	0.49
6:F:72:LYS:HB2	6:F:142:SER:HB3	1.94	0.49
7:G:25:TYR:HE2	7:G:29:LYS:HD2	1.77	0.49
8:H:58:THR:HB	8:H:143:LEU:HD13	1.94	0.49
9:I:113:ASP:O	9:I:114:GLN:CG	2.61	0.49
13:S:269:PHE:HE2	13:S:306:TRP:CZ2	2.30	0.49
1:A:1041:ALA:O	1:A:1044:TRP:HB3	2.12	0.49
1:A:1048:ASN:HD22	1:A:1048:ASN:N	2.10	0.49
1:A:838:GLN:O	1:A:842:VAL:HG23	2.13	0.49
1:A:903:ASN:C	1:A:903:ASN:ND2	2.65	0.49
1:A:90:VAL:CG1	1:A:91:PHE:H	2.23	0.49
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.47	0.49
2:B:261:ARG:HH11	2:B:261:ARG:HB3	1.76	0.49
2:B:882:THR:HB	2:B:934:LYS:O	2.11	0.49
3:C:186:LEU:N	3:C:186:LEU:CD1	2.75	0.49
3:C:69:LEU:HD12	3:C:69:LEU:N	2.27	0.49
5:E:164:LEU:CD2	5:E:211:TYR:CD2	2.95	0.49
5:E:23:VAL:O	5:E:28:TYR:HB2	2.12	0.49
1:A:1127:ASP:O	1:A:1128:GLN:C	2.50	0.49
1:A:1285:MET:HG3	1:A:1307:GLU:OE2	2.12	0.49
1:A:24:PRO:HG2	1:A:25:GLU:OE2	2.11	0.49
1:A:564:ALA:HB2	1:A:576:GLN:OE1	2.12	0.49
1:A:717:ASN:O	1:A:721:PHE:CD1	2.66	0.49
1:A:874:ASP:N	1:A:1058:VAL:HG23	2.27	0.49
1:A:997:LEU:HB3	1:A:1053:PHE:CE2	2.47	0.49
2:B:1165:ILE:HG22	2:B:1185:CYS:HB3	1.94	0.49
2:B:247:GLY:C	2:B:249:ARG:H	2.16	0.49
2:B:583:ASN:HD21	2:B:628:THR:CB	2.13	0.49
2:B:563:MET:HA	2:B:589:VAL:O	2.13	0.49
5:E:124:VAL:CG1	5:E:132:ILE:HD12	2.37	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:4:PHE:CE1	9:I:13:MET:HE1	2.47	0.49
1:A:1360:GLY:HA3	13:S:306:TRP:HA	1.94	0.49
1:A:1444:MET:HG2	7:G:60:ARG:CA	2.40	0.49
1:A:470:LEU:HD11	1:A:482:PHE:CZ	2.46	0.49
1:A:472:LEU:HD13	2:B:835:GLN:CD	2.33	0.49
1:A:821:ARG:HA	1:A:824:LEU:HD12	1.95	0.49
1:A:979:SER:HG	1:A:980:ASP:H	1.58	0.49
2:B:1177:HIS:O	2:B:1179:GLN:N	2.44	0.49
2:B:175:ARG:HH11	2:B:175:ARG:HG2	1.77	0.49
2:B:642:ASP:HA	2:B:649:LYS:HA	1.95	0.49
2:B:526:GLU:CD	2:B:752:ALA:HB2	2.32	0.49
2:B:497:ARG:NH2	2:B:775:LYS:NZ	2.60	0.49
5:E:72:PHE:CD1	5:E:72:PHE:N	2.80	0.49
4:D:147:TYR:CZ	7:G:103:VAL:HG13	2.47	0.49
1:A:37:PHE:N	1:A:37:PHE:CD1	2.81	0.49
1:A:601:LYS:HB2	1:A:603:ASN:ND2	2.27	0.49
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.78	0.49
1:A:869:GLY:O	1:A:870:GLU:HB2	2.11	0.49
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.47	0.49
3:C:73:GLN:HE21	3:C:74:SER:H	1.60	0.49
7:G:30:LEU:O	7:G:34:VAL:HG23	2.12	0.49
9:I:27:PHE:O	9:I:28:GLU:HB3	2.11	0.49
1:A:1090:ALA:O	1:A:1091:SER:CB	2.60	0.49
1:A:88:LYS:HE3	1:A:280:GLU:OE2	2.12	0.49
1:A:321:PRO:O	1:A:322:VAL:HB	2.13	0.49
1:A:387:ARG:O	1:A:390:GLN:HB3	2.13	0.49
1:A:809:THR:H	1:A:812:GLU:HB2	1.78	0.49
2:B:1002:THR:O	2:B:1005:GLY:N	2.32	0.49
2:B:1106:ARG:HD3	2:B:1126:GLY:O	2.12	0.49
2:B:54:PHE:O	2:B:59:LEU:HB2	2.12	0.49
2:B:693:ILE:HD11	2:B:740:HIS:NE2	2.27	0.49
2:B:757:PRO:O	2:B:758:PHE:HB2	2.13	0.49
2:B:899:ILE:HG22	2:B:900:ALA:H	1.75	0.49
4:D:127:ASP:O	4:D:131:GLU:HG3	2.13	0.49
4:D:56:ARG:NH2	4:D:155:ARG:HA	2.28	0.49
4:D:53:SER:O	4:D:57:LEU:HG	2.12	0.49
8:H:143:LEU:C	8:H:144:ILE:HG13	2.33	0.49
8:H:27:GLU:HA	8:H:38:LEU:O	2.12	0.49
9:I:13:MET:HG3	9:I:14:LEU:N	2.27	0.49
1:A:1086:PHE:HE2	13:S:261:ILE:CD1	2.24	0.49
1:A:3:GLY:O	1:A:4:GLN:O	2.31	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:ASN:O	1:A:628:GLY:N	2.42	0.49
1:A:711:ARG:HA	9:I:97:MET:HE1	1.95	0.49
1:A:877:HIS:C	1:A:878:ILE:HG13	2.33	0.49
2:B:1059:LEU:HD23	2:B:1065:GLN:O	2.12	0.49
1:A:433:GLU:OE2	2:B:1108:ARG:NH1	2.45	0.49
2:B:189:LEU:HD13	2:B:196:PRO:HA	1.94	0.49
2:B:247:GLY:H	2:B:418:LYS:NZ	2.10	0.49
2:B:361:LEU:N	2:B:362:PRO:CD	2.75	0.49
2:B:681:TRP:C	2:B:683:SER:N	2.66	0.49
2:B:910:VAL:CG1	2:B:911:ILE:N	2.76	0.49
2:B:97:VAL:CG1	2:B:178:ASN:ND2	2.74	0.49
4:D:170:THR:HG21	4:D:172:LEU:HG	1.94	0.49
4:D:173:HIS:O	4:D:177:VAL:HG23	2.13	0.49
12:L:31:CYS:HB3	12:L:35:SER:CA	2.42	0.49
1:A:1230:GLU:CD	13:S:201:ILE:CA	2.73	0.49
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.94	0.49
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.13	0.49
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.95	0.49
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.95	0.49
1:A:907:THR:CG2	1:A:908:LEU:N	2.75	0.49
2:B:1034:VAL:HG23	2:B:1059:LEU:HD12	1.95	0.49
2:B:234:ILE:HD12	2:B:234:ILE:N	2.27	0.49
2:B:446:LEU:O	2:B:447:ALA:CB	2.61	0.49
2:B:510:LYS:HG2	2:B:512:ARG:N	2.19	0.49
2:B:992:ILE:CG2	2:B:994:TYR:HE1	2.26	0.49
5:E:136:ASN:OD1	5:E:137:GLU:N	2.46	0.49
5:E:32:GLN:HG3	5:E:36:GLU:OE2	2.12	0.49
8:H:33:GLN:C	8:H:35:GLN:H	2.16	0.49
10:J:37:SER:OG	10:J:47:ARG:NH2	2.46	0.49
11:K:32:VAL:HG22	11:K:74:ARG:HG3	1.95	0.49
1:A:356:ASP:C	1:A:358:ASN:H	2.16	0.49
1:A:481:ASP:O	1:A:485:ASP:HB2	2.13	0.49
1:A:501:LEU:HD11	2:B:1146:PHE:CD2	2.48	0.49
2:B:594:ALA:CA	2:B:617:ARG:HH12	2.25	0.49
3:C:80:LEU:HD22	3:C:129:ILE:HD13	1.94	0.49
3:C:47:ASP:O	3:C:48:SER:HB2	2.13	0.49
5:E:25:ASP:C	5:E:27:GLY:N	2.63	0.49
8:H:142:LEU:C	8:H:143:LEU:HD12	2.33	0.49
1:A:618:GLU:CD	1:A:618:GLU:C	2.71	0.48
1:A:525:GLN:HB3	2:B:1015:HIS:CD2	2.48	0.48
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.33	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:760:ASP:O	2:B:761:HIS:CD2	2.66	0.48
6:F:72:LYS:O	6:F:73:ALA:CB	2.61	0.48
7:G:101:VAL:CG1	7:G:102:GLN:N	2.76	0.48
1:A:1329:THR:O	1:A:1330:ASN:C	2.50	0.48
2:B:102:VAL:CG2	2:B:112:LEU:HD22	2.43	0.48
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.95	0.48
2:B:498:THR:HG22	2:B:537:LYS:H	1.78	0.48
2:B:811:TYR:N	2:B:811:TYR:CD1	2.80	0.48
2:B:845:SER:HB3	10:J:8:PHE:O	2.13	0.48
3:C:136:ASP:OD1	3:C:138:GLU:N	2.45	0.48
3:C:111:THR:O	3:C:147:LEU:HD23	2.12	0.48
3:C:168:ALA:C	3:C:170:TRP:H	2.17	0.48
5:E:17:ARG:O	5:E:20:LYS:HB2	2.13	0.48
1:A:852:TYR:CE1	6:F:136:ARG:HB3	2.48	0.48
7:G:15:PRO:O	7:G:18:PHE:HB2	2.12	0.48
12:L:30:ILE:CG2	12:L:31:CYS:N	2.75	0.48
1:A:1263:ILE:O	1:A:1263:ILE:HG22	2.14	0.48
1:A:1308:THR:O	1:A:1309:ASP:HB2	2.12	0.48
1:A:503:GLN:O	1:A:504:LEU:HD12	2.13	0.48
1:A:543:LEU:O	1:A:544:ASP:C	2.52	0.48
1:A:348:SER:HB2	2:B:1128:LEU:HD12	1.93	0.48
2:B:1208:MET:HA	2:B:1212:ILE:O	2.13	0.48
2:B:38:PHE:HD1	2:B:811:TYR:CD2	2.31	0.48
1:A:472:LEU:HD13	2:B:835:GLN:OE1	2.13	0.48
2:B:899:ILE:HG23	2:B:903:VAL:HG21	1.95	0.48
4:D:60:LYS:O	4:D:61:GLU:C	2.51	0.48
5:E:204:THR:HG23	5:E:205:SER:N	2.29	0.48
8:H:10:PHE:N	8:H:10:PHE:CD1	2.81	0.48
10:J:36:LEU:HB2	10:J:47:ARG:NH1	2.28	0.48
10:J:61:LEU:C	10:J:63:TYR:H	2.16	0.48
1:A:780:VAL:O	1:A:780:VAL:HG12	2.14	0.48
1:A:877:HIS:O	1:A:878:ILE:CG1	2.61	0.48
1:A:929:LEU:HD23	1:A:983:ILE:HG21	1.95	0.48
2:B:579:ARG:HG2	2:B:579:ARG:HH11	1.79	0.48
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.41	0.48
2:B:616:ILE:N	2:B:625:LYS:O	2.37	0.48
2:B:760:ASP:OD1	2:B:1046:PRO:HA	2.12	0.48
2:B:976:ILE:O	2:B:990:ILE:HB	2.12	0.48
3:C:164:ALA:O	3:C:167:HIS:N	2.43	0.48
6:F:99:LEU:O	6:F:103:MET:HG2	2.14	0.48
10:J:3:VAL:HG12	10:J:4:PRO:N	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.96	0.48
13:S:254:TYR:C	13:S:256:ALA:H	2.17	0.48
13:S:274:CYS:O	13:S:276:GLU:HG3	2.13	0.48
1:A:1072:ILE:C	1:A:1075:PRO:HD2	2.33	0.48
1:A:1272:THR:C	1:A:1273:LEU:HD12	2.34	0.48
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.96	0.48
1:A:1372:VAL:HG12	1:A:1373:ASP:H	1.78	0.48
1:A:22:PHE:CD1	2:B:1213:THR:HG22	2.49	0.48
2:B:112:LEU:CD1	2:B:113:TYR:N	2.71	0.48
2:B:293:PRO:C	2:B:294:ASP:O	2.47	0.48
2:B:508:LEU:CA	2:B:510:LYS:H	2.24	0.48
2:B:658:ILE:HG22	2:B:659:ALA:N	2.28	0.48
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.44	0.48
3:C:173:ALA:O	3:C:174:ALA:HB3	2.13	0.48
3:C:8:VAL:HG12	3:C:9:LYS:N	2.28	0.48
4:D:190:GLU:O	4:D:194:LEU:HG	2.14	0.48
4:D:208:GLU:O	4:D:212:LYS:HG3	2.13	0.48
5:E:163:GLU:O	5:E:164:LEU:C	2.51	0.48
5:E:16:PHE:CE2	5:E:20:LYS:HE2	2.48	0.48
7:G:145:VAL:CG1	7:G:146:LYS:H	2.27	0.48
7:G:6:ASP:C	7:G:7:LEU:HD23	2.33	0.48
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.23	0.48
1:A:1029:ARG:HG3	1:A:1029:ARG:NH1	2.17	0.48
1:A:1051:ALA:O	1:A:1054:LEU:N	2.47	0.48
1:A:122:MET:O	1:A:123:ARG:C	2.51	0.48
1:A:228:PHE:CD2	1:A:228:PHE:N	2.81	0.48
1:A:817:ALA:O	1:A:818:MET:C	2.52	0.48
1:A:863:VAL:HG12	1:A:864:ILE:H	1.77	0.48
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.96	0.48
1:A:896:ARG:CD	1:A:897:TYR:HE1	2.12	0.48
1:A:814:PHE:CD1	2:B:519:TRP:HE3	2.32	0.48
2:B:583:ASN:OD1	2:B:628:THR:N	2.47	0.48
2:B:976:ILE:CD1	2:B:992:ILE:HA	2.41	0.48
3:C:116:LYS:HD3	3:C:140:ASN:HB3	1.95	0.48
3:C:263:THR:O	3:C:265:MET:N	2.47	0.48
8:H:83:GLN:O	8:H:85:GLY:N	2.44	0.48
2:B:992:ILE:HD11	11:K:66:PRO:HB2	1.96	0.48
11:K:65:HIS:CD2	11:K:66:PRO:N	2.81	0.48
1:A:1057:VAL:CG1	1:A:1058:VAL:N	2.76	0.48
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.96	0.48
1:A:335:ARG:NH1	2:B:1206:GLU:CD	2.65	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ASP:OD1	1:A:45:GLN:HA	2.13	0.48
1:A:821:ARG:CB	1:A:821:ARG:HH11	2.25	0.48
1:A:939:ASP:O	1:A:940:ARG:C	2.50	0.48
2:B:371:GLU:H	2:B:371:GLU:CD	2.17	0.48
2:B:525:ALA:O	2:B:527:THR:HG22	2.13	0.48
2:B:764:SER:N	2:B:765:PRO:HD2	2.29	0.48
2:B:797:TYR:HB3	2:B:798:TYR:CD2	2.49	0.48
3:C:168:ALA:C	3:C:170:TRP:N	2.67	0.48
6:F:111:LEU:O	6:F:113:GLY:N	2.47	0.48
8:H:82:PRO:O	8:H:83:GLN:HB2	2.13	0.48
8:H:89:LEU:O	8:H:91:ASP:N	2.39	0.48
11:K:81:TYR:OH	11:K:86:ALA:HA	2.13	0.48
13:S:236:LEU:CA	13:S:242:LYS:NZ	2.77	0.48
13:S:254:TYR:O	13:S:256:ALA:N	2.47	0.48
1:A:1059:HIS:O	1:A:1061:GLY:N	2.46	0.48
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.29	0.48
1:A:329:LEU:N	1:A:329:LEU:HD23	2.28	0.48
1:A:375:THR:HA	1:A:434:ARG:O	2.14	0.48
1:A:437:MET:O	1:A:438:ASP:C	2.50	0.48
1:A:821:ARG:O	1:A:821:ARG:HG3	2.12	0.48
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.95	0.48
2:B:1149:GLU:C	2:B:1151:LEU:N	2.67	0.48
2:B:458:LYS:O	2:B:459:TYR:C	2.50	0.48
2:B:509:ALA:O	2:B:510:LYS:O	2.32	0.48
2:B:619:ILE:C	2:B:621:GLU:H	2.17	0.48
2:B:825:VAL:CG1	2:B:826:ALA:N	2.77	0.48
3:C:22:LEU:HD13	3:C:230:MET:CE	2.44	0.48
4:D:196:PRO:C	4:D:198:LEU:N	2.67	0.48
5:E:46:TYR:CD2	5:E:58:MET:HG2	2.48	0.48
1:A:1265:ASN:O	1:A:1267:MET:N	2.47	0.48
1:A:1313:LEU:O	1:A:1314:SER:C	2.52	0.48
1:A:14:VAL:HG21	1:A:1430:LEU:HD13	1.96	0.48
1:A:590:ARG:HD3	1:A:604:GLY:CA	2.41	0.48
1:A:68:GLN:NE2	1:A:80:HIS:CD2	2.79	0.48
1:A:823:GLY:C	1:A:825:ILE:N	2.66	0.48
2:B:1135:ARG:NH2	2:B:1136:ASP:OD1	2.38	0.48
2:B:294:ASP:C	2:B:296:GLU:N	2.68	0.48
2:B:295:GLY:H	2:B:298:LEU:CD2	2.13	0.48
2:B:273:LEU:HD21	2:B:360:PHE:CD1	2.48	0.48
2:B:617:ARG:NE	2:B:619:ILE:HG12	2.29	0.48
2:B:681:TRP:O	2:B:683:SER:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.44	0.48
6:F:109:VAL:HG12	6:F:110:ASP:N	2.29	0.48
8:H:106:GLU:HG2	8:H:112:ILE:HG12	1.96	0.48
11:K:21:ILE:HG23	11:K:31:VAL:CG1	2.44	0.48
12:L:39:SER:O	12:L:40:LEU:HG	2.14	0.48
1:A:1293:SER:OG	1:A:1295:THR:CG2	2.62	0.48
