



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:43 AM UTC

PDB ID : 3PXI / pdb_00003pxi
Title : Structure of MecA108:ClpC
Authors : Wang, F.; Mei, Z.Q.; Wang, J.W.; Shi, Y.G.
Deposited on : 2010-12-09
Resolution : 6.93 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

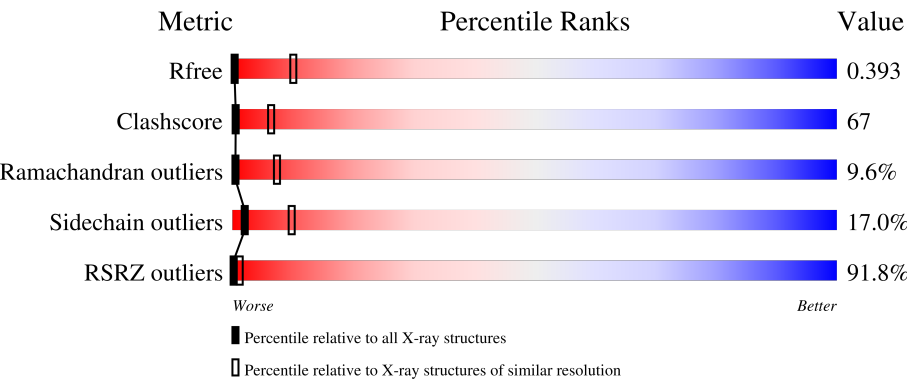
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 6.93 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1166 (9.70-4.00)
Clashscore	190562	1007 (9.70-4.04)
Ramachandran outliers	187476	1053 (9.70-4.00)
Sidechain outliers	187428	1016 (9.70-4.00)
RSRZ outliers	180081	1159 (9.70-4.00)

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

Mol	Chain	Length	Quality of chain
1	a	111	80% 25% 44% 14% • 15%
1	b	111	78% 26% 41% 16% • 15%
1	c	111	79% 23% 46% 15% • 15%
2	A	758	87% 31% 45% 16% • 7%
2	B	758	85% 27% 45% 18% • 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	C	758	84% 31%46%15%6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18645 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 Adapter protein mecA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	a	94	Total	C	N	O	S	0	0	0
			755	486	118	149	2			
1	b	94	Total	C	N	O	S	0	0	0
			756	485	120	149	2			
1	c	94	Total	C	N	O	S	0	0	0
			763	491	120	150	2			

- Molecule 2 is a protein called Negative regulator of genetic competence ClpC/MecB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	708	Total	C	N	O	S	0	0	0
			5455	3394	993	1055	13			
2	B	704	Total	C	N	O	S	0	0	0
			5437	3385	985	1054	13			
2	C	711	Total	C	N	O	S	0	0	0
			5479	3410	993	1063	13			

There are 162 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP P37571
A	?	-	VAL	deletion	UNP P37571
A	?	-	ALA	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571
A	?	-	THR	deletion	UNP P37571
A	280	ALA	GLU	engineered mutation	UNP P37571
A	?	-	LEU	deletion	UNP P37571
A	?	-	HIS	deletion	UNP P37571
A	?	-	THR	deletion	UNP P37571
A	?	-	LEU	deletion	UNP P37571
A	?	-	ILE	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571
A	?	-	ALA	deletion	UNP P37571
A	?	-	GLU	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571
A	?	-	ARG	deletion	UNP P37571
A	?	-	LEU	deletion	UNP P37571
A	?	-	VAL	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571
A	?	-	SER	deletion	UNP P37571
A	?	-	PRO	deletion	UNP P37571
A	?	-	PRO	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571
A	?	-	TYR	deletion	UNP P37571
A	?	-	VAL	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571
A	?	-	TYR	deletion	UNP P37571
A	?	-	ASP	deletion	UNP P37571
A	?	-	GLU	deletion	UNP P37571
A	618	ALA	GLU	engineered mutation	UNP P37571
A	?	-	LEU	deletion	UNP P37571
A	?	-	LYS	deletion	UNP P37571
A	?	-	ARG	deletion	UNP P37571
A	?	-	ASN	deletion	UNP P37571
A	?	-	LYS	deletion	UNP P37571
A	?	-	TYR	deletion	UNP P37571
A	?	-	VAL	deletion	UNP P37571
A	?	-	GLY	deletion	UNP P37571
A	?	-	PHE	deletion	UNP P37571
A	?	-	ASN	deletion	UNP P37571
A	?	-	VAL	deletion	UNP P37571
A	?	-	GLN	deletion	UNP P37571
A	?	-	ASP	deletion	UNP P37571
A	?	-	GLU	deletion	UNP P37571
A	?	-	THR	deletion	UNP P37571
A	?	-	GLN	deletion	UNP P37571
A	?	-	ASN	deletion	UNP P37571
A	?	-	HIS	deletion	UNP P37571
A	?	-	LYS	deletion	UNP P37571
A	?	-	ASP	deletion	UNP P37571
A	?	-	MET	deletion	UNP P37571

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	VAL	deletion	UNP P37571
B	?	-	VAL	deletion	UNP P37571
B	?	-	ALA	deletion	UNP P37571
B	?	-	GLY	deletion	UNP P37571
B	?	-	THR	deletion	UNP P37571
B	280	ALA	GLU	engineered mutation	UNP P37571
B	?	-	LEU	deletion	UNP P37571
B	?	-	HIS	deletion	UNP P37571
B	?	-	THR	deletion	UNP P37571
B	?	-	LEU	deletion	UNP P37571
B	?	-	ILE	deletion	UNP P37571
B	?	-	GLY	deletion	UNP P37571
B	?	-	ALA	deletion	UNP P37571
B	?	-	GLY	deletion	UNP P37571
B	?	-	GLY	deletion	UNP P37571
B	?	-	ALA	deletion	UNP P37571
B	?	-	GLU	deletion	UNP P37571
B	?	-	GLY	deletion	UNP P37571
B	?	-	ARG	deletion	UNP P37571
B	?	-	LEU	deletion	UNP P37571
B	?	-	VAL	deletion	UNP P37571
B	?	-	GLY	deletion	UNP P37571
B	?	-	SER	deletion	UNP P37571
B	?	-	PRO	deletion	UNP P37571
B	?	-	PRO	deletion	UNP P37571
B	?	-	GLY	deletion	UNP P37571
B	?	-	TYR	deletion	UNP P37571
B	?	-	VAL	deletion	UNP P37571
B	?	-	GLY	deletion	UNP P37571
B	?	-	TYR	deletion	UNP P37571
B	?	-	ASP	deletion	UNP P37571
B	?	-	GLU	deletion	UNP P37571
B	618	ALA	GLU	engineered mutation	UNP P37571
B	?	-	LEU	deletion	UNP P37571
B	?	-	LYS	deletion	UNP P37571
B	?	-	ARG	deletion	UNP P37571
B	?	-	ASN	deletion	UNP P37571
B	?	-	LYS	deletion	UNP P37571
B	?	-	TYR	deletion	UNP P37571
B	?	-	VAL	deletion	UNP P37571
B	?	-	GLY	deletion	UNP P37571
B	?	-	PHE	deletion	UNP P37571

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASN	deletion	UNP P37571
B	?	-	VAL	deletion	UNP P37571
B	?	-	GLN	deletion	UNP P37571
B	?	-	ASP	deletion	UNP P37571
B	?	-	GLU	deletion	UNP P37571
B	?	-	THR	deletion	UNP P37571
B	?	-	GLN	deletion	UNP P37571
B	?	-	ASN	deletion	UNP P37571
B	?	-	HIS	deletion	UNP P37571
B	?	-	LYS	deletion	UNP P37571
B	?	-	ASP	deletion	UNP P37571
B	?	-	MET	deletion	UNP P37571
C	?	-	VAL	deletion	UNP P37571
C	?	-	VAL	deletion	UNP P37571
C	?	-	ALA	deletion	UNP P37571
C	?	-	GLY	deletion	UNP P37571
C	?	-	THR	deletion	UNP P37571
C	280	ALA	GLU	engineered mutation	UNP P37571
C	?	-	LEU	deletion	UNP P37571
C	?	-	HIS	deletion	UNP P37571
C	?	-	THR	deletion	UNP P37571
C	?	-	LEU	deletion	UNP P37571
C	?	-	ILE	deletion	UNP P37571
C	?	-	GLY	deletion	UNP P37571
C	?	-	ALA	deletion	UNP P37571
C	?	-	GLY	deletion	UNP P37571
C	?	-	GLY	deletion	UNP P37571
C	?	-	ALA	deletion	UNP P37571
C	?	-	GLU	deletion	UNP P37571
C	?	-	GLY	deletion	UNP P37571
C	?	-	ARG	deletion	UNP P37571
C	?	-	LEU	deletion	UNP P37571
C	?	-	VAL	deletion	UNP P37571
C	?	-	GLY	deletion	UNP P37571
C	?	-	SER	deletion	UNP P37571
C	?	-	PRO	deletion	UNP P37571
C	?	-	PRO	deletion	UNP P37571
C	?	-	GLY	deletion	UNP P37571
C	?	-	TYR	deletion	UNP P37571
C	?	-	VAL	deletion	UNP P37571
C	?	-	GLY	deletion	UNP P37571
C	?	-	TYR	deletion	UNP P37571

Continued on next page...

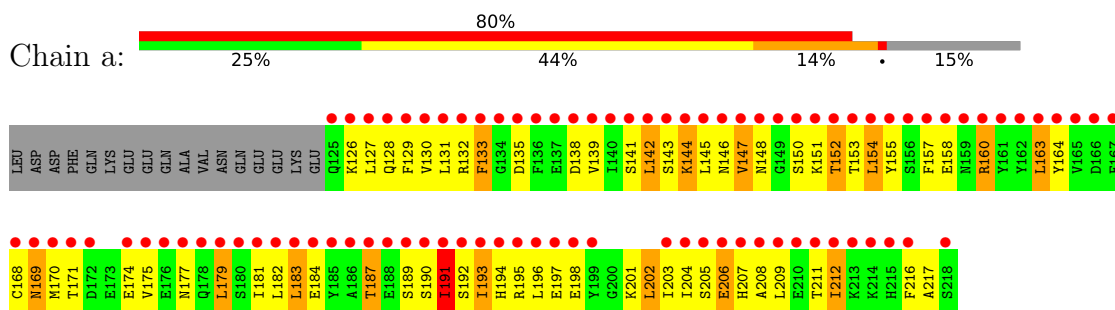
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASP	deletion	UNP P37571
C	?	-	GLU	deletion	UNP P37571
C	618	ALA	GLU	engineered mutation	UNP P37571
C	?	-	LEU	deletion	UNP P37571
C	?	-	LYS	deletion	UNP P37571
C	?	-	ARG	deletion	UNP P37571
C	?	-	ASN	deletion	UNP P37571
C	?	-	LYS	deletion	UNP P37571
C	?	-	TYR	deletion	UNP P37571
C	?	-	VAL	deletion	UNP P37571
C	?	-	GLY	deletion	UNP P37571
C	?	-	PHE	deletion	UNP P37571
C	?	-	ASN	deletion	UNP P37571
C	?	-	VAL	deletion	UNP P37571
C	?	-	GLN	deletion	UNP P37571
C	?	-	ASP	deletion	UNP P37571
C	?	-	GLU	deletion	UNP P37571
C	?	-	THR	deletion	UNP P37571
C	?	-	GLN	deletion	UNP P37571
C	?	-	ASN	deletion	UNP P37571
C	?	-	HIS	deletion	UNP P37571
C	?	-	LYS	deletion	UNP P37571
C	?	-	ASP	deletion	UNP P37571
C	?	-	MET	deletion	UNP P37571

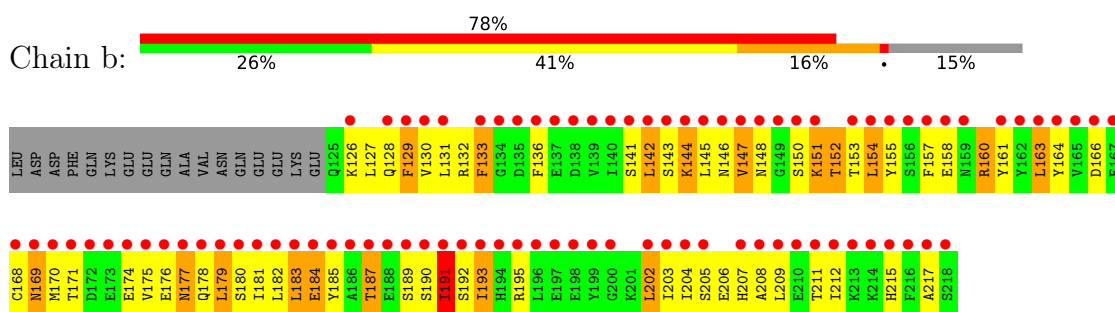
3 Residue-property plots [i](#)

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

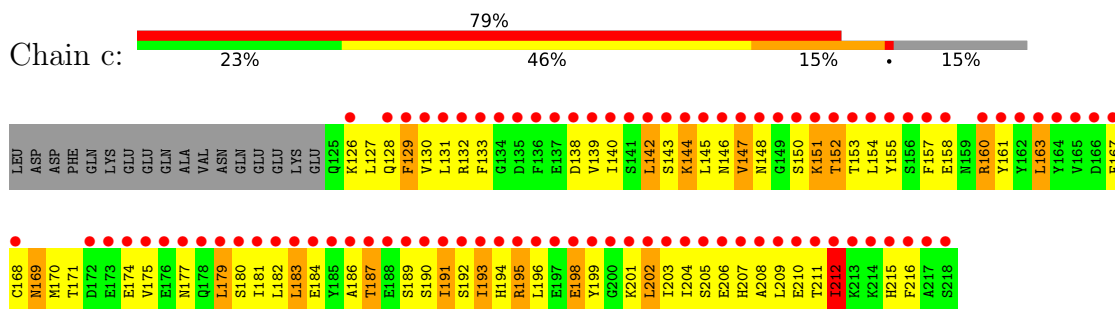
- Molecule 1: Adapter protein mecA 1



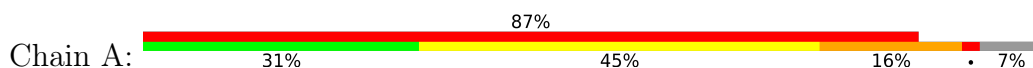
- Molecule 1: Adapter protein mecA 1

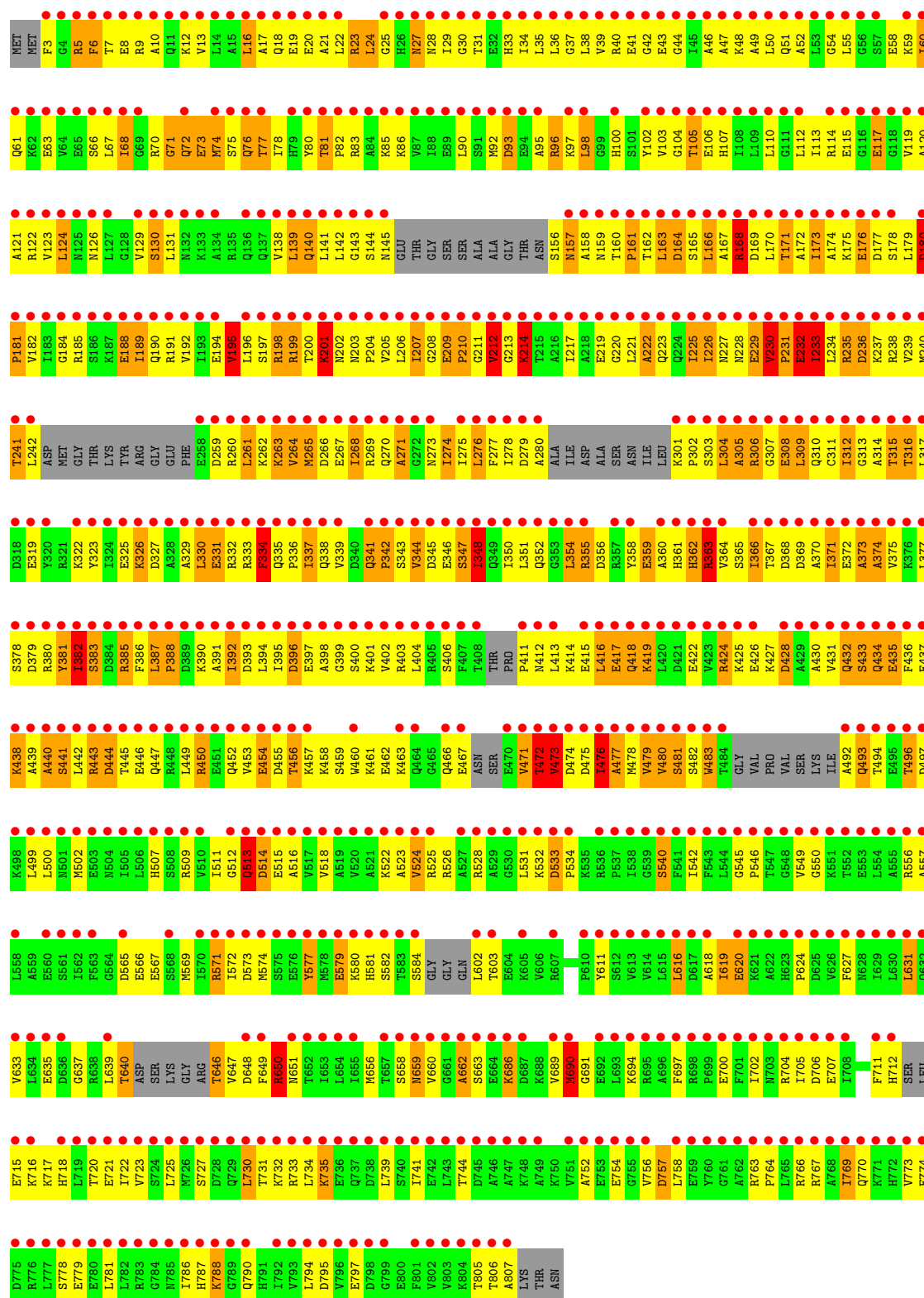


- Molecule 1: Adapter protein mecA 1

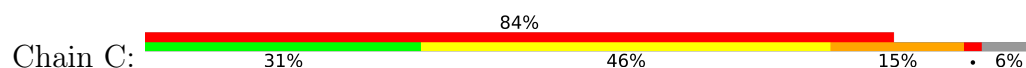


- Molecule 2: Negative regulator of genetic competence ClpC/MecB





● Molecule 2: Negative regulator of genetic competence ClpC/MecB



S778	S779	E779	E780	E781	E782	E783	E784	E785	E786	E787	E788	E789	E790	E791	E792	E793	E794	E795	E796	E797	E798	E799	E800	E801	E802	E803	E804	E805	E806	E807	LYS	THR	ASN																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
Q632	V633	L634	E635	S636	I637	G638	L639	T640	ASP	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
L558	A559	E560	L561	S562	I563	G564	D565	E566	E567	S568	S569	M570	L571	R572	D573	M574	S575	E576	E577	M578	E579	L580	H581	S582	T583	S584	GLY	GLN	L602	T603	E604	K605	K606	K607	K608	K609	P610	E611	L612	S613	G614	E615	L616	D617	A618	E619	O620	K621	A622	H623	L624	G625	E626	E627	E628	E629	E630	E631	E632	E633	E634	E635	E636	E637	E638	E639	E640	E641	E642	E643	E644	E645	E646	E647	E648	E649	E650	E651	E652	E653	E654	E655	E656	E657	E658	E659	E660	E661	E662	E663	E664	E665	E666	E667	E668	E669	E670	E671	E672	E673	E674	E675	E676	E677	E678	E679	E680	E681	E682	E683	E684	E685	E686	E687	E688	E689	E690	E691	E692	E693	E694	E695	E696	E697	E698	E699	E700	E701	E702	E703	E704	E705	E706	E707	E708	E709	E710	E711	E712	E713	E714	E715	E716	E717	E718	E719	E720	E721	E722	E723	E724	E725	E726	E727	E728	E729	E730	E731	E732	E733	E734	E735	E736	E737	E738	E739	E740	E741	E742	E743	E744	E745	E746	E747	E748	E749	E750	E751	E752	E753	E754	E755	E756	E757	E758	E759	E760	E761	E762	E763	E764	E765	E766	E767	E768	E769	E770	E771	E772	E773	E774	E775	E776	E777	E778	E779	E780	E781	E782	E783	E784	E785	E786	E787	E788	E789	E790	E791	E792	E793	E794	E795	E796	E797	E798	E799	E800	E801	E802	E803	E804	E805	E806	E807	E808	E809	E810	E811	E812	E813	E814	E815	E816	E817	E818	E819	E820	E821	E822	E823	E824	E825	E826	E827	E828	E829	E830	E831	E832	E833	E834	E835	E836	E837	E838	E839	E840	E841	E842	E843	E844	E845	E846	E847	E848	E849	E850	E851	E852	E853	E854	E855	E856	E857	E858	E859	E860	E861	E862	E863	E864	E865	E866	E867	E868	E869	E870	E871	E872	E873	E874	E875	E876	E877	E878	E879	E880	E881	E882	E883	E884	E885	E886	E887	E888	E889	E890	E891	E892	E893	E894	E895	E896	E897	E898	E899	E900	E901	E902	E903	E904	E905	E906	E907	E908	E909	E910	E911	E912	E913	E914	E915	E916	E917	E918	E919	E920	E921	E922	E923	E924	E925	E926	E927	E928	E929	E930	E931	E932	E933	E934	E935	E936	E937	E938	E939	E940	E941	E942	E943	E944	E945	E946	E947	E948	E949	E950	E951	E952	E953	E954	E955	E956	E957	E958	E959	E960	E961	E962	E963	E964	E965	E966	E967	E968	E969	E970	E971	E972	E973	E974	E975	E976	E977	E978	E979	E980	E981	E982	E983	E984	E985	E986	E987	E988	E989	E990	E991	E992	E993	E994	E995	E996	E997	E998	E999	E1000	E1001	E1002	E1003	E1004	E1005	E1006	E1007	E1008	E1009	E1010	E1011	E1012	E1013	E1014	E1015	E1016	E1017	E1018	E1019	E1020	E1021	E1022	E1023	E1024	E1025	E1026	E1027	E1028	E1029	E1030	E1031	E1032	E1033	E1034	E1035	E1036	E1037	E1038	E1039	E1040	E1041	E1042	E1043	E1044	E1045	E1046	E1047	E1048	E1049	E1050	E1051	E1052	E1053	E1054	E1055	E1056	E1057	E1058	E1059	E1060	E1061	E1062	E1063	E1064	E1065	E1066	E1067	E1068	E1069	E1070	E1071	E1072	E1073	E1074	E1075	E1076	E1077	E1078	E1079	E1080	E1081	E1082	E1083	E1084	E1085	E1086	E1087	E1088	E1089	E1090	E1091	E1092	E1093	E1094	E1095	E1096	E1097	E1098	E1099	E1100	E1101	E1102	E1103	E1104	E1105	E1106	E1107	E1108	E1109	E1110	E1111	E1112	E1113	E1114	E1115	E1116	E1117	E1118	E1119	E1120	E1121	E1122	E1123	E1124	E1125	E1126	E1127	E1128	E1129	E1130	E1131	E1132	E1133	E1134	E1135	E1136	E1137	E1138	E1139	E1140	E1141	E1142	E1143	E1144	E1145	E1146	E1147	E1148	E1149	E1150	E1151	E1152	E1153	E1154	E1155	E1156	E1157	E1158	E1159	E1160	E1161	E1162	E1163	E1164	E1165	E1166	E1167	E1168	E1169	E1170	E1171	E1172	E1173	E1174	E1175	E1176	E1177	E1178	E1179	E1180	E1181	E1182	E1183	E1184	E1185	E1186	E1187	E1188	E1189	E1190	E1191	E1192	E1193	E1194	E1195	E1196	E1197	E1198	E1199	E1200	E1201	E1202	E1203	E1204	E1205	E1206	E1207	E1208	E1209	E1210	E1211	E1212	E1213	E1214	E1215	E1216	E1217	E1218	E1219	E1220	E1221	E1222	E1223	E1224	E1225	E1226	E1227	E1228	E1229	E1230	E1231	E1232	E1233	E1234	E1235	E1236	E1237	E1238	E1239	E1240	E1241	E1242	E1243	E1244	E1245	E1246	E1247	E1248	E1249	E1250	E1251	E1252	E1253	E1254	E1255	E1256	E1257	E1258	E1259	E1260	E1261	E1262	E1263	E1264	E1265	E1266	E1267	E1268	E1269	E1270	E1271	E1272	E1273	E1274	E1275	E1276	E1277	E1278	E1279	E1280	E1281	E1282	E1283	E1284	E1285	E1286	E1287	E1288	E1289	E1290	E1291	E1292	E1293	E1294	E1295	E1296	E1297	E1298	E1299	E1300	E1301	E1302	E1303	E1304	E1305	E1306	E1307	E1308	E1309	E1310	E1311	E1312	E1313	E1314	E1315	E1316	E1317	E1318	E1319	E1320	E1321	E1322	E1323	E1324	E1325	E1326	E1327	E1328	E1329	E1330	E1331	E1332	E1333	E1334	E1335	E1336	E1337	E1338	E1339	E1340	E1341	E1342	E1343	E1344	E1345	E1346	E1347	E1348	E1349	E1350	E1351	E1352	E1353	E1354	E1355	E1356	E1357	E1358	E1359	E1360	E1361	E1362	E1363	E1364	E1365	E1366	E1367	E1368	E1369	E1370	E1371	E1372	E1373	E1374	E1375	E1376	E1377	E1378	E1379	E1380	E1381	E1382	E1383	E1384	E1385	E1386	E1387	E1388	E1389	E1390	E1391	E1392	E1393	E1394	E1395	E1396	E1397	E1398	E1399	E1400	E1401	E1402	E1403	E1404	E1405	E1406	E1407	E1408	E1409	E1410	E1411	E1412	E1413	E1414	E1415	E1416	E1417	E1418	E1419	E1420	E1421	E1422	E1423	E1424	E1425	E1426	E1427	E1428	E1429	E1430	E1431	E1432	E1433	E1434	E1435	E1436	E1437	E1438	E1439	E1440	E1441	E1442	E1443	E1444	E1445	E1446	E1447	E1448	E1449	E1450	E1451	E1452	E1453	E1454	E1455	E1456	E1457	E1458	E1459	E1460	E1461	E1462	E1463	E1464	E1465	E1466	E1467	E1468	E1469	E1470	E1471	E1472	E1473	E1474	E1475	E1476	E1477	E1478	E1479	E1480	E1481	E1482	E1483	E1484	E1485	E1486	E1487	E1488	E1489	E1490	E1491	E1492	E1493	E1494	E1495	E1496	E1497	E1498	E1499	E1500	E1501	E1502	E1503	E1504	E1505	E1506	E1507	E1508	E1509	E1510	E1511	E1512	E1513	E1514	E1515	E1516	E1517	E1518	E1519	E1520	E1521	E1522	E1523	E1524	E1525	E1526	E1527	E1528	E1529	E1530	E1531	E1532	E1533	E1534	E1535	E1536	E1537	E1538	E1539	E1540	E1541	E1542	E1543	E1544	E1545	E1546	E1547	E1548	E1549	E1550	E1551	E1552	E1553	E1554	E1555	E1556	E1557	E1558	E1559	E1560	E1561	E1562	E1563	E1564	E1565	E1566	E1567	E1568	E1569	E1570	E1571	E1572	E1573	E1574	E1575	E1576	E1577	E1578	E1579	E1580	E1581	E1582	E1583	E1584	E1585	E1586	E1587	E1588	E1589	E1590	E1591	E1592	E1593	E1594	E1595	E1596	E1597	E1598	E1599	E1600	E1601	E1602	E1603	E1604	E1605	E1606	E1607	E1608	E1609	E1610	E1611	E1612	E1613	E1614	E1615	E1616	E1617	E1618	E1619	E1620	E1621	E1622	E1623	E1624	E1625	E1626	E1627	E1628	E1629	E1630	E1631	E1632	E1633	E1634	E1635	E1636	E1637	E1638	E1639	E1640	E1641	E1642	E1643	E1644	E1645	E1646	E1647	E1648	E1649	E1650	E1651	E1652	E1653	E1654	E1655	E1656	E1657	E1658	E1659	E1660	E1661	E1662	E1663	E1664	E1665	E1666	E1667	E1668	E1669	E1670	E1671	E1672	E1673	E1674	E1675	E1676	E1677	E1678	E1679	E1680	E1681	E1682	E1683	E1684	E1685	E1686	E1687	E1688	E1689	E1690	E1691	E1692	E1693	E1694	E1695	E1696	E1697	E1698	E1699	E1700	E1701	E1702	E1703	E1704	E1705	E1706	E1707	E1708	E1709	E1710	E1711	E1712	E1713	E1714	E1715	E1716	E1717	E1718	E1719	E1720	E1721	E1722	E1723	E1724	E1725	E1726	E1727	E1728	E1729	E1730	E1731	E1732	E1733	E1734	E1735	E1736	E1737	E1738	E1739	E1740	E1741	E1742	E1743	E1744	E1745	E1746	E1747	E1748	E1749	E1750	E1751	E1752	E1753	E1754	E1755	E1756	E1757	E1758	E1759	E1760	E1761	E1762	E1763	E1764	E1765	E1766	E1767	E1768	E1769	E1770	E1771	E1772	E1773	E1774	E1775	E1776	E1777	E1778	E1779	E1780	E1781	E1782	E1783	E1784	E1785	E1786	E1787	E1788	E1789	E1790	E1791	E1792	E1793	E1794	E1795	E1796	E1797	E1798	E1799	E1800	E1801	E1802	E1803	E1804	E1805	E1806	E1807	E1808	E1809	E1810	E1811	E1812	E1813	E1814	E1815	E1816	E1817	E1818	E1819	E1820	E1821	E1822	E1823	E1824	E1825	E1826	E1827	E1828	E1829	E1830	E1831	E1832	E1833	E1834	E1835	E1836	E1837	E1838	E1839	E1840	E1841	E1842	E1843	E1844	E1845	E1846	E1847	E1848	E1849	E1850	E1851	E1852	E1853	E1854	E1855	E1856	E1857	E1858	E1859	E1860	E1861	E1862	E1863	E1864	E1865	E1866	E1867	E1868	E1869	E1870	E1871	E1872	E1873	E1874	E1875	E1876	E1877	E1878	E1879	E1880	E1881	E1882	E1883	E1884	E1885	E1886	E1887	E1888	E1889	E1890	E1891	E1892	E1893	E1894	E1895	E1896	E1897	E1898	E1899	E1900	E1901	E1902	E1903	E1904	E1905	E1906	E1907	E1908	E1909	E1910	E1911	E1912	E1913	E1914	E1915	E1916	E1917	E1918	E1919	E1920	E1921	E1922	E1923	E

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	141.81Å 141.81Å 656.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.15 – 6.93 49.15 – 6.93	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.15-6.93) 99.2 (49.15-6.93)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.84 (at 6.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_596)	Depositor
R, R_{free}	0.407 , 0.422 0.373 , 0.393	Depositor DCC
R_{free} test set	333 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	188.0	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 992.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.15	EDS
Total number of atoms	18645	wwPDB-VP
Average B, all atoms (Å ²)	642.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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

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	0.62	0/768	0.94	2/1035 (0.2%)
1	b	0.73	0/768	0.99	4/1035 (0.4%)
1	c	0.83	1/776 (0.1%)	0.99	2/1046 (0.2%)
2	A	0.67	3/5498 (0.1%)	1.05	27/7386 (0.4%)
2	B	0.76	1/5483 (0.0%)	1.16	36/7369 (0.5%)
2	C	0.71	1/5526 (0.0%)	1.06	24/7431 (0.3%)
All	All	0.72	6/18819 (0.0%)	1.08	95/25302 (0.4%)

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	A	0	1
2	C	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	334	PHE	CA-CB	7.13	1.65	1.53
2	A	334	PHE	CA-CB	5.46	1.62	1.53
1	c	212	ILE	CA-CB	-5.38	1.47	1.54
2	C	119	VAL	CA-CB	-5.33	1.47	1.54
2	A	366	ILE	CA-C	5.29	1.59	1.52
2	A	366	ILE	CA-CB	5.03	1.61	1.54

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	230	VAL	CA-C-N	-10.47	106.75	119.84
2	B	230	VAL	C-N-CA	-10.47	106.75	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	203	ASN	CA-C-N	8.68	128.82	120.31
2	A	203	ASN	C-N-CA	8.68	128.82	120.31
2	B	209	GLU	CA-C-N	8.47	130.43	119.84
2	B	209	GLU	C-N-CA	8.47	130.43	119.84
2	C	203	ASN	CA-C-N	8.47	128.61	120.31
2	C	203	ASN	C-N-CA	8.47	128.61	120.31
2	B	96	ARG	N-CA-C	-7.97	101.69	111.33
2	A	96	ARG	N-CA-C	-7.44	102.33	111.33
2	C	199	ARG	N-CA-C	-7.25	106.36	114.62
2	C	461	LYS	N-CA-C	-7.15	104.56	113.28
2	C	96	ARG	N-CA-C	-6.97	102.75	111.11
2	B	441	SER	N-CA-C	-6.95	102.54	111.02
2	A	161	PRO	N-CA-CB	6.85	110.61	103.15
2	B	434	GLN	N-CA-C	6.84	119.57	111.02
2	A	461	LYS	N-CA-C	-6.83	104.95	113.28
2	A	274	ILE	N-CA-C	6.77	118.47	108.45
2	B	480	VAL	N-CA-C	6.77	117.56	110.72
2	B	8	GLU	N-CA-C	-6.74	102.80	111.02
2	C	161	PRO	N-CA-CB	6.61	110.35	103.15
2	A	210	PRO	N-CA-C	6.51	123.23	114.18
2	B	81	THR	CA-C-N	-6.43	112.37	119.19
2	B	81	THR	C-N-CA	-6.43	112.37	119.19
2	A	199	ARG	N-CA-C	-6.39	107.33	114.62
2	A	241	THR	N-CA-C	6.35	117.81	108.86
2	A	8	GLU	N-CA-C	-6.16	103.50	111.02
2	C	8	GLU	N-CA-C	-6.14	103.53	111.02
2	C	210	PRO	N-CA-C	6.13	122.70	114.18
2	B	241	THR	N-CA-C	6.10	123.78	110.80
2	A	513	GLN	N-CA-C	6.06	119.90	111.90
2	B	161	PRO	N-CA-CB	6.05	109.60	103.25
2	B	513	GLN	N-CA-C	6.05	119.88	111.90
2	C	274	ILE	N-CA-C	6.03	116.97	108.17
2	C	513	GLN	N-CA-C	6.01	119.83	111.90
1	c	195	ARG	N-CA-C	-5.98	104.67	111.07
2	C	496	THR	N-CA-C	-5.96	106.01	113.28
2	A	496	THR	N-CA-C	-5.88	106.11	113.28
2	B	496	THR	N-CA-C	-5.85	106.15	113.28
1	b	191	ILE	N-CA-C	5.84	116.56	108.84
2	B	329	ALA	N-CA-C	-5.79	105.10	111.82
2	B	516	ALA	N-CA-C	5.77	117.25	111.07
2	A	516	ALA	N-CA-C	5.77	117.24	111.07
1	b	154	LEU	N-CA-C	5.74	117.76	108.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	516	ALA	N-CA-C	5.73	117.20	111.07
2	B	444	ASP	N-CA-C	-5.73	104.41	111.75
2	A	403	ARG	N-CA-C	-5.72	106.01	112.87
2	C	545	GLY	CA-C-N	5.67	125.65	120.21
2	C	545	GLY	C-N-CA	5.67	125.65	120.21
2	A	448	ARG	N-CA-C	-5.66	104.12	111.02
2	C	241	THR	N-CA-C	5.64	116.81	108.86
2	B	545	GLY	CA-C-N	5.62	125.60	120.21
2	B	545	GLY	C-N-CA	5.62	125.60	120.21
2	B	348	ILE	CB-CA-C	-5.58	104.56	111.70
2	A	545	GLY	CA-C-N	5.58	125.56	120.21
2	A	545	GLY	C-N-CA	5.58	125.56	120.21
2	C	269	ARG	N-CA-C	-5.56	104.64	111.75
2	A	112	LEU	N-CA-C	5.56	117.02	111.07
2	A	269	ARG	N-CA-C	-5.55	104.65	111.75
2	B	341	GLN	CA-C-N	5.55	126.77	119.84
2	B	341	GLN	C-N-CA	5.55	126.77	119.84
2	A	329	ALA	N-CA-C	-5.54	105.39	111.82
2	A	209	GLU	CA-C-N	5.52	125.22	119.64
2	A	209	GLU	C-N-CA	5.52	125.22	119.64
2	C	448	ARG	N-CA-C	-5.47	104.35	111.02
1	c	129	PHE	N-CA-C	5.44	117.95	109.52
2	C	60	ILE	CB-CA-C	-5.42	104.88	111.87
2	C	533	ASP	CA-C-N	5.42	125.24	119.28
2	C	533	ASP	C-N-CA	5.42	125.24	119.28
2	A	533	ASP	CA-C-N	5.41	125.23	119.28
2	A	533	ASP	C-N-CA	5.41	125.23	119.28
2	B	315	THR	N-CA-C	5.39	117.04	108.79
2	B	477	ALA	N-CA-C	5.38	117.89	111.71
2	B	180	ASP	CA-C-N	5.37	126.56	119.84
2	B	180	ASP	C-N-CA	5.37	126.56	119.84
2	B	195	VAL	CB-CA-C	-5.37	105.04	112.24
2	C	81	THR	CA-C-N	-5.37	113.50	119.19
2	C	81	THR	C-N-CA	-5.37	113.50	119.19
2	C	303	SER	N-CA-C	-5.37	107.28	112.97
2	B	533	ASP	CA-C-N	5.34	125.16	119.28
2	B	533	ASP	C-N-CA	5.34	125.16	119.28
1	a	191	ILE	N-CA-C	5.26	115.78	108.84
2	A	414	LYS	N-CA-C	-5.24	105.98	112.38
2	B	326	LYS	N-CA-C	-5.23	106.00	112.38
2	B	60	ILE	CB-CA-C	-5.17	105.20	111.87
2	B	219	GLU	N-CA-C	-5.14	106.27	112.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	129	PHE	N-CA-C	5.12	117.45	109.52
2	A	463	LYS	N-CA-C	-5.11	106.88	113.01
2	B	214	LYS	N-CA-C	5.10	121.67	110.80
2	C	19	GLU	N-CA-C	-5.09	105.00	111.11
1	b	184	GLU	N-CA-C	-5.09	105.92	111.82
2	A	125	ASN	N-CA-C	-5.06	106.80	112.87
2	B	274	ILE	N-CA-C	5.04	119.82	109.34
1	a	154	LEU	N-CA-C	5.04	116.62	108.41
2	B	461	LYS	N-CA-C	-5.01	107.00	113.01

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	210	PRO	Peptide
2	C	210	PRO	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	755	0	728	82	17
1	b	756	0	736	162	0
1	c	763	0	743	141	0
2	A	5455	0	5489	671	34
2	B	5437	0	5491	1053	1
2	C	5479	0	5524	814	24
All	All	18645	0	18711	2510	41

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 67.