1:A:315:LEU:HD22	1:A:319:GLY:O	2.13	0.48
1:A:779:PHE:O	1:A:780:VAL:C	2.52	0.48
2:B:1002:THR:HG22	2:B:1006:ILE:O	2.14	0.48
2:B:223:VAL:HG11	2:B:381:MET:HG2	1.96	0.48
2:B:465:ASN:HD22	2:B:465:ASN:N	2.12	0.48
2:B:910:VAL:HG12	2:B:911:ILE:H	1.79	0.48
3:C:143:LEU:HD21	3:C:146:LYS:CE	2.43	0.48
4:D:185:CYS:HB3	4:D:211:LEU:HD13	1.95	0.48
7:G:88:ASP:HB3	7:G:144:ARG:HB2	1.95	0.48
10:J:7:CYS:HA	10:J:49:MET:HE3	1.95	0.48
13:S:253:LEU:O	13:S:256:ALA:HB3	2.14	0.48
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.14	0.47
1:A:261:ASP:O	1:A:264:PHE:HB2	2.13	0.47
1:A:393:ARG:O	1:A:395:GLY:N	2.47	0.47
1:A:418:SER:O	1:A:421:ALA:N	2.46	0.47
1:A:356:ASP:HB2	1:A:469:ARG:HG2	1.96	0.47
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.96	0.47
2:B:540:SER:HA	2:B:749:LEU:O	2.14	0.47
2:B:806:THR:HG22	2:B:808:ALA:HB3	1.94	0.47
3:C:42:PRO:HA	3:C:163:ILE:CG2	2.44	0.47
5:E:44:ALA:O	5:E:45:LYS:HB2	2.13	0.47
6:F:132:LEU:O	6:F:148:VAL:HG22	2.14	0.47
10:J:57:ILE:CA	10:J:60:PHE:CD2	2.90	0.47
1:A:1116:LEU:HA	1:A:1329:THR:HA	1.96	0.47
1:A:1283:VAL:CG1	1:A:1284:MET:H	2.24	0.47
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.27	0.47
1:A:928:LEU:O	1:A:931:GLU:N	2.47	0.47
2:B:1017:ILE:HG22	2:B:1018:PRO:CD	2.44	0.47
2:B:486:TYR:CG	2:B:1096:ARG:NH2	2.82	0.47
2:B:1150:ARG:HE	2:B:1150:ARG:HA	1.79	0.47
2:B:1159:ARG:CD	2:B:1193:GLN:HE21	2.26	0.47
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.95	0.47
2:B:457:LEU:O	2:B:461:LEU:CD1	2.61	0.47
2:B:689:LEU:O	2:B:690:VAL:HG23	2.14	0.47
2:B:810:GLU:HG3	2:B:815:ARG:HH22	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:942:ARG:O	2:B:944:THR:N	2.48	0.47
3:C:79:GLN:O	3:C:127:ARG:NH1	2.46	0.47
3:C:242:GLN:CA	3:C:245:VAL:HG23	2.43	0.47
3:C:27:LEU:O	3:C:30:ALA:N	2.47	0.47
5:E:157:SER:C	5:E:159:ASP:N	2.68	0.47
8:H:84:ALA:HB2	8:H:87:ARG:HD2	1.96	0.47
9:I:2:THR:HG22	9:I:2:THR:O	2.14	0.47
1:A:1104:ILE:O	1:A:1105:LEU:C	2.53	0.47
1:A:81:PHE:CE2	1:A:242:PRO:HA	2.48	0.47
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.50	0.47
1:A:419:LYS:HG3	1:A:420:ARG:N	2.28	0.47
1:A:993:LEU:HD11	1:A:997:LEU:HD21	1.96	0.47
2:B:168:GLY:N	2:B:450:ALA:HB1	2.14	0.47
2:B:510:LYS:HD3	2:B:510:LYS:O	2.13	0.47
2:B:846:ILE:HG23	2:B:974:PRO:CG	2.36	0.47
2:B:992:ILE:HG21	2:B:994:TYR:HE1	1.79	0.47
3:C:191:TYR:CD2	3:C:201:TRP:CD1	2.97	0.47
7:G:1:MET:HE1	7:G:80:LYS:H	1.79	0.47
1:A:1090:ALA:CB	1:A:1093:LYS:HE3	2.43	0.47
1:A:1263:ILE:O	1:A:1267:MET:HG3	2.15	0.47
1:A:789:LYS:HE3	9:I:67:THR:HB	1.97	0.47
1:A:852:TYR:CD2	1:A:1060:PRO:CB	2.97	0.47
1:A:944:ARG:NE	1:A:1298:TYR:HE1	2.12	0.47
2:B:413:LEU:O	2:B:414:ALA:C	2.52	0.47
1:A:1006:ILE:HD11	5:E:163:GLU:CG	2.44	0.47
8:H:128:ASN:CG	8:H:128:ASN:O	2.52	0.47
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.94	0.47
1:A:1157:ASP:C	1:A:1159:ARG:H	2.18	0.47
1:A:1193:LEU:HD12	1:A:1193:LEU:C	2.35	0.47
1:A:125:ALA:O	1:A:127:ALA:N	2.48	0.47
1:A:1335:ILE:O	1:A:1335:ILE:CG2	2.63	0.47
2:B:1033:LYS:HB2	2:B:1089:PRO:HD2	1.97	0.47
4:D:51:ASN:O	4:D:52:LEU:O	2.33	0.47
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.96	0.47
10:J:48:ARG:HE	10:J:49:MET:CE	2.28	0.47
11:K:65:HIS:CD2	11:K:65:HIS:C	2.87	0.47
12:L:27:LEU:HD13	12:L:37:LYS:HE2	1.96	0.47
12:L:58:LYS:HG2	12:L:58:LYS:O	2.15	0.47
1:A:1051:ALA:C	1:A:1053:PHE:N	2.67	0.47
1:A:1057:VAL:CG1	1:A:1058:VAL:H	2.26	0.47
1:A:1216:ILE:O	1:A:1219:THR:HB	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1280:GLU:O	1:A:1281:ARG:C	2.52	0.47
1:A:399:HIS:CB	1:A:400:PRO:CD	2.87	0.47
1:A:447:GLN:HB3	1:A:448:PRO:HA	1.97	0.47
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.96	0.47
1:A:606:LEU:CB	1:A:614:PHE:CE2	2.97	0.47
1:A:814:PHE:C	1:A:814:PHE:CD2	2.88	0.47
1:A:962:ARG:O	1:A:964:ILE:N	2.47	0.47
2:B:1210:MET:O	2:B:1212:ILE:N	2.47	0.47
2:B:314:LEU:O	2:B:315:LYS:C	2.53	0.47
2:B:363:HIS:NE2	2:B:364:ILE:HG13	2.29	0.47
2:B:619:ILE:O	2:B:621:GLU:N	2.47	0.47
2:B:752:ALA:HB1	2:B:771:SER:HB3	1.96	0.47
2:B:798:TYR:CD2	2:B:798:TYR:N	2.83	0.47
2:B:903:VAL:CG1	2:B:904:ARG:N	2.76	0.47
3:C:227:THR:C	3:C:228:PHE:CD1	2.87	0.47
9:I:58:VAL:HG13	9:I:62:ILE:CD1	2.44	0.47
1:A:711:ARG:HA	9:I:97:MET:CE	2.44	0.47
1:A:1102:LYS:C	1:A:1106:ASN:HD22	2.18	0.47
1:A:1129:GLU:C	1:A:1131:ALA:N	2.67	0.47
1:A:1330:ASN:C	1:A:1330:ASN:OD1	2.52	0.47
1:A:650:GLN:O	1:A:654:ASN:HB2	2.14	0.47
2:B:221:ASN:OD1	2:B:242:SER:HA	2.14	0.47
2:B:298:LEU:H	2:B:298:LEU:CD2	2.27	0.47
2:B:371:GLU:OE1	2:B:371:GLU:N	2.48	0.47
2:B:544:CYS:O	2:B:545:ILE:HG13	2.15	0.47
1:A:253:ASN:OD1	2:B:884:ARG:HD2	2.14	0.47
3:C:206:ASN:OD1	3:C:229:TYR:CD2	2.67	0.47
5:E:167:ARG:O	5:E:168:TYR:HD2	1.97	0.47
7:G:62:LEU:HB3	7:G:63:PRO:HD2	1.95	0.47
8:H:102:TYR:HD2	8:H:102:TYR:H	1.51	0.47
9:I:5:ARG:O	9:I:14:LEU:HD12	2.13	0.47
1:A:1081:LEU:HD21	1:A:1098:VAL:CB	2.44	0.47
1:A:1227:ILE:O	1:A:1228:TRP:HB3	2.14	0.47
1:A:1311:VAL:HG21	1:A:1329:THR:HG23	1.96	0.47
1:A:1388:GLY:O	1:A:1391:ARG:HG2	2.15	0.47
1:A:302:THR:HA	1:A:305:ASP:O	2.14	0.47
1:A:53:LEU:HD23	1:A:54:ASN:CB	2.45	0.47
1:A:794:PRO:C	1:A:796:SER:H	2.18	0.47
1:A:814:PHE:O	1:A:817:ALA:HB3	2.15	0.47
1:A:897:TYR:HD2	1:A:936:LEU:CD1	2.28	0.47
1:A:451:HIS:O	2:B:1137:CYS:SG	2.73	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1191:ILE:C	2:B:1192:TYR:CD1	2.88	0.47
2:B:847:ASP:OD2	11:K:6:ARG:NH2	2.48	0.47
4:D:220:LEU:O	4:D:221:TYR:HD1	1.97	0.47
6:F:124:GLU:HB3	6:F:130:ILE:HG12	1.95	0.47
6:F:124:GLU:O	6:F:130:ILE:HG13	2.14	0.47
8:H:39:THR:HB	8:H:124:ARG:HB3	1.97	0.47
11:K:113:THR:O	11:K:114:LEU:CB	2.58	0.47
1:A:795:GLU:CD	1:A:795:GLU:N	2.59	0.47
1:A:937:VAL:C	1:A:939:ASP:N	2.68	0.47
1:A:95:PHE:HD1	1:A:234:MET:CG	2.25	0.47
2:B:1155:SER:OG	2:B:1156:ASP:N	2.47	0.47
2:B:51:PHE:O	2:B:52:ASN:C	2.53	0.47
2:B:831:SER:HB2	2:B:833:TYR:HD1	1.79	0.47
2:B:899:ILE:HG22	2:B:903:VAL:HG21	1.95	0.47
1:A:254:GLU:H	2:B:935:ARG:HH12	1.63	0.47
3:C:109:SER:O	3:C:110:THR:O	2.32	0.47
5:E:143:ASN:OD1	5:E:187:TYR:CE1	2.68	0.47
5:E:177:ARG:O	5:E:212:ARG:HD3	2.15	0.47
5:E:93:MET:C	5:E:95:THR:N	2.68	0.47
6:F:128:LYS:HD3	6:F:149:GLU:O	2.15	0.47
9:I:65:ASP:OD1	9:I:67:THR:OG1	2.21	0.47
10:J:8:PHE:CE1	10:J:49:MET:SD	3.08	0.47
11:K:12:LEU:HD23	11:K:16:GLU:O	2.14	0.47
1:A:1282:VAL:O	1:A:1283:VAL:HG22	2.14	0.47
1:A:254:GLU:O	2:B:935:ARG:NH1	2.45	0.47
1:A:543:LEU:HD11	1:A:547:LEU:HD11	1.96	0.47
1:A:759:ALA:O	1:A:761:MET:N	2.47	0.47
1:A:7:SER:O	1:A:8:SER:C	2.54	0.47
2:B:781:PHE:CD1	2:B:781:PHE:C	2.88	0.47
2:B:839:MET:HE2	2:B:1010:LEU:HD21	1.95	0.47
2:B:850:LEU:HD12	2:B:851:PHE:N	2.30	0.47
4:D:51:ASN:C	4:D:52:LEU:O	2.52	0.47
5:E:124:VAL:CG1	5:E:132:ILE:HB	2.43	0.47
6:F:77:ASP:O	6:F:79:ARG:N	2.47	0.47
6:F:90:ARG:CG	6:F:91:ALA:N	2.78	0.47
6:F:94:LEU:HD23	6:F:94:LEU:HA	1.64	0.47
1:A:1162:VAL:HG12	1:A:1162:VAL:O	2.15	0.47
1:A:1398:MET:O	1:A:1401:SER:OG	2.22	0.47
1:A:1402:PHE:CD1	1:A:1403:GLU:HG3	2.50	0.47
1:A:222:LEU:O	1:A:224:PHE:N	2.48	0.47
1:A:335:ARG:NE	1:A:339:ASN:ND2	2.57	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:VAL:HG12	1:A:947:PHE:N	2.29	0.47
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.48	0.47
2:B:834:ASN:HA	2:B:838:SER:O	2.15	0.47
2:B:95:ILE:HG13	2:B:130:VAL:CG2	2.44	0.47
2:B:97:VAL:CG1	2:B:178:ASN:HD21	2.28	0.47
3:C:107:SER:C	3:C:109:SER:N	2.69	0.47
3:C:112:ASN:CB	3:C:114:TYR:CE1	2.98	0.47
4:D:130:LEU:O	4:D:132:GLN:N	2.48	0.47
4:D:189:ASP:O	4:D:193:THR:HB	2.14	0.47
5:E:192:ARG:NH1	5:E:192:ARG:HG3	2.26	0.47
6:F:103:MET:CE	7:G:65:ASP:HB2	2.44	0.47
10:J:14:VAL:O	10:J:16:ASP:N	2.48	0.47
10:J:18:TRP:HA	10:J:18:TRP:CE3	2.49	0.47
10:J:23:ASN:C	10:J:25:LEU:N	2.68	0.47
1:A:551:TYR:CE2	11:K:62:LYS:HE2	2.50	0.47
11:K:78:THR:O	11:K:79:GLU:C	2.53	0.47
1:A:1283:VAL:CG1	1:A:1284:MET:N	2.78	0.46
1:A:1342:GLU:CG	5:E:198:ILE:HG21	2.45	0.46
1:A:24:PRO:HG2	1:A:25:GLU:CD	2.35	0.46
1:A:500:GLU:O	1:A:504:LEU:HB2	2.15	0.46
1:A:548:ASN:HA	11:K:60:ALA:HB1	1.97	0.46
1:A:626:ASN:O	1:A:631:HIS:CB	2.63	0.46
1:A:809:THR:HG23	1:A:812:GLU:OE1	2.15	0.46
1:A:830:LYS:HB2	1:A:1081:LEU:CD2	2.43	0.46
1:A:928:LEU:O	1:A:929:LEU:C	2.53	0.46
1:A:936:LEU:H	1:A:936:LEU:HD23	1.78	0.46
2:B:1204:PHE:CE1	2:B:1216:LEU:HD11	2.50	0.46
2:B:202:TYR:CE1	2:B:209:GLU:HG2	2.50	0.46
2:B:285:ILE:O	2:B:288:ALA:HB3	2.15	0.46
2:B:43:LEU:HD11	2:B:811:TYR:O	2.15	0.46
2:B:654:ARG:H	2:B:657:HIS:CD2	2.28	0.46
5:E:7:ARG:CG	5:E:8:ASN:N	2.76	0.46
5:E:90:VAL:HG23	5:E:120:ALA:HA	1.97	0.46
6:F:135:ARG:HD3	6:F:143:PHE:CD2	2.51	0.46
6:F:85:MET:HE1	6:F:148:VAL:CG1	2.45	0.46
13:S:269:PHE:CZ	13:S:308:PHE:CE1	3.03	0.46
1:A:1327:ILE:HG22	5:E:147:HIS:CE1	2.51	0.46
1:A:370:ILE:HG23	2:B:1105:ALA:CB	2.41	0.46
1:A:535:THR:O	1:A:536:LEU:O	2.34	0.46
1:A:549:MET:O	1:A:550:LEU:C	2.53	0.46
1:A:647:GLY:O	1:A:650:GLN:HB2	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:GLU:HG2	1:A:696:GLU:O	2.15	0.46
1:A:808:LEU:N	1:A:808:LEU:CD1	2.78	0.46
1:A:80:HIS:O	1:A:243:PRO:HB3	2.16	0.46
1:A:863:VAL:O	1:A:864:ILE:CG1	2.63	0.46
1:A:894:GLU:C	1:A:896:ARG:H	2.18	0.46
1:A:881:GLN:NE2	1:A:958:VAL:O	2.42	0.46
2:B:1034:VAL:CG1	2:B:1035:ALA:N	2.78	0.46
2:B:58:THR:O	2:B:62:ILE:HG13	2.14	0.46
2:B:785:TYR:HA	2:B:788:ARG:HG3	1.97	0.46
8:H:89:LEU:C	8:H:91:ASP:N	2.68	0.46
9:I:99:LEU:C	9:I:100:PHE:HD1	2.18	0.46
9:I:83:ASN:HA	9:I:102:VAL:O	2.16	0.46
11:K:83:PRO:O	11:K:86:ALA:HB3	2.15	0.46
13:S:236:LEU:CA	13:S:242:LYS:CE	2.93	0.46
1:A:1220:PHE:CE2	1:A:1263:ILE:HG23	2.50	0.46
1:A:1311:VAL:HG11	1:A:1329:THR:HG21	1.96	0.46
1:A:317:LYS:O	1:A:318:SER:HB3	2.14	0.46
1:A:43:GLU:O	1:A:44:THR:HB	2.15	0.46
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.98	0.46
2:B:27:ALA:O	2:B:30:SER:OG	2.29	0.46
2:B:753:ALA:O	2:B:756:ILE:N	2.46	0.46
2:B:834:ASN:O	2:B:838:SER:O	2.34	0.46
3:C:95:CYS:O	3:C:96:SER:HB3	2.15	0.46
5:E:144:ILE:C	5:E:146:HIS:H	2.19	0.46
5:E:7:ARG:C	5:E:9:ILE:H	2.19	0.46
7:G:81:PRO:HA	7:G:85:GLU:OE1	2.15	0.46
1:A:567:LYS:HZ1	8:H:46:LEU:HB2	1.77	0.46
9:I:73:ARG:HD2	9:I:101:PHE:CE2	2.50	0.46
10:J:36:LEU:HB2	10:J:47:ARG:HH12	1.81	0.46
12:L:48:CYS:O	12:L:50:ASP:N	2.47	0.46
13:S:269:PHE:CE2	13:S:297:CYS:CB	2.96	0.46
1:A:100:LYS:O	1:A:101:LYS:C	2.54	0.46
1:A:103:CYS:SG	1:A:108:MET:CE	3.04	0.46
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.46	0.46
1:A:414:ASP:O	1:A:416:ARG:N	2.48	0.46
1:A:618:GLU:O	1:A:621:THR:N	2.46	0.46
2:B:1079:LYS:HE3	3:C:188:HIS:CE1	2.51	0.46
2:B:281:PRO:O	2:B:283:VAL:N	2.48	0.46
2:B:293:PRO:O	2:B:294:ASP:O	2.33	0.46
2:B:313:MET:HE2	2:B:390:LEU:HD21	1.96	0.46
2:B:378:LEU:HD12	2:B:378:LEU:C	2.35	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:579:ARG:HA	2:B:589:VAL:HG13	1.96	0.46
2:B:788:ARG:HE	2:B:788:ARG:HB3	1.52	0.46