All (2510) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:694:LYS:HG3	2:C:760:TYR:CE2	1.20	1.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:694:LYS:CG	2:C:760:TYR:CE2	1.79	1.58
2:B:694:LYS:CD	2:C:760:TYR:HD2	1.05	1.57
2:B:694:LYS:CD	2:C:760:TYR:CD2	1.90	1.55
2:B:694:LYS:HD2	2:C:760:TYR:CD2	1.41	1.53
2:B:500:LEU:CD2	2:C:783:ARG:HG3	1.33	1.53
1:b:177:ASN:CG	2:B:67:LEU:HD22	1.25	1.52
2:A:374:ALA:CB	2:A:476:ILE:HD13	1.29	1.52
2:A:374:ALA:CA	2:A:476:ILE:HG21	1.31	1.52
1:b:187:THR:CG2	2:B:83:ARG:HH22	1.18	1.51
2:A:374:ALA:CA	2:A:476:ILE:CG2	1.86	1.49
2:B:394:LEU:HD23	2:B:483:TRP:CZ3	1.48	1.49
2:B:306:ARG:NH2	2:C:242:LEU:CD2	1.75	1.47
2:B:306:ARG:NH2	2:C:242:LEU:CD1	1.76	1.47
2:B:500:LEU:HD22	2:C:783:ARG:CG	1.43	1.47
1:b:177:ASN:CG	2:B:67:LEU:CD2	1.88	1.46
2:B:306:ARG:CD	2:C:168:ARG:HH22	1.29	1.45
2:C:377:LEU:CD1	2:C:476:ILE:CG2	1.94	1.44
2:B:690:MET:C	2:C:760:TYR:HH	1.21	1.43
2:B:511:ILE:CD1	2:B:721:GLU:OE1	1.67	1.43
2:B:694:LYS:CG	2:C:760:TYR:CD2	2.01	1.42
2:B:306:ARG:HD3	2:C:168:ARG:NH2	1.29	1.41
2:A:374:ALA:HB2	2:A:476:ILE:CD1	1.48	1.41
2:B:511:ILE:HG22	2:B:718:HIS:ND1	1.28	1.41
1:b:187:THR:HG22	2:B:83:ARG:NH2	1.08	1.40
2:C:377:LEU:HD12	2:C:476:ILE:CG2	1.50	1.39
2:A:374:ALA:N	2:A:476:ILE:HG21	1.15	1.38
2:B:306:ARG:CZ	2:C:242:LEU:CD2	2.01	1.37
1:c:138:ASP:OD1	2:C:82:PRO:CG	1.72	1.36
2:B:306:ARG:CZ	2:C:242:LEU:HD21	1.56	1.35
2:B:511:ILE:CG2	2:B:718:HIS:ND1	1.89	1.35
2:B:142:LEU:CA	1:c:195:ARG:HD2	1.57	1.34
2:B:367:THR:CG2	2:B:472:THR:HA	1.56	1.33
2:B:522:LYS:O	2:C:775:ASP:CB	1.75	1.33
2:A:374:ALA:HA	2:A:476:ILE:CG2	1.52	1.33
2:B:306:ARG:NH1	2:C:242:LEU:HD22	1.39	1.32
2:B:306:ARG:HH22	2:C:242:LEU:CG	1.41	1.32
2:B:367:THR:OG1	2:B:472:THR:HA	1.30	1.31
2:B:142:LEU:HA	1:c:195:ARG:CD	1.61	1.31
2:B:522:LYS:O	2:C:775:ASP:CG	1.73	1.31
2:A:199:ARG:CD	2:B:358:TYR:OH	1.79	1.30
2:B:199:ARG:HH22	2:C:357:ARG:NH2	1.29	1.29