2:B:871:THR:HG22	2:B:872:GLU:N	2.31	0.46
2:B:956:THR:CG2	2:B:960:GLY:HA2	2.45	0.46
2:B:789:MET:CE	2:B:965:LYS:HB3	2.46	0.46
4:D:29:LEU:N	4:D:29:LEU:HD23	2.30	0.46
7:G:1:MET:HE3	7:G:80:LYS:O	2.14	0.46
11:K:63:VAL:O	11:K:63:VAL:HG23	2.15	0.46
1:A:1169:ILE:O	1:A:1170:ILE:C	2.54	0.46
1:A:563:PRO:HB2	1:A:565:ILE:O	2.16	0.46
1:A:645:LEU:O	1:A:646:PHE:C	2.54	0.46
1:A:647:GLY:O	1:A:648:ASN:C	2.54	0.46
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.18	0.46
2:B:760:ASP:O	2:B:761:HIS:CG	2.69	0.46
2:B:770:GLN:CD	2:B:983:ARG:HA	2.36	0.46
3:C:228:PHE:N	3:C:228:PHE:CD1	2.83	0.46
4:D:154:PHE:HB2	4:D:160:VAL:HG22	1.97	0.46
5:E:16:PHE:O	5:E:17:ARG:C	2.54	0.46
5:E:197:LYS:O	5:E:199:ILE:HG13	2.16	0.46
5:E:24:LYS:HG3	5:E:25:ASP:N	2.30	0.46
6:F:87:LYS:HG3	6:F:88:TYR:CD1	2.51	0.46
1:A:567:LYS:HE3	8:H:46:LEU:HD12	1.97	0.46
8:H:76:THR:HG22	8:H:76:THR:O	2.14	0.46
9:I:99:LEU:HB2	9:I:101:PHE:CE1	2.50	0.46
10:J:61:LEU:O	10:J:63:TYR:N	2.48	0.46
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.80	0.46
12:L:30:ILE:O	12:L:56:LEU:HD23	2.15	0.46
1:A:460:VAL:CG1	1:A:461:LYS:N	2.79	0.46
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.97	0.46
1:A:715:GLU:O	1:A:718:VAL:N	2.48	0.46
1:A:867:ILE:CG2	1:A:872:GLY:H	2.29	0.46
1:A:896:ARG:CD	1:A:897:TYR:CE1	2.93	0.46
1:A:897:TYR:HB3	1:A:936:LEU:CD1	2.45	0.46
2:B:999:MET:HB3	2:B:1007:VAL:CG2	2.45	0.46
2:B:1023:VAL:HG12	2:B:1027:ILE:HG13	1.97	0.46
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.98	0.46
2:B:281:PRO:HG2	2:B:284:ILE:CG1	2.44	0.46
2:B:510:LYS:HD3	2:B:513:GLN:H	1.80	0.46
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.96	0.46
2:B:863:GLU:O	2:B:961:LEU:HD22	2.15	0.46
1:A:738:LYS:HZ1	3:C:194:GLU:C	2.18	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:251:LEU:O	3:C:254:LYS:N	2.49	0.46
5:E:22:MET:HE3	5:E:26:ARG:CZ	2.42	0.46
8:H:31:THR:O	8:H:31:THR:HG22	2.15	0.46
12:L:54:ARG:HG3	12:L:54:ARG:NH1	2.29	0.46
1:A:351:THR:HB	2:B:1103:ILE:CD1	2.43	0.46
1:A:399:HIS:O	1:A:400:PRO:C	2.54	0.46
1:A:550:LEU:HD11	1:A:561:PRO:HD2	1.98	0.46
1:A:907:THR:HG22	1:A:908:LEU:N	2.30	0.46
2:B:20:ASP:C	2:B:22:SER:H	2.19	0.46
2:B:69:LEU:HD13	2:B:429:PHE:HD1	1.80	0.46
2:B:63:ILE:HD12	2:B:421:PHE:CE2	2.51	0.46
2:B:994:TYR:HB2	2:B:999:MET:CE	2.46	0.46
4:D:53:SER:HB3	4:D:153:ARG:H	1.81	0.46
6:F:132:LEU:HD22	7:G:61:ILE:HD11	1.97	0.46
7:G:27:LYS:O	7:G:31:LEU:HG	2.16	0.46
8:H:143:LEU:O	8:H:144:ILE:HG13	2.16	0.46
9:I:11:ASN:O	9:I:12:ASN:ND2	2.48	0.46
9:I:69:PRO:O	9:I:84:VAL:HA	2.14	0.46
1:A:100:LYS:O	1:A:103:CYS:N	2.49	0.46
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.56	0.46
1:A:1083:THR:O	1:A:1084:PHE:O	2.34	0.46
1:A:1116:LEU:HB2	1:A:1329:THR:OG1	2.16	0.46
1:A:285:PRO:CG	1:A:288:ALA:HB3	2.40	0.46
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.72	0.46
1:A:707:GLY:O	1:A:708:MET:O	2.34	0.46
1:A:76:GLU:O	1:A:76:GLU:CG	2.63	0.46
2:B:189:LEU:O	2:B:192:LEU:HB2	2.15	0.46
2:B:558:LEU:C	2:B:560:GLU:N	2.70	0.46
2:B:683:SER:O	2:B:687:GLU:HB2	2.16	0.46
2:B:882:THR:O	2:B:883:LEU:CB	2.63	0.46
2:B:992:ILE:HD13	2:B:994:TYR:HE1	1.81	0.46
3:C:114:TYR:CD1	3:C:114:TYR:N	2.83	0.46
3:C:147:LEU:N	3:C:147:LEU:HD23	2.31	0.46
4:D:33:PHE:CZ	7:G:80:LYS:NZ	2.84	0.46
5:E:90:VAL:HB	5:E:119:SER:HB2	1.98	0.46
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	2.19	0.46
1:A:1385:THR:CG2	1:A:1386:ARG:N	2.79	0.46
1:A:385:ILE:HG22	1:A:386:ASP:N	2.29	0.46
1:A:63:ARG:HA	1:A:74:MET:CE	2.45	0.46
1:A:646:PHE:O	1:A:647:GLY:C	2.55	0.46
1:A:697:ALA:HB2	1:A:702:LEU:CD1	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:ILE:HG22	1:A:983:ILE:O	2.15	0.46
2:B:274:PRO:O	2:B:275:TYR:HB2	2.16	0.46
2:B:385:LEU:O	2:B:385:LEU:HD12	2.15	0.46
2:B:510:LYS:HD3	2:B:513:GLN:N	2.31	0.46
2:B:613:VAL:HG22	2:B:628:THR:HA	1.98	0.46
3:C:163:ILE:O	3:C:164:ALA:C	2.54	0.46
3:C:15:LYS:O	3:C:240:VAL:HG22	2.16	0.46
5:E:153:HIS:C	5:E:154:ILE:HG13	2.34	0.46
7:G:18:PHE:HA	7:G:22:MET:CE	2.45	0.46
7:G:56:ILE:O	7:G:57:GLN:HB2	2.15	0.46
8:H:98:TYR:HE1	8:H:139:ASN:HA	1.80	0.46
9:I:34:TYR:C	9:I:34:TYR:CD2	2.90	0.46
1:A:1067:LEU:O	1:A:1068:ALA:C	2.54	0.46
1:A:1119:TYR:CD2	1:A:1305:VAL:HG21	2.51	0.46
1:A:1129:GLU:HG3	1:A:1132:LYS:HE3	1.97	0.46
1:A:1227:ILE:CG2	1:A:1228:TRP:N	2.78	0.46
1:A:243:PRO:CB	1:A:244:PRO:HD2	2.46	0.46
1:A:566:ILE:O	1:A:567:LYS:O	2.34	0.46
1:A:642:CYS:O	1:A:643:ALA:C	2.54	0.46
1:A:695:LYS:C	1:A:697:ALA:N	2.69	0.46
1:A:809:THR:HB	1:A:810:PRO:HD2	1.97	0.46
1:A:921:GLY:O	1:A:922:ASP:C	2.55	0.46
2:B:546:SER:HA	2:B:612:GLU:CD	2.35	0.46
3:C:80:LEU:O	3:C:80:LEU:HG	2.16	0.46
7:G:80:LYS:HA	7:G:81:PRO:HD2	1.74	0.46
9:I:15:TYR:O	9:I:28:GLU:HG2	2.16	0.46
11:K:10:PHE:CD2	11:K:10:PHE:N	2.84	0.46
1:A:1081:LEU:CD1	1:A:1099:PRO:HD3	2.46	0.45
1:A:1170:ILE:HG23	1:A:1174:PHE:HE1	1.77	0.45
1:A:1191:TRP:HB3	1:A:1260:LEU:HD23	1.97	0.45
1:A:1330:ASN:OD1	1:A:1331:SER:N	2.49	0.45
1:A:871:ASP:CG	1:A:1366:ARG:HH22	2.19	0.45
1:A:1437:GLY:CA	6:F:88:TYR:CD2	2.97	0.45
1:A:811:GLN:O	1:A:812:GLU:C	2.55	0.45
1:A:512:VAL:HG11	1:A:876:ALA:O	2.16	0.45
2:B:1020:ARG:HH12	13:S:291:GLU:HA	1.81	0.45
2:B:1111:MET:O	2:B:1112:GLN:C	2.54	0.45
2:B:1182:CYS:O	2:B:1183:LYS:C	2.53	0.45
1:A:18:GLN:CB	2:B:1215:ARG:HB2	2.45	0.45
2:B:570:VAL:HG21	2:B:573:GLN:CD	2.36	0.45
3:C:94:LYS:HB2	3:C:94:LYS:HE3	1.67	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:48:ILE:CG2	7:G:4:ILE:HB	2.46	0.45
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.99	0.45
11:K:70:ARG:HG3	11:K:70:ARG:O	2.16	0.45
1:A:321:PRO:O	1:A:322:VAL:CG2	2.63	0.45
1:A:33:ALA:O	1:A:83:HIS:HD2	1.99	0.45
1:A:353:ILE:HG13	1:A:482:PHE:CD2	2.51	0.45
1:A:915:SER:O	1:A:919:ILE:HG13	2.16	0.45
2:B:172:ILE:CG2	2:B:173:MET:N	2.79	0.45
2:B:313:MET:CE	2:B:390:LEU:HD21	2.46	0.45
2:B:386:LEU:O	2:B:388:CYS:N	2.50	0.45
2:B:838:SER:HA	2:B:989:THR:O	2.17	0.45
2:B:880:THR:HB	2:B:934:LYS:CD	2.36	0.45
2:B:906:SER:O	2:B:907:GLY:O	2.34	0.45
3:C:43:THR:HG22	3:C:44:LEU:H	1.81	0.45
3:C:46:ILE:HD13	3:C:157:CYS:CB	2.46	0.45
5:E:202:SER:HB3	5:E:205:SER:O	2.15	0.45
5:E:25:ASP:C	5:E:27:GLY:H	2.17	0.45
8:H:91:ASP:C	8:H:93:TYR:N	2.70	0.45
1:A:1213:GLY:O	1:A:1214:GLU:C	2.54	0.45
1:A:44:THR:HG22	1:A:44:THR:O	2.16	0.45
1:A:515:GLN:O	1:A:516:SER:CB	2.58	0.45
1:A:556:TRP:CE2	1:A:558:GLY:HA2	2.51	0.45
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.29	0.45
1:A:791:ASP:C	1:A:791:ASP:OD1	2.55	0.45
2:B:551:PRO:HG2	2:B:552:MET:H	1.81	0.45
2:B:520:GLY:H	2:B:748:ILE:HG22	1.81	0.45
2:B:806:THR:HG22	2:B:808:ALA:CB	2.46	0.45
3:C:22:LEU:CD2	3:C:25:VAL:HG21	2.47	0.45
10:J:21:TYR:C	10:J:23:ASN:N	2.70	0.45
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.50	0.45
11:K:88:LYS:O	11:K:91:CYS:N	2.49	0.45
12:L:59:ALA:O	12:L:60:ARG:O	2.34	0.45
1:A:1210:GLY:O	1:A:1214:GLU:HB2	2.16	0.45
1:A:1329:THR:O	1:A:1331:SER:N	2.49	0.45
1:A:1359:ASP:HB2	1:A:1361:SER:OG	2.16	0.45
1:A:1451:VAL:C	1:A:1453:TYR:H	2.19	0.45
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.99	0.45
1:A:362:ASP:N	1:A:362:ASP:OD2	2.48	0.45
2:B:1026:LEU:HD23	2:B:1086:PHE:CE2	2.52	0.45
2:B:1115:THR:HG22	2:B:1117:GLN:CG	2.46	0.45
2:B:1164:GLY:HA3	2:B:1190:ASP:OD2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1169:MET:CE	2:B:1201:LYS:CA	2.89	0.45
2:B:170:LEU:HG	2:B:170:LEU:O	2.14	0.45
2:B:202:TYR:N	2:B:202:TYR:CD2	2.84	0.45
2:B:284:ILE:HG12	2:B:324:ILE:HD12	1.98	0.45
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.16	0.45
3:C:118:LEU:HB2	3:C:132:PRO:HG2	1.97	0.45
11:K:33:ILE:HB	11:K:35:PHE:HE1	1.81	0.45
1:A:1115:SER:OG	1:A:1116:LEU:N	2.49	0.45
1:A:1242:VAL:O	1:A:1243:VAL:HB	2.17	0.45
1:A:19:PHE:O	1:A:1416:ALA:HA	2.17	0.45
1:A:298:PHE:HZ	1:A:314:ALA:HB2	1.80	0.45
1:A:777:PHE:CE2	1:A:782:ARG:HA	2.51	0.45
1:A:937:VAL:HG12	1:A:938:LYS:N	2.30	0.45
2:B:255:GLN:O	2:B:271:ALA:HB1	2.17	0.45
2:B:293:PRO:HG2	2:B:296:GLU:OE1	2.16	0.45
2:B:615:MET:HA	2:B:625:LYS:O	2.16	0.45
2:B:816:GLU:O	2:B:817:LEU:CD2	2.59	0.45
3:C:158:VAL:O	3:C:158:VAL:HG12	2.17	0.45
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.98	0.45
6:F:143:PHE:C	6:F:143:PHE:CD1	2.90	0.45
7:G:126:ASN:HA	7:G:127:PRO:C	2.36	0.45
1:A:560:ILE:CG1	8:H:78:SER:HB2	2.36	0.45
12:L:28:LYS:HG3	12:L:39:SER:OG	2.15	0.45
12:L:52:GLY:O	12:L:53:HIS:C	2.54	0.45
1:A:1016:THR:O	1:A:1018:PHE:N	2.49	0.45
1:A:834:THR:CG2	1:A:1077:THR:HA	2.46	0.45
1:A:1122:PRO:O	1:A:1123:GLY:C	2.54	0.45
1:A:1151:GLU:HB3	1:A:1153:TYR:CE1	2.50	0.45
1:A:1173:HIS:CG	1:A:1227:ILE:HG23	2.51	0.45
1:A:42:ASP:CG	1:A:45:GLN:HA	2.37	0.45
1:A:688:LYS:O	1:A:690:VAL:N	2.50	0.45
1:A:95:PHE:CD1	1:A:234:MET:CG	2.96	0.45
2:B:1181:GLU:OE1	2:B:1183:LYS:HG3	2.17	0.45
2:B:217:ARG:C	2:B:217:ARG:HD2	2.37	0.45
2:B:901:PRO:O	2:B:902:GLY:C	2.53	0.45
2:B:984:HIS:CD2	2:B:1025:HIS:HA	2.51	0.45
3:C:46:ILE:HD13	3:C:157:CYS:HB3	1.99	0.45
4:D:122:GLU:HA	4:D:125:SER:OG	2.17	0.45
5:E:135:PHE:CB	5:E:140:LEU:HD11	2.47	0.45
7:G:132:SER:HB3	7:G:135:ASP:HB2	1.97	0.45
9:I:88:SER:C	9:I:90:GLN:N	2.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1115:SER:O	1:A:1329:THR:HG23	2.17	0.45
1:A:1121:GLU:O	1:A:1122:PRO:O	2.35	0.45
1:A:1271:ILE:CG2	1:A:1271:ILE:O	2.65	0.45
1:A:1293:SER:OG	1:A:1295:THR:HG23	2.17	0.45
1:A:760:GLN:O	1:A:804:TYR:CD1	2.70	0.45
1:A:849:MET:O	1:A:851:HIS:HD2	1.99	0.45
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.98	0.45
2:B:280:ILE:HG23	2:B:281:PRO:HD2	1.99	0.45
2:B:578:THR:HG23	2:B:622:LYS:CA	2.47	0.45
2:B:638:PHE:HD2	2:B:690:VAL:HG22	1.82	0.45
2:B:975:GLN:HG2	2:B:976:ILE:H	1.82	0.45
4:D:176:GLU:O	4:D:180:LEU:HB2	2.17	0.45
5:E:117:THR:O	5:E:120:ALA:N	2.45	0.45
5:E:171:LYS:O	5:E:172:GLU:C	2.55	0.45
7:G:1:MET:HE3	7:G:80:LYS:H	1.81	0.45
7:G:82:PHE:O	7:G:84:GLY:N	2.50	0.45
3:C:66:ARG:HH21	10:J:5:VAL:HG23	1.80	0.45
11:K:90:ALA:O	11:K:94:ILE:HG13	2.17	0.45
13:S:273:LYS:C	13:S:275:LYS:H	2.18	0.45
1:A:1011:GLN:NE2	1:A:1015:VAL:CG2	2.65	0.45
1:A:1143:LEU:HD12	1:A:1146:VAL:HG23	1.99	0.45
1:A:1313:LEU:HD11	1:A:1327:ILE:HD13	1.99	0.45
1:A:30:ILE:HD11	2:B:1168:LEU:HD13	1.99	0.45
1:A:353:ILE:HG23	1:A:485:ASP:O	2.16	0.45
1:A:52:GLY:O	1:A:56:PRO:HG2	2.17	0.45
1:A:668:ASP:HA	1:A:741:ASN:OD1	2.17	0.45
1:A:783:THR:O	1:A:784:LEU:HD23	2.16	0.45
2:B:1178:ASN:O	2:B:1179:GLN:C	2.55	0.45
2:B:489:SER:OG	2:B:490:SER:N	2.49	0.45
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.17	0.45
2:B:958:GLN:C	2:B:960:GLY:H	2.19	0.45
3:C:214:ASN:HB3	3:C:217:ASP:OD2	2.16	0.45
3:C:44:LEU:HG	3:C:159:ALA:HB1	1.99	0.45
3:C:88:CYS:SG	3:C:91:HIS:N	2.90	0.45
5:E:117:THR:HG22	5:E:119:SER:N	2.20	0.45
5:E:198:ILE:CD1	5:E:212:ARG:NH1	2.78	0.45
8:H:95:TYR:HE2	8:H:97:MET:CG	2.29	0.45
11:K:35:PHE:HD1	11:K:35:PHE:N	2.15	0.45
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.51	0.45
1:A:244:PRO:CG	1:A:245:PRO:HD3	2.47	0.45
1:A:324:SER:O	1:A:325:ILE:C	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:LEU:C	1:A:927:VAL:H	2.20	0.45
2:B:1006:ILE:HG13	2:B:1006:ILE:H	1.19	0.45
2:B:710:LEU:O	2:B:711:GLU:HG2	2.17	0.45
2:B:851:PHE:O	2:B:974:PRO:HD3	2.17	0.45
2:B:855:PHE:CD1	2:B:856:PHE:N	2.85	0.45
2:B:964:VAL:HG12	2:B:965:LYS:N	2.32	0.45
6:F:135:ARG:HG2	6:F:137:TYR:CE1	2.52	0.45
7:G:39:THR:C	7:G:41:LYS:N	2.70	0.45
8:H:100:THR:HG22	8:H:101:ALA:H	1.79	0.45
8:H:23:VAL:HG22	8:H:43:ASN:HA	1.99	0.45
9:I:55:THR:HG22	9:I:56:ALA:N	2.32	0.45
11:K:53:ASP:OD1	11:K:55:LYS:HB2	2.17	0.45
13:S:260:THR:CA	13:S:260:THR:HB	2.20	0.45
1:A:1081:LEU:CD2	1:A:1098:VAL:HG21	2.45	0.45
1:A:1261:LYS:C	1:A:1264:GLU:H	2.20	0.45
1:A:125:ALA:C	1:A:127:ALA:H	2.20	0.45
1:A:1115:SER:HA	1:A:1308:THR:HG23	1.99	0.45
1:A:563:PRO:HB3	1:A:571:LEU:O	2.17	0.45
2:B:1183:LYS:CE	2:B:1183:LYS:H	2.27	0.45
2:B:563:MET:HE3	2:B:580:VAL:HB	1.99	0.45
2:B:598:GLU:HG2	2:B:598:GLU:O	2.17	0.45
2:B:745:PRO:O	2:B:748:ILE:CG1	2.61	0.45
2:B:758:PHE:O	2:B:760:ASP:N	2.49	0.45
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.99	0.45
2:B:824:ILE:CD1	10:J:48:ARG:NH1	2.80	0.45
2:B:843:GLN:O	2:B:844:SER:C	2.56	0.45
2:B:975:GLN:HG2	2:B:976:ILE:N	2.32	0.45
2:B:990:ILE:HG22	2:B:992:ILE:H	1.81	0.45
3:C:170:TRP:O	3:C:171:GLY:C	2.54	0.45
4:D:51:ASN:OD1	4:D:52:LEU:O	2.34	0.45
1:A:866:PHE:HD2	5:E:168:TYR:CE1	2.33	0.45
8:H:95:TYR:CE2	8:H:97:MET:CG	3.00	0.45
9:I:15:TYR:CD1	9:I:15:TYR:N	2.85	0.45
1:A:789:LYS:HD2	9:I:67:THR:OG1	2.17	0.45
10:J:2:ILE:HG12	10:J:57:ILE:CD1	2.46	0.45
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.52	0.45
1:A:706:HIS:ND1	13:S:257:GLN:HB2	2.32	0.45
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.37	0.44
1:A:1101:LEU:HD12	1:A:1101:LEU:O	2.17	0.44
1:A:384:ASN:O	1:A:386:ASP:N	2.50	0.44
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:GLY:O	1:A:676:MET:HB2	2.16	0.44
2:B:828:ALA:HB2	2:B:1085:ILE:HG21	2.00	0.44
2:B:977:GLY:CA	2:B:1099:VAL:HB	2.44	0.44
2:B:1160:VAL:CG1	2:B:1161:HIS:H	2.30	0.44
2:B:390:LEU:O	2:B:391:ASP:C	2.54	0.44
2:B:615:MET:C	2:B:616:ILE:HD12	2.36	0.44
2:B:753:ALA:HA	2:B:756:ILE:HG13	1.99	0.44
3:C:77:ILE:HG23	3:C:161:LYS:HE3	2.00	0.44
4:D:141:LEU:O	4:D:144:THR:HB	2.16	0.44
4:D:40:HIS:CE1	4:D:41:GLN:HE21	2.34	0.44
6:F:88:TYR:N	6:F:88:TYR:CD1	2.85	0.44
2:B:785:TYR:CE2	10:J:60:PHE:CE1	3.04	0.44
1:A:465:TYR:N	11:K:2:ASN:HB3	2.32	0.44
3:C:52:GLU:HA	12:L:64:LEU:HD22	1.99	0.44
1:A:108:MET:O	1:A:109:HIS:HB2	2.16	0.44
1:A:1170:ILE:O	1:A:1174:PHE:HD1	2.00	0.44
1:A:1226:VAL:C	1:A:1227:ILE:HG13	2.37	0.44
1:A:576:GLN:O	1:A:579:SER:HB2	2.18	0.44
1:A:78:PRO:O	1:A:78:PRO:HG2	2.17	0.44
2:B:186:GLU:O	2:B:187:SER:C	2.55	0.44
1:A:814:PHE:CD1	2:B:519:TRP:CE3	3.05	0.44
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.47	0.44
2:B:981:ALA:CB	2:B:987:LYS:HA	2.46	0.44
3:C:73:GLN:NE2	3:C:75:MET:N	2.54	0.44
1:A:1132:LYS:CE	13:S:253:LEU:HD21	2.43	0.44
1:A:1161:THR:HG1	1:A:1170:ILE:HD11	1.82	0.44
1:A:1436:ILE:HD13	2:B:1139:ILE:CG2	2.45	0.44
1:A:381:THR:O	1:A:384:ASN:N	2.45	0.44
1:A:470:LEU:HD11	1:A:482:PHE:CE2	2.52	0.44
1:A:573:SER:CB	8:H:119:GLY:O	2.65	0.44
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.53	0.44
2:B:373:ARG:HG3	2:B:566:LEU:HD23	2.00	0.44
2:B:408:LEU:HA	2:B:408:LEU:HD12	1.76	0.44
2:B:555:ILE:HD11	2:B:587:HIS:NE2	2.32	0.44
2:B:542:MET:CG	2:B:747:MET:HB3	2.48	0.44
4:D:147:TYR:CE1	7:G:103:VAL:HG13	2.53	0.44
7:G:14:HIS:CG	7:G:15:PRO:HD2	2.53	0.44
10:J:3:VAL:CG2	10:J:18:TRP:CG	2.99	0.44
13:S:283:GLN:HG2	13:S:295:THR:OG1	2.17	0.44
1:A:1209:MET:O	1:A:1210:GLY:C	2.55	0.44
1:A:1354:ASN:O	1:A:1355:VAL:C	2.54	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1437:GLY:O	1:A:1438:THR:C	2.56	0.44
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.53	0.44
1:A:666:ILE:N	2:B:1026:LEU:HD22	2.32	0.44
2:B:1150:ARG:NE	2:B:1150:ARG:HA	2.33	0.44
2:B:287:ARG:NH1	2:B:324:ILE:O	2.50	0.44
2:B:372:SER:O	2:B:376:PHE:HD1	2.00	0.44
2:B:604:ARG:O	2:B:606:LYS:N	2.50	0.44
2:B:806:THR:C	2:B:808:ALA:N	2.68	0.44
3:C:178:PHE:O	3:C:179:GLU:HB2	2.16	0.44
3:C:91:HIS:HB2	3:C:96:SER:OG	2.18	0.44
8:H:24:CYS:CB	8:H:44:VAL:HG21	2.46	0.44
1:A:967:ALA:N	1:A:1044:TRP:HZ3	2.16	0.44
1:A:12:ARG:NE	2:B:1192:TYR:HE2	2.15	0.44
1:A:1434:ALA:HA	1:A:1435:PRO:HD3	1.91	0.44
1:A:786:HIS:CE1	2:B:519:TRP:CZ2	3.05	0.44
1:A:843:LYS:HD2	1:A:843:LYS:HA	1.89	0.44
2:B:1107:ALA:O	2:B:1108:ARG:O	2.36	0.44
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.44	0.44
2:B:233:PRO:HG2	2:B:234:ILE:CD1	2.47	0.44
2:B:371:GLU:N	2:B:371:GLU:CD	2.70	0.44
2:B:642:ASP:C	2:B:644:GLU:H	2.19	0.44
2:B:806:THR:O	2:B:808:ALA:N	2.51	0.44
2:B:821:GLN:HE22	2:B:851:PHE:N	2.09	0.44
1:A:483:ASP:HB2	2:B:987:LYS:HG3	1.99	0.44
3:C:80:LEU:HD11	3:C:95:CYS:CA	2.47	0.44
7:G:101:VAL:HG12	7:G:102:GLN:N	2.32	0.44
7:G:96:GLN:HA	7:G:121:PHE:CD2	2.52	0.44
2:B:394:ASP:OD2	9:I:91:ARG:HD2	2.17	0.44
10:J:1:MET:N	10:J:56:LEU:N	2.65	0.44
13:S:269:PHE:HZ	13:S:308:PHE:CE1	2.35	0.44
1:A:896:ARG:NH2	1:A:1030:ARG:NH2	2.66	0.44
1:A:834:THR:CG2	1:A:1077:THR:HG23	2.29	0.44
1:A:1099:PRO:O	1:A:1102:LYS:HB3	2.17	0.44
1:A:384:ASN:CG	1:A:388:LEU:HD12	2.37	0.44
1:A:76:GLU:O	1:A:76:GLU:HG3	2.18	0.44
1:A:847:ASP:N	1:A:847:ASP:OD1	2.48	0.44
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.17	0.44
2:B:1182:CYS:O	2:B:1183:LYS:O	2.36	0.44
2:B:324:ILE:CG2	2:B:325:GLN:N	2.81	0.44
2:B:360:PHE:CD2	2:B:360:PHE:C	2.91	0.44
2:B:67:SER:O	2:B:68:THR:C	2.56	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:798:TYR:HD2	2:B:798:TYR:N	2.16	0.44
2:B:882:THR:O	2:B:883:LEU:HB2	2.17	0.44
2:B:874:PHE:HA	2:B:913:GLY:O	2.17	0.44
2:B:999:MET:HE3	2:B:999:MET:HA	2.00	0.44
3:C:50:GLU:HB3	3:C:156:THR:HB	1.98	0.44
3:C:21:ILE:HG22	3:C:21:ILE:O	2.17	0.44
3:C:75:MET:HE2	3:C:239:PRO:HD3	1.99	0.44
4:D:47:LEU:CD1	4:D:48:ILE:N	2.81	0.44
1:A:164:ARG:CG	1:A:165:GLY:H	2.01	0.44
1:A:475:THR:CG2	1:A:476:SER:N	2.81	0.44
2:B:129:PHE:CD2	2:B:166:PHE:HA	2.53	0.44
2:B:230:ALA:N	2:B:231:PRO:CD	2.81	0.44
2:B:293:PRO:O	2:B:296:GLU:HB3	2.18	0.44
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.52	0.44
3:C:44:LEU:HD23	3:C:72:LEU:CB	2.48	0.44
1:A:1343:ALA:HB2	5:E:150:VAL:HG22	1.98	0.44
1:A:1342:GLU:HG2	5:E:198:ILE:HD13	1.99	0.44
5:E:177:ARG:HD3	5:E:215:MET:HG3	1.99	0.44
7:G:14:HIS:CD2	7:G:16:SER:H	2.34	0.44
8:H:38:LEU:HD12	8:H:39:THR:H	1.82	0.44
1:A:1206:ASP:HB2	1:A:1274:ARG:HH22	1.83	0.44
1:A:1210:GLY:O	1:A:1211:GLN:C	2.56	0.44
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.18	0.44
1:A:1313:LEU:HD12	1:A:1327:ILE:HD13	1.99	0.44
1:A:43:GLU:O	1:A:44:THR:CB	2.66	0.44
1:A:525:GLN:O	1:A:526:ASP:C	2.56	0.44
1:A:718:VAL:O	1:A:721:PHE:HB2	2.18	0.44
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.83	0.44
3:C:175:ALA:HB3	10:J:43:ARG:NH2	2.33	0.44
5:E:117:THR:C	5:E:119:SER:H	2.21	0.44
7:G:1:MET:CE	7:G:80:LYS:O	2.66	0.44
10:J:45:CYS:SG	10:J:46:CYS:N	2.91	0.44
12:L:47:ARG:NH2	12:L:54:ARG:HE	2.16	0.44
1:A:1104:ILE:C	1:A:1106:ASN:N	2.71	0.44
1:A:55:ASP:O	1:A:57:ARG:N	2.51	0.44
1:A:668:ASP:CG	1:A:742:ASN:HD22	2.19	0.44
2:B:952:VAL:CG1	2:B:953:LEU:N	2.79	0.44
3:C:211:ASP:HA	3:C:212:PRO:HD3	1.84	0.44
3:C:247:GLY:C	3:C:249:ASP:N	2.72	0.44
3:C:80:LEU:HD11	3:C:96:SER:N	2.33	0.44
4:D:146:GLN:O	4:D:150:ASN:N	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:207:ARG:NH1	5:E:207:ARG:HB3	2.28	0.44
5:E:80:VAL:HG12	5:E:81:GLU:N	2.33	0.44
11:K:7:PHE:O	11:K:11:LEU:HB2	2.18	0.44
12:L:40:LEU:HD22	12:L:44:ASP:CB	2.47	0.44
1:A:135:PHE:CE1	1:A:222:LEU:HD22	2.53	0.43
1:A:185:TRP:O	1:A:197:PRO:HA	2.18	0.43
1:A:449:SER:O	2:B:1133:MET:HB3	2.18	0.43
1:A:49:LYS:HZ1	1:A:60:SER:CA	2.31	0.43
1:A:64:ASN:O	1:A:65:LEU:C	2.56	0.43
1:A:814:PHE:CE1	2:B:519:TRP:HA	2.52	0.43
1:A:98:LYS:O	1:A:99:ILE:C	2.56	0.43
2:B:1085:ILE:CG2	2:B:1086:PHE:N	2.80	0.43
2:B:781:PHE:HD1	2:B:782:LEU:HG	1.83	0.43
2:B:1084:GLN:OE1	3:C:191:TYR:HA	2.17	0.43
3:C:98:VAL:O	3:C:99:LEU:HD23	2.18	0.43
5:E:138:ALA:HA	5:E:141:VAL:CG2	2.47	0.43
8:H:38:LEU:HD12	8:H:124:ARG:O	2.18	0.43
1:A:1152:ILE:HG13	9:I:44:TYR:HD2	1.83	0.43
9:I:71:SER:O	9:I:83:ASN:ND2	2.51	0.43
11:K:88:LYS:O	11:K:89:ASN:C	2.56	0.43
12:L:30:ILE:CD1	12:L:59:ALA:HB2	2.42	0.43
1:A:708:MET:HE3	1:A:1090:ALA:O	2.18	0.43
1:A:1189:SER:OG	1:A:1190:PRO:HD2	2.18	0.43
1:A:1329:THR:C	1:A:1331:SER:N	2.71	0.43
1:A:1406:VAL:HG12	1:A:1410:PHE:CD1	2.52	0.43
1:A:396:PRO:HB3	1:A:402:ALA:O	2.18	0.43
1:A:693:VAL:O	1:A:693:VAL:HG12	2.18	0.43
1:A:877:HIS:C	1:A:878:ILE:CG1	2.86	0.43
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.34	0.43
2:B:546:SER:HG	2:B:631:GLY:H	1.56	0.43
3:C:62:PHE:O	3:C:65:HIS:HB3	2.17	0.43
5:E:21:GLU:O	5:E:24:LYS:HG2	2.19	0.43
5:E:92:THR:HG22	5:E:92:THR:O	2.18	0.43
7:G:47:CYS:O	7:G:76:ALA:HB1	2.19	0.43
1:A:971:PHE:CE2	1:A:1040:GLN:HG2	2.53	0.43
1:A:1116:LEU:HD12	1:A:1116:LEU:C	2.38	0.43
1:A:1239:ARG:HB3	1:A:1239:ARG:NH1	2.33	0.43
1:A:218:ASP:HA	1:A:221:SER:HG	1.83	0.43
1:A:43:GLU:HB2	1:A:46:THR:HB	2.00	0.43
1:A:814:PHE:HE1	2:B:519:TRP:HA	1.83	0.43
2:B:1202:LEU:HD22	2:B:1206:GLU:CD	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:GLN:HG2	2:B:396:ASP:H	1.83	0.43
2:B:465:ASN:N	2:B:465:ASN:ND2	2.65	0.43
2:B:482:VAL:O	2:B:483:LEU:C	2.57	0.43
2:B:789:MET:CE	2:B:965:LYS:O	2.65	0.43
2:B:911:ILE:HG23	2:B:966:VAL:HG11	2.00	0.43
2:B:987:LYS:HG2	2:B:987:LYS:O	2.18	0.43
5:E:29:PHE:O	5:E:30:ILE:HG13	2.18	0.43
7:G:119:LEU:HD12	7:G:131:GLN:O	2.18	0.43
11:K:32:VAL:HA	11:K:73:LEU:O	2.18	0.43
11:K:30:ALA:HA	11:K:75:ILE:O	2.18	0.43
12:L:38:LEU:O	12:L:39:SER:CB	2.58	0.43
2:B:901:PRO:HB2	12:L:60:ARG:HA	2.00	0.43
3:C:169:LYS:NZ	12:L:69:ALA:CB	2.81	0.43
1:A:720:ARG:HD2	13:S:262:GLU:HB3	1.99	0.43
13:S:293:LEU:CD2	13:S:293:LEU:N	2.81	0.43
1:A:353:ILE:HD13	1:A:487:MET:HG3	2.00	0.43
1:A:477:PRO:HG2	1:A:521:MET:HG2	1.99	0.43
1:A:962:ARG:O	1:A:965:GLN:N	2.51	0.43
2:B:214:ALA:HA	2:B:408:LEU:HD12	2.00	0.43
2:B:59:LEU:CD1	2:B:417:PHE:CE2	3.01	0.43
2:B:215:GLN:OE1	2:B:499:ASN:HB3	2.18	0.43
3:C:144:ILE:O	3:C:145:CYS:CB	2.66	0.43
7:G:1:MET:HE3	7:G:80:LYS:N	2.33	0.43
8:H:12:VAL:HA	8:H:28:ALA:HB2	1.99	0.43
8:H:38:LEU:HD13	8:H:125:LEU:HD13	2.00	0.43
1:A:567:LYS:HD3	8:H:95:TYR:HA	1.99	0.43
10:J:25:LEU:O	10:J:29:GLU:HA	2.18	0.43
10:J:7:CYS:SG	10:J:49:MET:CE	3.01	0.43
11:K:106:GLU:O	11:K:107:THR:C	2.56	0.43
13:S:296:PHE:CD1	13:S:296:PHE:N	2.86	0.43
1:A:1001:ARG:HH11	1:A:1001:ARG:HG2	1.83	0.43
1:A:1121:GLU:O	1:A:1122:PRO:C	2.57	0.43
1:A:1202:MET:HE1	1:A:1212:VAL:HG21	2.00	0.43