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:LEU:CD2	2:B:483:TRP:CZ3	2.15	1.29
2:B:367:THR:CB	2:B:472:THR:HA	1.62	1.29
2:B:306:ARG:HH22	2:C:242:LEU:CD1	1.34	1.29
2:B:143:GLY:N	1:c:195:ARG:HH21	1.30	1.28
1:b:184:GLU:O	2:B:81:THR:HB	1.29	1.28
2:B:145:ASN:CB	1:c:158:GLU:OE1	1.83	1.26
2:B:511:ILE:HD11	2:B:721:GLU:OE1	1.08	1.25
2:A:373:ALA:HB2	2:A:473:VAL:CG1	1.66	1.25
1:b:203:ILE:CD1	2:B:432:GLN:HB3	1.68	1.23
2:B:143:GLY:H	1:c:195:ARG:NH2	1.34	1.23
2:C:374:ALA:N	2:C:476:ILE:CD1	2.00	1.23
2:B:690:MET:C	2:C:760:TYR:OH	1.73	1.23
2:B:199:ARG:NH2	2:C:357:ARG:NH2	1.85	1.22
2:A:380:ARG:O	2:A:611:TYR:OH	1.53	1.21
2:A:181:PRO:HB2	2:A:182:VAL:HA	1.24	1.20
2:A:233:ILE:CG2	2:B:361:HIS:HE2	1.52	1.20
2:B:367:THR:CG2	2:B:472:THR:CA	2.19	1.20
2:A:373:ALA:CB	2:A:473:VAL:HG12	1.71	1.20
2:B:511:ILE:CD1	2:B:721:GLU:CD	2.14	1.20
2:A:408:THR:C	2:A:414:LYS:CE	2.16	1.19
2:B:230:VAL:HG12	2:B:231:PRO:CD	1.71	1.18
2:C:377:LEU:CD1	2:C:476:ILE:HG22	1.60	1.18
2:B:522:LYS:O	2:C:775:ASP:HB3	1.29	1.18
2:B:306:ARG:HH22	2:C:242:LEU:CD2	1.43	1.18
2:B:199:ARG:NH2	2:C:357:ARG:HH21	1.39	1.17
2:B:304:LEU:HD22	2:B:305:ALA:N	1.58	1.17
1:b:184:GLU:HB3	2:B:81:THR:HG21	1.21	1.17
2:B:181:PRO:HB2	2:B:182:VAL:HA	1.18	1.17
2:B:694:LYS:HG2	2:C:760:TYR:CE2	1.76	1.17
2:B:363:ARG:O	2:B:471:VAL:HB	1.43	1.17
2:B:367:THR:HG21	2:B:472:THR:CB	1.75	1.17
2:B:690:MET:O	2:C:760:TYR:OH	1.61	1.17
2:B:394:LEU:CD2	2:B:483:TRP:CE3	2.27	1.16
2:B:169:ASP:O	2:B:173:ILE:HB	1.44	1.16
2:B:306:ARG:NH1	2:C:242:LEU:CD2	2.01	1.16
2:B:515:GLU:OE1	2:B:712:HIS:NE2	1.78	1.16
2:A:374:ALA:N	2:A:476:ILE:CG2	1.96	1.16
2:A:199:ARG:NE	2:B:358:TYR:OH	1.78	1.16
2:B:306:ARG:NH2	2:C:242:LEU:HD21	1.48	1.15
2:C:515:GLU:OE1	2:C:712:HIS:NE2	1.78	1.15
2:A:394:LEU:HG	2:A:480:VAL:HG23	1.16	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:515:GLU:OE1	2:A:712:HIS:NE2	1.78	1.15
2:B:13:VAL:HG21	2:B:38:LEU:HD23	1.22	1.14
2:B:439:ALA:O	2:B:442:LEU:N	1.79	1.14
2:B:511:ILE:HG22	2:B:718:HIS:CG	1.80	1.14
2:B:694:LYS:HG3	2:C:760:TYR:CD2	1.73	1.14
2:A:394:LEU:HG	2:A:480:VAL:CG2	1.78	1.13
2:B:531:LEU:O	2:C:733:ARG:NH2	1.80	1.13
2:C:13:VAL:HG21	2:C:38:LEU:HD23	1.23	1.13
2:B:363:ARG:HH12	2:B:476:ILE:N	1.45	1.13
2:B:694:LYS:CG	2:C:760:TYR:HE2	1.32	1.13
1:a:184:GLU:CD	2:A:119:VAL:HG23	1.72	1.12
2:A:374:ALA:HA	2:A:476:ILE:HG23	1.17	1.12
2:B:180:ASP:HB2	2:B:181:PRO:HD2	1.31	1.12
2:B:526:ARG:HH21	2:C:771:LYS:HG3	1.07	1.11
1:c:138:ASP:OD1	2:C:82:PRO:HG3	0.93	1.11
2:A:373:ALA:HB2	2:A:473:VAL:HG12	1.19	1.11
2:B:231:PRO:HG2	2:B:232:GLU:HG2	1.22	1.11
2:C:374:ALA:N	2:C:476:ILE:HD13	1.65	1.11
1:a:184:GLU:HG3	2:A:119:VAL:CG2	1.81	1.10
2:B:369:ASP:HB3	2:B:473:VAL:CG2	1.81	1.10
1:b:185:TYR:CE1	2:B:28:ASN:HB2	1.86	1.10
2:A:13:VAL:HG21	2:A:38:LEU:HD23	1.25	1.10
1:a:184:GLU:HG3	2:A:119:VAL:HG22	1.32	1.09
1:b:177:ASN:ND2	2:B:67:LEU:CD2	2.13	1.09
1:c:138:ASP:CG	2:C:82:PRO:HG3	1.77	1.09
2:C:394:LEU:HD13	2:C:479:VAL:HG11	1.11	1.09
2:B:511:ILE:HD12	2:B:721:GLU:CD	1.76	1.09
2:B:525:ARG:O	2:C:778:SER:HB2	1.49	1.09
2:C:181:PRO:HB2	2:C:182:VAL:HA	1.21	1.08
2:C:394:LEU:HD13	2:C:479:VAL:CG1	1.82	1.08
2:B:145:ASN:CB	1:c:158:GLU:CD	2.26	1.08
2:A:394:LEU:CG	2:A:480:VAL:HG23	1.82	1.08
2:A:408:THR:C	2:A:414:LYS:NZ	2.12	1.08
2:C:377:LEU:HD12	2:C:476:ILE:HG21	1.11	1.08
2:A:382:ILE:HA	2:A:383:SER:HB3	1.32	1.07
2:C:382:ILE:HA	2:C:383:SER:HB3	1.33	1.07
2:B:200:THR:CG2	2:C:392:ILE:HG22	1.85	1.07
2:B:500:LEU:CD1	2:C:783:ARG:HG2	1.84	1.07
2:A:233:ILE:HG23	2:B:361:HIS:NE2	1.31	1.07
2:A:408:THR:O	2:A:414:LYS:HE3	1.52	1.07
2:B:500:LEU:HD11	2:C:783:ARG:HA	1.32	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:203:ILE:HD13	2:B:432:GLN:CB	1.85	1.07
2:C:242:LEU:HB3	2:C:243:ASP:HA	1.28	1.07
1:b:177:ASN:CB	2:B:67:LEU:HD22	1.84	1.06
2:B:500:LEU:HD13	2:C:783:ARG:CG	1.85	1.06
2:A:526:ARG:HG2	2:B:778:SER:HB3	1.30	1.06
1:b:177:ASN:OD1	2:B:67:LEU:CD2	2.03	1.06
2:B:363:ARG:NH1	2:B:476:ILE:HD12	1.69	1.06
2:B:367:THR:OG1	2:B:472:THR:CA	2.02	1.06
2:A:374:ALA:CB	2:A:476:ILE:HG21	1.84	1.06
2:B:305:ALA:HA	2:B:309:LEU:HD21	1.30	1.06
1:b:185:TYR:HE1	2:B:28:ASN:CB	1.66	1.06
1:b:187:THR:CG2	2:B:83:ARG:NH2	1.89	1.06
2:B:526:ARG:NH2	2:C:771:LYS:HG3	1.65	1.06
2:B:200:THR:HG21	2:C:392:ILE:CG2	1.86	1.05
2:B:370:ALA:HB1	2:B:476:ILE:HD13	1.37	1.05
1:c:183:LEU:HB3	2:C:117:GLU:HG3	1.35	1.05
1:b:184:GLU:CD	2:B:31:THR:H	1.63	1.05
2:A:199:ARG:HD3	2:B:358:TYR:OH	1.55	1.05
2:A:374:ALA:HB3	2:A:476:ILE:HD13	1.39	1.05
1:b:180:SER:OG	2:B:119:VAL:HA	1.56	1.04
2:B:200:THR:HG21	2:C:392:ILE:HG22	1.05	1.04
2:B:525:ARG:O	2:C:778:SER:CB	2.03	1.04
2:A:373:ALA:CB	2:A:473:VAL:CG1	2.31	1.04
2:B:526:ARG:N	2:C:775:ASP:HA	1.38	1.03
2:B:306:ARG:NH2	2:C:242:LEU:HD11	1.50	1.03
2:B:500:LEU:HD13	2:C:783:ARG:HG2	1.06	1.03
2:B:512:GLY:H	2:B:718:HIS:CE1	1.76	1.03
2:C:373:ALA:HB3	2:C:476:ILE:HD12	1.41	1.03
1:b:136:PHE:CZ	2:B:431:VAL:HG21	1.94	1.02
2:B:306:ARG:NH2	2:C:242:LEU:CG	2.10	1.02
2:A:374:ALA:CB	2:A:476:ILE:CG2	2.36	1.02
2:A:171:THR:HG22	2:A:175:LYS:HE3	1.41	1.01
2:A:233:ILE:CG2	2:B:361:HIS:NE2	2.10	1.00
2:A:367:THR:CB	2:A:472:THR:HG23	1.92	1.00
2:B:230:VAL:CG1	2:B:231:PRO:HD3	1.90	1.00
2:B:305:ALA:HA	2:B:309:LEU:CD2	1.91	1.00
2:C:171:THR:HG22	2:C:175:LYS:HE3	1.44	1.00
2:B:441:SER:O	2:B:445:THR:HG23	1.62	1.00
2:B:526:ARG:NH2	2:C:771:LYS:CG	2.05	1.00
2:C:366:ILE:HG22	2:C:367:THR:HA	1.44	0.99
2:B:512:GLY:HA2	2:B:718:HIS:NE2	1.78	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:ARG:HH11	2:B:476:ILE:HD12	1.23	0.99
2:B:402:VAL:HG13	2:B:467:GLU:OE2	1.61	0.99
2:B:306:ARG:CZ	2:C:242:LEU:HD22	1.75	0.99
2:A:439:ALA:HA	2:A:442:LEU:HB2	1.44	0.99
2:B:230:VAL:HG12	2:B:231:PRO:HD3	1.02	0.99
2:B:379:ASP:HA	2:B:387:LEU:HD21	1.45	0.99
2:B:439:ALA:HA	2:B:442:LEU:HD12	1.44	0.99
2:B:476:ILE:O	2:B:479:VAL:HB	1.61	0.99
2:B:500:LEU:CD1	2:C:783:ARG:HA	1.90	0.98
2:B:512:GLY:CA	2:B:718:HIS:NE2	2.27	0.98
2:C:367:THR:OG1	2:C:471:VAL:CG1	2.11	0.98
2:C:377:LEU:CD1	2:C:476:ILE:HG21	1.73	0.98
2:C:556:ARG:HG2	2:C:569:MET:HE1	1.45	0.98
2:B:185:ARG:HG2	2:B:188:GLU:HG2	1.46	0.98
2:C:439:ALA:HA	2:C:442:LEU:HB2	1.44	0.98
2:B:306:ARG:NH2	2:C:242:LEU:HD13	1.78	0.98
2:A:397:GLU:CB	2:A:479:VAL:HG13	1.93	0.98
2:C:367:THR:OG1	2:C:471:VAL:HG11	1.63	0.98
2:A:397:GLU:HB2	2:A:479:VAL:HG13	0.98	0.97
1:a:184:GLU:CD	2:A:119:VAL:CG2	2.35	0.97
2:B:394:LEU:HD22	2:B:483:TRP:CE3	1.98	0.97
1:c:180:SER:OG	2:C:122:ARG:HB2	1.63	0.97
1:b:185:TYR:CE1	2:B:28:ASN:CB	2.44	0.97
2:B:200:THR:CG2	2:C:392:ILE:CG2	2.41	0.97
2:B:240:MET:HG3	2:B:274:ILE:HD11	1.43	0.97
1:b:177:ASN:CG	2:B:67:LEU:HD21	1.87	0.97
1:a:184:GLU:CG	2:A:119:VAL:CG2	2.42	0.96
1:b:203:ILE:HD11	2:B:432:GLN:HB3	1.44	0.96
2:B:556:ARG:HG2	2:B:569:MET:HE1	1.46	0.96
1:b:177:ASN:OD1	2:B:67:LEU:HD21	1.62	0.96
1:b:144:LYS:O	2:B:27:ASN:ND2	1.98	0.96
2:C:377:LEU:HD11	2:C:476:ILE:HG22	1.43	0.96
2:B:185:ARG:HH11	2:B:185:ARG:HB2	1.31	0.96
2:A:700:GLU:OE1	2:B:763:ARG:NH1	1.99	0.95
2:B:306:ARG:HH21	2:C:242:LEU:HD11	1.02	0.95
2:A:366:ILE:HG22	2:A:367:THR:HA	1.44	0.95
2:A:556:ARG:HG2	2:A:569:MET:HE1	1.46	0.95
2:B:512:GLY:N	2:B:718:HIS:CE1	2.33	0.95
2:A:397:GLU:HB2	2:A:479:VAL:CG1	1.94	0.95
2:C:377:LEU:HD11	2:C:476:ILE:CG2	1.93	0.95
1:a:184:GLU:CG	2:A:119:VAL:HG23	1.97	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:185:TYR:CZ	2:B:28:ASN:HB2	2.00	0.95
2:B:190:GLN:OE1	2:C:404:LEU:HD21	1.67	0.94
1:b:184:GLU:CD	2:B:31:THR:N	2.25	0.94
2:B:367:THR:HG23	2:B:472:THR:CA	1.95	0.94
2:A:371:ILE:HA	2:A:476:ILE:HD12	1.46	0.94
2:B:265:MET:HE1	2:B:269:ARG:HH21	1.31	0.94
2:B:359:GLU:HG2	2:B:365:SER:N	1.81	0.94
1:a:187:THR:HG23	2:A:83:ARG:HH22	1.33	0.94
1:b:147:VAL:HG23	1:b:150:SER:HB2	1.50	0.94
1:b:184:GLU:OE2	2:B:30:GLY:CA	2.15	0.94
2:B:276:LEU:N	2:B:310:GLN:O	2.00	0.94
1:b:185:TYR:OH	2:B:28:ASN:HB2	1.67	0.94
2:B:694:LYS:HG2	2:C:760:TYR:HE2	1.13	0.94
2:A:394:LEU:CG	2:A:480:VAL:CG2	2.45	0.93
2:B:394:LEU:HA	2:B:483:TRP:CH2	2.03	0.93
2:A:363:ARG:HH12	2:A:475:ASP:CB	1.82	0.93
2:C:98:LEU:HB3	2:C:100:HIS:HD2	1.33	0.93
2:C:379:ASP:HA	2:C:387:LEU:HD21	1.50	0.93
2:B:367:THR:HG23	2:B:472:THR:N	1.82	0.93
2:A:374:ALA:HB2	2:A:476:ILE:CG1	1.99	0.93
2:A:374:ALA:CB	2:A:476:ILE:CD1	2.24	0.93
2:B:367:THR:HG21	2:B:472:THR:CG2	1.97	0.93
2:B:306:ARG:HH12	2:C:242:LEU:CD2	1.74	0.93
1:b:184:GLU:OE2	2:B:31:THR:N	2.02	0.93
2:B:168:ARG:NH1	2:B:242:LEU:HB2	1.82	0.92
2:A:408:THR:O	2:A:414:LYS:CE	2.17	0.92
1:b:203:ILE:HD13	2:B:432:GLN:HB3	1.40	0.92
2:B:359:GLU:HA	2:B:364:VAL:O	1.70	0.92
1:b:181:ILE:HD11	2:B:67:LEU:O	1.70	0.92
1:c:147:VAL:HG23	1:c:150:SER:HB2	1.49	0.91
1:c:184:GLU:HA	2:C:118:GLY:HA2	1.49	0.91
2:A:374:ALA:H	2:A:476:ILE:HG21	1.13	0.91
1:b:203:ILE:CD1	2:B:432:GLN:CB	2.42	0.91
2:B:526:ARG:NE	2:C:775:ASP:HB2	1.85	0.91
2:B:194:GLU:HA	2:C:400:SER:OG	1.70	0.91
2:B:370:ALA:HB1	2:B:476:ILE:CD1	1.99	0.91
2:B:185:ARG:HB2	2:B:185:ARG:NH1	1.86	0.91
2:C:402:VAL:CG1	2:C:467:GLU:OE1	2.19	0.91
1:b:184:GLU:O	2:B:81:THR:CB	2.18	0.91
2:B:306:ARG:HH12	2:C:242:LEU:HD22	0.93	0.91
2:B:382:ILE:HA	2:B:383:SER:HB3	1.53	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:181:PRO:HB2	2:C:182:VAL:CA	2.01	0.91
2:C:439:ALA:O	2:C:442:LEU:N	2.04	0.91
2:A:394:LEU:CD1	2:A:480:VAL:HG23	2.01	0.90
2:A:500:LEU:CD1	2:A:500:LEU:CB	2.49	0.90
2:A:379:ASP:HA	2:A:387:LEU:HD21	1.51	0.90
2:A:394:LEU:HD21	2:A:480:VAL:HA	1.53	0.90
2:B:378:SER:HB3	2:B:390:LYS:HE2	1.52	0.90
2:A:500:LEU:CD1	2:A:500:LEU:CD2	2.49	0.90
2:B:98:LEU:HB3	2:B:100:HIS:HD2	1.37	0.90
2:B:369:ASP:C	2:B:473:VAL:HG22	1.96	0.90
2:B:265:MET:CE	2:B:269:ARG:HH21	1.85	0.90
2:B:402:VAL:HG13	2:B:467:GLU:CD	1.95	0.89
2:B:511:ILE:HG21	2:B:718:HIS:HA	1.53	0.89
2:B:145:ASN:CB	1:c:158:GLU:OE2	2.21	0.89
2:A:370:ALA:CB	2:A:471:VAL:O	2.20	0.89
2:C:374:ALA:CA	2:C:476:ILE:HD13	2.02	0.89
2:B:434:GLN:O	2:B:434:GLN:HG2	1.72	0.89
2:A:98:LEU:HB3	2:A:100:HIS:HD2	1.37	0.89
1:c:183:LEU:CB	2:C:117:GLU:HG3	2.03	0.89
2:A:181:PRO:HB2	2:A:182:VAL:CA	2.01	0.88
1:b:180:SER:C	2:B:119:VAL:HG22	1.98	0.88
2:B:367:THR:HG23	2:B:472:THR:HA	1.53	0.88
2:C:382:ILE:HG13	2:C:484:THR:HG23	1.52	0.88
2:A:371:ILE:HA	2:A:476:ILE:CD1	2.04	0.88
1:c:138:ASP:OD1	2:C:82:PRO:CB	2.20	0.88
1:b:180:SER:OG	2:B:119:VAL:HG13	1.74	0.87
2:B:369:ASP:HB3	2:B:473:VAL:HG21	1.54	0.87
2:B:370:ALA:O	2:B:476:ILE:HG21	1.74	0.87
2:B:532:LYS:C	2:C:733:ARG:NH2	2.32	0.87
2:A:500:LEU:CB	2:A:500:LEU:CD2	2.52	0.87
1:b:184:GLU:OE1	2:B:31:THR:N	2.07	0.87
2:B:180:ASP:CB	2:B:181:PRO:HD2	2.04	0.86
2:A:374:ALA:CA	2:A:476:ILE:HG23	1.83	0.86
2:B:428:ASP:O	2:B:431:VAL:HG12	1.75	0.86
2:B:367:THR:HG21	2:B:472:THR:HG23	1.56	0.86
1:c:216:PHE:O	2:C:443:ARG:CZ	2.23	0.86
2:B:233:ILE:O	2:B:233:ILE:HD13	1.76	0.86
2:B:523:ALA:O	2:C:775:ASP:OD1	1.93	0.86
1:c:180:SER:HB2	2:C:122:ARG:HD3	1.57	0.86
2:B:198:ARG:HB3	2:C:396:ASP:OD2	1.75	0.85
2:C:206:LEU:HD12	2:C:313:GLY:O	1.76	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:408:THR:C	2:A:414:LYS:HE3	1.93	0.85
2:B:180:ASP:HB2	2:B:181:PRO:CD	2.00	0.85
2:B:367:THR:OG1	2:B:472:THR:C	2.18	0.85
2:C:374:ALA:H	2:C:476:ILE:CD1	1.90	0.85
2:A:165:SER:N	2:A:166:LEU:O	2.09	0.85
2:B:370:ALA:CB	2:B:476:ILE:HD13	2.06	0.85
2:C:373:ALA:CB	2:C:476:ILE:HD12	2.06	0.85
2:C:321:ARG:O	2:C:325:GLU:HB2	1.75	0.85
2:B:143:GLY:O	1:c:195:ARG:NH2	2.09	0.85
1:a:126:LYS:HE3	1:a:129:PHE:HE1	1.39	0.85
2:B:500:LEU:HD11	2:C:783:ARG:CA	2.07	0.85
2:C:165:SER:N	2:C:166:LEU:O	2.10	0.85
1:b:187:THR:CG2	2:B:83:ARG:CZ	2.54	0.84
1:b:215:HIS:O	2:B:440:ALA:HB2	1.76	0.84
2:B:306:ARG:HH22	2:C:242:LEU:HD13	1.35	0.84
1:c:216:PHE:O	2:C:443:ARG:NH2	2.10	0.84
2:B:181:PRO:CB	2:B:182:VAL:HA	2.05	0.84
2:B:522:LYS:HA	2:C:779:GLU:OE2	1.77	0.84
2:A:374:ALA:HB2	2:A:476:ILE:CG2	2.03	0.84
2:B:456:THR:HA	2:B:459:SER:HB3	1.60	0.84
1:c:184:GLU:CA	2:C:118:GLY:HA2	2.08	0.84
2:C:377:LEU:HD13	2:C:476:ILE:HG22	1.59	0.84
2:B:365:SER:O	2:B:366:ILE:HG12	1.78	0.84
2:C:185:ARG:HH21	2:C:342:PRO:HG3	1.42	0.83
2:B:367:THR:HG21	2:B:472:THR:OG1	1.78	0.83
1:c:201:LYS:HE2	2:C:432:GLN:HE21	1.43	0.83
1:c:215:HIS:O	2:C:440:ALA:HA	1.78	0.83
2:B:512:GLY:HA2	2:B:718:HIS:HE2	1.41	0.83
1:c:126:LYS:HE3	1:c:129:PHE:HE1	1.43	0.83
2:A:526:ARG:CG	2:B:778:SER:HB3	2.07	0.83
2:A:321:ARG:O	2:A:325:GLU:HB2	1.76	0.83
1:a:147:VAL:HG23	1:a:150:SER:HB2	1.59	0.83
1:b:144:LYS:C	1:b:145:LEU:HD12	2.04	0.83
2:B:365:SER:O	2:B:471:VAL:HG21	1.78	0.83
2:C:382:ILE:HG13	2:C:484:THR:CG2	2.08	0.83
2:B:335:GLN:HG2	2:B:336:PRO:HD3	1.61	0.82
2:B:367:THR:HG21	2:B:472:THR:CA	1.97	0.82
2:C:300:LEU:CB	2:C:302:PRO:HD3	2.09	0.82
2:A:603:THR:HB	2:A:647:VAL:HG21	1.61	0.82
2:B:500:LEU:CD1	2:C:783:ARG:CG	2.50	0.82
2:C:444:ASP:O	2:C:448:ARG:HG3	1.79	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:136:PHE:CE2	2:B:431:VAL:HG21	2.14	0.82
2:B:366:ILE:HB	2:B:367:THR:HA	1.60	0.82
2:A:272:GLY:HA2	2:A:308:GLU:HG3	1.62	0.82
2:C:374:ALA:CA	2:C:476:ILE:CD1	2.57	0.82
2:C:706:ASP:O	2:C:707:GLU:HG2	1.80	0.82
2:B:526:ARG:N	2:C:775:ASP:CA	2.24	0.82
2:C:9:ARG:HD2	2:C:41:GLU:OE2	1.79	0.82
1:b:184:GLU:CD	2:B:30:GLY:HA3	2.04	0.82
2:B:706:ASP:O	2:B:707:GLU:HG2	1.80	0.81
2:A:341:GLN:HG3	2:A:387:LEU:H	1.45	0.81
2:A:526:ARG:HD3	2:B:778:SER:CB	2.10	0.81
1:b:126:LYS:HE3	1:b:129:PHE:HE1	1.44	0.81
2:B:306:ARG:NH2	2:C:242:LEU:HD22	1.77	0.81
2:B:363:ARG:NH1	2:B:476:ILE:N	2.28	0.81
2:C:423:VAL:O	2:C:424:ARG:C	2.21	0.81
2:A:366:ILE:CG2	2:A:367:THR:HA	2.09	0.81
2:A:434:GLN:HG2	2:A:434:GLN:O	1.77	0.81
2:A:439:ALA:O	2:A:442:LEU:N	2.13	0.81
2:B:496:THR:CG2	2:C:782:LEU:HD22	2.10	0.81
2:C:366:ILE:CG2	2:C:367:THR:HA	2.10	0.81
2:A:323:TYR:O	2:A:326:LYS:HB2	1.79	0.81
2:A:382:ILE:CA	2:A:383:SER:HB3	2.10	0.81
2:B:304:LEU:HD22	2:B:305:ALA:H	1.41	0.81
2:B:603:THR:HB	2:B:647:VAL:HG21	1.61	0.81
2:B:167:ALA:HB1	2:B:241:THR:O	1.81	0.81
2:C:427:LYS:O	2:C:431:VAL:HG23	1.81	0.81
2:A:185:ARG:HH21	2:A:342:PRO:HG3	1.43	0.81
2:A:394:LEU:HD12	2:A:476:ILE:O	1.79	0.81
2:B:240:MET:CG	2:B:274:ILE:HD11	2.11	0.81
2:B:308:GLU:O	2:B:309:LEU:HG	1.81	0.81
2:A:394:LEU:CD1	2:A:480:VAL:CG2	2.54	0.80
2:A:444:ASP:O	2:A:448:ARG:HG3	1.81	0.80
2:B:370:ALA:HB1	2:B:476:ILE:CG1	2.09	0.80
2:A:427:LYS:O	2:A:431:VAL:HG23	1.81	0.80
2:C:603:THR:HB	2:C:647:VAL:HG21	1.61	0.80
1:b:177:ASN:ND2	2:B:67:LEU:HD22	1.88	0.80
2:B:511:ILE:HD12	2:B:721:GLU:OE2	1.80	0.80
2:A:394:LEU:CD2	2:A:480:VAL:HA	2.10	0.80
2:C:272:GLY:HA2	2:C:308:GLU:HG3	1.62	0.80
2:B:346:GLU:O	2:B:350:ILE:HG13	1.81	0.80
2:C:242:LEU:CB	2:C:243:ASP:HA	2.11	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:706:ASP:O	2:A:707:GLU:HG2	1.80	0.80
2:B:262:LYS:NZ	2:C:260:ARG:HH22	1.79	0.80
2:B:359:GLU:HG2	2:B:365:SER:H	1.44	0.80
2:B:690:MET:O	2:C:760:TYR:CZ	2.35	0.80
2:A:21:ALA:HB3	2:A:22:LEU:HD22	1.64	0.80
2:A:199:ARG:HD3	2:B:358:TYR:HH	1.46	0.80
1:c:203:ILE:HG12	2:C:432:GLN:HG3	1.63	0.80
2:A:74:MET:HB3	2:A:76:GLN:NE2	1.97	0.79
2:A:363:ARG:HH12	2:A:475:ASP:HB3	1.45	0.79
2:B:500:LEU:CG	2:C:783:ARG:HG3	2.12	0.79
2:A:411:PRO:HB2	2:A:413:LEU:HG	1.64	0.79
2:B:496:THR:HB	2:C:782:LEU:HB3	1.65	0.79
2:B:511:ILE:HG23	2:B:718:HIS:ND1	1.95	0.79
2:C:203:ASN:O	2:C:334:PHE:HA	1.81	0.79
2:C:227:ASN:HA	2:C:228:ASN:HB2	1.64	0.79
2:B:90:LEU:HD22	2:B:114:ARG:HD3	1.65	0.79
2:B:367:THR:OG1	2:B:473:VAL:N	2.15	0.79
2:B:394:LEU:HD23	2:B:483:TRP:HZ3	1.39	0.79
2:C:300:LEU:C	2:C:302:PRO:HD3	2.07	0.79
2:C:434:GLN:HG2	2:C:434:GLN:O	1.80	0.79
2:B:191:ARG:HG2	2:B:337:ILE:HG21	1.64	0.79
2:B:305:ALA:CA	2:B:309:LEU:HD21	2.13	0.79
2:B:363:ARG:O	2:B:471:VAL:CB	2.29	0.79
1:a:184:GLU:CG	2:A:119:VAL:HG22	2.08	0.79
2:B:184:GLY:HA3	2:B:185:ARG:C	2.08	0.79
2:B:584:SER:HB3	2:B:602:LEU:HB3	1.63	0.79
2:C:74:MET:HB3	2:C:76:GLN:NE2	1.97	0.79
2:C:402:VAL:HG12	2:C:467:GLU:OE1	1.83	0.79
2:B:522:LYS:O	2:C:775:ASP:OD2	2.01	0.79
2:A:584:SER:HB3	2:A:602:LEU:HB3	1.63	0.79
2:C:13:VAL:HG23	2:C:37:GLY:O	1.83	0.79
2:C:584:SER:HB3	2:C:602:LEU:HB3	1.63	0.79
2:A:227:ASN:HA	2:A:228:ASN:HB2	1.64	0.78
2:B:185:ARG:HG2	2:B:188:GLU:CG	2.12	0.78
2:A:405:ARG:NH2	2:A:478:MET:HE1	1.98	0.78
2:A:199:ARG:CZ	2:B:358:TYR:OH	2.31	0.78
2:B:200:THR:HG23	2:C:358:TYR:OH	1.83	0.78
2:A:83:ARG:HD2	2:A:115:GLU:HG2	1.66	0.78
1:b:185:TYR:HE1	2:B:28:ASN:CG	1.90	0.78
2:B:74:MET:HB3	2:B:76:GLN:NE2	1.99	0.78
2:B:430:ALA:HB1	2:B:435:GLU:HG2	1.64	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:184:GLU:O	2:C:83:ARG:HB2	1.84	0.78
1:b:184:GLU:HB3	2:B:81:THR:CG2	2.07	0.78
2:B:511:ILE:HD12	2:B:721:GLU:OE1	1.66	0.78
2:A:369:ASP:HB2	2:A:472:THR:HG22	1.64	0.78
1:c:186:ALA:O	2:C:83:ARG:NH2	2.17	0.78
1:c:144:LYS:C	1:c:145:LEU:HD12	2.09	0.78
2:A:526:ARG:HD3	2:B:778:SER:HB2	1.66	0.78
2:C:181:PRO:CB	2:C:182:VAL:HA	2.07	0.78
2:C:394:LEU:CD1	2:C:479:VAL:HG11	2.06	0.78
2:B:21:ALA:HB3	2:B:22:LEU:HD22	1.65	0.77
2:B:358:TYR:C	2:B:360:ALA:H	1.91	0.77
2:B:690:MET:HB3	2:C:760:TYR:OH	1.84	0.77
2:C:402:VAL:HG13	2:C:467:GLU:OE1	1.84	0.77
2:C:35:LEU:HD21	2:C:60:ILE:HD13	1.67	0.77
2:C:373:ALA:C	2:C:476:ILE:HD13	2.09	0.77
2:A:183:ILE:HD12	2:A:350:ILE:HG12	1.65	0.77
2:B:129:VAL:O	2:B:129:VAL:HG12	1.83	0.77
2:A:546:PRO:HG2	2:A:549:VAL:HG21	1.67	0.77
2:B:355:ARG:HB3	2:B:355:ARG:HH11	1.47	0.77
2:B:546:PRO:HG2	2:B:549:VAL:HG21	1.67	0.77
2:A:423:VAL:O	2:A:424:ARG:C	2.28	0.77
2:A:763:ARG:HB2	2:A:764:PRO:HD3	1.67	0.77
2:B:345:ASP:HA	2:B:348:ILE:HD11	1.66	0.77
1:c:203:ILE:CD1	2:C:432:GLN:HG3	2.15	0.77
2:C:374:ALA:N	2:C:476:ILE:HD11	1.99	0.77
2:B:500:LEU:CG	2:C:783:ARG:CG	2.62	0.76
2:C:204:PRO:HG2	2:C:312:ILE:HG12	1.65	0.76
2:A:31:THR:HB	2:A:112:LEU:HD21	1.67	0.76
2:A:90:LEU:HD22	2:A:114:ARG:HD3	1.66	0.76
2:A:140:GLN:O	2:A:141:LEU:HD23	1.84	0.76
2:B:140:GLN:O	2:B:141:LEU:HD23	1.85	0.76
2:A:374:ALA:HB2	2:A:476:ILE:HD13	0.76	0.76
2:A:443:ARG:O	2:A:446:GLU:HB3	1.86	0.76
2:B:143:GLY:N	1:c:195:ARG:NH2	2.06	0.76
2:B:159:ASN:O	2:B:163:LEU:CB	2.34	0.76
2:C:13:VAL:HG23	2:C:37:GLY:C	2.11	0.76
2:C:341:GLN:HG3	2:C:387:LEU:H	1.50	0.76
2:A:371:ILE:CA	2:A:476:ILE:HD12	2.16	0.76
2:B:763:ARG:HB2	2:B:764:PRO:HD3	1.67	0.76
2:A:185:ARG:HG2	2:A:188:GLU:HG2	1.68	0.76
2:C:367:THR:H	2:C:471:VAL:HG21	1.51	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:394:LEU:CD1	2:C:479:VAL:CG1	2.63	0.76
2:B:5:ARG:H	2:B:5:ARG:NH1	1.84	0.75
2:B:379:ASP:HB2	2:B:387:LEU:HD11	1.68	0.75
2:C:230:VAL:HG13	2:C:231:PRO:HD2	1.67	0.75
2:C:546:PRO:HG2	2:C:549:VAL:HG21	1.67	0.75
2:C:411:PRO:HB2	2:C:413:LEU:HG	1.67	0.75
1:c:201:LYS:HE2	2:C:432:GLN:NE2	2.01	0.75
2:C:382:ILE:CD1	2:C:484:THR:HG21	2.17	0.75
2:A:206:LEU:HD12	2:A:313:GLY:O	1.87	0.75
2:B:31:THR:HB	2:B:112:LEU:HD21	1.67	0.75
2:B:276:LEU:O	2:B:311:CYS:HA	1.86	0.75
2:C:323:TYR:O	2:C:326:LYS:HB2	1.86	0.75
1:b:176:GLU:OE1	2:B:122:ARG:HD3	1.87	0.75
1:b:203:ILE:HD13	2:B:432:GLN:CA	2.17	0.75
2:B:198:ARG:O	2:B:199:ARG:HB2	1.85	0.75
2:B:395:ILE:O	2:B:399:GLY:N	2.19	0.75
1:c:216:PHE:CD1	2:C:443:ARG:HD3	2.21	0.75
2:A:441:SER:O	2:A:445:THR:HG23	1.87	0.75
2:C:5:ARG:H	2:C:5:ARG:NH1	1.85	0.75
2:C:183:ILE:HD12	2:C:350:ILE:HG12	1.69	0.75
2:A:181:PRO:CB	2:A:182:VAL:HA	2.10	0.75
2:B:411:PRO:C	2:B:413:LEU:H	1.94	0.75
2:C:377:LEU:HD12	2:C:476:ILE:HG23	1.67	0.75
2:A:408:THR:C	2:A:414:LYS:HZ1	1.92	0.74
2:B:483:TRP:CD1	2:B:483:TRP:H	2.05	0.74
2:B:48:LYS:NZ	1:c:194:HIS:HB3	2.01	0.74
2:C:382:ILE:CA	2:C:383:SER:HB3	2.13	0.74
2:B:364:VAL:HG22	2:B:366:ILE:O	1.87	0.74
2:B:526:ARG:H	2:C:775:ASP:CG	1.91	0.74
2:A:13:VAL:HG23	2:A:37:GLY:O	1.87	0.74
1:b:184:GLU:OE2	2:B:30:GLY:HA3	1.86	0.74
2:B:232:GLU:O	2:B:233:ILE:HD13	1.86	0.74
2:B:365:SER:C	2:B:471:VAL:HG21	2.13	0.74
2:B:369:ASP:HB3	2:B:473:VAL:HG22	1.66	0.74
1:b:180:SER:HG	2:B:119:VAL:HA	1.51	0.74
2:B:363:ARG:HH12	2:B:476:ILE:H	1.34	0.74
2:B:402:VAL:CG1	2:B:467:GLU:OE2	2.34	0.74
1:c:216:PHE:HD1	2:C:443:ARG:HD3	1.53	0.73
2:A:9:ARG:HD2	2:A:41:GLU:OE2	1.86	0.73
2:A:203:ASN:O	2:A:334:PHE:HA	1.88	0.73
2:B:179:LEU:HB3	2:B:223:GLN:NE2	2.03	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:6:PHE:HB2	2:A:10:ALA:HB3	1.70	0.73
2:A:703:ASN:HB3	2:B:767:ARG:CB	2.18	0.73
2:B:241:THR:HG22	2:B:277:PHE:HD1	1.53	0.73
1:b:180:SER:OG	2:B:119:VAL:CA	2.32	0.73
2:B:181:PRO:HB2	2:B:182:VAL:CA	2.09	0.73
2:B:200:THR:O	2:B:202:ASN:N	2.21	0.73
2:B:358:TYR:C	2:B:360:ALA:N	2.41	0.73
2:C:140:GLN:O	2:C:141:LEU:HD23	1.88	0.73
1:c:180:SER:OG	2:C:122:ARG:CB	2.36	0.73
2:C:60:ILE:HG22	2:C:61:GLN:N	2.03	0.73
2:C:242:LEU:HB3	2:C:243:ASP:CA	2.15	0.73
2:C:415:GLU:HA	2:C:418:GLN:CD	2.13	0.73
2:C:441:SER:O	2:C:445:THR:HG23	1.88	0.73
2:B:361:HIS:O	2:B:362:HIS:HB2	1.88	0.73
2:B:500:LEU:HD21	2:C:783:ARG:N	2.03	0.73
2:A:355:ARG:NE	2:A:366:ILE:H	1.87	0.73
2:A:204:PRO:HG2	2:A:312:ILE:HG12	1.71	0.73
1:b:185:TYR:HA	2:B:82:PRO:HD2	1.69	0.72
1:b:203:ILE:HG23	2:B:432:GLN:HA	1.69	0.72
2:C:129:VAL:O	2:C:129:VAL:HG12	1.87	0.72
2:B:483:TRP:H	2:B:483:TRP:HD1	1.37	0.72
2:A:13:VAL:HG23	2:A:37:GLY:C	2.14	0.72
2:A:166:LEU:CB	2:A:167:ALA:HB2	2.20	0.72
2:C:21:ALA:HB3	2:C:22:LEU:HD22	1.70	0.72
2:C:103:VAL:HG12	2:C:104:GLY:N	2.04	0.72
2:C:6:PHE:HB2	2:C:10:ALA:HB3	1.71	0.72
2:C:166:LEU:CB	2:C:167:ALA:HB2	2.19	0.72
1:a:217:ALA:HB1	2:A:74:MET:HE1	1.72	0.72
2:A:366:ILE:CB	2:A:367:THR:HA	2.19	0.72
1:b:187:THR:CG2	2:B:83:ARG:NH1	2.53	0.72
2:B:260:ARG:HA	2:B:263:LYS:HD3	1.71	0.72
2:B:367:THR:O	2:B:370:ALA:HB3	1.90	0.72
2:B:214:LYS:NZ	2:B:314:ALA:HA	2.04	0.72
1:c:154:LEU:HB2	1:c:163:LEU:HD23	1.72	0.72
2:A:21:ALA:HB2	2:A:29:ILE:CG2	2.19	0.72
2:A:129:VAL:O	2:A:129:VAL:HG12	1.88	0.72
2:A:367:THR:CB	2:A:472:THR:CG2	2.66	0.72
2:A:373:ALA:HB3	2:A:473:VAL:CG1	2.20	0.72
2:B:145:ASN:CA	1:c:158:GLU:OE2	2.38	0.71
2:B:142:LEU:HA	1:c:195:ARG:HD2	0.77	0.71
2:B:189:ILE:HG22	2:B:190:GLN:N	2.05	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:5:ARG:NH1	2:A:5:ARG:H	1.88	0.71
2:B:6:PHE:HB2	2:B:10:ALA:HB3	1.72	0.71
2:B:377:LEU:CD2	2:B:480:VAL:HG21	2.20	0.71
2:A:355:ARG:HD3	2:A:365:SER:HB2	1.72	0.71
2:B:21:ALA:HB2	2:B:29:ILE:CG2	2.20	0.71
2:C:382:ILE:HD11	2:C:484:THR:HG21	1.70	0.71
2:C:185:ARG:HG2	2:C:188:GLU:HG2	1.73	0.71
2:B:269:ARG:HH12	2:B:306:ARG:HB3	1.54	0.71
2:B:13:VAL:HG23	2:B:37:GLY:C	2.15	0.71
2:B:694:LYS:HD2	2:C:760:TYR:HD2	0.54	0.71
2:B:437:GLU:C	2:B:439:ALA:H	1.96	0.71
2:B:479:VAL:HG12	2:B:480:VAL:N	2.05	0.71
2:B:500:LEU:CD1	2:C:783:ARG:CA	2.66	0.71
2:A:526:ARG:HG2	2:B:778:SER:CB	2.14	0.71
2:B:190:GLN:OE1	2:C:404:LEU:CD2	2.38	0.71
2:B:397:GLU:O	2:B:401:LYS:HB2	1.90	0.71
2:B:402:VAL:CG1	2:B:467:GLU:CD	2.63	0.71
2:B:542:ILE:HG13	2:B:705:ILE:HD13	1.71	0.71
2:A:378:SER:HB3	2:A:390:LYS:HD3	1.73	0.71
2:B:214:LYS:HZ3	2:B:314:ALA:HA	1.55	0.71
2:A:373:ALA:HB3	2:A:473:VAL:HG12	1.68	0.70
2:A:542:ILE:HG13	2:A:705:ILE:HD13	1.71	0.70
2:B:185:ARG:HH11	2:B:185:ARG:CB	2.04	0.70
2:A:627:PHE:O	2:A:631:LEU:HB2	1.92	0.70
1:b:144:LYS:C	2:B:27:ASN:HD21	1.98	0.70
2:B:145:ASN:C	1:c:158:GLU:OE2	2.33	0.70
1:c:138:ASP:CG	2:C:82:PRO:CG	2.51	0.70
1:c:179:LEU:O	1:c:183:LEU:HD12	1.92	0.70
2:C:373:ALA:C	2:C:476:ILE:CD1	2.64	0.70
2:C:374:ALA:HA	2:C:476:ILE:HD13	1.72	0.70
2:A:341:GLN:HG2	2:A:387:LEU:HB2	1.74	0.70
2:C:648:ASP:OD1	2:C:650:ARG:HG2	1.91	0.70
2:C:54:GLY:O	2:C:55:LEU:HD23	1.91	0.70
2:B:648:ASP:OD1	2:B:650:ARG:HG2	1.91	0.70
2:C:542:ILE:HG13	2:C:705:ILE:HD13	1.71	0.70
2:C:565:ASP:C	2:C:567:GLU:H	2.00	0.70
2:C:627:PHE:O	2:C:631:LEU:HB2	1.92	0.70
2:B:207:ILE:O	2:B:338:GLN:HA	1.92	0.70
2:C:90:LEU:HD22	2:C:114:ARG:HD3	1.73	0.70
1:a:157:PHE:CE1	1:a:158:GLU:HG3	2.27	0.70
2:A:648:ASP:OD1	2:A:650:ARG:HG2	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:MET:HE1	2:B:269:ARG:NH2	2.05	0.70
2:B:499:LEU:HD13	2:C:782:LEU:CD1	2.22	0.70
1:c:203:ILE:CG1	2:C:432:GLN:HG3	2.21	0.70
2:A:367:THR:H	2:A:471:VAL:CA	2.05	0.69
2:B:9:ARG:HD2	2:B:41:GLU:OE2	1.92	0.69
2:B:176:GLU:C	2:B:178:SER:H	2.00	0.69
2:A:359:GLU:HG2	2:A:364:VAL:CG1	2.23	0.69
2:B:201:LYS:HZ1	2:B:335:GLN:CG	2.05	0.69
2:B:565:ASP:C	2:B:567:GLU:H	2.00	0.69
2:C:341:GLN:HG2	2:C:387:LEU:HB2	1.75	0.69
2:C:355:ARG:HD3	2:C:365:SER:HB2	1.74	0.69
2:A:565:ASP:C	2:A:567:GLU:H	2.00	0.69
2:C:31:THR:HB	2:C:112:LEU:HD21	1.73	0.69
2:C:66:SER:O	2:C:67:LEU:HD23	1.92	0.69
2:A:107:HIS:HA	2:A:110:LEU:HD12	1.74	0.69
2:A:411:PRO:C	2:A:413:LEU:H	1.99	0.69
1:b:187:THR:CG2	2:B:83:ARG:HH12	2.04	0.69
2:B:400:SER:OG	2:B:401:LYS:N	2.25	0.69
2:C:366:ILE:CB	2:C:367:THR:HA	2.23	0.69
1:a:154:LEU:HB2	1:a:163:LEU:HD23	1.73	0.69
2:B:306:ARG:HD3	2:C:168:ARG:HH22	0.56	0.69
2:C:443:ARG:O	2:C:446:GLU:HB3	1.92	0.69
2:A:382:ILE:HG13	2:A:484:THR:HB	1.73	0.69
2:B:206:LEU:HB2	2:B:313:GLY:O	1.93	0.69
1:c:205:SER:O	1:c:207:HIS:N	2.24	0.69
2:A:212:VAL:HG13	2:A:342:PRO:HD3	1.75	0.69
2:B:191:ARG:HD2	2:B:337:ILE:HG22	1.75	0.69
2:B:364:VAL:HA	2:B:365:SER:C	2.17	0.69
2:B:627:PHE:O	2:B:631:LEU:HB2	1.91	0.69
1:c:215:HIS:O	2:C:440:ALA:CA	2.39	0.69
2:C:359:GLU:HG2	2:C:364:VAL:CG1	2.22	0.69
2:A:341:GLN:CG	2:A:387:LEU:H	2.05	0.69
2:A:624:PRO:HA	2:A:627:PHE:HD2	1.57	0.69
2:B:142:LEU:HA	1:c:195:ARG:CG	2.22	0.69
2:B:315:THR:OG1	2:B:319:GLU:HB3	1.92	0.69
2:C:46:ALA:O	2:C:50:LEU:HD12	1.92	0.69
2:C:624:PRO:HA	2:C:627:PHE:HD2	1.58	0.69
2:A:10:ALA:HB2	2:A:104:GLY:HA2	1.73	0.68
2:A:494:THR:HA	2:A:497:ASP:HB2	1.75	0.68
1:c:203:ILE:HG23	2:C:432:GLN:HA	1.73	0.68
2:C:21:ALA:HB2	2:C:29:ILE:CG2	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:373:ALA:CB	2:A:473:VAL:HG13	2.19	0.68
2:C:212:VAL:HG13	2:C:342:PRO:HD3	1.76	0.68
2:C:364:VAL:HG13	2:C:365:SER:HA	1.75	0.68
2:B:197:SER:HB3	2:C:361:HIS:CD2	2.28	0.68
2:B:330:LEU:O	2:B:332:ARG:N	2.26	0.68
2:A:221:LEU:O	2:A:222:ALA:C	2.36	0.68
2:B:233:ILE:O	2:B:233:ILE:CD1	2.40	0.68
2:B:449:LEU:O	2:B:452:GLN:HB3	1.93	0.68
2:C:371:ILE:HG22	2:C:372:GLU:N	2.08	0.68
2:B:168:ARG:HH12	2:B:242:LEU:HD13	1.57	0.68
2:B:335:GLN:HG2	2:B:336:PRO:CD	2.23	0.68
2:A:199:ARG:CD	2:B:358:TYR:CZ	2.77	0.68
2:A:415:GLU:HA	2:A:418:GLN:CD	2.18	0.68
2:B:439:ALA:O	2:B:442:LEU:CA	2.41	0.68
1:c:157:PHE:HD1	1:c:158:GLU:N	1.92	0.68
1:b:145:LEU:HD11	2:B:27:ASN:OD1	1.94	0.68
2:B:222:ALA:O	2:B:226:ILE:HG13	1.94	0.68
1:c:180:SER:CB	2:C:122:ARG:HD3	2.23	0.68
2:B:46:ALA:O	2:B:50:LEU:HD12	1.94	0.68
2:B:200:THR:CG2	2:C:392:ILE:HG21	2.22	0.68
2:B:382:ILE:CA	2:B:383:SER:HB3	2.24	0.68
2:B:624:PRO:HA	2:B:627:PHE:HD2	1.58	0.68
2:C:411:PRO:C	2:C:413:LEU:H	2.01	0.68
2:B:306:ARG:HD3	2:C:168:ARG:CZ	2.18	0.68
2:C:5:ARG:HE	2:C:102:TYR:HE1	1.42	0.68
2:A:364:VAL:HG13	2:A:365:SER:HA	1.76	0.67
2:A:342:PRO:HD2	2:A:388:PRO:HD3	1.74	0.67
2:C:301:LYS:N	2:C:302:PRO:HD3	2.09	0.67
2:B:143:GLY:C	1:c:195:ARG:NH2	2.52	0.67
2:B:194:GLU:CA	2:C:400:SER:OG	2.42	0.67
2:B:204:PRO:HG2	2:B:312:ILE:HG13	1.75	0.67
2:A:233:ILE:HD11	2:B:399:GLY:O	1.94	0.67
1:b:179:LEU:O	1:b:183:LEU:HD12	1.94	0.67
2:B:48:LYS:HZ2	1:c:194:HIS:HB3	1.58	0.67
2:B:330:LEU:C	2:B:332:ARG:H	2.02	0.67
2:B:369:ASP:CB	2:B:473:VAL:CG2	2.67	0.67
2:A:445:THR:HG22	2:A:448:ARG:NH1	2.09	0.67
2:B:167:ALA:HB1	2:B:241:THR:C	2.19	0.67
1:a:146:ASN:HB3	1:a:148:ASN:OD1	1.95	0.67
2:A:382:ILE:HA	2:A:383:SER:CB	2.13	0.67
1:a:126:LYS:HE3	1:a:129:PHE:CE1	2.28	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:6:PHE:N	2:A:6:PHE:CD2	2.62	0.67
2:A:233:ILE:CD1	2:B:399:GLY:O	2.43	0.67
2:A:377:LEU:HD11	2:A:477:ALA:HB2	1.77	0.67
2:B:167:ALA:O	2:B:168:ARG:O	2.12	0.67
2:B:301:LYS:N	2:B:302:PRO:CD	2.58	0.67
2:A:66:SER:O	2:A:67:LEU:HD23	1.95	0.66
2:A:231:PRO:HD3	2:B:404:LEU:HD13	1.75	0.66
2:A:354:LEU:HB3	2:A:357:ARG:NH1	2.09	0.66
2:B:169:ASP:N	2:B:173:ILE:HD12	2.10	0.66
2:B:494:THR:HA	2:B:497:ASP:HB2	1.75	0.66
2:C:355:ARG:NE	2:C:366:ILE:H	1.92	0.66
2:A:197:SER:OG	2:B:400:SER:HB3	1.95	0.66
2:A:408:THR:C	2:A:414:LYS:HE2	2.17	0.66
2:B:355:ARG:HD2	2:B:365:SER:HA	1.78	0.66
2:A:565:ASP:O	2:A:567:GLU:N	2.27	0.66
2:B:13:VAL:CG2	2:B:38:LEU:HD23	2.14	0.66
2:B:229:GLU:O	2:B:230:VAL:HG22	1.95	0.66
2:B:396:ASP:O	2:B:397:GLU:C	2.37	0.66
2:B:437:GLU:O	2:B:439:ALA:N	2.27	0.66
2:C:445:THR:HG22	2:C:448:ARG:NH1	2.10	0.66
2:B:620:GLU:HG3	2:B:658:SER:OG	1.96	0.66
2:B:706:ASP:CG	2:C:770:GLN:OE1	2.38	0.66
2:C:509:ARG:HD3	2:C:557:ALA:HB2	1.77	0.66
2:B:262:LYS:NZ	2:C:260:ARG:NH2	2.42	0.66
2:B:499:LEU:HD12	2:C:782:LEU:HD13	1.77	0.66
2:C:10:ALA:HB2	2:C:104:GLY:HA2	1.76	0.66
2:C:494:THR:HA	2:C:497:ASP:HB2	1.75	0.66
2:C:515:GLU:OE1	2:C:712:HIS:CD2	2.49	0.66
1:b:177:ASN:HB3	2:B:67:LEU:HD22	1.75	0.66
2:B:367:THR:CG2	2:B:472:THR:CB	2.55	0.66
2:B:500:LEU:CD2	2:C:783:ARG:CG	2.22	0.66
2:B:565:ASP:O	2:B:567:GLU:N	2.27	0.66
2:B:707:GLU:OE2	2:C:771:LYS:HD2	1.96	0.66
2:C:10:ALA:O	2:C:13:VAL:HG12	1.96	0.66
2:C:183:ILE:HG22	2:C:184:GLY:N	2.09	0.66
1:a:201:LYS:HE2	2:A:432:GLN:NE2	2.10	0.66
2:A:371:ILE:HG22	2:A:372:GLU:N	2.11	0.66
2:B:499:LEU:CD1	2:C:782:LEU:CD1	2.74	0.66
2:B:766:ARG:HH11	2:B:766:ARG:HG3	1.61	0.66
1:c:146:ASN:HB3	1:c:148:ASN:OD1	1.96	0.66
2:C:354:LEU:HB3	2:C:357:ARG:NH1	2.10	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:THR:HA	2:B:264:VAL:HG11	1.78	0.65
2:B:171:THR:OG1	2:B:238:ARG:HA	1.95	0.65
2:B:262:LYS:HZ2	2:C:260:ARG:HH22	1.45	0.65
2:B:509:ARG:HD3	2:B:557:ALA:HB2	1.77	0.65
1:c:157:PHE:CD1	1:c:158:GLU:N	2.64	0.65
2:C:359:GLU:HG2	2:C:364:VAL:HG12	1.76	0.65
2:A:515:GLU:OE1	2:A:712:HIS:CD2	2.49	0.65
2:A:766:ARG:HH11	2:A:766:ARG:HG3	1.62	0.65
2:B:511:ILE:CG1	2:B:721:GLU:CD	2.69	0.65
2:C:351:LEU:HD11	2:C:375:VAL:HG23	1.77	0.65
2:A:103:VAL:HG12	2:A:104:GLY:N	2.10	0.65
2:A:355:ARG:HE	2:A:366:ILE:H	1.44	0.65
1:a:216:PHE:HZ	2:A:431:VAL:HG21	1.60	0.65
2:A:5:ARG:HE	2:A:102:TYR:HE1	1.44	0.65
2:A:110:LEU:HD21	2:A:138:VAL:HG11	1.78	0.65
2:A:394:LEU:HG	2:A:480:VAL:HG22	1.75	0.65
1:b:180:SER:OG	2:B:119:VAL:CG1	2.45	0.65
2:B:174:ALA:CB	2:B:179:LEU:HD22	2.26	0.65
2:B:345:ASP:HA	2:B:348:ILE:CD1	2.26	0.65
2:B:394:LEU:HD21	2:B:483:TRP:CE3	2.29	0.65
1:a:153:THR:HG23	1:a:205:SER:HA	1.78	0.65
2:A:509:ARG:HD3	2:A:557:ALA:HB2	1.77	0.65
2:B:66:SER:O	2:B:67:LEU:HD23	1.97	0.65
2:B:306:ARG:CD	2:C:168:ARG:NH2	2.14	0.65
2:C:204:PRO:HA	2:C:335:GLN:O	1.96	0.65
2:C:343:SER:HB2	2:C:346:GLU:HG3	1.78	0.65
2:A:172:ALA:HA	2:A:175:LYS:HD2	1.78	0.65
2:A:620:GLU:HG3	2:A:658:SER:OG	1.96	0.65
2:B:142:LEU:C	1:c:195:ARG:HD2	2.22	0.65
2:C:299:ILE:C	2:C:323:TYR:OH	2.39	0.65
2:C:620:GLU:HG3	2:C:658:SER:OG	1.96	0.65
2:A:46:ALA:O	2:A:50:LEU:HD12	1.96	0.65
2:A:54:GLY:O	2:A:55:LEU:HD23	1.97	0.65
2:B:305:ALA:C	2:B:307:GLY:H	2.04	0.65
2:C:46:ALA:HB2	2:C:105:THR:O	1.96	0.65
2:B:54:GLY:O	2:B:55:LEU:HD23	1.97	0.65
2:A:363:ARG:NH1	2:A:475:ASP:CB	2.59	0.65
1:b:146:ASN:HB3	1:b:148:ASN:OD1	1.97	0.65
2:B:512:GLY:CA	2:B:718:HIS:CD2	2.80	0.65
1:a:144:LYS:C	1:a:145:LEU:HD12	2.22	0.64
2:B:727:SER:O	2:B:731:THR:HG23	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:164:ASP:C	2:C:166:LEU:O	2.41	0.64
2:B:5:ARG:HE	2:B:102:TYR:HE1	1.44	0.64
2:B:367:THR:CG2	2:B:472:THR:HG23	2.27	0.64
2:B:500:LEU:CG	2:C:783:ARG:HG2	2.27	0.64
2:C:727:SER:O	2:C:731:THR:HG23	1.98	0.64
2:A:727:SER:O	2:A:731:THR:HG23	1.98	0.64
1:b:205:SER:O	1:b:207:HIS:N	2.29	0.64
2:B:620:GLU:CG	2:B:658:SER:OG	2.46	0.64
1:a:179:LEU:O	1:a:183:LEU:HD12	1.98	0.64
1:b:126:LYS:HE3	1:b:129:PHE:CE1	2.31	0.64
1:b:153:THR:HG23	1:b:205:SER:HA	1.78	0.64
2:B:203:ASN:O	2:B:334:PHE:HA	1.98	0.64
2:B:445:THR:O	2:B:449:LEU:HD12	1.97	0.64
2:C:6:PHE:CD2	2:C:6:PHE:N	2.66	0.64
2:B:515:GLU:OE1	2:B:712:HIS:CD2	2.49	0.64
2:A:370:ALA:O	2:A:473:VAL:HA	1.91	0.64
2:A:620:GLU:CG	2:A:658:SER:OG	2.46	0.64
2:B:361:HIS:O	2:B:362:HIS:CB	2.45	0.64
2:B:363:ARG:HG3	2:B:471:VAL:HA	1.79	0.64
2:C:86:LYS:HG2	2:C:115:GLU:CD	2.23	0.64
2:C:122:ARG:O	2:C:126:ASN:HB2	1.98	0.64
2:A:359:GLU:HG2	2:A:364:VAL:HG12	1.79	0.64
2:B:164:ASP:CB	2:B:166:LEU:O	2.44	0.64
2:C:231:PRO:C	2:C:233:ILE:H	2.06	0.64
2:A:171:THR:CG2	2:A:175:LYS:HE3	2.24	0.64
2:A:363:ARG:NH1	2:A:475:ASP:CG	2.56	0.64
2:B:231:PRO:O	2:B:233:ILE:N	2.31	0.64
2:A:29:ILE:HA	2:A:33:HIS:ND1	2.13	0.63
2:A:230:VAL:HG13	2:A:231:PRO:HD2	1.79	0.63
2:A:415:GLU:O	2:A:419:LYS:HG3	1.98	0.63
2:C:30:GLY:HA2	2:C:81:THR:OG1	1.98	0.63
2:C:620:GLU:CG	2:C:658:SER:OG	2.46	0.63
2:B:13:VAL:HG23	2:B:37:GLY:O	1.97	0.63
2:C:172:ALA:HA	2:C:175:LYS:HD2	1.80	0.63
1:a:184:GLU:OE2	2:A:118:GLY:CA	2.44	0.63
2:A:41:GLU:O	2:A:43:GLU:N	2.30	0.63
2:A:60:ILE:HG22	2:A:61:GLN:N	2.12	0.63
1:b:147:VAL:CG2	1:b:150:SER:HB2	2.28	0.63
1:b:203:ILE:HD13	2:B:432:GLN:HA	1.80	0.63
2:B:201:LYS:NZ	2:B:335:GLN:HG3	2.13	0.63
2:B:525:ARG:C	2:C:775:ASP:HA	2.19	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:ALA:HB2	2:B:105:THR:O	1.99	0.63
2:B:170:LEU:HB2	2:B:239:VAL:HB	1.81	0.63
2:C:565:ASP:O	2:C:567:GLU:N	2.28	0.63
2:C:766:ARG:HG3	2:C:766:ARG:HH11	1.62	0.63
2:A:122:ARG:O	2:A:126:ASN:HB2	1.98	0.63
2:B:394:LEU:HD23	2:B:483:TRP:CH2	2.27	0.63
2:A:343:SER:HB2	2:A:346:GLU:HG3	1.79	0.63
2:B:122:ARG:O	2:B:126:ASN:HB2	1.97	0.63
2:B:232:GLU:HA	2:C:362:HIS:CD2	2.34	0.63
2:A:318:ASP:O	2:A:321:ARG:N	2.31	0.63
2:A:374:ALA:CB	2:A:476:ILE:HG23	2.18	0.63
2:B:10:ALA:HB2	2:B:104:GLY:HA2	1.80	0.63
2:C:74:MET:HB3	2:C:76:GLN:HE22	1.62	0.63
2:C:374:ALA:N	2:C:476:ILE:HD12	2.09	0.63
2:A:351:LEU:HD11	2:A:375:VAL:HG23	1.81	0.63
1:b:144:LYS:HD3	2:B:76:GLN:OE1	1.99	0.63
2:B:41:GLU:O	2:B:43:GLU:N	2.32	0.63
2:B:268:ILE:C	2:B:270:GLN:H	2.06	0.63
2:B:276:LEU:HD13	2:B:277:PHE:N	2.14	0.63
2:B:306:ARG:HH22	2:C:242:LEU:HD22	1.44	0.63
2:B:694:LYS:HD3	2:C:760:TYR:CD2	2.24	0.63
1:b:154:LEU:HB2	1:b:163:LEU:HD23	1.80	0.62
2:C:12:LYS:O	2:C:16:LEU:HB2	1.98	0.62
2:C:239:VAL:O	2:C:240:MET:HG2	1.99	0.62
2:C:276:LEU:HD13	2:C:277:PHE:H	1.63	0.62
2:C:307:GLY:H	2:C:309:LEU:HD21	1.64	0.62
2:A:164:ASP:C	2:A:166:LEU:O	2.42	0.62
2:B:191:ARG:O	2:B:195:VAL:HG22	1.99	0.62
2:B:369:ASP:CB	2:B:473:VAL:HG22	2.29	0.62
2:B:499:LEU:HD13	2:C:782:LEU:HD11	1.81	0.62
2:B:690:MET:O	2:C:760:TYR:CE2	2.51	0.62
1:b:187:THR:HG23	2:B:83:ARG:NH1	2.14	0.62
2:C:41:GLU:O	2:C:43:GLU:N	2.32	0.62
2:C:171:THR:CG2	2:C:175:LYS:HE3	2.26	0.62
2:A:307:GLY:H	2:A:309:LEU:HD21	1.64	0.62
1:c:153:THR:HG23	1:c:205:SER:HA	1.80	0.62
2:C:241:THR:HG22	2:C:277:PHE:HB3	1.81	0.62
2:A:74:MET:HB3	2:A:76:GLN:HE22	1.62	0.62
2:B:198:ARG:HD2	2:B:201:LYS:O	1.99	0.62
2:C:452:GLN:O	2:C:456:THR:HG23	2.00	0.62
2:A:35:LEU:HD21	2:A:60:ILE:HD13	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:231:PRO:C	2:A:233:ILE:H	2.05	0.62
2:B:107:HIS:HA	2:B:110:LEU:HD12	1.81	0.62
2:B:143:GLY:CA	1:c:195:ARG:HH21	2.11	0.62
2:C:426:GLU:O	2:C:430:ALA:CB	2.48	0.62
2:A:352:GLN:O	2:A:355:ARG:HB3	1.99	0.62
2:B:236:ASP:O	2:B:273:ASN:HB2	1.99	0.62
2:B:424:ARG:O	2:B:427:LYS:HB3	2.00	0.62
2:A:280:ALA:C	2:A:301:LYS:HE2	2.25	0.62
2:A:382:ILE:HG13	2:A:484:THR:CB	2.30	0.62
2:B:500:LEU:HD13	2:C:783:ARG:HA	1.81	0.62
2:B:500:LEU:HD21	2:C:783:ARG:H	1.62	0.62
1:c:126:LYS:HE3	1:c:129:PHE:CE1	2.32	0.62
2:A:439:ALA:O	2:A:440:ALA:C	2.43	0.62
2:B:330:LEU:C	2:B:332:ARG:N	2.54	0.62
1:a:205:SER:O	1:a:207:HIS:N	2.31	0.62
1:c:183:LEU:HB3	2:C:117:GLU:CG	2.23	0.62
2:C:300:LEU:CB	2:C:323:TYR:HE2	2.13	0.62
1:b:184:GLU:CB	2:B:81:THR:HG21	2.14	0.61
2:B:174:ALA:HB2	2:B:179:LEU:HD22	1.81	0.61
2:B:363:ARG:NH2	2:B:402:VAL:HG21	2.16	0.61
2:B:512:GLY:CA	2:B:718:HIS:CE1	2.82	0.61
1:c:204:ILE:HD13	1:c:211:THR:HB	1.82	0.61
1:a:157:PHE:HD1	1:a:158:GLU:N	1.98	0.61
2:A:355:ARG:HD3	2:A:365:SER:CB	2.31	0.61
2:B:204:PRO:HA	2:B:335:GLN:O	2.00	0.61
2:B:439:ALA:HA	2:B:442:LEU:CD1	2.26	0.61
2:A:197:SER:OG	2:B:400:SER:CB	2.48	0.61
2:B:129:VAL:O	2:B:130:SER:O	2.18	0.61
2:B:6:PHE:CD2	2:B:6:PHE:N	2.66	0.61
2:B:201:LYS:HA	2:B:332:ARG:O	2.00	0.61
2:B:351:LEU:HD21	2:B:392:ILE:HD13	1.83	0.61
2:B:366:ILE:CB	2:B:367:THR:HA	2.23	0.61
2:C:341:GLN:CG	2:C:387:LEU:H	2.12	0.61
2:A:199:ARG:HD2	2:B:358:TYR:OH	1.94	0.61
1:b:184:GLU:OE2	2:B:30:GLY:C	2.44	0.61
2:B:162:THR:HA	2:B:264:VAL:CG1	2.30	0.61
2:B:233:ILE:O	2:B:233:ILE:CG1	2.48	0.61
2:B:241:THR:HG22	2:B:277:PHE:CD1	2.35	0.61
1:b:161:TYR:OH	2:B:428:ASP:OD2	2.18	0.61
2:A:452:GLN:O	2:A:456:THR:HG23	1.99	0.61
2:B:119:VAL:O	2:B:123:VAL:HG23	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:342:PRO:HG2	2:B:388:PRO:HG3	1.82	0.61
2:A:10:ALA:O	2:A:13:VAL:HG12	2.01	0.61
2:A:697:PHE:HB2	2:A:702:ILE:HD11	1.83	0.61
2:B:74:MET:HB3	2:B:76:GLN:HE22	1.64	0.61
2:B:143:GLY:C	1:c:195:ARG:HH22	2.09	0.61
2:A:212:VAL:O	2:A:213:GLY:C	2.44	0.61
2:B:526:ARG:HE	2:C:775:ASP:HB2	1.63	0.61
2:B:271:ALA:HB1	2:C:96:ARG:NH1	2.15	0.60
2:B:531:LEU:C	2:C:733:ARG:NH2	2.57	0.60
1:a:184:GLU:OE2	2:A:119:VAL:HG23	2.00	0.60
1:b:144:LYS:HB3	2:B:27:ASN:HD22	1.66	0.60
1:b:193:ILE:O	1:b:193:ILE:HD12	2.00	0.60
2:B:74:MET:HE2	2:B:76:GLN:HE22	1.66	0.60
2:B:304:LEU:HD13	2:B:306:ARG:N	2.15	0.60
2:C:22:LEU:O	2:C:25:GLY:N	2.33	0.60
2:C:377:LEU:HB3	2:C:480:VAL:HG21	1.83	0.60
1:b:144:LYS:HZ1	2:B:443:ARG:HH22	1.49	0.60
2:B:195:VAL:HA	2:B:198:ARG:HE	1.66	0.60
2:B:201:LYS:HB3	2:B:335:GLN:HG3	1.82	0.60
2:B:342:PRO:HD2	2:B:388:PRO:HD3	1.82	0.60
2:B:356:ASP:HA	2:B:359:GLU:OE1	2.00	0.60
2:C:351:LEU:HD11	2:C:375:VAL:CG2	2.32	0.60
1:b:144:LYS:CB	2:B:27:ASN:ND2	2.65	0.60
2:B:305:ALA:HB2	2:B:309:LEU:HD11	1.82	0.60
2:A:374:ALA:N	2:A:476:ILE:HG22	2.10	0.60
2:B:482:SER:OG	2:B:483:TRP:HD1	1.84	0.60
2:A:119:VAL:O	2:A:123:VAL:HG23	2.01	0.60
1:b:203:ILE:CD1	2:B:432:GLN:CG	2.80	0.60
2:B:86:LYS:HG2	2:B:115:GLU:CD	2.26	0.60
2:B:198:ARG:HH11	2:C:396:ASP:HB3	1.66	0.60
2:B:466:GLN:O	2:B:467:GLU:HG3	2.02	0.60
2:A:74:MET:HE2	2:A:76:GLN:NE2	2.17	0.60
2:A:577:TYR:HE1	2:A:584:SER:HG	1.50	0.60
2:C:221:LEU:O	2:C:222:ALA:C	2.45	0.60
2:C:382:ILE:HA	2:C:383:SER:CB	2.13	0.60
2:C:449:LEU:O	2:C:452:GLN:HB3	2.01	0.60
2:C:697:PHE:HB2	2:C:702:ILE:HD11	1.83	0.60
2:A:74:MET:HE2	2:A:76:GLN:HE22	1.65	0.60
2:A:162:THR:O	2:A:164:ASP:N	2.35	0.60
2:A:430:ALA:HB1	2:A:435:GLU:HG2	1.83	0.60
2:B:194:GLU:HA	2:C:400:SER:CB	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:ILE:HD11	2:B:237:LYS:O	2.01	0.60
2:B:359:GLU:CG	2:B:365:SER:H	2.13	0.60
1:c:157:PHE:CE1	1:c:158:GLU:HG3	2.35	0.60
2:A:199:ARG:HD3	2:B:358:TYR:CZ	2.36	0.60
2:A:377:LEU:HD11	2:A:477:ALA:CB	2.32	0.60
2:B:766:ARG:HG3	2:B:766:ARG:NH1	2.17	0.60
2:A:12:LYS:O	2:A:16:LEU:HB2	2.00	0.60
2:B:472:THR:HG22	2:B:473:VAL:HG23	1.84	0.60
1:c:130:VAL:C	1:c:131:LEU:HD23	2.27	0.60
2:C:201:LYS:HD2	2:C:335:GLN:HG3	1.83	0.60
2:C:395:ILE:O	2:C:399:GLY:N	2.35	0.60
2:A:304:LEU:O	2:A:306:ARG:N	2.35	0.59
2:A:411:PRO:C	2:A:413:LEU:N	2.60	0.59
2:A:445:THR:HA	2:A:448:ARG:HD2	1.83	0.59
2:B:304:LEU:CD2	2:B:305:ALA:N	2.50	0.59
2:C:72:GLN:C	2:C:74:MET:H	2.08	0.59
2:C:74:MET:HE2	2:C:76:GLN:HE22	1.67	0.59
2:C:228:ASN:HD21	2:C:235:ARG:HH21	1.50	0.59
2:A:306:ARG:N	2:A:309:LEU:HD11	2.17	0.59
2:A:382:ILE:CA	2:A:383:SER:CB	2.76	0.59
1:b:177:ASN:ND2	2:B:67:LEU:HD23	2.15	0.59
2:B:396:ASP:O	2:B:399:GLY:N	2.34	0.59
2:B:168:ARG:HH12	2:B:242:LEU:HB2	1.64	0.59
2:B:306:ARG:HH21	2:C:242:LEU:CD1	1.72	0.59
2:B:525:ARG:CB	2:C:779:GLU:OE2	2.50	0.59
2:C:13:VAL:CG2	2:C:38:LEU:HD23	2.15	0.59
2:C:318:ASP:O	2:C:321:ARG:N	2.35	0.59
2:C:445:THR:HA	2:C:448:ARG:HD2	1.83	0.59
2:C:766:ARG:HG3	2:C:766:ARG:NH1	2.17	0.59
2:A:72:GLN:H	2:A:72:GLN:CD	2.11	0.59
2:B:192:VAL:HG12	2:B:221:LEU:HD21	1.83	0.59
2:C:90:LEU:HD11	2:C:115:GLU:HB2	1.83	0.59
2:A:165:SER:CB	2:A:166:LEU:CB	2.81	0.59
2:A:183:ILE:HG22	2:A:184:GLY:N	2.17	0.59
2:A:228:ASN:HD21	2:A:235:ARG:HH21	1.50	0.59
2:B:166:LEU:HA	2:B:167:ALA:HB2	1.85	0.59
2:B:203:ASN:HD21	2:B:310:GLN:HA	1.68	0.59
2:B:697:PHE:HB2	2:B:702:ILE:HD11	1.83	0.59
2:C:396:ASP:O	2:C:397:GLU:C	2.44	0.59
2:A:402:VAL:C	2:A:404:LEU:H	2.11	0.59
2:B:141:LEU:HA	1:c:192:SER:OG	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:LEU:HB3	2:B:223:GLN:HE22	1.67	0.59
2:B:306:ARG:HA	2:C:168:ARG:NH2	2.16	0.59
2:B:373:ALA:C	2:B:377:LEU:HD13	2.26	0.59
2:C:72:GLN:CD	2:C:72:GLN:H	2.09	0.59
2:C:439:ALA:O	2:C:440:ALA:C	2.46	0.59
2:A:169:ASP:O	2:A:172:ALA:HB3	2.02	0.59
2:A:199:ARG:CD	2:B:358:TYR:HH	2.00	0.59
2:A:232:GLU:HA	2:A:235:ARG:HG3	1.84	0.59
2:B:72:GLN:C	2:B:74:MET:H	2.10	0.59
2:B:231:PRO:HB2	2:C:403:ARG:HE	1.68	0.59
2:C:139:LEU:C	2:C:141:LEU:H	2.11	0.59
2:C:380:ARG:HG3	2:C:381:TYR:CD2	2.36	0.59
2:A:304:LEU:C	2:A:306:ARG:H	2.09	0.59
2:B:185:ARG:HD3	2:B:339:VAL:HG13	1.85	0.59
2:B:382:ILE:HA	2:B:383:SER:CB	2.22	0.59
2:B:706:ASP:O	2:C:767:ARG:CB	2.50	0.59
1:c:179:LEU:HG	1:c:183:LEU:HD11	1.84	0.59
2:C:367:THR:OG1	2:C:471:VAL:HG12	2.01	0.59
2:B:143:GLY:CA	1:c:195:ARG:NH2	2.65	0.59
2:B:496:THR:HG22	2:C:782:LEU:HD22	1.85	0.59
2:A:241:THR:HG22	2:A:277:PHE:HB3	1.84	0.58
2:A:424:ARG:HG2	2:A:446:GLU:OE2	2.03	0.58
1:c:157:PHE:CD1	1:c:157:PHE:C	2.80	0.58
1:b:184:GLU:CD	2:B:30:GLY:CA	2.69	0.58
2:B:72:GLN:H	2:B:72:GLN:CD	2.09	0.58
2:B:201:LYS:HZ1	2:B:335:GLN:HG2	1.68	0.58
2:B:370:ALA:HA	2:B:473:VAL:HG13	1.85	0.58
2:A:268:ILE:HD13	2:A:269:ARG:N	2.18	0.58
2:B:201:LYS:HZ1	2:B:335:GLN:HG3	1.67	0.58
2:B:241:THR:HG22	2:B:277:PHE:HB3	1.85	0.58
2:B:347:SER:HB3	2:B:375:VAL:HG11	1.84	0.58
1:c:154:LEU:HD12	1:c:155:TYR:N	2.18	0.58
2:C:439:ALA:CA	2:C:442:LEU:HB2	2.26	0.58
1:a:157:PHE:CD1	1:a:158:GLU:N	2.71	0.58
2:A:639:LEU:O	2:A:646:THR:HA	2.03	0.58
1:c:145:LEU:HD12	1:c:145:LEU:N	2.19	0.58
1:c:184:GLU:HA	2:C:118:GLY:CA	2.28	0.58
2:C:415:GLU:O	2:C:419:LYS:HG3	2.02	0.58
2:A:162:THR:C	2:A:164:ASP:N	2.60	0.58
2:A:394:LEU:CD1	2:A:479:VAL:HB	2.34	0.58
2:B:12:LYS:O	2:B:16:LEU:HB2	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:GLY:HA2	2:B:212:VAL:HG22	1.86	0.58
2:B:232:GLU:OE2	2:C:361:HIS:HB3	2.04	0.58
2:B:371:ILE:O	2:B:372:GLU:C	2.47	0.58
2:C:169:ASP:O	2:C:172:ALA:HB3	2.03	0.58
2:C:179:LEU:HD12	2:C:180:ASP:N	2.19	0.58
1:a:133:PHE:CD1	1:a:139:VAL:HG22	2.39	0.58
2:B:83:ARG:HD2	2:B:115:GLU:HG2	1.86	0.58
2:C:446:GLU:O	2:C:449:LEU:HB2	2.03	0.58
2:A:86:LYS:HG2	2:A:115:GLU:CD	2.29	0.58
2:A:167:ALA:C	2:A:168:ARG:HD2	2.29	0.58
1:b:203:ILE:HD11	2:B:432:GLN:CB	2.23	0.58
2:C:304:LEU:C	2:C:306:ARG:H	2.12	0.58
2:C:306:ARG:N	2:C:309:LEU:HD11	2.19	0.58
2:C:639:LEU:O	2:C:646:THR:HA	2.03	0.58
1:a:189:SER:C	1:a:191:ILE:H	2.12	0.58
2:A:200:THR:CB	2:B:393:ASP:CB	2.81	0.58
2:A:308:GLU:C	2:A:308:GLU:CD	2.72	0.58
2:A:526:ARG:CD	2:B:778:SER:CB	2.82	0.58
2:C:201:LYS:CD	2:C:335:GLN:HG3	2.34	0.58
2:C:203:ASN:OD1	2:C:310:GLN:HG3	2.03	0.58
2:B:74:MET:HE2	2:B:76:GLN:NE2	2.18	0.58
2:B:225:ILE:HA	2:B:230:VAL:HG21	1.85	0.58
2:B:316:THR:O	2:B:317:LEU:C	2.47	0.58
2:C:232:GLU:HA	2:C:235:ARG:HG3	1.85	0.58
2:A:162:THR:C	2:A:164:ASP:H	2.10	0.57
2:A:446:GLU:O	2:A:449:LEU:HB2	2.04	0.57
2:B:60:ILE:HG22	2:B:61:GLN:N	2.18	0.57
2:B:214:LYS:NZ	2:B:315:THR:H	2.02	0.57
1:c:201:LYS:CE	2:C:432:GLN:HE21	2.15	0.57
2:C:355:ARG:HE	2:C:366:ILE:H	1.51	0.57
2:A:47:ALA:O	2:A:51:GLN:HG2	2.05	0.57
2:A:72:GLN:C	2:A:74:MET:H	2.10	0.57
1:b:184:GLU:HG2	2:B:119:VAL:HG23	1.84	0.57
2:B:355:ARG:CD	2:B:366:ILE:H	2.17	0.57
2:B:380:ARG:HD2	2:B:380:ARG:C	2.29	0.57
2:C:167:ALA:C	2:C:168:ARG:HD2	2.30	0.57
1:a:187:THR:HG23	2:A:83:ARG:NH2	2.12	0.57
2:B:639:LEU:O	2:B:646:THR:HA	2.03	0.57
1:c:126:LYS:C	1:c:127:LEU:HD23	2.29	0.57
2:C:342:PRO:HD2	2:C:388:PRO:HD3	1.85	0.57
2:C:394:LEU:HD13	2:C:479:VAL:CB	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:204:ILE:CG2	1:a:208:ALA:HA	2.34	0.57
2:A:6:PHE:CB	2:A:10:ALA:HB3	2.33	0.57
2:A:402:VAL:C	2:A:404:LEU:N	2.61	0.57
2:A:426:GLU:O	2:A:430:ALA:CB	2.52	0.57
2:B:171:THR:OG1	2:B:239:VAL:N	2.35	0.57
2:A:204:PRO:HA	2:A:335:GLN:O	2.04	0.57
2:A:373:ALA:O	2:A:374:ALA:C	2.48	0.57
1:b:136:PHE:CZ	2:B:431:VAL:CG2	2.80	0.57
2:B:29:ILE:HA	2:B:33:HIS:ND1	2.19	0.57
2:C:29:ILE:HA	2:C:33:HIS:ND1	2.19	0.57
2:C:404:LEU:O	2:C:407:PHE:N	2.38	0.57
2:A:380:ARG:HG3	2:A:381:TYR:CD2	2.40	0.57
2:B:240:MET:HB2	2:B:276:LEU:CD2	2.35	0.57
2:A:198:ARG:HA	2:B:396:ASP:HB3	1.86	0.57
2:A:330:LEU:O	2:A:332:ARG:N	2.38	0.57
2:A:377:LEU:CD1	2:A:477:ALA:CB	2.82	0.57
2:B:138:VAL:O	2:B:142:LEU:HD12	2.05	0.57
2:B:207:ILE:O	2:B:207:ILE:HG13	2.05	0.57
2:B:511:ILE:CG2	2:B:718:HIS:CE1	2.83	0.57
2:C:74:MET:HE2	2:C:76:GLN:NE2	2.18	0.57
1:b:184:GLU:HG2	2:B:119:VAL:CG2	2.34	0.57
2:B:201:LYS:HD2	2:B:331:GLU:O	2.05	0.57
2:B:304:LEU:CD1	2:B:306:ARG:HG2	2.35	0.57
2:C:374:ALA:CA	2:C:476:ILE:HD11	2.32	0.57
2:A:233:ILE:HG23	2:B:361:HIS:HE2	0.58	0.57
2:B:103:VAL:HG12	2:B:104:GLY:N	2.19	0.57
2:C:6:PHE:CB	2:C:10:ALA:HB3	2.34	0.57
2:C:268:ILE:HD13	2:C:269:ARG:N	2.20	0.57
2:B:6:PHE:CB	2:B:10:ALA:HB3	2.34	0.57
2:B:198:ARG:O	2:B:199:ARG:CB	2.53	0.57
2:B:358:TYR:O	2:B:360:ALA:N	2.37	0.57
2:C:212:VAL:O	2:C:213:GLY:C	2.47	0.57
2:C:300:LEU:C	2:C:302:PRO:CD	2.77	0.57
2:C:347:SER:O	2:C:350:ILE:HG13	2.05	0.57
2:C:404:LEU:C	2:C:406:SER:N	2.63	0.57
2:C:781:LEU:HD23	2:C:786:ILE:HG13	1.87	0.57
1:a:157:PHE:CD1	1:a:157:PHE:C	2.83	0.56
2:A:201:LYS:HD2	2:A:335:GLN:HG3	1.86	0.56
2:A:259:ASP:O	2:A:261:LEU:HG	2.05	0.56
2:A:364:VAL:HA	2:A:365:SER:O	2.05	0.56
1:b:144:LYS:HB3	2:B:27:ASN:ND2	2.18	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:202:LEU:HD12	1:b:203:ILE:N	2.20	0.56
1:b:217:ALA:HB1	2:B:74:MET:CE	2.35	0.56
2:B:139:LEU:C	2:B:141:LEU:H	2.13	0.56
2:B:344:VAL:O	2:B:347:SER:HB2	2.05	0.56
2:B:525:ARG:HB3	2:C:779:GLU:OE2	2.05	0.56
2:A:781:LEU:HD23	2:A:786:ILE:HG13	1.86	0.56
1:b:126:LYS:C	1:b:127:LEU:HD23	2.30	0.56
2:B:265:MET:CE	2:B:269:ARG:NH2	2.64	0.56
2:B:270:GLN:O	2:B:271:ALA:CB	2.53	0.56
2:B:480:VAL:O	2:B:482:SER:N	2.39	0.56
2:B:781:LEU:HD23	2:B:786:ILE:HG13	1.86	0.56
2:C:301:LYS:N	2:C:302:PRO:CD	2.68	0.56
2:C:424:ARG:HG2	2:C:446:GLU:OE2	2.04	0.56
2:A:139:LEU:C	2:A:141:LEU:H	2.13	0.56
2:A:185:ARG:HG2	2:A:188:GLU:CG	2.36	0.56
1:b:189:SER:C	1:b:191:ILE:H	2.14	0.56
2:B:124:LEU:N	2:B:124:LEU:HD23	2.19	0.56
2:B:364:VAL:HG13	2:B:365:SER:HA	1.86	0.56
2:B:434:GLN:N	2:B:435:GLU:HB3	2.20	0.56
2:C:22:LEU:O	2:C:24:LEU:N	2.39	0.56
2:C:162:THR:C	2:C:164:ASP:N	2.62	0.56
2:C:317:LEU:H	2:C:317:LEU:HD23	1.69	0.56
2:B:227:ASN:O	2:B:227:ASN:OD1	2.24	0.56
2:B:363:ARG:HH11	2:B:476:ILE:CD1	2.09	0.56
2:B:523:ALA:C	2:C:775:ASP:OD1	2.47	0.56
2:B:525:ARG:O	2:C:778:SER:OG	2.24	0.56
2:B:526:ARG:N	2:C:775:ASP:CG	2.56	0.56
2:B:690:MET:CB	2:C:760:TYR:OH	2.52	0.56
1:c:147:VAL:CG2	1:c:150:SER:HB2	2.29	0.56
2:C:364:VAL:HA	2:C:365:SER:O	2.06	0.56
1:b:157:PHE:HD1	1:b:158:GLU:N	2.04	0.56
2:B:352:GLN:HA	2:B:355:ARG:HB2	1.87	0.56
2:B:385:ARG:HB2	2:B:390:LYS:HG2	1.87	0.56
2:C:98:LEU:HB3	2:C:100:HIS:CD2	2.26	0.56
2:C:169:ASP:HA	2:C:240:MET:HE3	1.87	0.56
2:C:355:ARG:HD3	2:C:365:SER:CB	2.35	0.56
2:C:382:ILE:CG1	2:C:484:THR:CG2	2.82	0.56
2:C:411:PRO:C	2:C:413:LEU:N	2.61	0.56
2:A:6:PHE:CB	2:A:10:ALA:CB	2.84	0.56
2:A:766:ARG:HG3	2:A:766:ARG:NH1	2.17	0.56
1:b:184:GLU:OE2	2:B:30:GLY:HA2	2.03	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:ASN:CA	1:c:158:GLU:CD	2.78	0.56
2:B:192:VAL:HG12	2:B:192:VAL:O	2.05	0.56
2:B:511:ILE:HG13	2:B:721:GLU:CG	2.36	0.56
2:C:162:THR:O	2:C:164:ASP:N	2.38	0.56
2:C:231:PRO:C	2:C:233:ILE:N	2.62	0.56
2:B:54:GLY:O	2:B:59:LYS:HD3	2.06	0.56
2:B:169:ASP:O	2:B:173:ILE:CB	2.37	0.56
2:B:511:ILE:HG13	2:B:721:GLU:CD	2.31	0.56
2:C:83:ARG:HD2	2:C:115:GLU:HG2	1.87	0.56
2:A:241:THR:O	2:A:242:LEU:HB2	2.04	0.56
2:B:476:ILE:HG22	2:B:477:ALA:N	2.21	0.56
2:A:203:ASN:OD1	2:A:310:GLN:HG3	2.06	0.56
2:A:405:ARG:HH22	2:A:478:MET:HE1	1.69	0.56
1:b:202:LEU:HD12	1:b:203:ILE:H	1.70	0.56
2:B:169:ASP:H	2:B:173:ILE:HD12	1.68	0.56
2:B:169:ASP:OD1	2:B:238:ARG:HB3	2.06	0.56
2:B:438:LYS:O	2:B:442:LEU:HD12	2.06	0.56
1:c:152:THR:OG1	1:c:208:ALA:HB3	2.06	0.56
1:c:157:PHE:HD1	1:c:158:GLU:H	1.51	0.56
2:C:103:VAL:CG1	2:C:104:GLY:N	2.68	0.56
2:A:201:LYS:CD	2:A:335:GLN:HG3	2.36	0.56
2:A:689:VAL:C	2:A:691:GLY:N	2.63	0.56
2:B:382:ILE:CA	2:B:383:SER:CB	2.84	0.56
2:C:9:ARG:HH11	2:C:9:ARG:HG3	1.70	0.56
2:C:162:THR:C	2:C:164:ASP:H	2.14	0.56
2:C:209:GLU:OE2	2:C:209:GLU:HA	2.06	0.56
2:B:379:ASP:CB	2:B:387:LEU:HD11	2.36	0.55
2:B:689:VAL:C	2:B:691:GLY:N	2.63	0.55
2:C:124:LEU:N	2:C:124:LEU:HD23	2.19	0.55
2:C:138:VAL:O	2:C:142:LEU:HD12	2.06	0.55
2:A:408:THR:C	2:A:414:LYS:HZ3	2.10	0.55
1:b:126:LYS:CE	1:b:129:PHE:HE1	2.17	0.55
2:B:367:THR:HG1	2:B:473:VAL:N	2.04	0.55
2:B:483:TRP:CD1	2:B:483:TRP:N	2.73	0.55
2:B:526:ARG:HH11	2:C:770:GLN:CG	2.18	0.55
2:B:526:ARG:HH11	2:C:770:GLN:HG2	1.71	0.55
2:B:640:THR:HA	2:B:646:THR:HA	1.88	0.55
2:C:212:VAL:O	2:C:212:VAL:HG12	2.07	0.55
2:C:382:ILE:CD1	2:C:484:THR:CG2	2.85	0.55
2:A:229:GLU:O	2:A:230:VAL:HG23	2.06	0.55
1:b:145:LEU:HD12	1:b:145:LEU:N	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:185:TYR:CE1	2:B:28:ASN:CG	2.77	0.55
2:C:374:ALA:H	2:C:476:ILE:HD11	1.65	0.55
2:A:54:GLY:O	2:A:59:LYS:HD3	2.06	0.55
2:B:211:GLY:HA3	2:B:212:VAL:O	2.05	0.55
2:B:269:ARG:HH22	2:B:306:ARG:HB2	1.72	0.55
2:C:74:MET:HB3	2:C:76:GLN:CD	2.32	0.55
2:C:445:THR:HA	2:C:448:ARG:CD	2.37	0.55
2:A:171:THR:OG1	2:A:238:ARG:HA	2.06	0.55
1:b:180:SER:O	2:B:119:VAL:HG22	2.06	0.55
2:B:47:ALA:O	2:B:51:GLN:HG2	2.06	0.55
2:B:176:GLU:C	2:B:178:SER:N	2.61	0.55
1:a:216:PHE:O	2:A:443:ARG:CZ	2.55	0.55
2:A:640:THR:HA	2:A:646:THR:HA	1.88	0.55
1:b:130:VAL:C	1:b:131:LEU:HD23	2.32	0.55
1:b:157:PHE:CD1	1:b:158:GLU:N	2.74	0.55
2:B:197:SER:CB	2:C:361:HIS:CD2	2.89	0.55
2:B:198:ARG:CB	2:C:396:ASP:OD2	2.53	0.55
2:B:402:VAL:HG13	2:B:467:GLU:OE1	2.05	0.55
2:B:511:ILE:HG22	2:B:718:HIS:CE1	2.26	0.55
2:A:363:ARG:NH2	2:A:402:VAL:HG21	2.21	0.55
2:B:35:LEU:HD21	2:B:60:ILE:HD13	1.88	0.55
2:B:499:LEU:CD1	2:C:782:LEU:HD13	2.35	0.55
2:A:98:LEU:HB3	2:A:100:HIS:CD2	2.29	0.55
2:A:185:ARG:O	2:A:189:ILE:HG13	2.07	0.55
2:B:166:LEU:HA	2:B:167:ALA:CB	2.36	0.55
2:B:367:THR:CG2	2:B:472:THR:OG1	2.52	0.55
2:C:165:SER:CB	2:C:166:LEU:CB	2.85	0.55
2:C:184:GLY:CA	2:C:185:ARG:C	2.80	0.55
1:a:193:ILE:HD12	1:a:193:ILE:O	2.07	0.55
2:A:184:GLY:CA	2:A:185:ARG:C	2.80	0.55
2:A:231:PRO:C	2:A:233:ILE:N	2.62	0.55
2:A:449:LEU:O	2:A:452:GLN:HB3	2.07	0.55
2:B:361:HIS:C	2:B:362:HIS:CD2	2.84	0.55
1:c:138:ASP:OD1	2:C:82:PRO:HB3	2.04	0.55
2:C:304:LEU:O	2:C:306:ARG:N	2.38	0.55
2:A:689:VAL:C	2:A:691:GLY:H	2.15	0.55
2:A:806:THR:O	2:A:807:ALA:C	2.50	0.55
2:B:806:THR:O	2:B:807:ALA:C	2.50	0.55
2:C:171:THR:OG1	2:C:238:ARG:HA	2.07	0.55
2:C:426:GLU:O	2:C:430:ALA:HB2	2.07	0.55
2:A:731:THR:HG22	2:A:741:ILE:HG13	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:180:SER:OG	2:B:119:VAL:CB	2.55	0.54
2:B:260:ARG:O	2:B:263:LYS:HB2	2.07	0.54
2:B:268:ILE:C	2:B:270:GLN:N	2.65	0.54
2:C:54:GLY:C	2:C:55:LEU:HD23	2.32	0.54
2:C:124:LEU:C	2:C:126:ASN:H	2.13	0.54
2:C:348:ILE:HA	2:C:351:LEU:HD12	1.89	0.54
2:A:424:ARG:O	2:A:428:ASP:N	2.26	0.54
2:A:445:THR:HA	2:A:448:ARG:CD	2.37	0.54
1:b:157:PHE:CD1	1:b:157:PHE:C	2.85	0.54
2:B:460:TRP:CZ3	2:B:463:LYS:HG2	2.41	0.54
2:B:689:VAL:C	2:B:691:GLY:H	2.15	0.54
2:B:731:THR:HG22	2:B:741:ILE:HG13	1.89	0.54
2:C:179:LEU:HD12	2:C:180:ASP:H	1.72	0.54
2:C:689:VAL:C	2:C:691:GLY:H	2.15	0.54
2:A:207:ILE:HG13	2:A:317:LEU:HA	1.90	0.54
2:A:276:LEU:HD13	2:A:277:PHE:H	1.72	0.54
1:b:203:ILE:HD13	2:B:432:GLN:CG	2.37	0.54
2:B:5:ARG:H	2:B:5:ARG:CZ	2.21	0.54
2:B:106:GLU:OE2	1:c:199:TYR:OH	2.18	0.54
1:c:203:ILE:HD13	2:C:432:GLN:HG3	1.89	0.54
2:C:107:HIS:HA	2:C:110:LEU:HD12	1.89	0.54
2:C:640:THR:HA	2:C:646:THR:HA	1.88	0.54
2:A:168:ARG:HD2	2:A:168:ARG:N	2.22	0.54
2:A:364:VAL:HG22	2:A:365:SER:C	2.33	0.54
1:b:127:LEU:C	1:b:128:GLN:HG3	2.31	0.54
1:b:204:ILE:HD13	1:b:211:THR:HB	1.89	0.54
2:B:304:LEU:HD22	2:B:304:LEU:C	2.28	0.54
2:B:378:SER:HB3	2:B:390:LYS:CE	2.31	0.54
2:B:571:ARG:HH21	2:B:573:ASP:HB2	1.72	0.54
2:A:381:TYR:HD2	2:A:381:TYR:N	2.06	0.54
2:B:382:ILE:HD13	2:B:611:TYR:OH	2.07	0.54
2:B:398:ALA:C	2:B:400:SER:H	2.15	0.54
2:C:129:VAL:O	2:C:129:VAL:CG1	2.56	0.54
2:C:210:PRO:N	2:C:211:GLY:HA3	2.23	0.54
2:C:241:THR:O	2:C:242:LEU:HB2	2.07	0.54
1:a:126:LYS:CE	1:a:129:PHE:HE1	2.15	0.54
2:A:348:ILE:HD13	2:A:372:GLU:HG2	1.89	0.54
1:b:157:PHE:CE1	1:b:158:GLU:HG3	2.42	0.54
2:B:129:VAL:O	2:B:130:SER:C	2.51	0.54
2:B:184:GLY:HA3	2:B:185:ARG:O	2.08	0.54
2:B:624:PRO:HA	2:B:627:PHE:CD2	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:73:GLU:O	2:C:74:MET:C	2.50	0.54
2:C:174:ALA:CB	2:C:222:ALA:HB1	2.38	0.54
2:C:806:THR:O	2:C:807:ALA:C	2.50	0.54
1:c:187:THR:HG23	2:C:83:ARG:HH22	1.73	0.54
1:c:204:ILE:CG2	1:c:208:ALA:HA	2.38	0.54
2:C:185:ARG:O	2:C:189:ILE:HG13	2.07	0.54
2:C:352:GLN:O	2:C:355:ARG:HB3	2.08	0.54
2:C:787:HIS:O	2:C:790:GLN:HG2	2.08	0.54
1:a:179:LEU:HG	1:a:183:LEU:HD11	1.90	0.54
2:A:6:PHE:HB2	2:A:10:ALA:CB	2.38	0.54
2:A:565:ASP:C	2:A:567:GLU:N	2.66	0.54
2:A:624:PRO:HA	2:A:627:PHE:CD2	2.41	0.54
2:B:74:MET:HB3	2:B:76:GLN:CD	2.32	0.54
2:C:572:ILE:HG22	2:C:573:ASP:N	2.23	0.54
2:C:689:VAL:C	2:C:691:GLY:N	2.63	0.54
2:C:758:LEU:HD22	2:C:758:LEU:H	1.73	0.54
2:A:46:ALA:HB2	2:A:105:THR:O	2.08	0.54
2:A:374:ALA:HB2	2:A:476:ILE:CB	2.37	0.54
2:B:30:GLY:HA2	2:B:81:THR:OG1	2.07	0.54
2:B:532:LYS:O	2:C:733:ARG:NH2	2.40	0.54
2:C:119:VAL:O	2:C:123:VAL:HG23	2.07	0.54
1:a:130:VAL:C	1:a:131:LEU:HD23	2.33	0.54
2:A:6:PHE:N	2:A:6:PHE:HD2	2.06	0.54
2:A:184:GLY:HA3	2:A:185:ARG:C	2.33	0.54
2:A:363:ARG:HH12	2:A:475:ASP:CG	2.16	0.54
2:A:398:ALA:H	2:A:479:VAL:HG22	1.73	0.54
2:A:572:ILE:HG22	2:A:573:ASP:N	2.23	0.54
1:b:187:THR:HG22	2:B:83:ARG:HH22	0.46	0.54
2:B:9:ARG:O	2:B:13:VAL:HG12	2.08	0.54
2:B:10:ALA:O	2:B:13:VAL:HG12	2.08	0.54
2:B:305:ALA:C	2:B:307:GLY:N	2.62	0.54
2:B:365:SER:O	2:B:471:VAL:CG2	2.54	0.54
2:B:526:ARG:NE	2:C:775:ASP:CB	2.65	0.54
2:B:787:HIS:O	2:B:790:GLN:HG2	2.08	0.54
2:C:124:LEU:C	2:C:126:ASN:N	2.65	0.54