1:A:108:MET:SD	1:A:210:ILE:HD13	2.59	0.43
1:A:42:ASP:HB3	1:A:45:GLN:N	2.33	0.43
1:A:540:PHE:CB	1:A:571:LEU:HD23	2.39	0.43
1:A:58:LEU:O	1:A:59:GLY:O	2.36	0.43
1:A:706:HIS:C	1:A:708:MET:H	2.22	0.43
1:A:735:VAL:HG12	1:A:735:VAL:O	2.18	0.43
1:A:845:LEU:HD22	1:A:1374:VAL:HG21	2.00	0.43
1:A:88:LYS:HA	1:A:89:PRO:HD2	1.72	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1145:SER:O	2:B:1147:LEU:N	2.51	0.43
2:B:258:LEU:HG	2:B:258:LEU:O	2.18	0.43
2:B:509:ALA:C	2:B:510:LYS:HD2	2.36	0.43
2:B:591:ARG:O	2:B:592:ASN:C	2.57	0.43
2:B:634:TYR:CE1	2:B:692:TYR:CD1	3.06	0.43
2:B:695:ALA:O	2:B:698:GLU:HB3	2.18	0.43
2:B:540:SER:HB3	2:B:747:MET:O	2.18	0.43
2:B:787:VAL:HG12	2:B:787:VAL:O	2.19	0.43
2:B:847:ASP:C	2:B:849:GLY:N	2.72	0.43
2:B:976:ILE:HG22	2:B:977:GLY:N	2.34	0.43
3:C:237:SER:O	3:C:238:ILE:HG13	2.18	0.43
3:C:242:GLN:HA	3:C:245:VAL:CG2	2.45	0.43
3:C:44:LEU:HG	3:C:45:ALA:N	2.34	0.43
4:D:56:ARG:CB	4:D:148:LEU:HD22	2.37	0.43
7:G:1:MET:SD	7:G:79:PHE:CD1	3.12	0.43
1:A:1080:THR:HG22	1:A:1081:LEU:H	1.81	0.43
1:A:1101:LEU:HD11	1:A:1105:LEU:HD11	2.00	0.43
1:A:1192:LEU:CG	1:A:1193:LEU:N	2.81	0.43
2:B:287:ARG:NH2	2:B:325:GLN:HE22	2.16	0.43
2:B:390:LEU:O	2:B:392:ARG:N	2.51	0.43
2:B:460:ALA:HB1	2:B:466:TRP:CE3	2.52	0.43
2:B:508:LEU:O	2:B:509:ALA:C	2.51	0.43
2:B:644:GLU:C	2:B:646:LEU:N	2.71	0.43
2:B:777:ALA:HA	2:B:1095:LEU:CA	2.45	0.43
2:B:780:VAL:HG21	10:J:56:LEU:HD11	1.99	0.43
2:B:952:VAL:CG1	2:B:953:LEU:H	2.31	0.43
3:C:242:GLN:HB3	3:C:246:ARG:HG3	1.99	0.43
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	2.00	0.43
1:A:862:ASN:HA	5:E:174:GLN:O	2.19	0.43
5:E:198:ILE:HD11	5:E:212:ARG:HH11	1.84	0.43
12:L:63:ARG:O	12:L:63:ARG:HG3	2.19	0.43
1:A:115:LEU:O	1:A:122:MET:HE2	2.18	0.43
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.54	0.43
1:A:416:ARG:C	1:A:417:TYR:CD2	2.92	0.43
1:A:464:PRO:HG2	1:A:465:TYR:HD1	1.83	0.43
1:A:353:ILE:HG13	1:A:482:PHE:HD2	1.83	0.43
1:A:703:THR:HB	1:A:705:LYS:HE2	2.01	0.43
1:A:989:GLY:C	1:A:991:LYS:N	2.69	0.43
2:B:1099:VAL:CG1	2:B:1100:ASP:H	2.24	0.43
1:A:2:VAL:HG21	2:B:1158:PHE:N	2.34	0.43
2:B:597:MET:O	2:B:599:THR:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:758:PHE:C	2:B:760:ASP:N	2.72	0.43
1:A:525:GLN:CD	2:B:836:GLU:HG2	2.39	0.43
6:F:86:THR:O	6:F:89:GLU:HB2	2.18	0.43
8:H:145:ARG:O	8:H:146:ARG:HB2	2.18	0.43
11:K:62:LYS:O	11:K:62:LYS:HG3	2.19	0.43
1:A:1064:VAL:O	1:A:1065:GLY:C	2.55	0.43
1:A:1208:THR:O	1:A:1211:GLN:N	2.52	0.43
1:A:1319:VAL:O	1:A:1322:ILE:HG12	2.19	0.43
1:A:157:ASP:C	1:A:159:THR:H	2.22	0.43
1:A:231:PRO:C	1:A:233:TRP:N	2.72	0.43
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.49	0.43
1:A:426:LEU:O	1:A:427:GLN:HG2	2.19	0.43
1:A:49:LYS:NZ	1:A:60:SER:CA	2.81	0.43
1:A:722:LEU:O	1:A:725:ALA:HB3	2.19	0.43
2:B:486:TYR:CD1	2:B:1096:ARG:NH2	2.86	0.43
2:B:114:PRO:O	2:B:115:GLN:C	2.57	0.43
2:B:20:ASP:O	2:B:22:SER:N	2.48	0.43
2:B:376:PHE:HE2	2:B:569:TYR:HD2	1.65	0.43
2:B:545:ILE:C	2:B:634:TYR:HE2	2.22	0.43
2:B:624:LEU:HA	2:B:624:LEU:HD12	1.79	0.43
2:B:872:GLU:CD	2:B:914:LYS:HE2	2.39	0.43
3:C:97:VAL:HG12	3:C:98:VAL:H	1.84	0.43
6:F:134:ILE:N	6:F:146:TRP:O	2.50	0.43
2:B:1076:HIS:CD2	11:K:40:HIS:NE2	2.86	0.43
11:K:55:LYS:HB2	11:K:81:TYR:HE1	1.84	0.43
1:A:1051:ALA:O	1:A:1052:GLN:C	2.56	0.43
1:A:1230:GLU:C	1:A:1232:ASN:N	2.71	0.43
1:A:1373:ASP:HA	1:A:1376:THR:CG2	2.49	0.43
1:A:253:ASN:HB2	2:B:935:ARG:NH1	2.34	0.43
1:A:496:GLU:OE1	7:G:63:PRO:O	2.37	0.43
1:A:582:ILE:O	1:A:583:PRO:O	2.36	0.43
1:A:858:ASN:O	1:A:860:LEU:N	2.52	0.43
1:A:955:PRO:HG2	1:A:955:PRO:O	2.18	0.43
2:B:236:HIS:O	2:B:237:VAL:HG23	2.18	0.43
2:B:485:ARG:HH11	2:B:485:ARG:HG3	1.83	0.43
2:B:526:GLU:HG2	2:B:538:ASN:HB2	2.01	0.43
2:B:758:PHE:HB2	2:B:1024:ALA:HB1	2.00	0.43
2:B:995:ARG:O	2:B:997:GLU:N	2.52	0.43
2:B:798:TYR:HE2	3:C:62:PHE:CE2	2.37	0.43
1:A:1450:LEU:HD11	6:F:108:PHE:CZ	2.54	0.43
9:I:111:THR:CG2	9:I:112:SER:N	2.74	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:54:VAL:HG12	10:J:56:LEU:HD23	2.00	0.43
1:A:1021:LEU:O	1:A:1024:SER:HB3	2.19	0.43
1:A:841:LEU:HD13	1:A:1072:ILE:HB	2.00	0.43
1:A:1074:GLU:N	1:A:1075:PRO:CD	2.82	0.43
1:A:1098:VAL:N	1:A:1099:PRO:CD	2.81	0.43
1:A:1348:LEU:HG	1:A:1372:VAL:HG23	2.01	0.43
1:A:536:LEU:HG	1:A:536:LEU:H	1.51	0.43
1:A:919:ILE:O	1:A:920:LEU:C	2.57	0.43
1:A:751:SER:OG	2:B:1015:HIS:CE1	2.72	0.43
2:B:166:PHE:C	2:B:167:ILE:HG13	2.39	0.43
2:B:63:ILE:O	2:B:67:SER:HB3	2.19	0.43
2:B:936:ASP:CG	2:B:938:SER:H	2.23	0.43
3:C:76:ASP:HB2	3:C:128:ASN:O	2.18	0.43
3:C:41:ILE:HD11	3:C:247:GLY:CA	2.49	0.43
3:C:59:ALA:O	3:C:62:PHE:CB	2.67	0.43
4:D:26:THR:O	4:D:28:GLN:N	2.52	0.43
5:E:129:PRO:O	5:E:130:ALA:C	2.57	0.43
8:H:97:MET:SD	8:H:121:LEU:HD12	2.59	0.43
8:H:115:TYR:CE2	8:H:124:ARG:HG3	2.54	0.43
12:L:32:ALA:CB	12:L:55:ILE:HG13	2.49	0.43
12:L:50:ASP:O	12:L:52:GLY:N	2.52	0.43
13:S:281:TYR:CD1	13:S:281:TYR:C	2.93	0.43
1:A:1169:ILE:HD11	1:A:1229:SER:HB3	2.01	0.42
1:A:1384:VAL:O	1:A:1384:VAL:HG12	2.19	0.42
1:A:1444:MET:HG2	7:G:59:GLY:O	2.19	0.42
1:A:1446:ASP:HB3	1:A:1449:SER:HG	1.84	0.42
1:A:261:ASP:O	1:A:264:PHE:N	2.51	0.42
1:A:343:LYS:HE2	2:B:1156:ASP:HB2	2.01	0.42
1:A:366:VAL:O	1:A:463:ILE:HG12	2.19	0.42
1:A:715:GLU:C	1:A:717:ASN:N	2.71	0.42
1:A:727:ASP:O	1:A:731:ARG:HG3	2.18	0.42
1:A:784:LEU:HD11	1:A:815:PHE:CE2	2.54	0.42
1:A:996:ASN:C	1:A:998:LEU:H	2.22	0.42
2:B:1017:ILE:HG22	2:B:1018:PRO:HD3	2.01	0.42
2:B:1106:ARG:HD3	2:B:1126:GLY:C	2.39	0.42
2:B:1159:ARG:CD	2:B:1193:GLN:HG3	2.31	0.42
2:B:324:ILE:HG22	2:B:325:GLN:N	2.34	0.42
3:C:241:ASP:O	3:C:244:VAL:HB	2.19	0.42
5:E:154:ILE:HG22	5:E:155:ARG:O	2.19	0.42
8:H:27:GLU:HG2	8:H:39:THR:HG23	2.00	0.42
10:J:64:ASN:CB	10:J:65:PRO:CD	2.74	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:35:PHE:HD1	11:K:35:PHE:H	1.67	0.42
1:A:1129:GLU:O	1:A:1131:ALA:N	2.52	0.42
1:A:1282:VAL:C	1:A:1283:VAL:CG2	2.88	0.42
1:A:304:MET:O	1:A:326:ARG:HB3	2.19	0.42
1:A:533:LYS:HE3	1:A:745:GLN:NE2	2.34	0.42
1:A:600:PRO:HA	8:H:25:ARG:NH2	2.34	0.42
1:A:705:LYS:C	1:A:707:GLY:H	2.23	0.42
1:A:8:SER:O	1:A:9:ALA:C	2.57	0.42
2:B:1073:TYR:N	2:B:1073:TYR:CD1	2.87	0.42
2:B:1076:HIS:ND1	2:B:1076:HIS:N	2.66	0.42
2:B:1085:ILE:HD12	2:B:1085:ILE:N	2.34	0.42
2:B:176:SER:O	2:B:182:SER:HB3	2.19	0.42
2:B:292:ILE:N	2:B:293:PRO:HD2	2.34	0.42
2:B:597:MET:C	2:B:599:THR:H	2.22	0.42
3:C:197:SER:O	3:C:198:ALA:C	2.58	0.42
3:C:63:ILE:O	3:C:67:LEU:HG	2.19	0.42
5:E:182:ASP:O	5:E:185:ALA:HB3	2.19	0.42
5:E:205:SER:O	5:E:206:GLY:C	2.56	0.42
6:F:100:GLN:HG2	7:G:66:GLY:HA3	2.01	0.42
9:I:111:THR:HG21	9:I:113:ASP:HB2	2.00	0.42
1:A:1272:THR:HG22	1:A:1273:LEU:N	2.34	0.42
1:A:107:CYS:HB2	1:A:171:GLN:HG2	2.01	0.42
1:A:47:ARG:CZ	1:A:255:SER:H	2.31	0.42
1:A:472:LEU:O	1:A:475:THR:HG22	2.19	0.42
1:A:515:GLN:HB3	1:A:1071:SER:OG	2.20	0.42
1:A:526:ASP:HB3	1:A:657:LEU:HD23	2.01	0.42
1:A:527:THR:O	1:A:653:VAL:HG11	2.19	0.42
1:A:783:THR:HG21	1:A:815:PHE:CE2	2.53	0.42
2:B:222:ILE:O	2:B:240:ILE:HA	2.19	0.42
2:B:431:TYR:CD2	2:B:447:ALA:HB2	2.54	0.42
2:B:549:THR:CG2	2:B:550:ASP:H	2.17	0.42
2:B:912:ILE:HD11	2:B:966:VAL:HG23	1.99	0.42
1:A:483:ASP:HB2	2:B:987:LYS:CG	2.48	0.42
2:B:1003:ALA:HA	3:C:178:PHE:O	2.19	0.42
8:H:58:THR:HG22	8:H:59:ILE:N	2.35	0.42
13:S:254:TYR:C	13:S:256:ALA:N	2.73	0.42
1:A:1067:LEU:O	1:A:1067:LEU:HD12	2.20	0.42
1:A:370:ILE:O	1:A:371:ALA:C	2.57	0.42
1:A:608:ILE:O	1:A:609:ASP:C	2.58	0.42
1:A:928:LEU:C	1:A:930:ASP:N	2.70	0.42
2:B:295:GLY:HA2	2:B:298:LEU:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:546:SER:HG	2:B:630:ALA:CA	2.33	0.42
2:B:702:LEU:C	2:B:703:ILE:HG13	2.39	0.42
2:B:949:VAL:HG12	2:B:950:ASP:N	2.34	0.42
4:D:63:LEU:HD13	4:D:133:THR:OG1	2.19	0.42
5:E:147:HIS:HD2	5:E:149:LEU:H	1.67	0.42
5:E:25:ASP:O	5:E:27:GLY:N	2.52	0.42
10:J:52:THR:O	10:J:53:HIS:C	2.57	0.42
12:L:32:ALA:CB	12:L:55:ILE:HD12	2.48	0.42
1:A:1007:ILE:C	1:A:1009:ASN:N	2.71	0.42
1:A:1213:GLY:O	1:A:1215:ARG:N	2.53	0.42
1:A:1453:TYR:CE2	6:F:129:LYS:HA	2.54	0.42
1:A:40:THR:CG2	1:A:259:GLU:OE2	2.65	0.42
1:A:52:GLY:N	1:A:56:PRO:HG3	2.35	0.42
2:B:235:SER:OG	2:B:236:HIS:CD2	2.72	0.42
2:B:259:TYR:N	2:B:259:TYR:CD1	2.88	0.42
2:B:603:LEU:HD13	2:B:608:ASP:HB2	2.00	0.42
2:B:615:MET:HA	2:B:626:ILE:HA	2.01	0.42
2:B:744:HIS:HD2	2:B:746:SER:CB	2.32	0.42
3:C:236:GLY:C	3:C:238:ILE:N	2.73	0.42
3:C:245:VAL:C	3:C:247:GLY:N	2.73	0.42
3:C:258:ILE:N	3:C:258:ILE:HD12	2.35	0.42
6:F:103:MET:CE	7:G:66:GLY:H	2.32	0.42
9:I:73:ARG:HH12	9:I:112:SER:HB2	1.83	0.42
10:J:6:ARG:HB3	10:J:11:GLY:O	2.20	0.42
11:K:105:PHE:O	11:K:106:GLU:C	2.57	0.42
1:A:873:MET:C	1:A:1058:VAL:HG23	2.40	0.42
1:A:1081:LEU:HA	1:A:1081:LEU:HD13	1.84	0.42
1:A:1164:PRO:O	1:A:1167:GLU:HG3	2.19	0.42
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.18	0.42
1:A:231:PRO:O	1:A:233:TRP:N	2.52	0.42
1:A:252:PHE:HB2	1:A:256:GLN:HB3	2.01	0.42
1:A:695:LYS:O	1:A:697:ALA:N	2.53	0.42
1:A:929:LEU:HD13	1:A:929:LEU:O	2.19	0.42
2:B:1162:ILE:HG22	2:B:1163:CYS:O	2.19	0.42
2:B:283:VAL:O	2:B:284:ILE:C	2.57	0.42
2:B:533:CYS:C	2:B:535:LEU:N	2.72	0.42
2:B:843:GLN:HA	2:B:846:ILE:HG13	2.02	0.42
3:C:86:CYS:C	3:C:88:CYS:N	2.72	0.42
6:F:97:ARG:O	6:F:98:ALA:C	2.57	0.42
7:G:30:LEU:HD13	7:G:72:VAL:HG11	2.01	0.42
9:I:26:LEU:CD2	9:I:37:GLU:HA	2.41	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:LEU:HD23	5:E:204:THR:O	2.18	0.42
1:A:1134:ILE:O	1:A:1137:ALA:N	2.48	0.42
1:A:282:ASN:O	1:A:284:ALA:N	2.53	0.42
1:A:325:ILE:O	1:A:328:ARG:HB2	2.20	0.42
1:A:532:ARG:HD3	1:A:749:ALA:HB2	2.00	0.42
1:A:900:ASP:HA	1:A:926:GLN:HE22	1.84	0.42
1:A:962:ARG:O	1:A:963:ILE:C	2.58	0.42
2:B:1031:LEU:HD13	2:B:1055:ILE:HD11	2.00	0.42
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.83	0.42
2:B:582:VAL:HG23	2:B:626:ILE:CB	2.39	0.42
2:B:680:THR:HB	2:B:681:TRP:H	1.58	0.42
2:B:634:TYR:HE1	2:B:692:TYR:CD1	2.38	0.42
1:A:526:ASP:OD2	2:B:829:CYS:HB3	2.20	0.42
4:D:146:GLN:O	4:D:147:TYR:C	2.58	0.42
5:E:135:PHE:CD1	5:E:135:PHE:N	2.88	0.42
5:E:147:HIS:O	5:E:148:GLU:C	2.57	0.42
5:E:162:ARG:CG	5:E:162:ARG:HH11	2.32	0.42
5:E:185:ALA:O	5:E:190:LEU:HG	2.18	0.42
7:G:106:MET:HG2	7:G:107:LYS:N	2.34	0.42
7:G:145:VAL:HG12	7:G:146:LYS:H	1.82	0.42
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.54	0.42
1:A:1080:THR:C	1:A:1081:LEU:HD22	2.40	0.42
1:A:117:GLU:H	1:A:117:GLU:CD	2.23	0.42
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	2.02	0.42
1:A:322:VAL:CG1	1:A:323:LYS:N	2.82	0.42
1:A:523:ILE:HD12	1:A:622:VAL:CG2	2.49	0.42
1:A:566:ILE:O	1:A:567:LYS:C	2.57	0.42
1:A:605:MET:HE2	1:A:605:MET:HB2	1.78	0.42
1:A:853:ASP:OD2	1:A:857:ARG:NH2	2.52	0.42
1:A:893:PHE:CD2	1:A:893:PHE:C	2.92	0.42
1:A:933:TYR:C	1:A:935:GLN:N	2.72	0.42
2:B:315:LYS:HE2	9:I:4:PHE:CD2	2.55	0.42
2:B:515:HIS:HD2	2:B:517:THR:OG1	2.03	0.42
2:B:730:ARG:O	2:B:731:VAL:O	2.38	0.42
2:B:865:LYS:HZ2	2:B:869:SER:HA	1.84	0.42
3:C:183:TRP:O	3:C:184:ASN:C	2.58	0.42
3:C:91:HIS:O	3:C:91:HIS:CD2	2.73	0.42
5:E:144:ILE:C	5:E:146:HIS:N	2.72	0.42
6:F:138:LEU:O	6:F:140:ASP:N	2.52	0.42
7:G:21:ARG:HD3	7:G:21:ARG:HA	1.92	0.42
11:K:40:HIS:O	11:K:41:THR:C	2.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:LEU:O	1:A:1308:THR:HG22	2.19	0.42
1:A:1348:LEU:HG	1:A:1372:VAL:CG2	2.50	0.42
1:A:542:GLU:HG2	1:A:542:GLU:H	1.66	0.42
1:A:870:GLU:HG2	5:E:208:TYR:CE2	2.55	0.42
1:A:886:ILE:HG13	1:A:943:LEU:HD13	2.00	0.42
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.35	0.42
1:A:92:HIS:HB3	1:A:95:PHE:HB2	2.02	0.42
2:B:1090:THR:O	2:B:1091:TYR:C	2.57	0.42
2:B:23:ALA:CB	2:B:24:PRO:CD	2.95	0.42
2:B:515:HIS:CD2	2:B:517:THR:HG23	2.54	0.42
2:B:628:THR:O	2:B:629:ASP:O	2.38	0.42
2:B:642:ASP:HB3	2:B:649:LYS:CE	2.49	0.42
2:B:644:GLU:O	2:B:646:LEU:N	2.53	0.42
3:C:181:ASP:N	3:C:182:PRO:CD	2.83	0.42
7:G:44:TYR:HE1	7:G:157:ILE:HB	1.83	0.42
8:H:95:TYR:HB3	8:H:144:ILE:HB	2.00	0.42
1:A:598:LEU:CD2	8:H:25:ARG:NH1	2.83	0.42
11:K:58:PHE:CB	11:K:76:GLN:HE21	2.32	0.42
12:L:54:ARG:HH11	12:L:54:ARG:HG3	1.85	0.42
1:A:1131:ALA:O	1:A:1132:LYS:C	2.58	0.42
1:A:1215:ARG:HA	1:A:1215:ARG:HD2	1.87	0.42
1:A:216:VAL:O	1:A:219:PHE:HB2	2.20	0.42
1:A:254:GLU:N	2:B:935:ARG:HH22	2.17	0.42
1:A:419:LYS:HG3	1:A:420:ARG:H	1.84	0.42
1:A:483:ASP:OD2	1:A:485:ASP:OD1	2.38	0.42
1:A:552:TRP:O	1:A:554:PRO:HD3	2.20	0.42
1:A:518:LYS:HE2	1:A:624:SER:O	2.20	0.42
1:A:70:CYS:O	1:A:71:GLN:C	2.58	0.42
1:A:716:ASP:O	1:A:716:ASP:OD1	2.37	0.42
1:A:825:ILE:O	1:A:827:THR:N	2.52	0.42
2:B:1115:THR:CG2	2:B:1117:GLN:HB2	2.50	0.42
2:B:591:ARG:O	2:B:593:PRO:HD3	2.19	0.42
2:B:835:GLN:HE21	2:B:835:GLN:HB2	1.57	0.42
2:B:939:THR:HA	2:B:940:PRO:HD2	1.92	0.42
2:B:1073:TYR:HE2	3:C:180:TYR:CE2	2.37	0.42
4:D:33:PHE:CE1	7:G:80:LYS:CE	3.02	0.42
5:E:197:LYS:O	5:E:197:LYS:CG	2.64	0.42
7:G:27:LYS:HE2	7:G:54:ILE:HB	2.02	0.42
12:L:53:HIS:O	12:L:55:ILE:HG12	2.20	0.42
12:L:66:GLN:C	12:L:67:PHE:CD1	2.94	0.42
1:A:874:ASP:HA	1:A:1058:VAL:HG23	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1125:ALA:C	1:A:1127:ASP:N	2.72	0.41
1:A:114:LEU:O	1:A:115:LEU:HG	2.20	0.41
1:A:1143:LEU:HD23	1:A:1267:MET:O	2.19	0.41
1:A:1282:VAL:HG22	1:A:1308:THR:HA	2.01	0.41
1:A:324:SER:O	1:A:327:ALA:HB3	2.19	0.41
1:A:675:THR:O	1:A:675:THR:HG22	2.19	0.41
1:A:726:ARG:O	1:A:729:ALA:N	2.53	0.41
2:B:1098:MET:O	2:B:1099:VAL:C	2.59	0.41
2:B:172:ILE:HG22	2:B:173:MET:N	2.35	0.41
2:B:31:TRP:CE3	2:B:31:TRP:HA	2.55	0.41
2:B:373:ARG:CG	2:B:566:LEU:HD23	2.50	0.41
2:B:419:THR:HG21	2:B:468:GLU:OE2	2.20	0.41
2:B:487:THR:CG2	2:B:488:TYR:N	2.82	0.41
2:B:492:LEU:O	2:B:495:LEU:N	2.42	0.41
2:B:57:TYR:HD1	2:B:57:TYR:H	1.67	0.41
2:B:593:PRO:O	2:B:594:ALA:C	2.59	0.41
2:B:616:ILE:CD1	2:B:616:ILE:N	2.81	0.41
2:B:637:LEU:HD21	2:B:742:GLU:OE2	2.20	0.41
2:B:785:TYR:HE2	10:J:60:PHE:CZ	2.38	0.41
3:C:249:ASP:O	3:C:252:GLN:N	2.53	0.41
3:C:75:MET:O	3:C:246:ARG:NH2	2.31	0.41
6:F:86:THR:O	6:F:89:GLU:N	2.51	0.41
12:L:62:LYS:O	12:L:63:ARG:C	2.58	0.41
1:A:1092:LYS:HD2	1:A:1092:LYS:HA	1.82	0.41
1:A:1450:LEU:HD21	7:G:19:GLY:O	2.20	0.41
1:A:209:ASN:O	1:A:210:ILE:C	2.58	0.41
1:A:320:ARG:HH21	1:A:323:LYS:NZ	2.17	0.41
1:A:408:ASP:C	1:A:410:GLY:H	2.23	0.41
1:A:546:VAL:HG21	1:A:572:TRP:CD2	2.55	0.41
1:A:901:LEU:CG	1:A:926:GLN:HE21	2.28	0.41
2:B:1098:MET:O	2:B:1101:ASP:HB2	2.20	0.41
2:B:510:LYS:HE2	2:B:513:GLN:OE1	2.21	0.41
2:B:544:CYS:O	2:B:545:ILE:CG1	2.68	0.41
2:B:806:THR:N	2:B:809:MET:HE3	2.35	0.41
2:B:866:TYR:O	2:B:868:MET:N	2.53	0.41
3:C:164:ALA:O	3:C:165:LYS:C	2.57	0.41
3:C:18:VAL:O	3:C:20:PHE:CD2	2.73	0.41
1:A:567:LYS:CE	8:H:46:LEU:HB2	2.50	0.41
9:I:16:PRO:HA	9:I:26:LEU:O	2.21	0.41
9:I:55:THR:HG22	9:I:56:ALA:H	1.84	0.41
1:A:1397:LEU:HA	1:A:1400:CYS:HB2	1.99	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:LEU:HB3	1:A:614:PHE:CD2	2.55	0.41
2:B:1032:SER:O	2:B:1034:VAL:N	2.53	0.41
2:B:1102:LYS:C	2:B:1103:ILE:O	2.58	0.41
1:A:7:SER:HB2	2:B:1175:LEU:CD2	2.49	0.41
2:B:1201:LYS:HE2	2:B:1205:GLN:NE2	2.35	0.41
2:B:170:LEU:HA	2:B:171:PRO:HD2	1.87	0.41
2:B:174:LEU:HD11	2:B:204:ILE:CD1	2.49	0.41
2:B:233:PRO:HG2	2:B:234:ILE:HD12	2.02	0.41
2:B:303:TYR:HD2	2:B:303:TYR:N	2.18	0.41
2:B:45:SER:O	2:B:46:GLN:C	2.58	0.41
2:B:849:GLY:O	2:B:852:ARG:HG3	2.20	0.41
3:C:8:VAL:CG1	3:C:9:LYS:N	2.83	0.41
4:D:149:THR:O	4:D:149:THR:HG23	2.20	0.41
4:D:151:PHE:O	4:D:152:SER:O	2.38	0.41
4:D:195:ILE:O	4:D:198:LEU:HG	2.21	0.41
4:D:217:LEU:O	4:D:219:THR:N	2.54	0.41
5:E:117:THR:C	5:E:119:SER:N	2.73	0.41
5:E:16:PHE:CD1	5:E:58:MET:HE2	2.55	0.41
11:K:12:LEU:HD11	11:K:18:LYS:HE2	2.02	0.41
1:A:1260:LEU:HG	1:A:1260:LEU:O	2.20	0.41
1:A:550:LEU:HD22	1:A:556:TRP:CD1	2.55	0.41
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.73	0.41
1:A:630:ILE:HG23	1:A:642:CYS:SG	2.60	0.41
1:A:784:LEU:C	1:A:786:HIS:H	2.23	0.41
1:A:809:THR:O	1:A:810:PRO:C	2.58	0.41
2:B:1060:ARG:C	2:B:1062:HIS:H	2.22	0.41
2:B:121:ASN:HA	2:B:207:GLY:HA2	2.02	0.41
2:B:34:ILE:O	2:B:35:SER:C	2.58	0.41
2:B:515:HIS:CG	2:B:516:ASN:N	2.88	0.41
2:B:700:SER:C	2:B:701:ILE:CG2	2.89	0.41
2:B:770:GLN:OE1	2:B:983:ARG:HA	2.20	0.41
2:B:809:MET:O	2:B:811:TYR:N	2.54	0.41
1:A:254:GLU:H	2:B:935:ARG:NH1	2.18	0.41
3:C:187:LYS:HG3	3:C:219:PHE:CE1	2.55	0.41
3:C:255:VAL:HG21	11:K:94:ILE:HG21	2.03	0.41
3:C:80:LEU:HD12	3:C:95:CYS:HA	2.01	0.41
4:D:40:HIS:CG	4:D:41:GLN:N	2.89	0.41
5:E:124:VAL:HG13	5:E:132:ILE:CG1	2.50	0.41
5:E:112:TYR:CE1	5:E:136:ASN:HB2	2.56	0.41
5:E:143:ASN:ND2	5:E:146:HIS:ND1	2.68	0.41
7:G:7:LEU:O	7:G:73:LYS:HD2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:101:PHE:O	9:I:102:VAL:CG2	2.67	0.41
10:J:43:ARG:HG2	10:J:46:CYS:SG	2.61	0.41
11:K:85:ASP:O	11:K:89:ASN:ND2	2.54	0.41
13:S:269:PHE:CE2	13:S:306:TRP:CZ2	3.08	0.41
1:A:1377:THR:O	1:A:1378:GLN:C	2.57	0.41
1:A:266:LEU:O	1:A:267:ALA:C	2.58	0.41
1:A:324:SER:O	1:A:327:ALA:N	2.53	0.41
1:A:44:THR:O	1:A:45:GLN:CB	2.65	0.41
1:A:618:GLU:O	1:A:619:LYS:C	2.59	0.41
1:A:703:THR:O	1:A:704:ALA:C	2.59	0.41
1:A:889:SER:C	1:A:891:ALA:N	2.72	0.41
2:B:365:THR:CG2	2:B:367:LEU:HG	2.38	0.41
2:B:282:ILE:HD13	2:B:382:ILE:HD13	2.01	0.41
2:B:62:ILE:HG23	2:B:418:LYS:CG	2.49	0.41
2:B:575:PRO:HG2	2:B:576:ASP:H	1.84	0.41
2:B:635:ARG:HG3	2:B:635:ARG:NH1	2.35	0.41
2:B:702:LEU:HA	2:B:702:LEU:HD12	1.85	0.41
2:B:952:VAL:O	2:B:953:LEU:HB3	2.20	0.41
2:B:956:THR:HG22	2:B:960:GLY:HA2	2.02	0.41
2:B:995:ARG:O	2:B:996:ARG:C	2.59	0.41
3:C:215:GLU:O	3:C:216:GLY:C	2.59	0.41
3:C:249:ASP:O	3:C:250:THR:C	2.58	0.41
5:E:116:ILE:HG22	5:E:117:THR:N	2.35	0.41
5:E:33:GLU:C	5:E:35:VAL:N	2.72	0.41
6:F:150:GLU:O	6:F:151:LEU:C	2.59	0.41
6:F:75:PRO:C	6:F:77:ASP:N	2.74	0.41
1:A:1260:LEU:CG	1:A:1260:LEU:O	2.68	0.41
1:A:1279:ILE:CD1	1:A:1316:VAL:HG21	2.48	0.41
1:A:1362:TYR:CE1	1:A:1364:ASN:HA	2.56	0.41
1:A:1397:LEU:H	1:A:1397:LEU:HG	1.64	0.41
1:A:151:ASP:OD1	1:A:163:SER:CB	2.68	0.41
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.86	0.41
1:A:361:LEU:HG	1:A:507:VAL:CG1	2.51	0.41
1:A:368:LYS:O	1:A:369:SER:C	2.58	0.41
1:A:445:ASN:ND2	1:A:455:MET:HE3	2.35	0.41
1:A:475:THR:O	1:A:479:ASN:N	2.53	0.41
1:A:598:LEU:O	1:A:599:SER:C	2.58	0.41
1:A:960:ILE:O	1:A:960:ILE:HG22	2.20	0.41
2:B:129:PHE:HE2	2:B:166:PHE:CD1	2.35	0.41
2:B:274:PRO:CG	2:B:359:GLU:HB3	2.51	0.41
2:B:700:SER:O	2:B:701:ILE:HG22	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:830:TYR:HD1	2:B:830:TYR:HA	1.68	0.41
4:D:167:LEU:C	4:D:169:SER:H	2.24	0.41
5:E:114:ASN:O	5:E:115:ASN:CB	2.68	0.41
5:E:165:LEU:O	5:E:166:LYS:C	2.58	0.41
6:F:138:LEU:O	6:F:139:PRO:C	2.59	0.41
7:G:1:MET:SD	7:G:79:PHE:CE1	3.14	0.41
8:H:83:GLN:C	8:H:85:GLY:N	2.74	0.41
9:I:40:SER:HB2	9:I:41:PRO:HD2	2.03	0.41
3:C:241:ASP:HB3	11:K:109:TRP:CH2	2.55	0.41
11:K:55:LYS:O	11:K:77:THR:HG22	2.20	0.41
12:L:31:CYS:SG	12:L:34:CYS:N	2.93	0.41
1:A:1116:LEU:H	1:A:1308:THR:CG2	2.18	0.41
1:A:1120:LEU:N	1:A:1120:LEU:HD12	2.36	0.41
1:A:1187:GLN:HG3	1:A:1188:GLN:H	1.85	0.41
1:A:1419:ASP:OD1	1:A:1426:GLU:OE1	2.39	0.41
1:A:1427:ASN:O	1:A:1430:LEU:N	2.43	0.41
1:A:231:PRO:C	1:A:233:TRP:H	2.23	0.41
1:A:443:LEU:HB2	1:A:501:LEU:HD21	2.03	0.41
1:A:541:ILE:CD1	1:A:577:ILE:HD11	2.51	0.41
1:A:78:PRO:O	1:A:79:GLY:C	2.58	0.41
1:A:825:ILE:O	1:A:828:ALA:N	2.49	0.41
1:A:839:ARG:O	1:A:842:VAL:HB	2.21	0.41
2:B:293:PRO:CG	2:B:296:GLU:OE1	2.68	0.41
2:B:599:THR:O	2:B:603:LEU:HB2	2.20	0.41
2:B:604:ARG:C	2:B:606:LYS:H	2.24	0.41
3:C:8:VAL:HG12	3:C:10:ILE:H	1.86	0.41
3:C:229:TYR:CD1	3:C:229:TYR:N	2.89	0.41
4:D:50:LEU:HD11	7:G:4:ILE:CG1	2.51	0.41
4:D:59:ILE:O	4:D:60:LYS:C	2.58	0.41
5:E:211:TYR:HD1	5:E:211:TYR:N	2.19	0.41
5:E:66:GLU:HA	5:E:69:ILE:HD12	2.02	0.41
7:G:5:LYS:HG3	7:G:7:LEU:HD21	2.02	0.41
9:I:86:PHE:HB2	9:I:87:GLN:H	1.67	0.41
10:J:57:ILE:CG2	10:J:58:GLU:N	2.84	0.41
11:K:71:PHE:C	11:K:71:PHE:CD1	2.94	0.41
1:A:1018:PHE:O	1:A:1019:CYS:C	2.59	0.41
1:A:1167:GLU:O	1:A:1168:GLU:C	2.58	0.41
1:A:135:PHE:O	1:A:137:ALA:N	2.54	0.41
1:A:24:PRO:HG2	1:A:25:GLU:OE1	2.20	0.41
1:A:582:ILE:HA	1:A:583:PRO:HD2	1.84	0.41
1:A:883:LEU:HA	1:A:883:LEU:HD23	1.87	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:824:ILE:HG22	2:B:1087:PHE:CE2	2.55	0.41
2:B:114:PRO:CG	2:B:115:GLN:H	2.25	0.41
1:A:7:SER:HB2	2:B:1175:LEU:HD22	2.02	0.41
2:B:360:PHE:CE2	2:B:361:LEU:HB2	2.55	0.41
2:B:386:LEU:C	2:B:388:CYS:N	2.73	0.41
2:B:401:PHE:C	2:B:403:LYS:H	2.24	0.41
2:B:526:GLU:CD	2:B:752:ALA:CB	2.89	0.41
2:B:543:SER:C	2:B:544:CYS:SG	2.99	0.41
5:E:11:ARG:C	5:E:13:TRP:N	2.74	0.41
7:G:97:HIS:CD2	7:G:97:HIS:N	2.89	0.41
8:H:104:PHE:HZ	8:H:135:LEU:O	2.04	0.41
8:H:96:VAL:HA	8:H:142:LEU:O	2.21	0.41
8:H:3:ASN:HB3	8:H:4:THR:H	1.61	0.41
9:I:45:ARG:HE	9:I:47:GLU:HG3	1.85	0.41
13:S:308:PHE:O	13:S:309:SER:CB	2.69	0.41
1:A:1027:ALA:O	1:A:1030:ARG:N	2.54	0.41
1:A:103:CYS:SG	1:A:108:MET:HE3	2.61	0.41
1:A:1114:PRO:O	1:A:1115:SER:O	2.38	0.41
1:A:1308:THR:OG1	1:A:1309:ASP:N	2.53	0.41
1:A:130:ASP:C	1:A:132:LYS:H	2.24	0.41
1:A:49:LYS:HZ1	1:A:60:SER:C	2.23	0.41
1:A:544:ASP:CG	1:A:545:GLN:N	2.74	0.41
1:A:562:THR:HA	1:A:563:PRO:HD3	1.84	0.41
1:A:73:GLY:O	1:A:74:MET:C	2.59	0.41
1:A:971:PHE:N	1:A:971:PHE:CD1	2.88	0.41
2:B:1004:GLU:CB	2:B:1006:ILE:HD11	2.51	0.41
2:B:1152:MET:O	2:B:1154:ALA:N	2.54	0.41
2:B:23:ALA:CB	2:B:24:PRO:HD2	2.31	0.41
2:B:38:PHE:O	2:B:39:ARG:C	2.59	0.41
2:B:570:VAL:HA	2:B:571:PRO:HD2	1.78	0.41
2:B:857:ARG:O	2:B:858:SER:HB3	2.21	0.41
2:B:90:ILE:HD11	2:B:432:MET:SD	2.60	0.41
5:E:112:TYR:HE1	5:E:136:ASN:HD22	1.69	0.41