2:C:421:ASP:O	2:C:423:VAL:N	2.40	0.54
2:C:445:THR:HG22	2:C:448:ARG:CZ	2.38	0.54
2:A:194:GLU:C	2:A:196:LEU:H	2.15	0.53
2:B:73:GLU:O	2:B:74:MET:C	2.51	0.53
2:B:522:LYS:C	2:C:775:ASP:CG	2.57	0.53
1:c:171:THR:HG23	1:c:174:GLU:OE1	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:47:ALA:O	2:C:51:GLN:HG2	2.08	0.53
2:C:381:TYR:HD2	2:C:381:TYR:N	2.06	0.53
2:A:124:LEU:N	2:A:124:LEU:HD23	2.23	0.53
2:A:140:GLN:C	2:A:141:LEU:HD23	2.33	0.53
2:A:171:THR:O	2:A:175:LYS:HG3	2.07	0.53
2:A:341:GLN:HE21	2:A:386:PHE:HA	1.73	0.53
2:A:787:HIS:O	2:A:790:GLN:HG2	2.08	0.53
2:B:103:VAL:HG13	2:B:107:HIS:HB2	1.90	0.53
2:B:571:ARG:HG3	2:B:571:ARG:O	2.08	0.53
2:C:168:ARG:HD2	2:C:168:ARG:N	2.23	0.53
2:C:348:ILE:HD13	2:C:372:GLU:HG2	1.91	0.53
2:C:402:VAL:C	2:C:404:LEU:N	2.66	0.53
2:C:571:ARG:HH21	2:C:573:ASP:HB2	1.72	0.53
2:A:758:LEU:H	2:A:758:LEU:HD22	1.73	0.53
2:B:525:ARG:NE	2:C:779:GLU:OE2	2.21	0.53
2:C:6:PHE:CB	2:C:10:ALA:CB	2.87	0.53
2:C:103:VAL:HG12	2:C:104:GLY:H	1.73	0.53
2:C:308:GLU:CD	2:C:308:GLU:C	2.76	0.53
2:A:174:ALA:CB	2:A:222:ALA:HB1	2.37	0.53
2:A:533:ASP:HB2	2:B:733:ARG:CZ	2.39	0.53
2:A:571:ARG:HH21	2:A:573:ASP:HB2	1.72	0.53
2:B:512:GLY:HA3	2:B:718:HIS:CD2	2.43	0.53
2:C:5:ARG:H	2:C:5:ARG:CZ	2.21	0.53
2:A:235:ARG:CZ	2:A:235:ARG:HB3	2.38	0.53
2:B:231:PRO:CG	2:B:232:GLU:HG2	2.16	0.53
2:B:526:ARG:N	2:C:775:ASP:CB	2.71	0.53
2:C:103:VAL:HG13	2:C:107:HIS:HB2	1.91	0.53
2:C:307:GLY:C	2:C:309:LEU:H	2.14	0.53
2:C:377:LEU:O	2:C:381:TYR:HB2	2.07	0.53
2:C:415:GLU:O	2:C:418:GLN:HB2	2.08	0.53
2:A:74:MET:HB3	2:A:76:GLN:CD	2.33	0.53
2:A:381:TYR:CD2	2:A:381:TYR:N	2.77	0.53
2:B:572:ILE:HG22	2:B:573:ASP:N	2.23	0.53
2:A:445:THR:HG22	2:A:448:ARG:CZ	2.38	0.53
1:b:203:ILE:CG2	2:B:432:GLN:HA	2.35	0.53
2:B:203:ASN:HD22	2:B:311:CYS:H	1.55	0.53
2:C:72:GLN:C	2:C:74:MET:N	2.67	0.53
2:C:110:LEU:HD21	2:C:138:VAL:HG11	1.90	0.53
2:C:235:ARG:HB3	2:C:235:ARG:CZ	2.38	0.53
2:C:365:SER:C	2:C:366:ILE:CG1	2.82	0.53
2:C:394:LEU:CD1	2:C:479:VAL:HB	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:731:THR:HG22	2:C:741:ILE:HG13	1.89	0.53
1:a:126:LYS:C	1:a:127:LEU:HD23	2.34	0.53
2:B:229:GLU:O	2:B:230:VAL:CG2	2.56	0.53
2:B:278:ILE:O	2:B:314:ALA:HB2	2.08	0.53
2:B:301:LYS:N	2:B:302:PRO:HD2	2.23	0.53
2:A:571:ARG:HG3	2:A:571:ARG:O	2.08	0.53
1:b:141:SER:HB3	2:B:28:ASN:OD1	2.08	0.53
2:B:140:GLN:C	2:B:141:LEU:HD23	2.33	0.53
2:B:194:GLU:CB	2:C:400:SER:OG	2.57	0.53
2:C:382:ILE:CG1	2:C:484:THR:HG21	2.39	0.53
2:C:421:ASP:O	2:C:422:GLU:C	2.51	0.53
2:C:624:PRO:HA	2:C:627:PHE:CD2	2.41	0.53
2:C:635:GLU:HG2	2:C:704:ARG:HD3	1.90	0.53
1:a:184:GLU:OE2	2:A:118:GLY:HA2	2.05	0.53
2:B:635:GLU:HG2	2:B:704:ARG:HD3	1.90	0.53
2:B:758:LEU:HD22	2:B:758:LEU:H	1.73	0.53
2:C:259:ASP:O	2:C:261:LEU:HG	2.08	0.53
2:C:700:GLU:O	2:C:704:ARG:NH1	2.42	0.53
2:A:396:ASP:O	2:A:397:GLU:C	2.51	0.52
1:b:161:TYR:CZ	2:B:432:GLN:OE1	2.62	0.52
1:b:187:THR:HG21	2:B:83:ARG:HH22	1.50	0.52
2:B:266:ASP:C	2:B:268:ILE:H	2.16	0.52
2:C:363:ARG:NH2	2:C:402:VAL:HG21	2.23	0.52
2:A:13:VAL:CG2	2:A:38:LEU:HD23	2.18	0.52
2:A:63:GLU:O	2:A:67:LEU:HG	2.09	0.52
2:A:73:GLU:O	2:A:74:MET:C	2.52	0.52
2:A:395:ILE:O	2:A:399:GLY:N	2.42	0.52
2:A:635:GLU:HG2	2:A:704:ARG:HD3	1.90	0.52
2:B:6:PHE:CB	2:B:10:ALA:CB	2.88	0.52
2:B:145:ASN:CA	1:c:158:GLU:OE1	2.56	0.52
2:B:171:THR:CB	2:B:238:ARG:HA	2.38	0.52
2:B:572:ILE:N	2:B:572:ILE:HD12	2.24	0.52
2:B:752:ALA:C	2:B:754:GLU:H	2.18	0.52
2:C:381:TYR:CD2	2:C:381:TYR:N	2.77	0.52
1:a:204:ILE:HD13	1:a:211:THR:HB	1.89	0.52
2:A:90:LEU:CD1	2:A:115:GLU:HB2	2.39	0.52
2:A:317:LEU:HD23	2:A:317:LEU:H	1.74	0.52
1:b:177:ASN:ND2	2:B:67:LEU:HD21	2.04	0.52
2:B:565:ASP:C	2:B:567:GLU:N	2.66	0.52
2:C:430:ALA:HB1	2:C:435:GLU:HG2	1.91	0.52
2:A:138:VAL:O	2:A:142:LEU:HD12	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:303:SER:O	2:A:306:ARG:HB2	2.09	0.52
2:A:367:THR:H	2:A:471:VAL:C	2.18	0.52
2:A:370:ALA:HB2	2:A:471:VAL:O	2.08	0.52
2:A:475:ASP:O	2:A:478:MET:HB2	2.09	0.52
2:A:572:ILE:N	2:A:572:ILE:HD12	2.24	0.52
1:b:170:MET:HB2	1:b:175:VAL:HG23	1.92	0.52
2:B:305:ALA:HA	2:B:309:LEU:CD1	2.39	0.52
2:B:341:GLN:HB3	2:B:387:LEU:H	1.75	0.52
2:B:700:GLU:O	2:B:704:ARG:NH1	2.42	0.52
1:c:127:LEU:C	1:c:128:GLN:HG3	2.34	0.52
2:C:230:VAL:HG13	2:C:231:PRO:CD	2.36	0.52
2:A:29:ILE:HG13	2:A:80:TYR:CD1	2.44	0.52
2:A:103:VAL:CG1	2:A:104:GLY:N	2.73	0.52
1:b:126:LYS:O	1:b:127:LEU:HD23	2.09	0.52
2:B:221:LEU:O	2:B:222:ALA:C	2.52	0.52
2:C:378:SER:HB3	2:C:390:LYS:HD3	1.92	0.52
2:C:572:ILE:HD12	2:C:572:ILE:N	2.24	0.52
2:A:412:ASN:C	2:A:414:LYS:H	2.17	0.52
1:b:144:LYS:NZ	2:B:443:ARG:HH22	2.07	0.52
2:B:180:ASP:CB	2:B:181:PRO:CD	2.76	0.52
2:B:268:ILE:CG2	2:B:269:ARG:N	2.73	0.52
2:B:532:LYS:C	2:C:733:ARG:HH22	2.09	0.52
2:C:387:LEU:N	2:C:388:PRO:CD	2.72	0.52
2:A:344:VAL:O	2:A:347:SER:HB2	2.10	0.52
2:A:359:GLU:HG2	2:A:364:VAL:HG13	1.90	0.52
2:B:446:GLU:HG3	2:B:447:GLN:N	2.24	0.52
2:C:54:GLY:O	2:C:59:LYS:HD3	2.10	0.52
2:C:303:SER:O	2:C:306:ARG:HB2	2.10	0.52
2:C:571:ARG:HG3	2:C:571:ARG:O	2.08	0.52
2:A:502:MET:HE1	2:A:524:VAL:HG11	1.92	0.52
2:B:185:ARG:HB3	2:B:188:GLU:HB2	1.92	0.52
2:B:418:GLN:HG3	2:B:419:LYS:N	2.23	0.52
1:c:155:TYR:HE1	1:c:202:LEU:HD22	1.75	0.52
2:C:752:ALA:C	2:C:754:GLU:H	2.18	0.52
2:B:29:ILE:HG13	2:B:80:TYR:CD1	2.45	0.52
2:B:184:GLY:CA	2:B:185:ARG:C	2.81	0.52
2:C:171:THR:O	2:C:175:LYS:HG3	2.10	0.52
2:C:425:LYS:O	2:C:426:GLU:C	2.53	0.52
2:A:574:MET:HE3	2:A:616:LEU:HB3	1.92	0.52
2:A:686:LYS:HZ3	2:A:690:MET:HE1	1.75	0.52
2:A:700:GLU:O	2:A:704:ARG:NH1	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:413:LEU:HD11	2:B:456:THR:HG21	1.92	0.52
2:C:364:VAL:HG22	2:C:365:SER:C	2.35	0.52
2:C:442:LEU:O	2:C:445:THR:OG1	2.22	0.52
2:A:398:ALA:HB2	2:A:479:VAL:CG2	2.40	0.51
2:A:531:LEU:HD21	2:B:781:LEU:CD1	2.40	0.51
2:B:416:LEU:HD23	2:B:416:LEU:O	2.10	0.51
2:B:459:SER:O	2:B:462:GLU:HB2	2.10	0.51
2:C:482:SER:O	2:C:483:TRP:HD1	1.93	0.51
1:b:154:LEU:HD12	1:b:155:TYR:N	2.25	0.51
2:C:90:LEU:CD1	2:C:115:GLU:HB2	2.40	0.51
2:C:574:MET:HE3	2:C:616:LEU:HB3	1.92	0.51
2:A:330:LEU:C	2:A:332:ARG:N	2.66	0.51
2:B:225:ILE:CD1	2:B:237:LYS:O	2.57	0.51
2:B:304:LEU:HD12	2:B:306:ARG:HG2	1.93	0.51
2:A:276:LEU:O	2:A:312:ILE:N	2.38	0.51
2:A:439:ALA:CA	2:A:442:LEU:HB2	2.29	0.51
1:b:161:TYR:OH	2:B:432:GLN:OE1	2.16	0.51
2:B:268:ILE:HD11	2:B:274:ILE:CG2	2.40	0.51
2:C:183:ILE:CG2	2:C:184:GLY:N	2.71	0.51
2:C:359:GLU:HG2	2:C:364:VAL:HG13	1.92	0.51
2:C:402:VAL:C	2:C:404:LEU:H	2.18	0.51
2:C:414:LYS:O	2:C:418:GLN:HG3	2.10	0.51
2:C:580:LYS:HG2	2:C:580:LYS:O	2.11	0.51
2:A:363:ARG:NH1	2:A:475:ASP:HB3	2.18	0.51
2:B:356:ASP:HA	2:B:359:GLU:HG3	1.93	0.51
2:B:370:ALA:HB1	2:B:476:ILE:HG12	1.92	0.51
2:B:466:GLN:O	2:B:467:GLU:CG	2.58	0.51
2:B:513:GLN:OE1	2:B:513:GLN:N	2.44	0.51
2:C:382:ILE:CA	2:C:383:SER:CB	2.79	0.51
1:a:216:PHE:HD1	2:A:443:ARG:HD3	1.76	0.51
2:A:320:TYR:O	2:A:321:ARG:C	2.54	0.51
2:A:381:TYR:HA	2:A:611:TYR:OH	2.11	0.51
2:A:472:THR:O	2:A:474:ASP:N	2.43	0.51
2:B:48:LYS:HZ3	1:c:194:HIS:HB3	1.75	0.51
2:B:54:GLY:C	2:B:55:LEU:HD23	2.36	0.51
2:B:124:LEU:C	2:B:126:ASN:H	2.17	0.51
2:B:201:LYS:NZ	2:B:335:GLN:CG	2.72	0.51
2:B:203:ASN:ND2	2:B:310:GLN:HA	2.24	0.51
2:B:262:LYS:HZ3	2:C:260:ARG:NH2	2.08	0.51
2:B:649:PHE:O	2:B:651:ASN:N	2.44	0.51
2:C:13:VAL:HG21	2:C:38:LEU:HA	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:185:ARG:HG2	2:C:188:GLU:CG	2.39	0.51
2:A:307:GLY:C	2:A:309:LEU:H	2.17	0.51
2:A:365:SER:C	2:A:366:ILE:CG1	2.84	0.51
1:b:158:GLU:O	1:b:160:ARG:HG2	2.11	0.51
1:b:187:THR:HG23	2:B:83:ARG:CZ	2.39	0.51
2:B:22:LEU:O	2:B:24:LEU:N	2.44	0.51
2:B:124:LEU:C	2:B:126:ASN:N	2.68	0.51
2:B:336:PRO:O	2:B:337:ILE:HG23	2.11	0.51
2:B:482:SER:OG	2:B:483:TRP:CD1	2.64	0.51
2:C:205:VAL:O	2:C:336:PRO:HA	2.11	0.51
2:A:460:TRP:CZ3	2:A:463:LYS:HG2	2.46	0.51
1:b:145:LEU:HD12	2:B:27:ASN:HD21	1.75	0.51
2:B:72:GLN:C	2:B:74:MET:N	2.69	0.51
2:B:228:ASN:HD21	2:B:235:ARG:HE	1.59	0.51
2:B:304:LEU:HD22	2:B:305:ALA:CA	2.36	0.51
2:B:386:PHE:C	2:B:388:PRO:HD2	2.36	0.51
2:B:439:ALA:C	2:B:442:LEU:H	2.18	0.51
2:B:574:MET:HE3	2:B:616:LEU:HB3	1.92	0.51
1:c:193:ILE:HD12	1:c:193:ILE:O	2.11	0.51
2:C:380:ARG:HG3	2:C:381:TYR:HD2	1.76	0.51
2:A:30:GLY:HA2	2:A:81:THR:OG1	2.10	0.51
2:A:649:PHE:O	2:A:651:ASN:N	2.44	0.51
2:B:763:ARG:N	2:B:764:PRO:CD	2.74	0.51
1:c:126:LYS:O	1:c:127:LEU:HD23	2.10	0.51
2:C:330:LEU:O	2:C:332:ARG:N	2.44	0.51
2:C:412:ASN:C	2:C:414:LYS:H	2.18	0.51
2:A:209:GLU:HA	2:A:209:GLU:OE2	2.10	0.51
2:A:268:ILE:HD13	2:A:268:ILE:C	2.35	0.51
2:A:387:LEU:N	2:A:388:PRO:CD	2.74	0.51
2:B:46:ALA:HB2	2:B:105:THR:C	2.36	0.51
2:B:232:GLU:O	2:B:233:ILE:O	2.29	0.51
2:B:305:ALA:CA	2:B:309:LEU:HD11	2.40	0.51
2:B:480:VAL:O	2:B:481:SER:C	2.54	0.51
2:B:509:ARG:HD3	2:B:557:ALA:CB	2.41	0.51
2:C:365:SER:C	2:C:366:ILE:HG13	2.36	0.51
2:C:556:ARG:CG	2:C:569:MET:HE1	2.30	0.51
2:C:649:PHE:O	2:C:651:ASN:N	2.44	0.51
1:a:144:LYS:HD3	2:A:27:ASN:ND2	2.27	0.50
2:A:13:VAL:HG21	2:A:38:LEU:HA	1.92	0.50
2:A:142:LEU:HA	1:b:195:ARG:HD2	1.92	0.50
2:A:404:LEU:O	2:A:407:PHE:N	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:421:ASP:O	2:A:423:VAL:N	2.44	0.50
1:b:171:THR:HG23	1:b:174:GLU:OE1	2.11	0.50
2:A:305:ALA:C	2:A:309:LEU:HD11	2.36	0.50
2:A:346:GLU:O	2:A:350:ILE:HG13	2.11	0.50
2:A:404:LEU:C	2:A:406:SER:N	2.69	0.50
2:A:411:PRO:O	2:A:413:LEU:N	2.45	0.50
2:A:509:ARG:HD3	2:A:557:ALA:CB	2.41	0.50
2:A:513:GLN:OE1	2:A:513:GLN:N	2.44	0.50
2:A:763:ARG:N	2:A:764:PRO:CD	2.74	0.50
2:B:106:GLU:CD	2:B:106:GLU:H	2.19	0.50
2:B:270:GLN:O	2:B:271:ALA:HB2	2.12	0.50
2:B:305:ALA:CB	2:B:309:LEU:HD11	2.40	0.50
2:B:526:ARG:CZ	2:C:775:ASP:OD2	2.59	0.50
2:B:690:MET:HB3	2:C:760:TYR:CZ	2.46	0.50
1:c:140:ILE:O	1:c:143:SER:OG	2.16	0.50
2:C:167:ALA:HB1	2:C:241:THR:O	2.12	0.50
2:C:194:GLU:C	2:C:196:LEU:H	2.19	0.50
2:C:207:ILE:HG13	2:C:317:LEU:HA	1.93	0.50
2:C:470:GLU:O	2:C:471:VAL:HG23	2.11	0.50
2:A:169:ASP:HA	2:A:240:MET:HE3	1.93	0.50
2:A:179:LEU:HD12	2:A:180:ASP:N	2.27	0.50
2:A:210:PRO:N	2:A:211:GLY:HA3	2.26	0.50
2:A:370:ALA:HB3	2:A:471:VAL:O	2.07	0.50
2:A:421:ASP:O	2:A:422:GLU:C	2.54	0.50
2:A:428:ASP:O	2:A:431:VAL:N	2.44	0.50
2:A:580:LYS:HG2	2:A:580:LYS:O	2.10	0.50
2:B:90:LEU:CD1	2:B:115:GLU:HB2	2.42	0.50
2:B:169:ASP:OD2	2:B:172:ALA:HB3	2.11	0.50
2:B:341:GLN:HB3	2:B:387:LEU:HB2	1.93	0.50
2:B:502:MET:HE1	2:B:524:VAL:HG11	1.92	0.50
2:B:511:ILE:CG2	2:B:718:HIS:HA	2.33	0.50
2:B:689:VAL:O	2:B:691:GLY:N	2.44	0.50
1:c:202:LEU:HD12	1:c:203:ILE:N	2.27	0.50
2:C:67:LEU:C	2:C:68:ILE:HG13	2.35	0.50
2:C:428:ASP:O	2:C:431:VAL:N	2.45	0.50
2:C:513:GLN:OE1	2:C:513:GLN:N	2.44	0.50
2:A:414:LYS:O	2:A:418:GLN:HG3	2.10	0.50
2:A:752:ALA:C	2:A:754:GLU:H	2.18	0.50
2:B:98:LEU:HB3	2:B:100:HIS:CD2	2.30	0.50
2:B:192:VAL:O	2:B:192:VAL:CG1	2.58	0.50
2:B:212:VAL:HA	2:B:213:GLY:C	2.35	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:GLU:OE1	2:B:309:LEU:N	2.44	0.50
2:B:378:SER:O	2:B:390:LYS:NZ	2.39	0.50
2:B:402:VAL:HG21	2:B:475:ASP:HB3	1.93	0.50
2:B:694:LYS:HD2	2:C:760:TYR:CG	2.30	0.50
2:C:305:ALA:C	2:C:309:LEU:HD11	2.37	0.50
2:C:574:MET:CE	2:C:616:LEU:HB3	2.42	0.50
2:A:556:ARG:CG	2:A:569:MET:HE1	2.30	0.50
2:A:689:VAL:O	2:A:691:GLY:N	2.45	0.50
2:B:214:LYS:HZ1	2:B:315:THR:H	1.59	0.50
2:B:396:ASP:C	2:B:399:GLY:H	2.18	0.50
2:B:472:THR:HG22	2:B:473:VAL:H	1.76	0.50
2:C:9:ARG:HG3	2:C:9:ARG:NH1	2.25	0.50
2:C:184:GLY:HA3	2:C:185:ARG:C	2.36	0.50
1:a:127:LEU:C	1:a:128:GLN:HG3	2.37	0.50
1:a:154:LEU:HD12	1:a:155:TYR:N	2.26	0.50
2:A:226:ILE:HG22	2:A:227:ASN:N	2.26	0.50
2:B:201:LYS:CB	2:B:335:GLN:HG3	2.41	0.50
2:B:580:LYS:O	2:B:580:LYS:HG2	2.11	0.50
1:c:142:LEU:HD11	1:c:182:LEU:HD22	1.94	0.50
2:C:72:GLN:O	2:C:74:MET:N	2.45	0.50
2:C:425:LYS:O	2:C:429:ALA:N	2.45	0.50
2:C:475:ASP:O	2:C:478:MET:HB2	2.12	0.50
2:C:686:LYS:HZ3	2:C:690:MET:HE1	1.76	0.50
2:C:689:VAL:O	2:C:691:GLY:N	2.44	0.50
2:A:205:VAL:O	2:A:336:PRO:HA	2.11	0.50
2:B:211:GLY:HA3	2:B:212:VAL:C	2.36	0.50
2:B:240:MET:HB2	2:B:276:LEU:HD21	1.94	0.50
2:B:577:TYR:HE1	2:B:584:SER:HG	1.59	0.50
2:B:769:ILE:O	2:B:773:VAL:HB	2.12	0.50
2:C:29:ILE:HG13	2:C:80:TYR:CD1	2.47	0.50
2:A:347:SER:O	2:A:350:ILE:HG13	2.10	0.50
2:A:572:ILE:CG2	2:A:573:ASP:N	2.75	0.50
1:b:179:LEU:HG	1:b:183:LEU:HD11	1.94	0.50
2:C:169:ASP:CA	2:C:240:MET:HE3	2.41	0.50
2:C:175:LYS:C	2:C:177:ASP:H	2.20	0.50
2:C:269:ARG:HA	2:C:308:GLU:OE1	2.11	0.50
2:C:509:ARG:HD3	2:C:557:ALA:CB	2.41	0.50
2:A:415:GLU:O	2:A:418:GLN:HB2	2.11	0.50
2:A:649:PHE:C	2:A:651:ASN:H	2.20	0.50
1:c:147:VAL:HG22	1:c:148:ASN:N	2.26	0.50
2:C:377:LEU:HD13	2:C:476:ILE:CG2	2.19	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:502:MET:HE1	2:C:524:VAL:HG11	1.92	0.50
2:C:649:PHE:C	2:C:651:ASN:H	2.20	0.50
2:A:90:LEU:HD11	2:A:115:GLU:HB2	1.94	0.49
2:A:269:ARG:HA	2:A:308:GLU:OE1	2.11	0.49
2:A:351:LEU:HD11	2:A:375:VAL:CG2	2.42	0.49
2:A:364:VAL:HG23	2:A:366:ILE:O	2.12	0.49
2:A:366:ILE:HG22	2:A:367:THR:CA	2.30	0.49
2:A:574:MET:CE	2:A:616:LEU:HB3	2.41	0.49
2:B:48:LYS:HD3	1:c:194:HIS:CD2	2.47	0.49
2:B:574:MET:CE	2:B:616:LEU:HB3	2.41	0.49
2:B:619:ILE:HG21	2:B:656:MET:CE	2.42	0.49
1:a:212:ILE:HG23	1:a:216:PHE:HD2	1.77	0.49
2:A:619:ILE:HG21	2:A:656:MET:CE	2.42	0.49
1:b:181:ILE:HG12	2:B:68:ILE:HG12	1.94	0.49
2:B:22:LEU:O	2:B:25:GLY:N	2.44	0.49
2:B:70:ARG:HB3	2:B:71:GLY:HA3	1.94	0.49
2:B:176:GLU:O	2:B:177:ASP:HB3	2.12	0.49
2:B:382:ILE:HD13	2:B:611:TYR:CE2	2.46	0.49
2:B:454:GLU:O	2:B:457:LYS:N	2.39	0.49
2:C:6:PHE:HB2	2:C:10:ALA:CB	2.42	0.49
2:C:364:VAL:HG22	2:C:365:SER:HA	1.93	0.49
2:C:472:THR:O	2:C:474:ASP:N	2.45	0.49
2:C:769:ILE:O	2:C:773:VAL:HB	2.12	0.49
2:A:29:ILE:HG13	2:A:80:TYR:HD1	1.78	0.49
2:A:265:MET:HA	2:A:268:ILE:CG2	2.42	0.49
2:A:425:LYS:O	2:A:426:GLU:C	2.54	0.49
1:b:144:LYS:NZ	2:B:76:GLN:HG3	2.28	0.49
1:b:187:THR:HG21	2:B:83:ARG:HH12	1.76	0.49
2:B:436:PHE:O	2:B:437:GLU:C	2.53	0.49
2:B:439:ALA:O	2:B:440:ALA:C	2.55	0.49
2:B:500:LEU:HD13	2:C:783:ARG:CB	2.42	0.49
2:B:572:ILE:CG2	2:B:573:ASP:N	2.75	0.49
1:c:126:LYS:CE	1:c:129:PHE:HE1	2.20	0.49
2:C:268:ILE:C	2:C:270:GLN:N	2.69	0.49
2:B:265:MET:O	2:B:268:ILE:HG22	2.13	0.49
2:B:355:ARG:HB3	2:B:355:ARG:NH1	2.22	0.49
2:B:473:VAL:O	2:B:474:ASP:C	2.56	0.49
1:c:133:PHE:CD1	1:c:139:VAL:HG22	2.47	0.49
2:C:27:ASN:OD1	2:C:27:ASN:N	2.43	0.49
2:C:35:LEU:HD21	2:C:60:ILE:CD1	2.41	0.49
2:C:300:LEU:CB	2:C:323:TYR:CE2	2.96	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:314:ALA:O	2:C:315:THR:HG23	2.13	0.49
2:C:330:LEU:C	2:C:332:ARG:N	2.70	0.49
2:C:394:LEU:CD1	2:C:479:VAL:CB	2.90	0.49
2:A:140:GLN:O	2:A:140:GLN:HG3	2.11	0.49
2:A:769:ILE:O	2:A:773:VAL:HB	2.12	0.49
2:B:129:VAL:C	2:B:130:SER:O	2.55	0.49
2:B:363:ARG:HH12	2:B:475:ASP:C	2.15	0.49
2:C:763:ARG:N	2:C:764:PRO:CD	2.74	0.49
2:A:373:ALA:H	2:A:473:VAL:HG13	1.76	0.49
2:B:343:SER:HB2	2:B:346:GLU:CG	2.42	0.49
1:c:148:ASN:O	1:c:150:SER:OG	2.29	0.49
2:C:366:ILE:HG22	2:C:368:ASP:H	1.77	0.49
1:a:143:SER:C	1:a:145:LEU:H	2.21	0.49
2:A:72:GLN:C	2:A:74:MET:N	2.69	0.49
2:A:124:LEU:C	2:A:126:ASN:N	2.68	0.49
2:B:9:ARG:HH11	2:B:9:ARG:HG3	1.78	0.49
2:B:382:ILE:CD1	2:B:611:TYR:HE2	2.25	0.49
2:C:122:ARG:HG3	2:C:126:ASN:HD22	1.78	0.49
2:C:373:ALA:O	2:C:374:ALA:C	2.55	0.49
1:a:202:LEU:HD12	1:a:203:ILE:N	2.28	0.49
2:A:49:ALA:O	2:A:52:ALA:HB3	2.13	0.49
2:A:194:GLU:O	2:A:198:ARG:HG3	2.13	0.49
2:B:351:LEU:CD2	2:B:392:ILE:HD13	2.42	0.49
2:B:373:ALA:O	2:B:374:ALA:C	2.55	0.49
2:C:140:GLN:C	2:C:141:LEU:HD23	2.36	0.49
2:C:355:ARG:HH21	2:C:366:ILE:HA	1.78	0.49
2:A:103:VAL:HG13	2:A:107:HIS:HB2	1.94	0.49
2:A:365:SER:C	2:A:366:ILE:HG13	2.37	0.49
2:A:434:GLN:HA	2:A:435:GLU:C	2.37	0.49
1:b:145:LEU:CD1	2:B:27:ASN:OD1	2.61	0.49
2:B:279:ASP:O	2:B:280:ALA:HB2	2.13	0.49
2:B:411:PRO:C	2:B:413:LEU:N	2.62	0.49
1:c:189:SER:C	1:c:191:ILE:H	2.20	0.49
2:C:259:ASP:C	2:C:261:LEU:H	2.21	0.49
1:b:127:LEU:O	1:b:128:GLN:HG3	2.13	0.49
2:B:93:ASP:C	2:B:95:ALA:H	2.21	0.49
2:B:439:ALA:C	2:B:441:SER:N	2.69	0.49
2:C:6:PHE:N	2:C:6:PHE:HD2	2.09	0.49
2:C:38:LEU:HD11	2:C:108:ILE:HG22	1.94	0.49
2:C:265:MET:HA	2:C:268:ILE:CG2	2.43	0.49
2:C:424:ARG:O	2:C:425:LYS:C	2.56	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:443:ARG:O	2:C:446:GLU:N	2.45	0.49
1:a:141:SER:OG	2:A:28:ASN:OD1	2.30	0.48
2:A:5:ARG:H	2:A:5:ARG:CZ	2.26	0.48
2:A:9:ARG:HG3	2:A:9:ARG:HH11	1.77	0.48
2:A:212:VAL:O	2:A:212:VAL:HG12	2.12	0.48
2:C:72:GLN:CB	2:C:74:MET:HG3	2.43	0.48
2:C:276:LEU:O	2:C:312:ILE:N	2.43	0.48
2:C:386:PHE:C	2:C:388:PRO:HD2	2.38	0.48
2:C:411:PRO:O	2:C:413:LEU:N	2.46	0.48
2:A:366:ILE:HG22	2:A:368:ASP:H	1.78	0.48
2:C:44:GLY:HA3	2:C:105:THR:HG21	1.95	0.48
2:C:206:LEU:N	2:C:313:GLY:O	2.42	0.48
2:C:229:GLU:O	2:C:230:VAL:HG23	2.13	0.48
2:C:619:ILE:HG21	2:C:656:MET:CE	2.42	0.48
2:A:175:LYS:C	2:A:177:ASP:H	2.20	0.48
2:A:194:GLU:OE2	2:B:401:LYS:HE3	2.13	0.48
2:B:650:ARG:HG3	2:B:650:ARG:HH11	1.78	0.48
2:C:421:ASP:C	2:C:423:VAL:N	2.67	0.48
1:a:164:TYR:C	1:a:164:TYR:CD1	2.91	0.48
2:B:158:ALA:HB1	2:B:267:GLU:O	2.13	0.48
2:B:436:PHE:O	2:B:439:ALA:HB3	2.13	0.48
2:B:496:THR:HG21	2:C:782:LEU:HD22	1.93	0.48
2:B:649:PHE:C	2:B:651:ASN:H	2.20	0.48
1:c:155:TYR:CE1	1:c:202:LEU:HD22	2.48	0.48
1:c:216:PHE:O	2:C:443:ARG:NE	2.46	0.48
2:C:243:ASP:O	2:C:244:MET:CB	2.60	0.48
2:C:574:MET:HE3	2:C:616:LEU:HD13	1.95	0.48
2:A:129:VAL:O	2:A:129:VAL:CG1	2.60	0.48
2:A:165:SER:CA	2:A:166:LEU:O	2.61	0.48
2:B:90:LEU:HD11	2:B:115:GLU:HB2	1.94	0.48
2:B:416:LEU:HD21	2:B:449:LEU:HB3	1.96	0.48
2:C:22:LEU:C	2:C:24:LEU:N	2.70	0.48
2:C:35:LEU:CD2	2:C:60:ILE:HD13	2.41	0.48
2:C:129:VAL:O	2:C:130:SER:O	2.30	0.48
2:C:265:MET:HA	2:C:268:ILE:HG22	1.94	0.48
1:a:142:LEU:HD11	1:a:182:LEU:HD22	1.95	0.48
1:b:215:HIS:CB	2:B:436:PHE:CA	2.92	0.48
2:B:185:ARG:CB	2:B:188:GLU:HB2	2.43	0.48
2:B:577:TYR:CD2	2:B:577:TYR:N	2.82	0.48
2:C:9:ARG:O	2:C:13:VAL:HG12	2.13	0.48
2:A:348:ILE:CD1	2:A:372:GLU:HG2	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:VAL:HG21	2:B:38:LEU:CD2	2.16	0.48
2:B:156:SER:O	2:B:157:ASN:O	2.31	0.48
2:A:199:ARG:NE	2:B:358:TYR:HH	2.00	0.48
2:A:265:MET:HA	2:A:268:ILE:HG22	1.94	0.48
2:A:359:GLU:HA	2:A:364:VAL:HG12	1.95	0.48
2:A:577:TYR:N	2:A:577:TYR:CD2	2.82	0.48
2:A:647:VAL:HG12	2:A:648:ASP:N	2.29	0.48
1:b:204:ILE:CG2	1:b:208:ALA:HA	2.43	0.48
2:B:29:ILE:HG13	2:B:80:TYR:HD1	1.79	0.48
2:B:194:GLU:CD	2:C:401:LYS:HB2	2.38	0.48
2:B:305:ALA:HA	2:B:309:LEU:HD11	1.95	0.48
2:C:13:VAL:CG2	2:C:37:GLY:C	2.82	0.48
2:C:650:ARG:HH11	2:C:650:ARG:HG3	1.78	0.48
1:b:187:THR:HG23	2:B:83:ARG:HH12	1.72	0.48
2:B:351:LEU:CB	2:B:371:ILE:HD13	2.44	0.48
2:B:415:GLU:O	2:B:418:GLN:HG3	2.14	0.48
1:c:212:ILE:CG2	1:c:216:PHE:HD2	2.26	0.48
2:C:70:ARG:HB3	2:C:71:GLY:HA3	1.96	0.48
2:C:385:ARG:HB2	2:C:390:LYS:CG	2.44	0.48
2:C:385:ARG:HB2	2:C:390:LYS:HG3	1.95	0.48
2:C:577:TYR:CD2	2:C:577:TYR:N	2.82	0.48
2:A:83:ARG:O	2:A:86:LYS:HB3	2.14	0.48
2:A:196:LEU:HD12	2:A:310:GLN:NE2	2.29	0.48
2:A:261:LEU:C	2:A:263:LYS:H	2.22	0.48
2:B:556:ARG:CG	2:B:569:MET:HE1	2.30	0.48
2:B:647:VAL:HG12	2:B:648:ASP:N	2.29	0.48
1:c:127:LEU:O	1:c:128:GLN:HG3	2.14	0.48
1:c:212:ILE:HG23	1:c:216:PHE:HD2	1.79	0.48
2:C:28:ASN:HD22	2:C:28:ASN:N	2.12	0.48
2:C:122:ARG:HG3	2:C:126:ASN:ND2	2.29	0.48
2:C:196:LEU:HD13	2:C:204:PRO:HD3	1.95	0.48
2:C:242:LEU:HD12	2:C:243:ASP:O	2.14	0.48
2:C:268:ILE:HD13	2:C:268:ILE:C	2.39	0.48
2:C:268:ILE:HD11	2:C:308:GLU:OE2	2.14	0.48
2:C:412:ASN:C	2:C:414:LYS:N	2.72	0.48
2:C:572:ILE:CG2	2:C:573:ASP:N	2.75	0.48
2:A:6:PHE:HB3	2:A:10:ALA:CB	2.43	0.47
2:A:16:LEU:HD13	2:A:41:GLU:HB2	1.96	0.47
2:A:179:LEU:HB3	2:A:223:GLN:NE2	2.29	0.47
2:A:201:LYS:HE2	2:B:385:ARG:HH12	1.79	0.47
2:A:239:VAL:O	2:A:240:MET:HG2	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:LYS:HZ3	2:B:314:ALA:CA	2.26	0.47
2:B:278:ILE:O	2:B:314:ALA:CB	2.62	0.47
1:c:202:LEU:HD12	1:c:203:ILE:H	1.79	0.47
2:C:98:LEU:C	2:C:100:HIS:H	2.22	0.47
2:A:54:GLY:C	2:A:55:LEU:HD23	2.39	0.47
2:A:355:ARG:HH21	2:A:366:ILE:HA	1.78	0.47
2:A:364:VAL:HG22	2:A:365:SER:HA	1.95	0.47
2:A:367:THR:N	2:A:471:VAL:CA	2.76	0.47
1:b:164:TYR:CD1	1:b:164:TYR:C	2.89	0.47
2:B:618:ALA:HA	2:B:620:GLU:OE2	2.14	0.47
2:A:44:GLY:HA3	2:A:105:THR:HG21	1.95	0.47
2:A:184:GLY:HA2	2:A:185:ARG:HB2	1.95	0.47
2:A:211:GLY:C	2:A:213:GLY:H	2.22	0.47
2:A:230:VAL:HG13	2:A:231:PRO:CD	2.44	0.47
2:A:259:ASP:C	2:A:261:LEU:H	2.22	0.47
2:A:348:ILE:HA	2:A:351:LEU:HD12	1.96	0.47
2:A:618:ALA:HA	2:A:620:GLU:OE2	2.14	0.47
1:b:180:SER:OG	2:B:119:VAL:HG22	2.14	0.47
2:B:5:ARG:NH1	2:B:5:ARG:N	2.59	0.47
2:B:67:LEU:C	2:B:68:ILE:HG13	2.39	0.47
2:B:72:GLN:O	2:B:74:MET:N	2.47	0.47
2:C:140:GLN:O	2:C:140:GLN:HG3	2.13	0.47
2:C:473:VAL:O	2:C:476:ILE:N	2.47	0.47
2:C:618:ALA:HA	2:C:620:GLU:OE2	2.14	0.47
1:a:201:LYS:CE	2:A:432:GLN:NE2	2.77	0.47
1:a:203:ILE:HG22	1:a:204:ILE:HG13	1.97	0.47
2:A:348:ILE:HG23	2:A:371:ILE:HG21	1.96	0.47
2:A:398:ALA:N	2:A:479:VAL:HG22	2.28	0.47
2:A:574:MET:HE3	2:A:616:LEU:HD13	1.95	0.47
2:B:268:ILE:HD11	2:B:274:ILE:HG23	1.96	0.47
2:B:359:GLU:HG2	2:B:364:VAL:C	2.36	0.47
2:B:364:VAL:HA	2:B:365:SER:O	2.14	0.47
2:C:18:GLN:O	2:C:21:ALA:N	2.48	0.47
2:C:93:ASP:C	2:C:95:ALA:H	2.21	0.47
2:C:341:GLN:HE21	2:C:386:PHE:HA	1.78	0.47
1:a:202:LEU:HD12	1:a:203:ILE:H	1.80	0.47
2:A:439:ALA:O	2:A:443:ARG:N	2.44	0.47
1:b:133:PHE:N	1:b:133:PHE:CD2	2.81	0.47
2:C:129:VAL:O	2:C:130:SER:C	2.57	0.47
2:C:261:LEU:HG	2:C:261:LEU:H	1.52	0.47
2:A:214:LYS:O	2:A:216:ALA:N	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:425:LYS:O	2:A:429:ALA:N	2.47	0.47
2:B:20:GLU:CD	2:B:40:ARG:NH1	2.72	0.47
2:B:20:GLU:O	2:B:21:ALA:C	2.55	0.47
2:B:201:LYS:HB3	2:B:335:GLN:HB2	1.97	0.47
2:B:229:GLU:H	2:B:229:GLU:HG3	1.39	0.47
2:B:233:ILE:O	2:B:234:LEU:HG	2.15	0.47
2:B:574:MET:HE3	2:B:616:LEU:HD13	1.95	0.47
2:C:22:LEU:C	2:C:24:LEU:H	2.22	0.47
2:C:123:VAL:HB	2:C:124:LEU:HD23	1.96	0.47
2:C:647:VAL:HG12	2:C:648:ASP:N	2.29	0.47
2:A:13:VAL:CG2	2:A:37:GLY:C	2.86	0.47
2:A:268:ILE:C	2:A:270:GLN:N	2.69	0.47
2:A:380:ARG:HG3	2:A:381:TYR:HD2	1.79	0.47
2:A:405:ARG:O	2:A:408:THR:HG22	2.14	0.47
1:b:126:LYS:HG3	1:b:129:PHE:CE1	2.50	0.47
2:B:13:VAL:HG21	2:B:38:LEU:HA	1.97	0.47
2:B:30:GLY:HA2	2:B:81:THR:CG2	2.43	0.47
2:B:129:VAL:O	2:B:129:VAL:CG1	2.54	0.47
2:B:356:ASP:CA	2:B:359:GLU:HG3	2.45	0.47
2:B:480:VAL:C	2:B:482:SER:N	2.72	0.47
2:C:18:GLN:O	2:C:19:GLU:C	2.58	0.47
2:C:179:LEU:HB3	2:C:223:GLN:NE2	2.30	0.47
2:C:204:PRO:HD2	2:C:311:CYS:O	2.15	0.47
2:C:396:ASP:C	2:C:399:GLY:H	2.21	0.47
2:C:633:VAL:O	2:C:637:GLY:N	2.47	0.47
2:A:378:SER:HB3	2:A:390:LYS:CD	2.43	0.47
2:A:650:ARG:HH11	2:A:650:ARG:HG3	1.79	0.47
2:B:6:PHE:HB2	2:B:10:ALA:CB	2.43	0.47
2:B:141:LEU:HA	1:c:192:SER:CB	2.45	0.47
2:B:739:LEU:HG	2:B:788:LYS:HE2	1.97	0.47
2:C:38:LEU:HD13	2:C:109:LEU:HB2	1.96	0.47
2:C:86:LYS:HG2	2:C:115:GLU:OE2	2.15	0.47
2:A:179:LEU:HD12	2:A:180:ASP:H	1.80	0.47
1:b:151:LYS:C	1:b:152:THR:HG22	2.39	0.47
1:b:184:GLU:CD	2:B:30:GLY:C	2.82	0.47
2:B:22:LEU:HD22	2:B:22:LEU:N	2.29	0.47
2:B:176:GLU:O	2:B:178:SER:N	2.48	0.47
2:B:633:VAL:O	2:B:637:GLY:N	2.47	0.47
2:C:22:LEU:HD22	2:C:22:LEU:N	2.30	0.47
2:C:374:ALA:HA	2:C:476:ILE:CD1	2.35	0.47
2:A:177:ASP:C	2:A:179:LEU:H	2.23	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:301:LYS:N	2:A:302:PRO:CD	2.77	0.47
2:A:365:SER:O	2:A:366:ILE:HG13	2.15	0.47
2:A:633:VAL:O	2:A:637:GLY:N	2.47	0.47
1:b:142:LEU:HD11	1:b:182:LEU:HD22	1.97	0.47
2:B:367:THR:OG1	2:B:370:ALA:HB2	2.15	0.47
2:C:435:GLU:HG3	2:C:438:LYS:CB	2.45	0.47
2:C:442:LEU:HD23	2:C:442:LEU:HA	1.51	0.47
1:a:126:LYS:O	1:a:127:LEU:HD23	2.14	0.46
1:a:145:LEU:HD12	1:a:145:LEU:N	2.30	0.46
1:a:179:LEU:CD2	1:a:183:LEU:HD11	2.45	0.46
2:A:370:ALA:O	2:A:476:ILE:HD12	2.15	0.46
2:A:619:ILE:HG12	2:A:656:MET:HB3	1.97	0.46
2:A:739:LEU:HG	2:A:788:LYS:HE2	1.97	0.46
2:B:10:ALA:HA	2:B:13:VAL:HG12	1.98	0.46
2:B:22:LEU:C	2:B:24:LEU:N	2.72	0.46
2:B:191:ARG:HG2	2:B:337:ILE:CG2	2.41	0.46
2:B:192:VAL:CG1	2:B:221:LEU:HD21	2.44	0.46
1:c:143:SER:C	1:c:145:LEU:H	2.23	0.46
1:c:184:GLU:CB	2:C:118:GLY:HA2	2.45	0.46
1:c:216:PHE:HZ	2:C:431:VAL:CG2	2.28	0.46
2:C:106:GLU:H	2:C:106:GLU:CD	2.22	0.46
2:C:359:GLU:HA	2:C:364:VAL:HG12	1.97	0.46
2:A:335:GLN:HG2	2:A:336:PRO:HD2	1.97	0.46
2:B:27:ASN:OD1	2:B:27:ASN:N	2.47	0.46
2:B:203:ASN:ND2	2:B:311:CYS:H	2.13	0.46
2:B:271:ALA:CB	2:C:96:ARG:NH1	2.78	0.46
2:C:165:SER:CA	2:C:166:LEU:O	2.62	0.46
2:C:270:GLN:O	2:C:271:ALA:HB2	2.15	0.46
2:C:335:GLN:CD	2:C:336:PRO:HD2	2.41	0.46
2:A:731:THR:HG22	2:A:741:ILE:CG1	2.45	0.46
2:B:202:ASN:C	2:B:202:ASN:OD1	2.57	0.46
2:B:262:LYS:HZ2	2:C:260:ARG:NH2	2.08	0.46
2:B:356:ASP:O	2:B:359:GLU:HG3	2.15	0.46
2:C:18:GLN:HA	2:C:21:ALA:HB2	1.98	0.46
2:C:434:GLN:HA	2:C:435:GLU:C	2.40	0.46
2:A:22:LEU:O	2:A:25:GLY:N	2.47	0.46
2:A:203:ASN:O	2:A:335:GLN:N	2.49	0.46
2:A:269:ARG:HG2	2:A:307:GLY:HA3	1.97	0.46
2:A:278:ILE:HG13	2:A:313:GLY:HA2	1.98	0.46
2:A:435:GLU:HG3	2:A:438:LYS:CB	2.46	0.46
2:B:435:GLU:HG3	2:B:438:LYS:CB	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:640:THR:HG22	2:B:646:THR:HB	1.98	0.46
2:C:103:VAL:CG1	2:C:104:GLY:H	2.27	0.46
2:C:203:ASN:O	2:C:335:GLN:N	2.48	0.46
2:C:226:ILE:HG22	2:C:227:ASN:N	2.29	0.46
2:A:70:ARG:HB3	2:A:71:GLY:HA3	1.98	0.46
2:A:377:LEU:CD1	2:A:477:ALA:HA	2.46	0.46
2:A:377:LEU:O	2:A:381:TYR:HB2	2.16	0.46
2:A:412:ASN:C	2:A:414:LYS:N	2.73	0.46
2:A:461:LYS:O	2:A:464:GLN:HB2	2.16	0.46
2:B:373:ALA:O	2:B:377:LEU:HD13	2.14	0.46
2:C:731:THR:HG22	2:C:741:ILE:CG1	2.45	0.46
2:C:752:ALA:C	2:C:754:GLU:N	2.73	0.46
2:C:763:ARG:CB	2:C:764:PRO:HD3	2.45	0.46
2:A:351:LEU:O	2:A:355:ARG:N	2.48	0.46
2:A:374:ALA:H	2:A:476:ILE:CG2	1.95	0.46
2:A:715:GLU:O	2:A:716:LYS:C	2.58	0.46
1:b:147:VAL:HG22	1:b:148:ASN:N	2.30	0.46
1:b:148:ASN:O	1:b:150:SER:OG	2.33	0.46
2:B:171:THR:CG2	2:B:226:ILE:HD11	2.46	0.46
2:B:450:ARG:C	2:B:452:GLN:N	2.74	0.46
2:C:20:GLU:CD	2:C:40:ARG:NH1	2.74	0.46
2:C:211:GLY:C	2:C:213:GLY:H	2.24	0.46
2:C:278:ILE:HG13	2:C:313:GLY:HA2	1.98	0.46
2:C:365:SER:O	2:C:366:ILE:HG13	2.16	0.46
2:C:640:THR:HG22	2:C:646:THR:HB	1.98	0.46
2:A:72:GLN:O	2:A:74:MET:N	2.49	0.46
2:A:124:LEU:C	2:A:126:ASN:H	2.21	0.46
2:B:190:GLN:HB3	2:C:404:LEU:HD21	1.98	0.46
2:B:230:VAL:O	2:C:407:PHE:CZ	2.69	0.46
2:C:377:LEU:O	2:C:381:TYR:N	2.42	0.46
2:C:460:TRP:CZ3	2:C:463:LYS:HG2	2.50	0.46
2:A:106:GLU:H	2:A:106:GLU:CD	2.24	0.46
2:A:526:ARG:CG	2:B:778:SER:CB	2.83	0.46
2:B:70:ARG:CB	2:B:71:GLY:HA3	2.45	0.46
2:B:170:LEU:N	2:B:239:VAL:O	2.49	0.46
2:B:422:GLU:O	2:B:426:GLU:N	2.38	0.46
1:c:151:LYS:C	1:c:152:THR:HG22	2.40	0.46
2:C:6:PHE:HB3	2:C:10:ALA:CB	2.45	0.46
2:A:394:LEU:CG	2:A:480:VAL:HG22	2.41	0.46
1:b:142:LEU:HD13	1:b:209:LEU:HD21	1.97	0.46
1:b:192:SER:HB3	1:b:195:ARG:HG3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:PHE:N	2:B:6:PHE:HD2	2.11	0.46
2:B:279:ASP:O	2:B:280:ALA:CB	2.64	0.46
2:B:369:ASP:O	2:B:473:VAL:HG13	2.16	0.46
2:B:731:THR:HG22	2:B:741:ILE:CG1	2.45	0.46
2:A:53:LEU:HD22	2:A:53:LEU:N	2.31	0.46
2:A:214:LYS:C	2:A:216:ALA:N	2.74	0.46
2:B:39:VAL:HG22	2:B:39:VAL:O	2.15	0.46
2:B:185:ARG:NH2	2:B:342:PRO:HG3	2.31	0.46
2:B:199:ARG:HH22	2:C:357:ARG:HH21	0.58	0.46
2:B:619:ILE:HG12	2:B:656:MET:HB3	1.97	0.46
2:C:739:LEU:HG	2:C:788:LYS:HE2	1.97	0.46
1:a:147:VAL:HG22	1:a:148:ASN:N	2.31	0.45
2:A:139:LEU:C	2:A:141:LEU:N	2.74	0.45
2:A:375:VAL:HG12	2:A:376:LYS:N	2.30	0.45
2:A:421:ASP:C	2:A:423:VAL:N	2.70	0.45
2:A:640:THR:HG22	2:A:646:THR:HB	1.98	0.45
2:B:275:ILE:HA	2:B:310:GLN:O	2.15	0.45
2:B:500:LEU:HD11	2:C:783:ARG:N	2.31	0.45
2:C:619:ILE:HG12	2:C:656:MET:HB3	1.97	0.45
1:a:171:THR:HG23	1:a:174:GLU:OE1	2.15	0.45
2:A:186:SER:HA	2:A:189:ILE:HD12	1.97	0.45
2:A:330:LEU:C	2:A:332:ARG:H	2.24	0.45
2:A:405:ARG:HH22	2:A:478:MET:CE	2.29	0.45
2:B:189:ILE:O	2:B:192:VAL:HB	2.16	0.45
2:B:233:ILE:O	2:B:233:ILE:HG12	2.16	0.45
2:B:269:ARG:HH12	2:B:306:ARG:CB	2.27	0.45
2:B:715:GLU:O	2:B:716:LYS:C	2.58	0.45
2:B:744:THR:HG21	2:B:795:ASP:CG	2.42	0.45
2:C:90:LEU:O	2:C:93:ASP:N	2.47	0.45
2:C:447:GLN:O	2:C:448:ARG:C	2.57	0.45
2:C:461:LYS:O	2:C:464:GLN:HB2	2.16	0.45
2:C:744:THR:HG21	2:C:795:ASP:CG	2.42	0.45
1:a:204:ILE:HG21	1:a:208:ALA:HA	1.98	0.45
2:A:170:LEU:HB2	2:A:239:VAL:HB	1.98	0.45
2:A:381:TYR:O	2:A:382:ILE:C	2.59	0.45
2:A:386:PHE:C	2:A:388:PRO:HD2	2.41	0.45
2:A:473:VAL:O	2:A:476:ILE:N	2.49	0.45
2:B:526:ARG:HD2	2:C:770:GLN:HG3	1.98	0.45
1:a:216:PHE:O	2:A:443:ARG:NH2	2.50	0.45
2:A:72:GLN:CB	2:A:74:MET:HG3	2.46	0.45
2:A:110:LEU:HD21	2:A:138:VAL:CG1	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:194:GLU:C	2:A:196:LEU:N	2.74	0.45
2:A:424:ARG:O	2:A:427:LYS:HB3	2.16	0.45
1:b:175:VAL:O	1:b:176:GLU:C	2.58	0.45
1:b:189:SER:C	1:b:191:ILE:N	2.75	0.45
2:B:191:ARG:O	2:B:195:VAL:CG2	2.65	0.45
2:B:306:ARG:CA	2:C:168:ARG:NH2	2.79	0.45
2:C:227:ASN:HA	2:C:228:ASN:CB	2.36	0.45
2:C:239:VAL:C	2:C:240:MET:HG2	2.41	0.45
2:C:348:ILE:HG23	2:C:371:ILE:HG21	1.99	0.45
2:C:715:GLU:O	2:C:716:LYS:C	2.58	0.45
1:a:189:SER:C	1:a:191:ILE:N	2.74	0.45
2:B:117:GLU:OE1	2:B:117:GLU:HA	2.15	0.45
2:B:161:PRO:C	2:B:264:VAL:HG22	2.42	0.45
1:c:184:GLU:CB	2:C:119:VAL:HG23	2.46	0.45
2:C:344:VAL:O	2:C:347:SER:HB2	2.17	0.45
2:C:404:LEU:C	2:C:406:SER:H	2.24	0.45
2:A:646:THR:O	2:A:646:THR:OG1	2.35	0.45
2:B:234:LEU:HD23	2:B:237:LYS:HD2	1.98	0.45
2:B:730:LEU:HD22	2:B:734:LEU:HG	1.99	0.45
2:C:67:LEU:C	2:C:68:ILE:CG1	2.89	0.45
2:C:117:GLU:OE1	2:C:117:GLU:HA	2.15	0.45
2:C:396:ASP:O	2:C:399:GLY:N	2.50	0.45
2:C:620:GLU:OE2	2:C:658:SER:HA	2.17	0.45
2:C:649:PHE:C	2:C:651:ASN:N	2.74	0.45
2:A:113:ILE:HG13	2:A:131:LEU:HD13	1.98	0.45
2:A:270:GLN:O	2:A:271:ALA:HB2	2.15	0.45
2:A:318:ASP:O	2:A:319:GLU:C	2.59	0.45
2:B:161:PRO:O	2:B:162:THR:C	2.60	0.45
2:B:214:LYS:NZ	2:B:315:THR:N	2.64	0.45
2:B:259:ASP:C	2:B:260:ARG:HG3	2.41	0.45
2:B:351:LEU:O	2:B:352:GLN:C	2.57	0.45
2:B:442:LEU:HA	2:B:445:THR:OG1	2.17	0.45
2:B:499:LEU:CD1	2:C:782:LEU:HD11	2.46	0.45
1:c:170:MET:HB2	1:c:175:VAL:HG23	1.97	0.45
2:C:476:ILE:O	2:C:479:VAL:N	2.50	0.45
1:a:184:GLU:HA	2:A:118:GLY:HA2	1.99	0.45
2:A:9:ARG:O	2:A:13:VAL:HG12	2.17	0.45
2:A:426:GLU:O	2:A:430:ALA:HB2	2.17	0.45
2:A:507:HIS:NE2	2:A:514:ASP:OD1	2.48	0.45
2:A:739:LEU:HD23	2:A:739:LEU:HA	1.61	0.45
2:A:744:THR:HG21	2:A:795:ASP:CG	2.42	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:LEU:HD21	2:B:138:VAL:HG11	1.99	0.45
2:B:140:GLN:O	2:B:140:GLN:HG3	2.15	0.45
2:B:174:ALA:HB1	2:B:179:LEU:HD22	1.98	0.45
2:B:179:LEU:HD12	2:B:179:LEU:HA	1.46	0.45
2:B:342:PRO:HG2	2:B:388:PRO:HB3	1.98	0.45
2:B:472:THR:O	2:B:473:VAL:C	2.58	0.45
2:C:5:ARG:NH1	2:C:5:ARG:N	2.61	0.45
2:C:228:ASN:OD1	2:C:228:ASN:O	2.34	0.45
2:C:261:LEU:C	2:C:263:LYS:H	2.24	0.45
2:C:49:ALA:O	2:C:52:ALA:HB3	2.16	0.45
2:C:192:VAL:O	2:C:196:LEU:HB2	2.17	0.45
2:C:507:HIS:NE2	2:C:514:ASP:OD1	2.48	0.45
2:A:18:GLN:O	2:A:21:ALA:HB3	2.17	0.45
2:A:169:ASP:CB	2:A:240:MET:HE3	2.47	0.45
2:A:214:LYS:C	2:A:216:ALA:H	2.25	0.45
2:A:730:LEU:HD22	2:A:734:LEU:HG	1.99	0.45
2:B:18:GLN:O	2:B:21:ALA:HB3	2.17	0.45
2:B:72:GLN:CB	2:B:74:MET:HG3	2.47	0.45
2:B:162:THR:O	2:B:164:ASP:N	2.49	0.45
2:B:351:LEU:O	2:B:354:LEU:N	2.49	0.45
2:B:526:ARG:CD	2:C:775:ASP:CG	2.86	0.45
2:C:268:ILE:O	2:C:269:ARG:C	2.59	0.45
2:C:385:ARG:HB3	2:C:386:PHE:H	1.53	0.45
2:C:416:LEU:O	2:C:419:LYS:N	2.50	0.45
1:a:151:LYS:C	1:a:152:THR:HG22	2.42	0.44
2:A:314:ALA:O	2:A:315:THR:HG23	2.16	0.44
2:A:394:LEU:HD13	2:A:479:VAL:CB	2.28	0.44
2:B:3:PHE:O	2:B:92:MET:HE1	2.17	0.44
2:B:28:ASN:HD22	2:B:28:ASN:N	2.15	0.44
2:B:231:PRO:CG	2:B:232:GLU:N	2.78	0.44
2:B:266:ASP:OD1	2:B:269:ARG:HD2	2.17	0.44
2:B:351:LEU:HB2	2:B:371:ILE:HD13	1.99	0.44
2:B:356:ASP:C	2:B:359:GLU:HG3	2.41	0.44
2:B:411:PRO:O	2:B:413:LEU:N	2.50	0.44
2:B:438:LYS:O	2:B:442:LEU:CD1	2.65	0.44
2:B:690:MET:CA	2:C:760:TYR:OH	2.58	0.44
2:C:91:SER:HB3	2:C:108:ILE:HA	1.98	0.44
2:C:169:ASP:CB	2:C:240:MET:HE3	2.47	0.44
2:C:194:GLU:O	2:C:198:ARG:HG3	2.16	0.44
2:C:320:TYR:O	2:C:321:ARG:C	2.58	0.44
2:C:424:ARG:O	2:C:427:LYS:HB3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:10:ALA:HA	2:A:13:VAL:HG12	2.00	0.44
2:A:95:ALA:O	2:A:96:ARG:C	2.60	0.44
2:A:620:GLU:OE2	2:A:658:SER:HA	2.16	0.44
1:b:184:GLU:O	2:B:82:PRO:HD2	2.17	0.44
2:B:143:GLY:N	1:c:195:ARG:HD2	2.31	0.44
2:B:175:LYS:C	2:B:177:ASP:H	2.25	0.44
2:B:342:PRO:HG2	2:B:388:PRO:CG	2.47	0.44
2:C:214:LYS:C	2:C:216:ALA:N	2.74	0.44
2:A:9:ARG:HG3	2:A:9:ARG:NH1	2.32	0.44
2:A:23:ARG:NH1	2:A:61:GLN:HE22	2.14	0.44
2:A:129:VAL:O	2:A:130:SER:C	2.61	0.44
2:A:179:LEU:HD23	2:A:223:GLN:HE21	1.83	0.44
2:A:213:GLY:O	2:A:214:LYS:C	2.60	0.44
2:B:23:ARG:NH1	2:B:61:GLN:HE22	2.14	0.44
2:B:143:GLY:H	1:c:195:ARG:CD	2.30	0.44
2:B:304:LEU:CD2	2:B:305:ALA:H	2.22	0.44
2:B:443:ARG:O	2:B:444:ASP:C	2.60	0.44
2:B:477:ALA:O	2:B:480:VAL:N	2.50	0.44
2:C:177:ASP:C	2:C:179:LEU:H	2.25	0.44
2:C:439:ALA:O	2:C:442:LEU:CA	2.65	0.44
2:A:22:LEU:HD22	2:A:22:LEU:N	2.31	0.44
2:A:210:PRO:HA	2:A:214:LYS:HE3	1.99	0.44
2:A:265:MET:O	2:A:268:ILE:CG2	2.66	0.44
2:A:752:ALA:C	2:A:754:GLU:N	2.73	0.44
2:B:63:GLU:O	2:B:67:LEU:HG	2.17	0.44
2:B:98:LEU:C	2:B:100:HIS:H	2.25	0.44
2:B:139:LEU:C	2:B:141:LEU:N	2.75	0.44
2:B:351:LEU:HG	2:B:392:ILE:CD1	2.48	0.44
2:B:531:LEU:C	2:C:733:ARG:HH22	2.24	0.44
2:B:691:GLY:N	2:C:760:TYR:OH	2.42	0.44
2:B:752:ALA:C	2:B:754:GLU:N	2.73	0.44
2:C:46:ALA:HB2	2:C:105:THR:C	2.41	0.44
2:C:196:LEU:HD12	2:C:310:GLN:NE2	2.32	0.44
2:A:209:GLU:C	2:A:211:GLY:HA3	2.43	0.44
1:b:168:CYS:O	1:b:169:ASN:C	2.60	0.44
2:C:95:ALA:O	2:C:96:ARG:C	2.58	0.44
2:C:182:VAL:HG12	2:C:183:ILE:N	2.32	0.44
2:C:204:PRO:CG	2:C:312:ILE:HG12	2.43	0.44
2:C:308:GLU:O	2:C:310:GLN:N	2.51	0.44
2:C:335:GLN:HG2	2:C:336:PRO:HD2	1.99	0.44
2:C:363:ARG:HH21	2:C:402:VAL:HG21	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:364:VAL:HA	2:C:365:SER:C	2.43	0.44
1:a:158:GLU:O	1:a:160:ARG:HG2	2.18	0.44
2:A:169:ASP:CA	2:A:240:MET:HE3	2.47	0.44
2:A:398:ALA:CB	2:A:479:VAL:CG2	2.95	0.44
1:b:144:LYS:HG2	2:B:74:MET:HE1	1.99	0.44
2:B:6:PHE:HB3	2:B:10:ALA:CB	2.46	0.44
2:B:103:VAL:CG1	2:B:104:GLY:N	2.80	0.44
2:B:276:LEU:O	2:B:311:CYS:CA	2.62	0.44
2:B:363:ARG:CG	2:B:471:VAL:HA	2.47	0.44
2:B:496:THR:CB	2:C:782:LEU:HD22	2.47	0.44
1:c:215:HIS:CB	2:C:436:PHE:O	2.66	0.44
2:C:29:ILE:HG13	2:C:80:TYR:HD1	1.82	0.44
2:C:382:ILE:HG13	2:C:484:THR:HG21	1.91	0.44
1:a:157:PHE:HD1	1:a:158:GLU:H	1.65	0.44
2:A:3:PHE:O	2:A:92:MET:HE1	2.18	0.44
2:A:261:LEU:HG	2:A:261:LEU:H	1.48	0.44
2:A:398:ALA:HA	2:A:401:LYS:HB3	2.00	0.44
2:B:85:LYS:HE3	2:B:85:LYS:HB2	1.76	0.44
2:B:180:ASP:OD1	2:B:180:ASP:N	2.46	0.44
1:c:155:TYR:CD2	1:c:196:LEU:HD13	2.52	0.44
2:C:170:LEU:HB2	2:C:239:VAL:HB	2.00	0.44
2:C:364:VAL:HG13	2:C:365:SER:CA	2.47	0.44
2:C:492:ALA:O	2:C:493:GLN:C	2.61	0.44
1:a:126:LYS:HG3	1:a:129:PHE:CE1	2.53	0.44
1:a:147:VAL:CG2	1:a:150:SER:HB2	2.39	0.44
2:A:18:GLN:HA	2:A:21:ALA:HB2	2.00	0.44
2:A:46:ALA:HB2	2:A:105:THR:C	2.43	0.44
2:A:122:ARG:O	2:A:123:VAL:C	2.61	0.44
2:A:167:ALA:HB1	2:A:241:THR:O	2.18	0.44
2:A:198:ARG:C	2:B:396:ASP:OD2	2.60	0.44
2:A:352:GLN:HA	2:A:355:ARG:CB	2.48	0.44
2:A:367:THR:CB	2:A:472:THR:HA	2.47	0.44
2:A:492:ALA:O	2:A:493:GLN:C	2.61	0.44
2:B:22:LEU:C	2:B:24:LEU:H	2.25	0.44
2:B:86:LYS:HG2	2:B:115:GLU:OE2	2.18	0.44
2:B:171:THR:O	2:B:172:ALA:C	2.61	0.44
2:B:620:GLU:OE2	2:B:658:SER:HA	2.16	0.44
2:B:633:VAL:O	2:B:637:GLY:HA2	2.18	0.44
1:c:187:THR:HG23	2:C:83:ARG:NH2	2.32	0.44
1:c:216:PHE:HZ	2:C:431:VAL:HG21	1.83	0.44
2:C:166:LEU:HA	2:C:167:ALA:HA	1.78	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:341:GLN:CG	2:C:387:LEU:HB2	2.46	0.44
2:C:355:ARG:C	2:C:357:ARG:N	2.76	0.44
2:C:364:VAL:HG23	2:C:366:ILE:O	2.17	0.44
2:A:20:GLU:O	2:A:21:ALA:C	2.59	0.44
2:A:265:MET:O	2:A:268:ILE:HG23	2.18	0.44
2:A:633:VAL:O	2:A:637:GLY:HA2	2.18	0.44
1:b:170:MET:HB2	1:b:175:VAL:CG2	2.48	0.44
2:B:209:GLU:HA	2:B:210:PRO:HD3	1.81	0.44
1:c:179:LEU:CG	1:c:183:LEU:HD11	2.48	0.44
1:c:201:LYS:CE	2:C:432:GLN:NE2	2.75	0.44
2:C:300:LEU:N	2:C:323:TYR:OH	2.51	0.44
2:C:302:PRO:HB2	2:C:304:LEU:HG	1.98	0.44
2:C:307:GLY:C	2:C:309:LEU:HG	2.43	0.44
2:C:403:ARG:O	2:C:406:SER:HB3	2.17	0.44
2:A:5:ARG:NH1	2:A:5:ARG:N	2.63	0.43
2:A:351:LEU:HD22	2:A:395:ILE:CD1	2.48	0.43
2:B:319:GLU:O	2:B:322:LYS:HB2	2.17	0.43
2:B:437:GLU:C	2:B:439:ALA:N	2.66	0.43
2:B:514:ASP:O	2:B:518:VAL:HG23	2.18	0.43
2:A:233:ILE:HD11	2:B:361:HIS:HB3	1.99	0.43
2:A:514:ASP:O	2:A:518:VAL:HG23	2.18	0.43
2:B:686:LYS:HZ3	2:B:690:MET:HE1	1.83	0.43
1:c:161:TYR:OH	2:C:428:ASP:OD2	2.34	0.43
1:c:209:LEU:O	1:c:210:GLU:C	2.61	0.43
2:C:72:GLN:HB3	2:C:74:MET:HG3	1.99	0.43
2:C:206:LEU:HD12	2:C:206:LEU:H	1.82	0.43
2:A:52:ALA:HB3	2:A:137:GLN:HG2	1.99	0.43
2:A:164:ASP:O	2:A:165:SER:C	2.61	0.43
2:A:182:VAL:HG12	2:A:183:ILE:N	2.33	0.43
2:A:199:ARG:HD2	2:B:358:TYR:CZ	2.53	0.43
2:A:335:GLN:CD	2:A:336:PRO:HD2	2.42	0.43
2:A:377:LEU:HD12	2:A:477:ALA:HA	2.00	0.43
2:A:546:PRO:HG2	2:A:549:VAL:CG2	2.44	0.43
1:b:177:ASN:O	1:b:178:GLN:C	2.59	0.43
1:b:203:ILE:HG22	1:b:204:ILE:HG13	2.00	0.43
2:B:18:GLN:HA	2:B:21:ALA:HB2	2.00	0.43
2:B:168:ARG:HH12	2:B:242:LEU:CD1	2.28	0.43
2:B:191:ARG:HD2	2:B:337:ILE:CG2	2.47	0.43
2:B:232:GLU:OE1	2:C:400:SER:HB2	2.18	0.43
2:B:646:THR:O	2:B:646:THR:OG1	2.34	0.43
2:B:649:PHE:C	2:B:651:ASN:N	2.74	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:215:HIS:CB	2:C:436:PHE:C	2.91	0.43
2:C:201:LYS:CE	2:C:335:GLN:HG3	2.49	0.43
2:C:300:LEU:O	2:C:301:LYS:C	2.60	0.43
2:C:324:ILE:HA	2:C:330:LEU:CB	2.48	0.43
2:C:386:PHE:CB	2:C:388:PRO:HD2	2.48	0.43
2:C:633:VAL:O	2:C:637:GLY:HA2	2.18	0.43
2:C:730:LEU:HD22	2:C:734:LEU:HG	1.99	0.43
1:a:155:TYR:CD2	1:a:196:LEU:HD13	2.53	0.43
2:A:53:LEU:HD22	2:A:53:LEU:H	1.84	0.43
2:A:649:PHE:C	2:A:651:ASN:N	2.74	0.43
1:b:144:LYS:C	2:B:27:ASN:ND2	2.68	0.43
2:B:507:HIS:NE2	2:B:514:ASP:OD1	2.48	0.43
1:c:192:SER:HB3	1:c:195:ARG:HG3	1.99	0.43
2:C:12:LYS:HG2	2:C:16:LEU:HD12	2.01	0.43
2:C:182:VAL:HG12	2:C:183:ILE:H	1.83	0.43
2:A:302:PRO:HB2	2:A:304:LEU:HG	2.01	0.43
2:A:339:VAL:O	2:A:339:VAL:HG12	2.18	0.43
2:A:426:GLU:O	2:A:430:ALA:HB3	2.18	0.43
1:b:166:ASP:C	1:b:166:ASP:OD1	2.62	0.43
1:b:193:ILE:O	1:b:193:ILE:CD1	2.64	0.43
2:B:229:GLU:C	2:B:230:VAL:CG2	2.91	0.43
2:C:70:ARG:CB	2:C:71:GLY:HA3	2.47	0.43
2:C:514:ASP:O	2:C:518:VAL:HG23	2.19	0.43
1:a:133:PHE:CD2	1:a:133:PHE:N	2.87	0.43
1:a:152:THR:OG1	1:a:208:ALA:HB3	2.18	0.43
2:A:116:GLY:O	2:A:121:ALA:CB	2.66	0.43
1:b:184:GLU:O	2:B:81:THR:CG2	2.67	0.43
2:B:492:ALA:O	2:B:493:GLN:C	2.61	0.43
2:C:186:SER:HA	2:C:189:ILE:HD12	2.00	0.43
2:C:210:PRO:HA	2:C:214:LYS:HE3	2.00	0.43
2:C:269:ARG:HG2	2:C:307:GLY:HA3	2.00	0.43
2:A:93:ASP:C	2:A:95:ALA:H	2.24	0.43
2:A:191:ARG:HG2	2:A:337:ILE:HG21	2.01	0.43
2:A:307:GLY:C	2:A:309:LEU:HG	2.43	0.43
2:A:330:LEU:O	2:A:331:GLU:C	2.62	0.43
2:A:364:VAL:HA	2:A:365:SER:C	2.42	0.43
2:B:339:VAL:O	2:B:339:VAL:HG12	2.18	0.43
2:B:382:ILE:CD1	2:B:611:TYR:CE2	3.00	0.43
2:C:318:ASP:O	2:C:319:GLU:C	2.61	0.43
2:C:346:GLU:O	2:C:350:ILE:HG13	2.19	0.43
2:C:419:LYS:O	2:C:420:LEU:C	2.60	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:170:MET:HB2	1:a:175:VAL:HG23	2.01	0.43
2:A:67:LEU:C	2:A:68:ILE:HG13	2.44	0.43
2:A:70:ARG:CB	2:A:71:GLY:HA3	2.48	0.43
2:A:204:PRO:HD2	2:A:311:CYS:O	2.18	0.43
2:A:321:ARG:HD2	2:A:325:GLU:OE1	2.18	0.43
2:A:478:MET:O	2:A:479:VAL:C	2.61	0.43
2:B:188:GLU:HB3	2:B:217:ILE:CD1	2.49	0.43
2:B:261:LEU:C	2:B:263:LYS:H	2.26	0.43
2:B:335:GLN:CG	2:B:336:PRO:CD	2.93	0.43
2:B:766:ARG:HH11	2:B:766:ARG:CG	2.31	0.43
1:c:179:LEU:O	1:c:180:SER:C	2.58	0.43
2:C:739:LEU:HA	2:C:739:LEU:HD23	1.61	0.43
1:a:127:LEU:O	1:a:128:GLN:HG3	2.18	0.43
2:A:32:GLU:HB3	2:A:119:VAL:CG1	2.49	0.43
2:A:279:ASP:OD2	2:A:279:ASP:N	2.51	0.43
2:A:324:ILE:HA	2:A:330:LEU:CB	2.48	0.43
2:A:473:VAL:O	2:A:474:ASP:C	2.61	0.43
2:B:198:ARG:NH1	2:C:396:ASP:HB3	2.33	0.43
2:C:67:LEU:O	2:C:68:ILE:CG1	2.67	0.43
2:C:330:LEU:C	2:C:332:ARG:H	2.27	0.43
2:C:424:ARG:O	2:C:428:ASP:N	2.30	0.43
2:C:473:VAL:O	2:C:474:ASP:C	2.62	0.43
2:C:735:LYS:HE3	2:C:735:LYS:HB2	1.88	0.43
2:A:359:GLU:CA	2:A:364:VAL:HG12	2.49	0.43
2:B:345:ASP:O	2:B:348:ILE:HG13	2.19	0.43
2:B:370:ALA:HB1	2:B:476:ILE:CB	2.49	0.43
2:B:528:ARG:HG3	2:B:528:ARG:O	2.19	0.43
1:c:181:ILE:O	1:c:182:LEU:C	2.61	0.43
2:C:183:ILE:CD1	2:C:349:GLN:HB2	2.49	0.43
2:A:98:LEU:C	2:A:100:HIS:H	2.26	0.42
2:A:117:GLU:OE1	2:A:117:GLU:HA	2.16	0.42
2:A:192:VAL:O	2:A:196:LEU:HB2	2.19	0.42
2:A:540:SER:HB2	2:A:706:ASP:H	1.85	0.42
2:C:23:ARG:NH1	2:C:61:GLN:HE22	2.16	0.42
2:C:304:LEU:C	2:C:306:ARG:N	2.77	0.42
2:C:307:GLY:C	2:C:309:LEU:N	2.77	0.42
2:C:471:VAL:HG12	2:C:472:THR:N	2.33	0.42
2:A:103:VAL:HG12	2:A:104:GLY:H	1.82	0.42
1:b:144:LYS:HB3	2:B:74:MET:SD	2.59	0.42
1:b:158:GLU:C	1:b:160:ARG:H	2.26	0.42
2:B:48:LYS:HD3	1:c:194:HIS:HD2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:ASN:O	2:B:335:GLN:N	2.51	0.42
2:B:458:LYS:C	2:B:460:TRP:H	2.27	0.42
2:C:722:ILE:O	2:C:723:VAL:C	2.61	0.42
1:a:142:LEU:HD13	1:a:209:LEU:HD21	2.01	0.42
1:a:181:ILE:O	1:a:182:LEU:C	2.62	0.42
2:A:341:GLN:CD	2:A:387:LEU:HD23	2.44	0.42
2:A:364:VAL:HG13	2:A:365:SER:CA	2.48	0.42
2:A:416:LEU:HD21	2:A:452:GLN:HE22	1.84	0.42
2:B:199:ARG:HH21	2:C:357:ARG:NH2	2.00	0.42
2:B:220:GLY:O	2:B:221:LEU:C	2.62	0.42
2:B:308:GLU:O	2:B:309:LEU:CG	2.61	0.42
2:B:533:ASP:OD1	2:B:534:PRO:HD2	2.20	0.42
2:C:139:LEU:O	2:C:141:LEU:N	2.52	0.42
2:A:32:GLU:OE2	2:A:32:GLU:N	2.53	0.42
2:A:393:ASP:O	2:A:479:VAL:CG1	2.68	0.42
2:A:416:LEU:O	2:A:419:LYS:N	2.52	0.42
2:B:9:ARG:HG3	2:B:9:ARG:NH1	2.33	0.42
2:B:443:ARG:C	2:B:445:THR:N	2.75	0.42
1:c:133:PHE:CD2	1:c:133:PHE:N	2.88	0.42
1:c:145:LEU:N	1:c:145:LEU:CD1	2.81	0.42
2:C:279:ASP:OD2	2:C:279:ASP:N	2.53	0.42
2:C:540:SER:HB2	2:C:706:ASP:H	1.85	0.42
2:A:72:GLN:HB3	2:A:74:MET:HG3	2.01	0.42
2:A:335:GLN:HG2	2:A:336:PRO:CD	2.50	0.42
2:A:732:LYS:HE3	2:A:732:LYS:HB2	1.85	0.42
2:B:341:GLN:OE1	2:B:387:LEU:HD23	2.20	0.42
2:B:343:SER:O	2:B:346:GLU:N	2.53	0.42
1:c:179:LEU:CD2	1:c:183:LEU:HD11	2.49	0.42
2:C:67:LEU:O	2:C:68:ILE:HG12	2.19	0.42
2:C:239:VAL:C	2:C:240:MET:CG	2.93	0.42
2:C:478:MET:O	2:C:479:VAL:C	2.62	0.42
2:A:362:HIS:O	2:A:363:ARG:HB2	2.18	0.42
2:A:377:LEU:O	2:A:381:TYR:N	2.47	0.42
2:A:420:LEU:HA	2:A:449:LEU:HD13	2.01	0.42
1:b:203:ILE:CD1	2:B:432:GLN:HG2	2.48	0.42
2:B:44:GLY:HA3	2:B:105:THR:HG21	2.01	0.42
2:B:75:SER:O	2:B:77:THR:N	2.52	0.42
2:B:261:LEU:HB3	2:B:262:LYS:H	1.29	0.42
2:B:360:ALA:C	2:B:361:HIS:ND1	2.78	0.42
2:B:500:LEU:CD2	2:C:779:GLU:O	2.67	0.42
2:B:511:ILE:CG2	2:B:718:HIS:CG	2.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:511:ILE:HG13	2:B:721:GLU:HB3	2.02	0.42
2:B:532:LYS:C	2:C:733:ARG:HH21	2.24	0.42
2:B:722:ILE:O	2:B:723:VAL:C	2.61	0.42
1:c:158:GLU:C	1:c:160:ARG:H	2.27	0.42
2:C:18:GLN:O	2:C:21:ALA:HB3	2.19	0.42
2:C:528:ARG:O	2:C:528:ARG:HG3	2.19	0.42
2:C:616:LEU:N	2:C:616:LEU:HD23	2.35	0.42
2:C:756:VAL:O	2:C:757:ASP:C	2.63	0.42
1:b:168:CYS:O	1:b:169:ASN:O	2.38	0.42
2:B:325:GLU:OE1	2:B:325:GLU:HA	2.19	0.42
2:B:382:ILE:O	2:B:382:ILE:HG22	2.19	0.42
2:B:540:SER:HB2	2:B:706:ASP:H	1.84	0.42
2:C:20:GLU:O	2:C:21:ALA:C	2.62	0.42
2:C:300:LEU:C	2:C:302:PRO:N	2.78	0.42
2:A:268:ILE:O	2:A:269:ARG:C	2.59	0.42
2:A:395:ILE:HG13	2:A:476:ILE:HG12	2.02	0.42
2:A:419:LYS:O	2:A:420:LEU:C	2.63	0.42
2:B:49:ALA:O	2:B:52:ALA:HB3	2.20	0.42
2:B:185:ARG:CZ	2:B:342:PRO:HG3	2.49	0.42
2:B:200:THR:HG23	2:C:392:ILE:CG2	2.42	0.42
2:B:206:LEU:HB3	2:B:214:LYS:HE3	2.02	0.42
2:B:363:ARG:HH11	2:B:363:ARG:HD3	1.67	0.42
2:B:367:THR:CB	2:B:472:THR:HG23	2.49	0.42
2:B:414:LYS:O	2:B:417:GLU:HB2	2.20	0.42
2:B:422:GLU:HA	2:B:425:LYS:HB2	2.01	0.42
1:c:158:GLU:O	1:c:160:ARG:HG2	2.20	0.42
2:C:439:ALA:O	2:C:443:ARG:N	2.47	0.42
1:a:158:GLU:C	1:a:160:ARG:H	2.28	0.42
2:A:528:ARG:HG3	2:A:528:ARG:O	2.19	0.42
1:b:217:ALA:HB1	2:B:74:MET:HE3	2.02	0.42
2:B:13:VAL:CG2	2:B:37:GLY:C	2.91	0.42
1:c:126:LYS:HG3	1:c:129:PHE:CE1	2.55	0.42
2:C:139:LEU:C	2:C:141:LEU:N	2.73	0.42
2:C:242:LEU:HD12	2:C:243:ASP:CA	2.50	0.42
2:C:335:GLN:HG2	2:C:336:PRO:CD	2.49	0.42
2:A:13:VAL:CG2	2:A:38:LEU:HA	2.50	0.42
2:A:180:ASP:CG	2:A:181:PRO:HD2	2.45	0.42
2:A:531:LEU:HD21	2:B:781:LEU:HD13	2.00	0.42
2:A:616:LEU:N	2:A:616:LEU:HD23	2.35	0.42
2:A:722:ILE:O	2:A:723:VAL:C	2.61	0.42
2:B:17:ALA:O	2:B:21:ALA:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:LEU:HD13	2:B:114:ARG:HB3	2.02	0.42
2:B:194:GLU:OE1	2:C:397:GLU:O	2.38	0.42
2:B:205:VAL:O	2:B:336:PRO:HA	2.20	0.42
2:B:325:GLU:C	2:B:327:ASP:N	2.76	0.42
2:B:336:PRO:C	2:B:337:ILE:HG12	2.44	0.42
2:B:363:ARG:NH1	2:B:475:ASP:C	2.72	0.42
2:B:496:THR:HB	2:C:782:LEU:HD22	2.00	0.42
2:B:500:LEU:HB3	2:C:783:ARG:CG	2.50	0.42
2:B:756:VAL:O	2:B:757:ASP:C	2.63	0.42
2:C:41:GLU:O	2:C:41:GLU:HG2	2.20	0.42
2:C:53:LEU:HD22	2:C:53:LEU:N	2.35	0.42
2:C:83:ARG:O	2:C:86:LYS:HB3	2.20	0.42
2:C:797:GLU:HB3	2:C:798:ASP:H	1.67	0.42
1:b:157:PHE:HD1	1:b:158:GLU:H	1.68	0.41
2:B:72:GLN:HB3	2:B:74:MET:HG3	2.02	0.41
2:B:112:LEU:HD23	2:B:112:LEU:HA	1.79	0.41
2:B:208:GLY:O	2:B:209:GLU:C	2.63	0.41
2:B:274:ILE:HG23	2:B:274:ILE:O	2.20	0.41
2:C:366:ILE:HG22	2:C:367:THR:CA	2.31	0.41
2:A:447:GLN:O	2:A:448:ARG:C	2.61	0.41
2:A:513:GLN:HG3	2:A:711:PHE:CD1	2.56	0.41
2:A:579:GLU:HB3	2:A:581:HIS:CE1	2.55	0.41
2:B:103:VAL:HA	2:B:107:HIS:ND1	2.34	0.41
2:B:198:ARG:HH12	2:C:397:GLU:N	2.17	0.41
2:C:9:ARG:HD3	2:C:9:ARG:HA	1.79	0.41
2:C:416:LEU:HD21	2:C:452:GLN:HE22	1.84	0.41
2:C:506:LEU:HA	2:C:506:LEU:HD23	1.87	0.41
2:C:619:ILE:HG12	2:C:656:MET:HE2	2.01	0.41
2:A:706:ASP:C	2:A:707:GLU:HG2	2.44	0.41
2:B:95:ALA:O	2:B:96:ARG:C	2.60	0.41
2:B:381:TYR:O	2:B:382:ILE:C	2.62	0.41
2:B:472:THR:O	2:B:474:ASP:N	2.53	0.41
2:B:616:LEU:HD23	2:B:616:LEU:N	2.35	0.41
2:B:647:VAL:HG12	2:B:648:ASP:H	1.85	0.41
2:C:355:ARG:C	2:C:357:ARG:H	2.28	0.41
2:C:533:ASP:OD1	2:C:534:PRO:HD2	2.19	0.41
2:A:22:LEU:C	2:A:24:LEU:N	2.75	0.41
2:A:370:ALA:HB1	2:A:471:VAL:O	2.11	0.41
2:A:434:GLN:HB2	2:A:436:PHE:CD1	2.55	0.41
2:A:662:ALA:O	2:A:663:SER:C	2.64	0.41
2:A:758:LEU:H	2:A:758:LEU:CD2	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:766:ARG:HH11	2:A:766:ARG:CG	2.32	0.41
2:B:195:VAL:HA	2:B:198:ARG:NE	2.31	0.41
2:B:225:ILE:HA	2:B:230:VAL:CG2	2.51	0.41
2:B:763:ARG:N	2:B:764:PRO:HD2	2.36	0.41
1:c:204:ILE:HG21	1:c:208:ALA:HA	2.02	0.41
2:C:112:LEU:HD23	2:C:112:LEU:HA	1.77	0.41
2:C:116:GLY:O	2:C:121:ALA:CB	2.68	0.41
2:C:374:ALA:HB2	2:C:476:ILE:HD11	2.01	0.41
2:C:462:GLU:C	2:C:464:GLN:N	2.77	0.41
2:A:28:ASN:HD22	2:A:28:ASN:N	2.18	0.41
2:A:166:LEU:HA	2:A:167:ALA:HA	1.77	0.41
2:A:355:ARG:C	2:A:357:ARG:N	2.78	0.41
2:A:619:ILE:HG12	2:A:656:MET:HE2	2.01	0.41
2:B:120:ALA:O	2:B:121:ALA:C	2.63	0.41
2:B:368:ASP:C	2:B:370:ALA:N	2.76	0.41
2:B:526:ARG:HG3	2:C:775:ASP:HB2	0.85	0.41
1:c:203:ILE:HD11	2:C:432:GLN:OE1	2.20	0.41
2:C:180:ASP:CG	2:C:181:PRO:HD2	2.45	0.41
2:C:339:VAL:O	2:C:339:VAL:HG12	2.20	0.41
2:C:355:ARG:NH2	2:C:366:ILE:HA	2.36	0.41
2:C:546:PRO:HG2	2:C:549:VAL:CG2	2.44	0.41
2:A:238:ARG:HB2	2:A:274:ILE:HD12	2.03	0.41
2:A:266:ASP:C	2:A:268:ILE:H	2.29	0.41
2:A:352:GLN:C	2:A:355:ARG:H	2.29	0.41
2:A:423:VAL:HG21	2:A:449:LEU:CD1	2.50	0.41
2:A:533:ASP:OD1	2:A:534:PRO:HD2	2.19	0.41
2:A:622:ALA:HB1	2:A:626:VAL:HG21	2.03	0.41
2:A:756:VAL:O	2:A:757:ASP:C	2.63	0.41
2:B:232:GLU:HB3	2:C:361:HIS:HA	2.03	0.41
2:B:758:LEU:H	2:B:758:LEU:CD2	2.33	0.41
1:c:146:ASN:HB3	1:c:148:ASN:CG	2.44	0.41
2:C:183:ILE:CG2	2:C:184:GLY:H	2.33	0.41
2:C:194:GLU:C	2:C:196:LEU:N	2.78	0.41
2:C:209:GLU:C	2:C:211:GLY:HA3	2.45	0.41
2:C:213:GLY:O	2:C:214:LYS:C	2.61	0.41
2:C:513:GLN:HG3	2:C:711:PHE:CD1	2.55	0.41
2:C:647:VAL:HG12	2:C:648:ASP:H	1.86	0.41
1:a:216:PHE:CD1	2:A:443:ARG:HD3	2.55	0.41
2:A:20:GLU:CD	2:A:40:ARG:NH1	2.78	0.41
2:A:123:VAL:HB	2:A:124:LEU:HD23	2.03	0.41
2:A:174:ALA:HB3	2:A:222:ALA:HB1	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:416:LEU:O	2:A:417:GLU:C	2.63	0.41
2:A:531:LEU:HD21	2:B:781:LEU:HD12	2.03	0.41
1:b:179:LEU:CD2	1:b:183:LEU:HD11	2.50	0.41
2:B:18:GLN:O	2:B:19:GLU:C	2.63	0.41
2:B:196:LEU:HD21	2:B:275:ILE:HD12	2.03	0.41
2:B:241:THR:HB	2:B:242:LEU:H	1.57	0.41
2:B:261:LEU:C	2:B:263:LYS:N	2.79	0.41
2:B:266:ASP:C	2:B:268:ILE:N	2.78	0.41
2:B:404:LEU:C	2:B:406:SER:H	2.28	0.41
2:B:513:GLN:HG3	2:B:711:PHE:CD1	2.56	0.41
1:c:181:ILE:H	1:c:181:ILE:HG13	1.71	0.41
2:C:3:PHE:O	2:C:92:MET:HE1	2.20	0.41
2:C:10:ALA:HA	2:C:13:VAL:HG12	2.03	0.41
2:C:375:VAL:HG12	2:C:376:LYS:N	2.36	0.41
2:C:622:ALA:HB1	2:C:626:VAL:HG21	2.03	0.41
2:A:405:ARG:NH2	2:A:478:MET:CE	2.78	0.41
2:B:97:LYS:O	2:B:98:LEU:HG	2.20	0.41
2:B:735:LYS:HE3	2:B:735:LYS:HB2	1.88	0.41
2:C:75:SER:O	2:C:77:THR:N	2.53	0.41
2:C:419:LYS:O	2:C:421:ASP:N	2.54	0.41
2:C:426:GLU:O	2:C:427:LYS:C	2.63	0.41
2:C:426:GLU:O	2:C:430:ALA:HB3	2.20	0.41
2:C:639:LEU:HD23	2:C:639:LEU:HA	1.92	0.41
1:a:153:THR:HA	1:a:208:ALA:HB2	2.03	0.41
2:A:27:ASN:OD1	2:A:27:ASN:N	2.54	0.41
2:A:122:ARG:HG3	2:A:126:ASN:HD22	1.85	0.41
2:A:261:LEU:C	2:A:263:LYS:N	2.78	0.41
2:A:269:ARG:NH2	2:A:306:ARG:HB3	2.36	0.41
2:A:453:VAL:HG12	2:A:454:GLU:N	2.35	0.41
2:A:462:GLU:C	2:A:464:GLN:N	2.77	0.41
2:A:506:LEU:HA	2:A:506:LEU:HD23	1.87	0.41
2:A:735:LYS:HB2	2:A:735:LYS:HE3	1.88	0.41
2:A:763:ARG:N	2:A:764:PRO:HD2	2.36	0.41
1:b:143:SER:C	1:b:145:LEU:H	2.27	0.41
1:b:145:LEU:N	1:b:145:LEU:CD1	2.83	0.41
1:b:153:THR:HA	1:b:208:ALA:HB2	2.03	0.41
2:B:169:ASP:O	2:B:170:LEU:C	2.63	0.41
2:B:192:VAL:HG21	2:B:217:ILE:CG2	2.50	0.41
2:B:207:ILE:O	2:B:207:ILE:CG1	2.66	0.41
2:B:304:LEU:HD13	2:B:306:ARG:HG2	2.03	0.41
2:B:316:THR:H	2:B:319:GLU:HB3	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:SER:O	2:B:344:VAL:C	2.63	0.41
2:B:358:TYR:O	2:B:359:GLU:C	2.62	0.41
2:B:364:VAL:CA	2:B:365:SER:C	2.93	0.41
2:B:385:ARG:CB	2:B:390:LYS:HG2	2.49	0.41
2:B:471:VAL:O	2:B:472:THR:O	2.39	0.41
2:B:511:ILE:HG22	2:B:718:HIS:CB	2.42	0.41
2:B:619:ILE:HG12	2:B:656:MET:HE2	2.01	0.41
2:B:662:ALA:O	2:B:663:SER:C	2.64	0.41
1:c:143:SER:O	1:c:145:LEU:N	2.52	0.41
1:c:145:LEU:HB3	1:c:146:ASN:H	1.66	0.41
2:C:13:VAL:CG2	2:C:38:LEU:HA	2.51	0.41
2:C:214:LYS:O	2:C:216:ALA:N	2.53	0.41
2:C:321:ARG:HD2	2:C:325:GLU:OE1	2.21	0.41
1:a:192:SER:HB3	1:a:195:ARG:HG3	2.03	0.41
2:A:75:SER:O	2:A:77:THR:N	2.54	0.41
1:b:193:ILE:O	1:b:193:ILE:CG1	2.68	0.41
1:b:203:ILE:HD11	2:B:432:GLN:CG	2.50	0.41
2:B:122:ARG:O	2:B:123:VAL:C	2.63	0.41
2:B:143:GLY:H	1:c:195:ARG:HH21	0.54	0.41
2:B:205:VAL:HG23	2:B:335:GLN:N	2.36	0.41
2:B:232:GLU:HA	2:C:362:HIS:NE2	2.36	0.41
2:C:476:ILE:HG22	2:C:477:ALA:N	2.36	0.41
2:C:577:TYR:N	2:C:577:TYR:HD2	2.19	0.41
2:A:433:SER:O	2:A:434:GLN:CD	2.64	0.40
2:A:476:ILE:HG22	2:A:477:ALA:N	2.36	0.40
2:A:577:TYR:N	2:A:577:TYR:HD2	2.19	0.40
2:A:773:VAL:HG22	2:A:794:LEU:HD12	2.03	0.40
1:b:152:THR:OG1	1:b:208:ALA:HB3	2.21	0.40
1:c:167:PHE:HD1	1:c:170:MET:HE1	1.85	0.40
1:c:198:GLU:HB3	1:c:199:TYR:CD2	2.56	0.40
2:C:83:ARG:HA	2:C:83:ARG:HD3	1.92	0.40
2:C:164:ASP:O	2:C:165:SER:C	2.65	0.40
2:C:184:GLY:HA2	2:C:185:ARG:HB2	2.03	0.40
2:C:201:LYS:HB3	2:C:335:GLN:HB2	2.03	0.40
2:C:209:GLU:HA	2:C:210:PRO:HD3	1.86	0.40
2:C:475:ASP:O	2:C:479:VAL:HG23	2.20	0.40
2:A:112:LEU:HD23	2:A:112:LEU:HA	1.83	0.40
2:A:122:ARG:HG3	2:A:126:ASN:ND2	2.37	0.40
2:A:620:GLU:HG2	2:A:658:SER:OG	2.21	0.40
2:B:36:LEU:O	2:B:40:ARG:HB2	2.21	0.40
2:B:93:ASP:C	2:B:95:ALA:N	2.79	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:387:LEU:N	2:B:388:PRO:CD	2.84	0.40
2:B:395:ILE:H	2:B:395:ILE:HD12	1.86	0.40
2:B:403:ARG:O	2:B:406:SER:HB3	2.20	0.40
2:B:434:GLN:O	2:B:434:GLN:CG	2.51	0.40
2:B:526:ARG:NH1	2:C:770:GLN:HG2	2.36	0.40
1:c:183:LEU:HB2	2:C:117:GLU:HG3	1.96	0.40
2:C:120:ALA:O	2:C:123:VAL:N	2.54	0.40
2:C:214:LYS:C	2:C:216:ALA:H	2.29	0.40
2:C:377:LEU:HD11	2:C:476:ILE:HG21	1.73	0.40
2:C:451:GLU:O	2:C:455:ASP:HB2	2.21	0.40
2:C:579:GLU:HB3	2:C:581:HIS:CE1	2.56	0.40
1:a:135:ASP:O	1:a:138:ASP:HB2	2.20	0.40
1:a:143:SER:O	1:a:145:LEU:N	2.52	0.40
2:A:66:SER:C	2:A:67:LEU:HD23	2.45	0.40
2:A:209:GLU:HA	2:A:210:PRO:HD3	1.81	0.40
2:A:368:ASP:O	2:A:369:ASP:C	2.63	0.40
2:A:446:GLU:HG2	2:A:447:GLN:N	2.36	0.40
2:B:188:GLU:HB3	2:B:217:ILE:HD11	2.04	0.40
2:B:197:SER:OG	2:B:232:GLU:HG3	2.21	0.40
2:B:330:LEU:O	2:B:331:GLU:C	2.64	0.40
2:B:373:ALA:O	2:B:375:VAL:N	2.54	0.40
2:B:500:LEU:HD13	2:C:783:ARG:CA	2.47	0.40
2:B:579:GLU:HB3	2:B:581:HIS:CE1	2.56	0.40
1:c:204:ILE:HD13	1:c:211:THR:CB	2.49	0.40
2:C:18:GLN:C	2:C:21:ALA:H	2.30	0.40
2:C:348:ILE:CD1	2:C:372:GLU:HG2	2.50	0.40
2:C:416:LEU:O	2:C:417:GLU:C	2.64	0.40
2:C:662:ALA:O	2:C:663:SER:C	2.64	0.40
1:a:146:ASN:HB3	1:a:148:ASN:CG	2.46	0.40
1:a:155:TYR:CE1	1:a:202:LEU:HD22	2.56	0.40
1:a:168:CYS:O	1:a:169:ASN:C	2.65	0.40
2:A:12:LYS:HG2	2:A:16:LEU:HD12	2.03	0.40
2:A:476:ILE:O	2:A:479:VAL:N	2.54	0.40
2:B:229:GLU:CB	2:C:407:PHE:CD1	3.05	0.40
2:B:390:LYS:O	2:B:391:ALA:C	2.65	0.40
2:B:439:ALA:CA	2:B:442:LEU:HD12	2.31	0.40
2:B:706:ASP:C	2:B:707:GLU:HG2	2.44	0.40
1:c:168:CYS:O	1:c:169:ASN:C	2.65	0.40
2:C:265:MET:O	2:C:268:ILE:HG23	2.22	0.40
2:C:354:LEU:H	2:C:354:LEU:HG	1.74	0.40
2:C:381:TYR:O	2:C:382:ILE:C	2.65	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:773:VAL:HG22	2:C:794:LEU:HD12	2.03	0.40
1:a:196:LEU:O	1:a:197:GLU:C	2.64	0.40
2:A:181:PRO:CB	2:A:182:VAL:CA	2.82	0.40
2:A:204:PRO:CG	2:A:312:ILE:HG12	2.47	0.40
2:A:207:ILE:HD12	2:A:317:LEU:O	2.21	0.40
2:B:659:ASN:O	2:B:662:ALA:HB3	2.22	0.40
2:C:63:GLU:O	2:C:67:LEU:HG	2.21	0.40
2:C:766:ARG:HH11	2:C:766:ARG:CG	2.32	0.40

All (41) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:194:HIS:CD2	2:C:48:LYS:NZ[10_445]	1.03	1.17
2:A:500:LEU:CB	2:A:500:LEU:CB[8_555]	1.04	1.16
1:a:128:GLN:NE2	2:A:787:HIS:NE2[8_545]	1.09	1.11
1:a:128:GLN:NE2	2:A:787:HIS:CD2[8_545]	1.25	0.95
1:a:128:GLN:CD	2:A:787:HIS:NE2[8_545]	1.38	0.82
2:A:797:GLU:OE2	2:C:58:GLU:OE2[6_454]	1.42	0.78
2:A:500:LEU:CA	2:A:500:LEU:CB[8_555]	1.44	0.76
1:a:128:GLN:CG	2:A:787:HIS:CE1[8_545]	1.50	0.70
2:A:361:HIS:NE2	2:C:197:SER:O[10_445]	1.51	0.69
2:A:404:LEU:CD2	2:C:190:GLN:NE2[10_445]	1.51	0.69
2:A:797:GLU:CD	2:C:58:GLU:OE2[6_454]	1.51	0.69
1:a:192:SER:OG	2:C:141:LEU:O[10_445]	1.53	0.67
2:A:763:ARG:NH2	2:C:699:PRO:CG[10_445]	1.54	0.66
1:a:194:HIS:CD2	2:C:48:LYS:CE[10_445]	1.55	0.65
1:a:194:HIS:CG	2:C:48:LYS:NZ[10_445]	1.62	0.58
1:a:194:HIS:NE2	2:C:48:LYS:CD[10_445]	1.63	0.57
2:A:503:GLU:OE2	2:A:504:ASN:OD1[8_555]	1.65	0.55
1:a:128:GLN:CG	2:A:787:HIS:NE2[8_545]	1.66	0.54
2:A:361:HIS:CD2	2:C:197:SER:O[10_445]	1.66	0.54
2:A:500:LEU:CD1	2:A:500:LEU:CD2[8_555]	1.71	0.49
1:a:168:CYS:SG	2:A:781:LEU:O[8_545]	1.75	0.45
1:a:194:HIS:CD2	2:C:48:LYS:CD[10_445]	1.78	0.42
2:A:500:LEU:CB	2:A:500:LEU:CD2[8_555]	1.83	0.37
2:A:797:GLU:OE1	2:C:58:GLU:OE2[6_454]	1.87	0.33
2:A:763:ARG:NH1	2:C:699:PRO:CB[10_445]	1.91	0.29
2:A:404:LEU:CD2	2:C:190:GLN:CD[10_445]	1.98	0.22
2:A:733:ARG:CZ	2:C:533:ASP:CB[10_445]	1.99	0.21