6:F:123:LYS:C	6:F:125:LEU:N	2.73	0.41
7:G:18:PHE:HA	7:G:22:MET:HE3	2.03	0.41
7:G:62:LEU:HB3	7:G:63:PRO:CD	2.50	0.41
10:J:18:TRP:HA	10:J:18:TRP:HE3	1.85	0.41
10:J:21:TYR:HB2	10:J:39:LEU:CD1	2.51	0.41
12:L:60:ARG:CG	12:L:61:THR:H	2.29	0.41
1:A:1451:VAL:O	1:A:1453:TYR:N	2.54	0.41
1:A:18:GLN:OE1	1:A:18:GLN:C	2.59	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASP:HA	1:A:221:SER:OG	2.21	0.41
1:A:35:ILE:HD12	1:A:241:VAL:CG2	2.50	0.41
1:A:393:ARG:C	1:A:395:GLY:N	2.75	0.41
1:A:420:ARG:O	1:A:424:ILE:HG13	2.21	0.41
1:A:556:TRP:CD2	1:A:558:GLY:HA2	2.55	0.41
1:A:996:ASN:CA	1:A:998:LEU:HD12	2.51	0.41
2:B:1064:TYR:O	2:B:1065:GLN:C	2.59	0.41
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.51	0.41
2:B:102:VAL:O	2:B:109:THR:HG23	2.21	0.41
2:B:1142:GLY:O	2:B:1144:ALA:N	2.54	0.41
2:B:408:LEU:O	2:B:412:LEU:HG	2.21	0.41
2:B:535:LEU:HA	2:B:535:LEU:HD23	1.87	0.41
2:B:635:ARG:HH11	2:B:635:ARG:CG	2.33	0.41
2:B:792:MET:O	2:B:793:ALA:HB2	2.20	0.41
3:C:26:ASP:O	3:C:27:LEU:C	2.58	0.41
3:C:61:GLU:HG2	3:C:62:PHE:N	2.36	0.41
3:C:69:LEU:H	3:C:69:LEU:CD1	2.32	0.41
4:D:34:GLN:O	4:D:47:LEU:HD23	2.21	0.41
5:E:24:LYS:CG	5:E:25:ASP:N	2.84	0.41
4:D:47:LEU:CD1	7:G:3:PHE:HD2	2.33	0.41
7:G:39:THR:HB	7:G:42:PHE:H	1.86	0.41
11:K:27:ALA:HB1	11:K:28:PRO:HD2	2.03	0.41
1:A:967:ALA:HA	1:A:1044:TRP:CZ3	2.56	0.41
1:A:1072:ILE:O	1:A:1075:PRO:CG	2.66	0.41
1:A:113:LEU:HA	1:A:113:LEU:HD23	1.96	0.41
1:A:1142:THR:O	1:A:1145:SER:OG	2.27	0.41
1:A:1191:TRP:HA	1:A:1191:TRP:CE3	2.56	0.41
1:A:704:ALA:O	1:A:705:LYS:CB	2.66	0.41
1:A:90:VAL:HG12	1:A:91:PHE:O	2.20	0.41
1:A:922:ASP:OD1	1:A:922:ASP:C	2.60	0.41
1:A:937:VAL:O	1:A:938:LYS:C	2.58	0.41
2:B:1168:LEU:HB2	2:B:1170:THR:OG1	2.21	0.41
1:A:7:SER:CB	2:B:1175:LEU:HD22	2.51	0.41
2:B:212:LEU:HA	2:B:212:LEU:HD23	1.73	0.41
2:B:351:TYR:O	2:B:355:ILE:HG13	2.20	0.41
2:B:483:LEU:HD12	2:B:484:ASN:N	2.35	0.41
3:C:27:LEU:HA	3:C:228:PHE:CE2	2.56	0.41
1:A:1318:THR:HB	5:E:141:VAL:HG11	2.03	0.41
5:E:59:SER:O	5:E:60:PHE:HB3	2.21	0.41
5:E:93:MET:O	5:E:94:LYS:C	2.59	0.41
10:J:48:ARG:C	10:J:48:ARG:HD2	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:65:HIS:NE2	11:K:67:PHE:CG	2.88	0.41
13:S:258:GLY:O	13:S:259:ALA:O	2.38	0.41
1:A:1037:LEU:HD23	1:A:1037:LEU:N	2.36	0.40
1:A:1147:THR:HG22	1:A:1148:ILE:N	2.36	0.40
1:A:1161:THR:CG2	1:A:1163:ILE:HG13	2.51	0.40
1:A:1165:GLU:H	1:A:1165:GLU:HG3	1.58	0.40
1:A:599:SER:HA	1:A:600:PRO:HD2	1.86	0.40
1:A:706:HIS:CD2	1:A:706:HIS:H	2.38	0.40
1:A:707:GLY:C	1:A:708:MET:HG3	2.41	0.40
1:A:848:ILE:O	1:A:1065:GLY:N	2.39	0.40
1:A:920:LEU:CD2	1:A:920:LEU:C	2.89	0.40
1:A:935:GLN:C	1:A:937:VAL:N	2.71	0.40
2:B:1023:VAL:O	2:B:1027:ILE:N	2.50	0.40
2:B:121:ASN:HA	2:B:207:GLY:CA	2.51	0.40
2:B:222:ILE:O	2:B:240:ILE:HG13	2.21	0.40
2:B:329:THR:O	2:B:332:ASP:HB3	2.21	0.40
2:B:878:GLN:O	2:B:879:ARG:C	2.58	0.40
3:C:22:LEU:HD13	3:C:230:MET:HE1	2.02	0.40
5:E:124:VAL:HA	5:E:132:ILE:CD1	2.47	0.40
5:E:124:VAL:HB	5:E:125:PRO:CD	2.50	0.40
1:A:1211:GLN:O	1:A:1214:GLU:HB2	2.21	0.40
1:A:130:ASP:C	1:A:132:LYS:N	2.75	0.40
1:A:445:ASN:HB2	1:A:455:MET:HG2	2.03	0.40
1:A:477:PRO:HG3	1:A:521:MET:HG2	2.03	0.40
1:A:626:ASN:HB3	1:A:627:GLY:H	1.71	0.40
1:A:639:PRO:HG2	1:A:640:GLN:H	1.85	0.40
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.99	0.40
1:A:942:PHE:C	1:A:942:PHE:CD2	2.94	0.40
2:B:1187:ASN:HD21	2:B:1190:ASP:HB3	1.86	0.40
2:B:1198:TYR:O	2:B:1199:ALA:C	2.59	0.40
2:B:114:PRO:HG3	2:B:194:GLU:HG3	2.03	0.40
2:B:247:GLY:N	2:B:418:LYS:HZ3	2.17	0.40
2:B:38:PHE:CE2	2:B:43:LEU:HD23	2.57	0.40
2:B:508:LEU:HB3	2:B:510:LYS:N	2.25	0.40
2:B:564:GLU:O	2:B:565:PRO:C	2.58	0.40
2:B:687:GLU:O	2:B:688:GLY:C	2.59	0.40
2:B:796:LEU:HA	2:B:796:LEU:HD12	1.82	0.40
2:B:842:ASN:O	2:B:846:ILE:HG13	2.21	0.40
2:B:847:ASP:O	2:B:849:GLY:N	2.55	0.40
2:B:873:THR:CG2	2:B:874:PHE:N	2.84	0.40
2:B:903:VAL:O	2:B:948:ILE:HG23	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:LEU:CD1	3:C:95:CYS:CA	2.99	0.40
5:E:144:ILE:H	5:E:144:ILE:HG12	1.68	0.40
1:A:1327:ILE:HG22	5:E:147:HIS:HE1	1.85	0.40
5:E:153:HIS:HB3	5:E:196:VAL:HG13	1.99	0.40
1:A:1004:ASN:HD22	5:E:167:ARG:HD2	1.78	0.40
6:F:88:TYR:HD1	6:F:88:TYR:H	1.67	0.40
7:G:132:SER:O	7:G:134:GLU:N	2.54	0.40
7:G:22:MET:O	7:G:23:LYS:C	2.59	0.40
8:H:47:PHE:CD2	8:H:95:TYR:HD1	2.39	0.40
9:I:34:TYR:HE2	9:I:36:GLU:CB	2.32	0.40
13:S:282:TYR:O	13:S:282:TYR:CG	2.73	0.40
1:A:1019:CYS:O	1:A:1022:LEU:CB	2.68	0.40
1:A:1435:PRO:C	1:A:1436:ILE:HG13	2.40	0.40
1:A:34:LYS:HD3	1:A:34:LYS:H	1.86	0.40
1:A:515:GLN:HB2	1:A:1071:SER:HB3	2.02	0.40
1:A:532:ARG:NH2	1:A:745:GLN:HG2	2.36	0.40
1:A:933:TYR:C	1:A:935:GLN:H	2.24	0.40
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.50	0.40
1:A:1438:THR:CG2	2:B:1144:ALA:HB3	2.51	0.40
2:B:1194:ILE:HD12	2:B:1196:ILE:CG2	2.52	0.40
2:B:213:ILE:HA	2:B:213:ILE:HD13	1.81	0.40
2:B:496:ARG:NH1	2:B:496:ARG:HB3	2.30	0.40
2:B:515:HIS:HD2	2:B:517:THR:N	2.12	0.40
2:B:996:ARG:HH22	3:C:175:ALA:CA	2.34	0.40
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.84	0.40
3:C:43:THR:CG2	3:C:44:LEU:H	2.34	0.40
4:D:188:ALA:O	4:D:191:ALA:N	2.55	0.40
4:D:29:LEU:O	4:D:30:GLY:O	2.39	0.40
5:E:60:PHE:HE2	5:E:80:VAL:CB	2.35	0.40
6:F:82:THR:HA	6:F:83:PRO:HD3	1.82	0.40
7:G:154:VAL:HB	7:G:155:SER:H	1.71	0.40
7:G:5:LYS:CG	7:G:7:LEU:HD21	2.51	0.40
10:J:13:VAL:HG12	10:J:14:VAL:H	1.86	0.40
10:J:47:ARG:HG2	10:J:47:ARG:HH11	1.85	0.40
11:K:101:LEU:O	11:K:102:LYS:C	2.58	0.40
12:L:32:ALA:HB3	12:L:55:ILE:CG1	2.52	0.40
1:A:1129:GLU:O	1:A:1130:GLN:C	2.60	0.40
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.52	0.40
1:A:42:ASP:O	1:A:44:THR:N	2.38	0.40
1:A:493:GLN:HE21	1:A:493:GLN:CA	2.33	0.40
1:A:757:ASN:O	1:A:761:MET:HG3	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:SER:C	1:A:805:LEU:N	2.75	0.40
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.25	0.40
1:A:932:GLU:HG3	1:A:936:LEU:HD21	2.02	0.40
2:B:1013:ASN:OD1	2:B:1014:PRO:HD2	2.21	0.40
2:B:1183:LYS:HA	2:B:1186:ASP:HA	2.04	0.40
2:B:216:GLU:HB2	2:B:406:LEU:CD2	2.51	0.40
2:B:349:ILE:HG22	2:B:349:ILE:O	2.20	0.40
2:B:236:HIS:HE1	2:B:389:ALA:HA	1.83	0.40
2:B:530:GLY:O	2:B:532:ALA:N	2.54	0.40
2:B:661:LEU:C	2:B:663:ALA:N	2.75	0.40
1:A:254:GLU:H	2:B:935:ARG:HH22	1.70	0.40
4:D:52:LEU:O	4:D:54:GLU:N	2.46	0.40
5:E:37:LEU:HA	5:E:38:PRO:HD2	1.94	0.40
6:F:97:ARG:O	6:F:100:GLN:N	2.54	0.40
7:G:13:LEU:HD12	7:G:26:LEU:HD21	2.03	0.40
4:D:50:LEU:HD11	7:G:4:ILE:HG13	2.03	0.40
6:F:99:LEU:HD21	7:G:66:GLY:N	2.37	0.40
10:J:21:TYR:HB2	10:J:39:LEU:HD13	2.02	0.40
2:B:763:GLN:OE1	13:S:292:PRO:HB3	2.21	0.40
1:A:1116:LEU:HG	1:A:1116:LEU:O	2.22	0.40
1:A:1138:ILE:CG2	1:A:1316:VAL:HG13	2.52	0.40
1:A:1347:ALA:O	1:A:1348:LEU:C	2.60	0.40
1:A:461:LYS:O	1:A:463:ILE:HG23	2.22	0.40
1:A:501:LEU:HD11	2:B:1146:PHE:CE2	2.56	0.40
1:A:599:SER:HB2	1:A:603:ASN:H	1.87	0.40
1:A:79:GLY:C	1:A:243:PRO:HG3	2.42	0.40
1:A:867:ILE:HG22	1:A:871:ASP:H	1.85	0.40
2:B:1192:TYR:N	2:B:1192:TYR:CD1	2.89	0.40
2:B:240:ILE:O	2:B:240:ILE:CG2	2.68	0.40
2:B:377:PHE:C	2:B:379:GLY:N	2.71	0.40
2:B:516:ASN:H	2:B:516:ASN:HD22	1.70	0.40
2:B:533:CYS:SG	2:B:534:GLY:N	2.95	0.40
5:E:93:MET:O	5:E:96:PHE:N	2.55	0.40
6:F:103:MET:HE3	7:G:15:PRO:HG2	2.03	0.40
2:B:800:GLN:CB	10:J:52:THR:CG2	2.98	0.40
11:K:20:LYS:HB2	11:K:20:LYS:HE3	1.89	0.40
12:L:61:THR:HG22	12:L:63:ARG:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1418/1733 (82%)	914 (64%)	316 (22%)	188 (13%)	0	4
2	B	1096/1224 (90%)	726 (66%)	223 (20%)	147 (13%)	0	4
3	C	264/318 (83%)	169 (64%)	62 (24%)	33 (12%)	0	6
4	D	173/221 (78%)	129 (75%)	27 (16%)	17 (10%)	0	10
5	E	212/215 (99%)	141 (66%)	50 (24%)	21 (10%)	0	10
6	F	82/155 (53%)	60 (73%)	15 (18%)	7 (8%)	1	12
7	G	169/171 (99%)	123 (73%)	34 (20%)	12 (7%)	1	17
8	H	129/146 (88%)	93 (72%)	26 (20%)	10 (8%)	1	15
9	I	117/122 (96%)	80 (68%)	22 (19%)	15 (13%)	0	5
10	J	63/70 (90%)	36 (57%)	14 (22%)	13 (21%)	0	2
11	K	112/120 (93%)	82 (73%)	25 (22%)	5 (4%)	2	25
12	L	44/70 (63%)	18 (41%)	14 (32%)	12 (27%)	0	0
13	S	68/179 (38%)	51 (75%)	10 (15%)	7 (10%)	0	9
All	All	3947/4744 (83%)	2622 (66%)	838 (21%)	487 (12%)	0	6

All (487) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	48	ALA
1	A	55	ASP
1	A	58	LEU
1	A	62	ASP
1	A	70	CYS
1	A	73	GLY
1	A	76	GLU
1	A	93	VAL
1	A	130	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	286	HIS
1	A	311	GLN
1	A	322	VAL
1	A	385	ILE
1	A	399	HIS
1	A	423	ASP
1	A	516	SER
1	A	525	GLN
1	A	536	LEU
1	A	567	LYS
1	A	583	PRO
1	A	626	ASN
1	A	709	THR
1	A	780	VAL
1	A	821	ARG
1	A	920	LEU
1	A	1002	GLY
1	A	1036	ARG
1	A	1115	SER
1	A	1122	PRO
1	A	1124	HIS
1	A	1165	GLU
1	A	1167	GLU
1	A	1212	VAL
1	A	1223	ASP
1	A	1231	ASP
1	A	1242	VAL
1	A	1281	ARG
1	A	1308	THR
1	A	1309	ASP
1	A	1335	ILE
1	A	1341	ILE
1	A	1366	ARG
1	A	1377	THR
1	A	1378	GLN
1	A	1386	ARG
1	A	1392	SER
1	A	1396	ALA
1	A	1397	LEU
1	A	1403	GLU
1	A	1405	THR
1	A	1424	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	43	LEU
2	B	45	SER
2	B	58	THR
2	B	67	SER
2	B	108	VAL
2	B	124	TYR
2	B	186	GLU
2	B	219	ALA
2	B	261	ARG
2	B	367	LEU
2	B	391	ASP
2	B	466	TRP
2	B	467	GLY
2	B	468	GLU
2	B	474	SER
2	B	510	LYS
2	B	530	GLY
2	B	531	GLN
2	B	571	PRO
2	B	591	ARG
2	B	620	ARG
2	B	629	ASP
2	B	636	PRO
2	B	643	ASP
2	B	648	HIS
2	B	709	ASP
2	B	727	LYS
2	B	731	VAL
2	B	751	VAL
2	B	752	ALA
2	B	818	PRO
2	B	901	PRO
2	B	943	SER
2	B	958	GLN
2	B	992	ILE
2	B	1046	PRO
2	B	1108	ARG
2	B	1157	ALA
2	B	1167	GLY
2	B	1171	VAL
2	B	1175	LEU
2	B	1181	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1188	LYS
2	B	1211	ASN
3	C	10	ILE
3	C	60	ASP
3	C	81	GLU
3	C	83	SER
3	C	87	PHE
3	C	110	THR
3	C	149	LYS
3	C	167	HIS
3	C	175	ALA
3	C	184	ASN
3	C	213	PRO
3	C	214	ASN
3	C	215	GLU
3	C	216	GLY
4	D	12	ARG
4	D	15	LEU
4	D	20	GLU
4	D	152	SER
5	E	130	ALA
5	E	158	SER
6	F	81	THR
7	G	118	ASP
8	H	81	PRO
8	H	84	ALA
8	H	140	ALA
9	I	9	ASP
9	I	11	ASN
9	I	84	VAL
10	J	6	ARG
10	J	15	GLY
10	J	53	HIS
10	J	64	ASN
12	L	50	ASP
12	L	53	HIS
12	L	59	ALA
12	L	60	ARG
13	S	275	LYS
13	S	292	PRO
1	A	42	ASP
1	A	44	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	45	GLN
1	A	54	ASN
1	A	57	ARG
1	A	61	ILE
1	A	74	MET
1	A	79	GLY
1	A	111	GLY
1	A	126	LEU
1	A	131	SER
1	A	154	SER
1	A	219	PHE
1	A	223	GLY
1	A	244	PRO
1	A	290	GLU
1	A	317	LYS
1	A	318	SER
1	A	331	GLY
1	A	332	LYS
1	A	335	ARG
1	A	400	PRO
1	A	415	LEU
1	A	418	SER
1	A	419	LYS
1	A	424	ILE
1	A	473	SER
1	A	557	ASP
1	A	594	GLY
1	A	598	LEU
1	A	619	LYS
1	A	708	MET
1	A	716	ASP
1	A	720	ARG
1	A	738	LYS
1	A	760	GLN
1	A	765	VAL
1	A	775	ILE
1	A	824	LEU
1	A	846	GLU
1	A	847	ASP
1	A	859	SER
1	A	864	ILE
1	A	875	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	929	LEU
1	A	968	GLN
1	A	979	SER
1	A	1006	ILE