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:763:ARG:CZ	2:C:699:PRO:CB[10_445]	1.99	0.21
1:a:206:GLU:OE2	2:A:783:ARG:CG[8_545]	2.02	0.18
2:A:404:LEU:CD2	2:C:190:GLN:CG[10_445]	2.02	0.18
2:A:763:ARG:CZ	2:C:699:PRO:CG[10_445]	2.03	0.17
1:a:127:LEU:O	2:A:787:HIS:ND1[8_545]	2.04	0.16
2:A:494:THR:CG2	2:B:781:LEU:O[8_555]	2.07	0.13
1:a:192:SER:CB	2:C:141:LEU:O[10_445]	2.08	0.12
2:A:242:LEU:CD2	2:C:306:ARG:NH2[10_445]	2.09	0.11
2:A:500:LEU:CA	2:A:500:LEU:CA[8_555]	2.09	0.11
2:A:733:ARG:NH2	2:C:533:ASP:N[10_445]	2.09	0.11
2:A:797:GLU:OE2	2:C:58:GLU:CD[6_454]	2.09	0.11
1:a:127:LEU:CD1	2:A:787:HIS:CB[8_545]	2.14	0.06
2:A:260:ARG:NH2	2:C:262:LYS:NZ[10_445]	2.15	0.05
1:a:128:GLN:CD	2:A:787:HIS:CE1[8_545]	2.17	0.03

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	92/111 (83%)	76 (83%)	12 (13%)	4 (4%)	2	17
1	b	92/111 (83%)	76 (83%)	12 (13%)	4 (4%)	2	17
1	c	92/111 (83%)	75 (82%)	13 (14%)	4 (4%)	2	17
2	A	686/758 (90%)	493 (72%)	127 (18%)	66 (10%)	0	7
2	B	682/758 (90%)	491 (72%)	115 (17%)	76 (11%)	0	5
2	C	691/758 (91%)	492 (71%)	130 (19%)	69 (10%)	0	7
All	All	2335/2607 (90%)	1703 (73%)	409 (18%)	223 (10%)	0	7

All (223) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	169	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	42	GLY
2	A	98	LEU
2	A	144	SER
2	A	183	ILE
2	A	261	LEU
2	A	271	ALA
2	A	306	ARG
2	A	309	LEU
2	A	333	ARG
2	A	363	ARG
2	A	366	ILE
2	A	382	ILE
2	A	471	VAL
2	A	473	VAL
2	A	566	GLU
2	B	42	GLY
2	B	98	LEU
2	B	130	SER
2	B	144	SER
2	B	157	ASN
2	B	164	ASP
2	B	168	ARG
2	B	180	ASP
2	B	181	PRO
2	B	198	ARG
2	B	201	LYS
2	B	210	PRO
2	B	214	LYS
2	B	231	PRO
2	B	232	GLU
2	B	233	ILE
2	B	261	LEU
2	B	271	ALA
2	B	305	ALA
2	B	308	GLU
2	B	333	ARG
2	B	363	ARG
2	B	366	ILE
2	B	373	ALA
2	B	382	ILE
2	B	412	ASN
2	B	438	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	472	THR
2	B	566	GLU
1	c	169	ASN
2	C	42	GLY
2	C	98	LEU
2	C	130	SER
2	C	144	SER
2	C	183	ILE
2	C	242	LEU
2	C	244	MET
2	C	261	LEU
2	C	271	ALA
2	C	299	ILE
2	C	306	ARG
2	C	309	LEU
2	C	333	ARG
2	C	363	ARG
2	C	366	ILE
2	C	382	ILE
2	C	391	ALA
2	C	392	ILE
2	C	471	VAL
2	C	473	VAL
2	C	566	GLU
1	a	144	LYS
1	a	177	ASN
2	A	156	SER
2	A	163	LEU
2	A	165	SER
2	A	166	LEU
2	A	229	GLU
2	A	383	SER
2	A	391	ALA
2	A	493	GLN
2	A	662	ALA
2	A	690	MET
1	b	169	ASN
2	B	166	LEU
2	B	171	THR
2	B	199	ARG
2	B	331	GLU
2	B	362	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	433	SER
2	B	440	ALA
2	B	455	ASP
2	B	493	GLN
2	B	662	ALA
2	B	690	MET
1	c	144	LYS
1	c	206	GLU
2	C	3	PHE
2	C	77	THR
2	C	163	LEU
2	C	165	SER
2	C	166	LEU
2	C	280	ALA
2	C	331	GLU
2	C	383	SER
2	C	493	GLN
2	C	662	ALA
2	C	690	MET
2	A	73	GLU
2	A	77	THR
2	A	130	SER
2	A	162	THR
2	A	168	ARG
2	A	181	PRO
2	A	200	THR
2	A	228	ASN
2	A	305	ALA
2	A	330	LEU
2	A	331	GLU
2	A	375	VAL
2	A	388	PRO
2	A	412	ASN
2	A	413	LEU
2	A	788	LYS
1	b	144	LYS
1	b	206	GLU
2	B	77	THR
2	B	263	LYS
2	B	334	PHE
2	B	388	PRO
2	B	481	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	788	LYS
1	c	177	ASN
2	C	23	ARG
2	C	68	ILE
2	C	73	GLU
2	C	140	GLN
2	C	145	ASN
2	C	162	THR
2	C	168	ARG
2	C	181	PRO
2	C	228	ASN
2	C	229	GLU
2	C	330	LEU
2	C	375	VAL
2	C	388	PRO
2	C	412	ASN
2	C	413	LEU
2	C	788	LYS
2	A	71	GLY
2	A	74	MET
2	A	145	ASN
2	A	148	GLY
2	A	212	VAL
2	A	215	THR
2	A	226	ILE
2	A	316	THR
2	A	400	SER
2	A	422	GLU
2	A	434	GLN
2	A	650	ARG
2	A	757	ASP
2	A	779	GLU
1	b	177	ASN
2	B	68	ILE
2	B	71	GLY
2	B	73	GLU
2	B	74	MET
2	B	140	GLN
2	B	163	LEU
2	B	165	SER
2	B	176	GLU
2	B	212	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	330	LEU
2	B	344	VAL
2	B	359	GLU
2	B	374	ALA
2	B	385	ARG
2	B	450	ARG
2	B	650	ARG
2	B	757	ASP
2	B	779	GLU
2	C	71	GLY
2	C	74	MET
2	C	200	THR
2	C	212	VAL
2	C	226	ILE
2	C	301	LYS
2	C	305	ALA
2	C	316	THR
2	C	422	GLU
2	C	434	GLN
2	C	650	ARG
2	C	757	ASP
2	C	779	GLU
1	a	206	GLU
2	A	68	ILE
2	A	140	GLN
2	A	774	GLU
2	B	23	ARG
2	B	160	THR
2	B	306	ARG
2	B	342	PRO
2	B	774	GLU
2	C	400	SER
2	C	774	GLU
2	A	440	ALA
2	B	222	ALA
2	B	383	SER
2	C	76	GLN
2	C	323	TYR
2	A	116	GLY
2	A	479	VAL
2	B	473	VAL
2	A	160	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	471	VAL
2	B	476	ILE
2	A	392	ILE
2	A	423	VAL
2	C	160	THR
2	C	387	LEU
2	A	387	LEU
2	B	392	ILE
2	A	550	GLY
2	B	550	GLY
2	C	479	VAL
2	C	550	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	83/104 (80%)	67 (81%)	16 (19%)	1	7
1	b	84/104 (81%)	68 (81%)	16 (19%)	1	8
1	c	85/104 (82%)	69 (81%)	16 (19%)	1	8
2	A	571/645 (88%)	481 (84%)	90 (16%)	2	12
2	B	573/645 (89%)	467 (82%)	106 (18%)	1	8
2	C	576/645 (89%)	484 (84%)	92 (16%)	2	11
All	All	1972/2247 (88%)	1636 (83%)	336 (17%)	2	10