1	A	1016	THR
1	A	1052	GLN
1	A	1084	PHE
1	A	1089	VAL
1	A	1104	ILE
1	A	1105	LEU
1	A	1126	ALA
1	A	1128	GLN
1	A	1164	PRO
1	A	1168	GLU
1	A	1169	ILE
1	A	1170	ILE
1	A	1224	LEU
1	A	1314	SER
1	A	1365	TYR
1	A	1376	THR
2	B	21	GLU
2	B	46	GLN
2	B	65	GLU
2	B	68	THR
2	B	114	PRO
2	B	229	ALA
2	B	258	LEU
2	B	260	GLY
2	B	266	ALA
2	B	294	ASP
2	B	322	PHE
2	B	504	ARG
2	B	509	ALA
2	B	526	GLU
2	B	534	GLY
2	B	559	SER
2	B	605	ARG
2	B	613	VAL
2	B	641	GLU
2	B	810	GLU
2	B	867	GLY
2	B	869	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	880	THR
2	B	881	ASN
2	B	891	ASP
2	B	902	GLY
2	B	903	VAL
2	B	907	GLY
2	B	1018	PRO
2	B	1041	GLU
2	B	1096	ARG
2	B	1099	VAL
2	B	1150	ARG
2	B	1156	ASP
2	B	1170	THR
2	B	1183	LYS
2	B	1186	ASP
2	B	1190	ASP
3	C	74	SER
3	C	141	GLY
3	C	161	LYS
4	D	6	SER
4	D	8	PHE
4	D	16	LYS
4	D	19	GLU
4	D	30	GLY
4	D	199	ASN
4	D	218	GLU
5	E	36	GLU
5	E	45	LYS
5	E	59	SER
5	E	106	GLN
5	E	145	THR
5	E	189	GLY
5	E	206	GLY
6	F	131	PRO
7	G	83	LYS
7	G	154	VAL
8	H	59	ILE
8	H	77	ARG
8	H	82	PRO
8	H	108	SER
8	H	128	ASN
9	I	3	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	34	TYR
9	I	62	ILE
9	I	89	GLN
9	I	106	CYS
9	I	107	SER
10	J	2	ILE
10	J	62	ARG
11	K	37	LYS
11	K	103	THR
12	L	43	THR
12	L	51	CYS
12	L	56	LEU
13	S	259	ALA
1	A	59	GLY
1	A	66	LYS
1	A	89	PRO
1	A	124	GLN
1	A	167	CYS
1	A	283	GLY
1	A	394	ASN
1	A	396	PRO
1	A	517	ASN
1	A	543	LEU
1	A	592	ASP
1	A	640	GLN
1	A	647	GLY
1	A	707	GLY
1	A	731	ARG
1	A	774	ARG
1	A	903	ASN
1	A	1017	LEU
1	A	1060	PRO
1	A	1062	GLU
1	A	1131	ALA
1	A	1221	LYS
1	A	1229	SER
1	A	1452	LYS
2	B	115	GLN
2	B	131	ASP
2	B	176	SER
2	B	206	ASN
2	B	295	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	308	TRP
2	B	334	ILE
2	B	365	THR
2	B	369	GLY
2	B	469	GLN
2	B	480	SER
2	B	551	PRO
2	B	598	GLU
2	B	645	SER
2	B	682	SER
2	B	688	GLY
2	B	711	GLU
2	B	712	PRO
2	B	738	PHE
2	B	761	HIS
2	B	792	MET
2	B	822	ASN
2	B	996	ARG
2	B	1017	ILE
2	B	1153	GLU
2	B	1155	SER
2	B	1189	ILE
3	C	6	PRO
3	C	28	ALA
3	C	91	HIS
3	C	169	LYS
3	C	202	PRO
3	C	212	PRO
3	C	218	PRO
3	C	264	GLN
4	D	52	LEU
5	E	8	ASN
5	E	44	ALA
5	E	56	LYS
5	E	74	ASP
5	E	192	ARG
7	G	17	PHE
7	G	139	ILE
7	G	147	ILE
9	I	7	CYS
9	I	113	ASP
10	J	22	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	35	SER
12	L	49	LYS
13	S	295	THR
1	A	35	ILE
1	A	67	CYS
1	A	100	LYS
1	A	196	GLU
1	A	253	ASN
1	A	312	PRO
1	A	465	TYR
1	A	526	ASP
1	A	605	MET
1	A	986	ILE
1	A	1040	GLN
1	A	1139	GLU
1	A	1206	ASP
1	A	1266	THR
1	A	1280	GLU
1	A	1302	PRO
2	B	387	LEU
2	B	409	ALA
2	B	430	ARG
2	B	754	SER
2	B	848	ARG
2	B	884	ARG
2	B	946	ASN
2	B	1029	CYS
2	B	1143	ALA
2	B	1178	ASN
2	B	1202	LEU
3	C	90	ASP
3	C	198	ALA
3	C	227	THR
3	C	240	VAL
4	D	131	GLU
4	D	168	LYS
5	E	73	PRO
5	E	115	ASN
6	F	73	ALA
6	F	112	GLU
7	G	133	SER
8	H	92	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	32	CYS
9	I	73	ARG
9	I	86	PHE
9	I	95	THR
10	J	9	SER
10	J	29	GLU
10	J	51	LEU
10	J	63	TYR
11	K	64	GLU
12	L	42	ARG
13	S	288	SER
1	A	84	ILE
1	A	197	PRO
1	A	696	GLU
1	A	759	ALA
1	A	789	LYS
1	A	795	GLU
1	A	808	LEU
1	A	817	ALA
1	A	958	VAL
1	A	1160	SER
1	A	1188	GLN
1	A	1435	PRO
2	B	22	SER
2	B	56	ASP
2	B	368	GLU
2	B	483	LEU
2	B	490	SER
2	B	565	PRO
2	B	878	GLN
2	B	879	ARG
2	B	883	LEU
2	B	1019	SER
2	B	1100	ASP
3	C	148	ARG
4	D	27	LEU
4	D	142	LYS
5	E	40	GLU
5	E	172	GLU
5	E	183	PRO
6	F	108	PHE
7	G	30	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	124	GLY
7	G	165	GLU
8	H	52	GLN
11	K	70	ARG
13	S	277	LYS
13	S	293	LEU
1	A	599	SER
1	A	641	VAL
1	A	719	VAL
1	A	1162	VAL
1	A	1338	VAL
2	B	171	PRO
2	B	282	ILE
2	B	450	ALA
2	B	543	SER
2	B	694	ASP
2	B	758	PHE
2	B	906	SER
2	B	1103	ILE
2	B	1118	PRO
3	C	126	GLY
3	C	171	GLY
4	D	201	LYS
6	F	139	PRO
10	J	18	TRP
12	L	26	THR
12	L	46	VAL
1	A	507	VAL
1	A	1057	VAL
2	B	635	ARG
3	C	142	VAL
6	F	93	ILE
1	A	9	ALA
1	A	653	VAL
1	A	886	ILE
1	A	963	ILE
1	A	1158	PRO
2	B	985	GLY
5	E	37	LEU
7	G	63	PRO
1	A	392	VAL
1	A	673	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1379	GLY
2	B	410	GLY
2	B	502	ILE
2	B	552	MET
2	B	974	PRO
1	A	250	ILE
1	A	649	ILE
1	A	1031	VAL
10	J	14	VAL
11	K	43	GLY
1	A	357	PRO
1	A	1061	GLY
2	B	575	PRO
7	G	157	ILE
5	E	129	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	1246/1520 (82%)	1133 (91%)	113 (9%)	9	36
2	B	964/1061 (91%)	880 (91%)	84 (9%)	10	38
3	C	234/274 (85%)	205 (88%)	29 (12%)	4	24
4	D	140/200 (70%)	126 (90%)	14 (10%)	7	32
5	E	196/197 (100%)	184 (94%)	12 (6%)	18	50
6	F	74/137 (54%)	63 (85%)	11 (15%)	3	18
7	G	152/152 (100%)	143 (94%)	9 (6%)	19	51
8	H	117/128 (91%)	110 (94%)	7 (6%)	19	50
9	I	113/116 (97%)	97 (86%)	16 (14%)	3	21
10	J	60/65 (92%)	55 (92%)	5 (8%)	11	40
11	K	99/102 (97%)	91 (92%)	8 (8%)	11	41
12	L	40/57 (70%)	33 (82%)	7 (18%)	2	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	S	62/156 (40%)	55 (89%)	7 (11%)	6	28
All	All	3497/4165 (84%)	3175 (91%)	322 (9%)	9	35

All (322) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	13	THR
1	A	14	VAL
1	A	18	GLN
1	A	34	LYS
1	A	41	MET
1	A	54	ASN
1	A	62	ASP
1	A	83	HIS
1	A	93	VAL
1	A	108	MET
1	A	167	CYS
1	A	195	ASP
1	A	200	ARG
1	A	208	LEU
1	A	215	SER
1	A	220	THR
1	A	270	LEU
1	A	303	TYR
1	A	308	ILE
1	A	326	ARG
1	A	329	LEU
1	A	335	ARG
1	A	354	SER
1	A	362	ASP
1	A	375	THR
1	A	381	THR
1	A	406	ILE
1	A	408	ASP
1	A	425	GLN
1	A	434	ARG
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	453	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	454	SER
1	A	466	SER
1	A	469	ARG
1	A	481	ASP
1	A	487	MET
1	A	489	LEU
1	A	493	GLN
1	A	498	ARG
1	A	501	LEU
1	A	503	GLN
1	A	523	ILE
1	A	524	VAL
1	A	560	ILE
1	A	562	THR
1	A	596	THR
1	A	618	GLU
1	A	626	ASN
1	A	629	LEU
1	A	734	GLU
1	A	739	ASP
1	A	754	SER
1	A	762	SER
1	A	774	ARG
1	A	786	HIS
1	A	791	ASP
1	A	816	HIS
1	A	821	ARG
1	A	831	THR
1	A	833	GLU
1	A	845	LEU
1	A	852	TYR
1	A	854	ASN
1	A	858	ASN
1	A	879	GLU
1	A	890	ASP
1	A	897	TYR
1	A	903	ASN
1	A	906	HIS
1	A	920	LEU
1	A	929	LEU
1	A	936	LEU
1	A	949	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	969	GLN
1	A	1029	ARG
1	A	1035	TYR
1	A	1048	ASN
1	A	1050	GLU
1	A	1058	VAL
1	A	1081	LEU
1	A	1082	ASN
1	A	1110	ASN
1	A	1111	MET
1	A	1114	PRO
1	A	1116	LEU
1	A	1122	PRO
1	A	1127	ASP
1	A	1142	THR
1	A	1155	ASP
1	A	1166	ASP
1	A	1236	LEU
1	A	1264	GLU
1	A	1271	ILE
1	A	1274	ARG
1	A	1291	VAL
1	A	1295	THR
1	A	1298	TYR
1	A	1300	LYS
1	A	1325	THR
1	A	1333	ILE
1	A	1353	TYR
1	A	1358	SER
1	A	1362	TYR
1	A	1364	ASN
1	A	1372	VAL
1	A	1376	THR
1	A	1445	ILE
1	A	1447	GLU
2	B	44	VAL
2	B	57	TYR
2	B	128	LEU
2	B	175	ARG
2	B	194	GLU
2	B	217	ARG
2	B	223	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	261	ARG
2	B	268	THR
2	B	286	PHE
2	B	294	ASP
2	B	298	LEU
2	B	365	THR
2	B	371	GLU
2	B	378	LEU
2	B	393	LYS
2	B	401	PHE
2	B	408	LEU
2	B	419	THR
2	B	427	ASP
2	B	429	PHE
2	B	463	THR
2	B	466	TRP
2	B	476	ARG
2	B	485	ARG
2	B	496	ARG
2	B	498	THR
2	B	510	LYS
2	B	511	PRO
2	B	582	VAL
2	B	603	LEU
2	B	615	MET
2	B	629	ASP
2	B	635	ARG
2	B	636	PRO
2	B	644	GLU
2	B	658	ILE
2	B	682	SER
2	B	724	ASP
2	B	737	THR
2	B	742	GLU
2	B	743	ILE
2	B	748	ILE
2	B	751	VAL
2	B	766	ARG
2	B	815	ARG
2	B	830	TYR
2	B	835	GLN
2	B	839	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	855	PHE
2	B	856	PHE
2	B	859	TYR
2	B	878	GLN
2	B	895	ASP
2	B	901	PRO
2	B	909	ASP
2	B	939	THR
2	B	953	LEU
2	B	986	GLN
2	B	987	LYS
2	B	993	THR
2	B	997	GLU
2	B	999	MET
2	B	1002	THR
2	B	1006	ILE
2	B	1026	LEU
2	B	1034	VAL
2	B	1047	PHE
2	B	1051	THR
2	B	1076	HIS
2	B	1084	GLN
2	B	1087	PHE
2	B	1092	TYR
2	B	1095	LEU
2	B	1096	ARG
2	B	1104	HIS
2	B	1137	CYS
2	B	1138	MET
2	B	1159	ARG
2	B	1170	THR
2	B	1183	LYS
2	B	1202	LEU
2	B	1212	ILE
2	B	1224	PHE
3	C	23	SER
3	C	44	LEU
3	C	54	ASN
3	C	55	THR
3	C	56	THR
3	C	57	VAL
3	C	58	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	62	PHE
3	C	74	SER
3	C	77	ILE
3	C	86	CYS
3	C	88	CYS
3	C	89	GLU
3	C	91	HIS
3	C	100	THR
3	C	104	PHE
3	C	108	GLU
3	C	129	ILE
3	C	138	GLU
3	C	140	ASN
3	C	143	LEU
3	C	147	LEU
3	C	186	LEU
3	C	193	TYR
3	C	214	ASN
3	C	240	VAL
3	C	245	VAL
3	C	250	THR
3	C	266	ASP
4	D	47	LEU
4	D	63	LEU
4	D	70	PHE
4	D	137	ASN
4	D	139	LYS
4	D	148	LEU
4	D	149	THR
4	D	152	SER
4	D	177	VAL
4	D	182	SER
4	D	187	THR
4	D	193	THR
4	D	197	SER
4	D	206	GLU
5	E	60	PHE
5	E	72	PHE
5	E	83	CYS
5	E	104	ASN
5	E	114	ASN
5	E	135	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	153	HIS
5	E	169	ARG
5	E	183	PRO
5	E	207	ARG
5	E	211	TYR
5	E	212	ARG
6	F	77	ASP
6	F	79	ARG
6	F	81	THR
6	F	84	TYR
6	F	86	THR
6	F	90	ARG
6	F	96	THR
6	F	119	ARG
6	F	143	PHE
6	F	148	VAL
6	F	153	VAL
7	G	1	MET
7	G	38	CYS
7	G	39	THR
7	G	70	PHE
7	G	78	VAL
7	G	80	LYS
7	G	96	GLN
7	G	126	ASN
7	G	171	ILE
8	H	10	PHE
8	H	86	ASP
8	H	95	TYR
8	H	102	TYR
8	H	130	ARG
8	H	134	ASN
8	H	141	TYR
9	I	6	PHE
9	I	8	ARG
9	I	9	ASP
9	I	10	CYS
9	I	13	MET
9	I	32	CYS
9	I	34	TYR
9	I	46	HIS
9	I	75	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	78	CYS
9	I	85	PHE
9	I	86	PHE
9	I	100	PHE
9	I	101	PHE
9	I	106	CYS
9	I	113	ASP
10	J	2	ILE
10	J	28	ASP
10	J	46	CYS
10	J	48	ARG
10	J	55	ASP
11	K	10	PHE
11	K	25	THR
11	K	35	PHE
11	K	47	ARG
11	K	70	ARG
11	K	78	THR
11	K	81	TYR
11	K	114	LEU
12	L	33	GLU
12	L	48	CYS
12	L	51	CYS
12	L	55	ILE
12	L	63	ARG
12	L	65	VAL
12	L	68	GLU
13	S	263	ARG
13	S	266	THR
13	S	267	ASP
13	S	283	GLN
13	S	288	SER
13	S	292	PRO
13	S	293	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	80	HIS
1	A	83	HIS
1	A	92	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	213	HIS
1	A	225	ASN
1	A	256	GLN
1	A	299	HIS
1	A	339	ASN
1	A	394	ASN
1	A	435	HIS
1	A	445	ASN
1	A	451	HIS
1	A	493	GLN
1	A	503	GLN
1	A	587	HIS
1	A	603	ASN
1	A	611	GLN
1	A	631	HIS
1	A	654	ASN
1	A	659	HIS
1	A	741	ASN
1	A	757	ASN
1	A	786	HIS
1	A	851	HIS
1	A	858	ASN
1	A	877	HIS
1	A	903	ASN
1	A	926	GLN
1	A	1048	ASN
1	A	1085	HIS
1	A	1106	ASN
1	A	1232	ASN
1	A	1432	GLN
2	B	52	ASN
2	B	60	GLN
2	B	121	ASN
2	B	178	ASN
2	B	236	HIS
2	B	325	GLN
2	B	366	GLN
2	B	465	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	657	HIS
2	B	744	HIS
2	B	821	GLN
2	B	835	GLN
2	B	957	ASN
2	B	984	HIS
2	B	1015	HIS
2	B	1065	GLN
2	B	1084	GLN
2	B	1117	GLN
2	B	1161	HIS
2	B	1179	GLN
2	B	1193	GLN
3	C	65	HIS
3	C	73	GLN
3	C	79	GLN
3	C	91	HIS
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	252	GLN
4	D	28	GLN
4	D	39	ASN
4	D	40	HIS
4	D	51	ASN
4	D	137	ASN
5	E	101	GLN
5	E	104	ASN
5	E	114	ASN
5	E	143	ASN
5	E	147	HIS
7	G	14	HIS
7	G	53	ASN
7	G	97	HIS
7	G	122	ASN
7	G	126	ASN
9	I	12	ASN
9	I	83	ASN
9	I	89	GLN
9	I	90	GLN
11	K	65	HIS
11	K	76	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	89	ASN
13	S	283	GLN
13	S	285	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	269:PHE	C	270:THR	N	0.95

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.