All (336) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	132	ARG
1	a	133	PHE
1	a	142	LEU
1	a	147	VAL
1	a	152	THR
1	a	160	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	163	LEU
1	a	179	LEU
1	a	183	LEU
1	a	187	THR
1	a	190	SER
1	a	191	ILE
1	a	193	ILE
1	a	198	GLU
1	a	202	LEU
1	a	212	ILE
2	A	5	ARG
2	A	6	PHE
2	A	7	THR
2	A	16	LEU
2	A	24	LEU
2	A	27	ASN
2	A	28	ASN
2	A	34	ILE
2	A	58	GLU
2	A	72	GLN
2	A	76	GLN
2	A	78	ILE
2	A	93	ASP
2	A	105	THR
2	A	117	GLU
2	A	124	LEU
2	A	131	LEU
2	A	139	LEU
2	A	176	GLU
2	A	180	ASP
2	A	188	GLU
2	A	206	LEU
2	A	207	ILE
2	A	215	THR
2	A	230	VAL
2	A	239	VAL
2	A	241	THR
2	A	242	LEU
2	A	261	LEU
2	A	268	ILE
2	A	274	ILE
2	A	276	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	278	ILE
2	A	279	ASP
2	A	304	LEU
2	A	308	GLU
2	A	309	LEU
2	A	315	THR
2	A	317	LEU
2	A	337	ILE
2	A	338	GLN
2	A	339	VAL
2	A	350	ILE
2	A	354	LEU
2	A	363	ARG
2	A	364	VAL
2	A	366	ILE
2	A	371	ILE
2	A	387	LEU
2	A	392	ILE
2	A	393	ASP
2	A	396	ASP
2	A	404	LEU
2	A	408	THR
2	A	424	ARG
2	A	428	ASP
2	A	456	THR
2	A	472	THR
2	A	473	VAL
2	A	513	GLN
2	A	514	ASP
2	A	524	VAL
2	A	531	LEU
2	A	540	SER
2	A	571	ARG
2	A	577	TYR
2	A	579	GLU
2	A	582	SER
2	A	616	LEU
2	A	619	ILE
2	A	620	GLU
2	A	631	LEU
2	A	640	THR
2	A	646	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	650	ARG
2	A	659	ASN
2	A	660	VAL
2	A	686	LYS
2	A	690	MET
2	A	717	LYS
2	A	720	THR
2	A	725	LEU
2	A	730	LEU
2	A	732	LYS
2	A	735	LYS
2	A	769	ILE
2	A	770	GLN
2	A	794	LEU
2	A	797	GLU
2	A	805	THR
1	b	132	ARG
1	b	133	PHE
1	b	142	LEU
1	b	147	VAL
1	b	151	LYS
1	b	152	THR
1	b	160	ARG
1	b	163	LEU
1	b	179	LEU
1	b	183	LEU
1	b	187	THR
1	b	190	SER
1	b	191	ILE
1	b	193	ILE
1	b	202	LEU
1	b	212	ILE
2	B	5	ARG
2	B	6	PHE
2	B	7	THR
2	B	16	LEU
2	B	24	LEU
2	B	27	ASN
2	B	34	ILE
2	B	58	GLU
2	B	72	GLN
2	B	76	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	78	ILE
2	B	93	ASP
2	B	105	THR
2	B	113	ILE
2	B	117	GLU
2	B	124	LEU
2	B	131	LEU
2	B	139	LEU
2	B	168	ARG
2	B	173	ILE
2	B	180	ASP
2	B	188	GLU
2	B	189	ILE
2	B	195	VAL
2	B	201	LYS
2	B	207	ILE
2	B	212	VAL
2	B	225	ILE
2	B	226	ILE
2	B	229	GLU
2	B	230	VAL
2	B	232	GLU
2	B	233	ILE
2	B	235	ARG
2	B	236	ASP
2	B	264	VAL
2	B	265	MET
2	B	268	ILE
2	B	276	LEU
2	B	303	SER
2	B	304	LEU
2	B	309	LEU
2	B	312	ILE
2	B	316	THR
2	B	323	TYR
2	B	326	LYS
2	B	337	ILE
2	B	347	SER
2	B	348	ILE
2	B	354	LEU
2	B	355	ARG
2	B	363	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	371	ILE
2	B	381	TYR
2	B	382	ILE
2	B	387	LEU
2	B	396	ASP
2	B	416	LEU
2	B	417	GLU
2	B	418	GLN
2	B	419	LYS
2	B	424	ARG
2	B	428	ASP
2	B	432	GLN
2	B	433	SER
2	B	435	GLU
2	B	443	ARG
2	B	453	VAL
2	B	454	GLU
2	B	456	THR
2	B	472	THR
2	B	473	VAL
2	B	476	ILE
2	B	478	MET
2	B	479	VAL
2	B	483	TRP
2	B	513	GLN
2	B	514	ASP
2	B	524	VAL
2	B	540	SER
2	B	571	ARG
2	B	577	TYR
2	B	579	GLU
2	B	582	SER
2	B	616	LEU
2	B	619	ILE
2	B	620	GLU
2	B	631	LEU
2	B	640	THR
2	B	646	THR
2	B	650	ARG
2	B	659	ASN
2	B	660	VAL
2	B	686	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	690	MET
2	B	717	LYS
2	B	720	THR
2	B	725	LEU
2	B	730	LEU
2	B	732	LYS
2	B	735	LYS
2	B	769	ILE
2	B	770	GLN
2	B	794	LEU
2	B	797	GLU
2	B	805	THR
1	c	132	ARG
1	c	142	LEU
1	c	147	VAL
1	c	151	LYS
1	c	152	THR
1	c	160	ARG
1	c	163	LEU
1	c	179	LEU
1	c	183	LEU
1	c	187	THR
1	c	190	SER
1	c	191	ILE
1	c	193	ILE
1	c	198	GLU
1	c	202	LEU
1	c	212	ILE
2	C	5	ARG
2	C	6	PHE
2	C	7	THR
2	C	16	LEU
2	C	27	ASN
2	C	28	ASN
2	C	29	ILE
2	C	34	ILE
2	C	58	GLU
2	C	72	GLN
2	C	76	GLN
2	C	78	ILE
2	C	93	ASP
2	C	105	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	117	GLU
2	C	124	LEU
2	C	131	LEU
2	C	139	LEU
2	C	176	GLU
2	C	180	ASP
2	C	188	GLU
2	C	206	LEU
2	C	207	ILE
2	C	230	VAL
2	C	239	VAL
2	C	241	THR
2	C	242	LEU
2	C	261	LEU
2	C	268	ILE
2	C	274	ILE
2	C	276	LEU
2	C	278	ILE
2	C	279	ASP
2	C	304	LEU
2	C	308	GLU
2	C	309	LEU
2	C	315	THR
2	C	317	LEU
2	C	337	ILE
2	C	338	GLN
2	C	339	VAL
2	C	350	ILE
2	C	354	LEU
2	C	364	VAL
2	C	366	ILE
2	C	371	ILE
2	C	387	LEU
2	C	392	ILE
2	C	393	ASP
2	C	394	LEU
2	C	395	ILE
2	C	396	ASP
2	C	404	LEU
2	C	408	THR
2	C	423	VAL
2	C	424	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	428	ASP
2	C	456	THR
2	C	471	VAL
2	C	472	THR
2	C	473	VAL
2	C	513	GLN
2	C	514	ASP
2	C	524	VAL
2	C	531	LEU
2	C	540	SER
2	C	571	ARG
2	C	577	TYR
2	C	579	GLU
2	C	582	SER
2	C	616	LEU
2	C	619	ILE
2	C	620	GLU
2	C	631	LEU
2	C	640	THR
2	C	646	THR
2	C	650	ARG
2	C	659	ASN
2	C	660	VAL
2	C	686	LYS
2	C	690	MET
2	C	717	LYS
2	C	720	THR
2	C	725	LEU
2	C	730	LEU
2	C	732	LYS
2	C	735	LYS
2	C	769	ILE
2	C	770	GLN
2	C	794	LEU
2	C	797	GLU
2	C	805	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	159	ASN
1	a	207	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	51	GLN
2	A	61	GLN
2	A	72	GLN
2	A	76	GLN
2	A	100	HIS
2	A	126	ASN
2	A	137	GLN
2	A	223	GLN
2	A	310	GLN
2	A	338	GLN
2	A	341	GLN
2	A	349	GLN
2	A	362	HIS
2	A	432	GLN
2	A	452	GLN
2	A	623	HIS
2	A	628	ASN
2	A	770	GLN
2	A	785	ASN
1	b	159	ASN
1	b	207	HIS
2	B	51	GLN
2	B	61	GLN
2	B	72	GLN
2	B	76	GLN
2	B	100	HIS
2	B	126	ASN
2	B	137	GLN
2	B	202	ASN
2	B	203	ASN
2	B	223	GLN
2	B	227	ASN
2	B	228	ASN
2	B	310	GLN
2	B	361	HIS
2	B	362	HIS
2	B	623	HIS
2	B	628	ASN
2	B	659	ASN
2	B	770	GLN
2	B	785	ASN
1	c	159	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	c	194	HIS
1	c	207	HIS
2	C	28	ASN
2	C	51	GLN
2	C	61	GLN
2	C	72	GLN
2	C	76	GLN
2	C	100	HIS
2	C	126	ASN
2	C	137	GLN
2	C	223	GLN
2	C	227	ASN
2	C	228	ASN
2	C	338	GLN
2	C	341	GLN
2	C	349	GLN
2	C	362	HIS
2	C	432	GLN
2	C	452	GLN
2	C	493	GLN
2	C	623	HIS
2	C	628	ASN
2	C	785	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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
2	A	1
2	B	1
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	664:GLU	C	686:LYS	N	7.77
1	B	664:GLU	C	686:LYS	N	7.77
1	C	664:GLU	C	686:LYS	N	7.77

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	a	94/111 (84%)	4.28	89 (94%) 0 1	583, 624, 738, 792	0
1	b	94/111 (84%)	4.96	87 (92%) 0 1	543, 603, 730, 756	0
1	c	94/111 (84%)	6.21	88 (93%) 0 1	523, 590, 707, 731	0
2	A	708/758 (93%)	5.14	660 (93%) 0 1	508, 632, 810, 849	0
2	B	704/758 (92%)	5.16	646 (91%) 0 1	523, 661, 747, 823	0
2	C	711/758 (93%)	5.07	637 (89%) 0 1	426, 601, 842, 889	0
All	All	2405/2607 (92%)	5.13	2207 (91%) 0 1	426, 636, 815, 889	0

All (2207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	104	GLY	25.0
2	C	807	ALA	24.3
2	C	276	LEU	21.3
1	c	140	ILE	21.3
2	A	654	LEU	20.3
2	A	582	SER	20.2
2	C	2	MET	19.3
2	B	8	GLU	19.2
1	c	203	ILE	19.1
1	c	164	TYR	19.0
2	A	145	ASN	18.3
2	B	561	SER	18.0
2	B	103	VAL	18.0
1	c	163	LEU	17.7
2	B	572	ILE	17.4
2	C	405	ARG	17.2
2	C	311	CYS	17.2
1	c	142	LEU	17.0
2	A	653	ILE	16.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	265	MET	16.5
1	c	165	VAL	16.3
2	C	806	THR	16.2
2	A	515	GLU	16.2
2	B	215	THR	16.2
2	A	313	GLY	16.1
2	A	134	ALA	16.1
2	B	236	ASP	16.0
2	A	18	GLN	15.7
2	A	575	SER	15.6
2	A	556	ARG	15.5
2	B	49	ALA	15.4
2	C	275	ILE	15.4
2	C	408	THR	15.4
2	A	712	HIS	14.9
2	C	209	GLU	14.7
2	A	774	GLU	14.6
2	C	116	GLY	14.6
2	B	280	ALA	14.6
2	B	698	ARG	14.3
2	A	660	VAL	14.3
2	C	577	TYR	14.3
2	B	80	TYR	14.1
2	B	333	ARG	13.7
2	B	723	VAL	13.5
2	A	66	SER	13.5
2	A	133	LYS	13.5
2	B	66	SER	13.4
2	B	580	LYS	13.4
2	B	457	LYS	13.4
2	A	496	THR	13.4
2	A	480	VAL	13.4
1	c	129	PHE	13.2
2	B	79	HIS	13.2
2	A	793	VAL	13.2
2	C	39	VAL	13.1
2	B	581	HIS	13.0
2	B	374	ALA	13.0
2	C	238	ARG	13.0
2	C	312	ILE	12.8
1	c	181	ILE	12.8
1	b	199	TYR	12.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	511	ILE	12.6
2	C	233	ILE	12.6
2	C	164	ASP	12.5
2	A	60	ILE	12.4
2	A	61	GLN	12.4
2	C	437	GLU	12.4
1	c	153	THR	12.3
2	B	137	GLN	12.2
2	C	634	LEU	12.1
2	C	510	VAL	12.1
2	C	414	LYS	12.1
2	A	655	ILE	12.1
2	A	217	ILE	12.0
2	A	517	VAL	12.0
2	A	528	ARG	12.0
2	C	576	GLU	12.0
2	B	407	PHE	11.9
2	A	477	ALA	11.9
2	A	721	GLU	11.8
2	A	314	ALA	11.8
2	C	305	ALA	11.8
2	C	258	GLU	11.7
2	C	231	PRO	11.7
1	a	194	HIS	11.6
2	C	628	ASN	11.6
2	B	402	VAL	11.5
1	c	197	GLU	11.5
2	C	688	LYS	11.5
2	C	466	GLN	11.5
2	C	219	GLU	11.4
2	B	629	ILE	11.3
2	B	62	LYS	11.3
2	C	357	ARG	11.3
2	A	553	GLU	11.3
2	C	85	LYS	11.2
2	B	161	PRO	11.2
2	A	614	VAL	11.1
2	C	401	LYS	11.0
1	c	141	SER	11.0
2	C	230	VAL	11.0
2	A	547	THR	11.0
2	B	761	GLY	10.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	495	GLU	10.9
2	C	45	ILE	10.9
2	C	189	ILE	10.9
2	A	499	LEU	10.8
2	B	420	LEU	10.8
2	B	218	ALA	10.8
2	C	467	GLU	10.8
2	C	205	VAL	10.7
2	B	578	MET	10.7
2	C	584	SER	10.7
2	C	805	THR	10.7
2	C	484	THR	10.7
2	A	392	ILE	10.6
1	c	182	LEU	10.6
2	A	367	THR	10.6
2	A	221	LEU	10.5
2	B	434	GLN	10.5
2	C	328	ALA	10.5
2	C	664	GLU	10.5
1	b	133	PHE	10.4
2	B	32	GLU	10.4
2	A	708	ILE	10.4
2	C	304	LEU	10.4
2	A	89	GLU	10.4
2	A	576	GLU	10.4
2	A	584	SER	10.3
1	c	137	GLU	10.3
1	c	185	TYR	10.3
2	A	546	PRO	10.3
2	B	751	VAL	10.3
2	A	220	GLY	10.2
2	C	180	ASP	10.2
2	B	549	VAL	10.2
2	C	700	GLU	10.2
2	B	416	LEU	10.2
2	B	726	MET	10.2
2	C	555	ALA	10.2
2	B	479	VAL	10.2
2	C	54	GLY	10.2
2	A	379	ASP	10.1
2	A	661	GLY	10.1
2	A	126	ASN	10.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	471	VAL	10.1
1	a	188	GLU	10.1
2	C	126	ASN	10.1
2	A	500	LEU	10.0
2	A	310	GLN	10.0
2	A	494	THR	9.9
2	C	131	LEU	9.9
2	B	120	ALA	9.9
1	c	130	VAL	9.9
1	c	214	LYS	9.9
2	B	43	GLU	9.8
2	B	211	GLY	9.8
2	C	183	ILE	9.8
2	C	528	ARG	9.8
2	A	67	LEU	9.7
2	B	309	LEU	9.7
2	A	315	THR	9.7
1	a	209	LEU	9.7
2	B	385	ARG	9.7
2	C	336	PRO	9.6
2	B	483	TRP	9.6
2	B	369	ASP	9.6
2	B	443	ARG	9.6
2	C	64	VAL	9.6
2	C	454	GLU	9.6
2	B	524	VAL	9.6
2	B	440	ALA	9.6
2	B	762	ALA	9.6
2	C	323	TYR	9.6
2	C	470	GLU	9.6
2	C	662	ALA	9.5
2	B	444	ASP	9.5
2	B	351	LEU	9.5
2	B	107	HIS	9.5
2	B	712	HIS	9.5
2	C	572	ILE	9.5
2	A	725	LEU	9.5
2	A	190	GLN	9.5
2	C	324	ILE	9.5
2	A	492	ALA	9.5
2	C	13	VAL	9.5
2	A	329	ALA	9.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	583	THR	9.4
2	A	224	GLN	9.4
2	A	512	GLY	9.4
2	A	219	GLU	9.4
2	A	571	ARG	9.4
2	C	350	ILE	9.4
2	B	621	LYS	9.4
2	C	50	LEU	9.4
2	C	117	GLU	9.3
2	B	139	LEU	9.3
1	b	165	VAL	9.3
2	A	497	ASP	9.3
2	C	300	LEU	9.3
2	C	398	ALA	9.3
2	A	493	GLN	9.2
2	B	46	ALA	9.2
2	A	436	PHE	9.1
2	A	385	ARG	9.1
2	B	477	ALA	9.1
2	C	301	LYS	9.1
1	c	207	HIS	9.1
1	a	182	LEU	9.1
2	B	108	ILE	9.1
2	B	319	GLU	9.1
2	B	722	ILE	9.1
2	B	182	VAL	9.0
2	B	803	VAL	9.0
2	C	552	THR	9.0
1	b	155	TYR	9.0
2	C	686	LYS	9.0
2	A	316	THR	9.0
1	b	148	ASN	9.0
2	A	470	GLU	9.0
2	A	35	LEU	9.0
2	B	35	LEU	9.0
2	A	194	GLU	9.0
2	C	32	GLU	9.0
2	A	210	PRO	9.0
1	b	176	GLU	9.0
2	B	785	ASN	9.0
2	B	317	LEU	9.0
2	B	528	ARG	9.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	567	GLU	8.9
2	B	498	LYS	8.9
2	C	329	ALA	8.8
2	C	511	ILE	8.8
1	a	180	SER	8.8
2	C	623	HIS	8.8
1	c	139	VAL	8.8
2	C	625	ASP	8.8
2	A	696	ALA	8.8
2	B	199	ARG	8.8
2	A	68	ILE	8.7
2	C	136	GLN	8.7
2	A	507	HIS	8.7
1	c	154	LEU	8.7
2	B	378	SER	8.7
2	A	548	GLY	8.7
1	b	179	LEU	8.7
2	B	332	ARG	8.7
2	B	659	ASN	8.7
2	B	620	GLU	8.6
1	a	137	GLU	8.6
2	B	311	CYS	8.6
1	b	145	LEU	8.6
2	A	360	ALA	8.6
2	C	240	MET	8.6
2	C	790	GLN	8.6
2	C	419	LYS	8.6
2	B	105	THR	8.6
2	A	794	LEU	8.6
2	B	554	LEU	8.6
2	C	375	VAL	8.5
2	C	493	GLN	8.5
2	C	704	ARG	8.5
2	B	406	SER	8.5
1	c	178	GLN	8.5
2	C	395	ILE	8.5
2	A	772	HIS	8.5
2	A	144	SER	8.5
2	C	51	GLN	8.5
2	C	504	ASN	8.4
2	C	38	LEU	8.4
1	c	149	GLY	8.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	117	GLU	8.4
2	B	727	SER	8.4
2	C	690	MET	8.4
2	B	546	PRO	8.4
2	A	777	LEU	8.4
2	A	7	THR	8.4
2	C	348	ILE	8.4
2	C	531	LEU	8.4
2	A	697	PHE	8.4
2	A	621	LYS	8.4
2	C	112	LEU	8.4
2	C	710	VAL	8.4
2	B	334	PHE	8.4
2	A	624	PRO	8.4
2	B	106	GLU	8.3
2	A	710	VAL	8.3
2	C	267	GLU	8.3
2	B	315	THR	8.3
2	B	395	ILE	8.3
2	B	562	ILE	8.3
2	B	327	ASP	8.3
2	B	510	VAL	8.3
2	A	351	LEU	8.3
2	B	538	ILE	8.3
2	A	122	ARG	8.3
2	B	782	LEU	8.3
1	b	181	ILE	8.2
1	b	147	VAL	8.2
2	B	59	LYS	8.2
2	C	121	ALA	8.2
2	C	389	ASP	8.2
2	A	304	LEU	8.2
2	B	109	LEU	8.2
2	C	160	THR	8.2
2	C	200	THR	8.2
2	B	50	LEU	8.2
2	B	787	HIS	8.2
2	A	802	VAL	8.2
2	C	87	VAL	8.2
2	B	398	ALA	8.2
2	B	557	ALA	8.2
2	B	141	LEU	8.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	773	VAL	8.2
2	C	191	ARG	8.2
2	A	361	HIS	8.2
2	B	68	ILE	8.2
2	C	708	ILE	8.2
2	B	86	LYS	8.1
2	C	48	LYS	8.1
2	C	705	ILE	8.1
1	b	182	LEU	8.1
2	A	303	SER	8.1
2	B	64	VAL	8.1
1	c	188	GLU	8.1
2	B	308	GLU	8.1
2	C	165	SER	8.1
2	B	730	LEU	8.1
1	b	210	GLU	8.1
2	A	380	ARG	8.1
2	A	743	LEU	8.1
2	C	106	GLU	8.1
2	A	564	GLY	8.1
2	B	630	LEU	8.0
2	C	483	TRP	8.0
2	C	787	HIS	8.0
2	B	88	ILE	8.0
2	A	389	ASP	8.0
2	B	336	PRO	8.0
2	C	432	GLN	8.0
2	A	182	VAL	8.0
2	A	629	ILE	8.0
2	B	183	ILE	8.0
1	c	136	PHE	8.0
2	B	765	LEU	8.0
2	B	6	PHE	8.0
1	c	216	PHE	7.9
2	B	781	LEU	7.9
2	A	80	TYR	7.9
2	B	515	GLU	7.9
2	C	431	VAL	7.9
2	C	580	LYS	7.9
1	a	179	LEU	7.9
2	A	36	LEU	7.9
2	B	273	ASN	7.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	323	TYR	7.8
2	A	447	GLN	7.8
2	A	277	PHE	7.8
2	C	270	GLN	7.8
2	B	437	GLU	7.8
2	B	778	SER	7.8
2	A	362	HIS	7.8
2	B	755	GLY	7.8
2	B	316	THR	7.8
2	C	215	THR	7.8
2	C	310	GLN	7.8
1	c	212	ILE	7.7
2	B	362	HIS	7.7
2	B	558	LEU	7.7
2	C	507	HIS	7.7
2	A	259	ASP	7.7
2	B	539	GLY	7.7
2	C	402	VAL	7.7
2	B	12	LYS	7.7
2	B	774	GLU	7.7
2	C	331	GLU	7.7
2	A	628	ASN	7.7
2	B	125	ASN	7.7
2	C	313	GLY	7.7
2	C	391	ALA	7.7
2	B	584	SER	7.7
2	C	525	ARG	7.6
2	C	206	LEU	7.6
2	C	743	LEU	7.6
2	A	514	ASP	7.6
2	B	138	VAL	7.6
2	A	100	HIS	7.6
2	B	85	LYS	7.6
2	A	449	LEU	7.6
2	A	23	ARG	7.6
2	A	63	GLU	7.6
2	B	700	GLU	7.6
2	C	184	GLY	7.6
2	B	266	ASP	7.6
2	A	754	GLU	7.6
2	B	550	GLY	7.6
2	B	754	GLU	7.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	552	THR	7.6
2	B	329	ALA	7.6
2	A	801	PHE	7.6
2	A	718	HIS	7.6
2	C	741	ILE	7.6
2	B	715	GLU	7.5
2	B	476	ILE	7.5
2	C	31	THR	7.5
1	b	218	SER	7.5
1	b	146	ASN	7.5
1	c	143	SER	7.5
2	C	602	LEU	7.5
2	A	659	ASN	7.5
2	A	773	VAL	7.5
2	B	780	GLU	7.5
2	C	33	HIS	7.5
2	B	426	GLU	7.4
2	C	457	LYS	7.4
2	C	57	SER	7.4
2	C	353	GLY	7.4
2	B	354	LEU	7.4
1	b	195	ARG	7.4
2	C	115	GLU	7.4
2	C	214	LYS	7.4
2	A	501	ASN	7.4
2	A	529	ALA	7.4
2	C	327	ASP	7.4
1	b	183	LEU	7.4
2	C	314	ALA	7.4
1	b	139	VAL	7.4
2	A	573	ASP	7.3
2	A	623	HIS	7.3
2	A	769	ILE	7.3
2	C	26	HIS	7.3
2	B	314	ALA	7.3
1	a	197	GLU	7.3
2	B	579	GLU	7.3
2	C	397	GLU	7.3
1	c	152	THR	7.3
2	B	123	VAL	7.3
2	C	98	LEU	7.3
2	B	769	ILE	7.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	363	ARG	7.2
2	C	403	ARG	7.2
2	B	664	GLU	7.2
2	C	727	SER	7.2
2	B	397	GLU	7.2
2	B	627	PHE	7.2
2	B	436	PHE	7.2
1	b	186	ALA	7.2
1	c	210	GLU	7.2
1	a	131	LEU	7.2
2	C	172	ALA	7.2
2	B	214	LYS	7.1
2	B	777	LEU	7.1
2	C	731	THR	7.1
1	b	204	ILE	7.1
2	C	661	GLY	7.1
2	A	129	VAL	7.1
2	B	100	HIS	7.1
2	A	92	MET	7.1
2	A	662	ALA	7.1
2	C	335	GLN	7.1
2	A	278	ILE	7.1
2	B	277	PHE	7.1
2	A	113	ILE	7.1
2	B	419	LYS	7.1
2	C	474	ASP	7.1
2	A	198	ARG	7.1
2	B	794	LEU	7.1
2	A	626	VAL	7.1
2	A	27	ASN	7.0
2	A	327	ASP	7.0
2	A	120	ALA	7.0
2	C	508	SER	7.0
2	A	520	VAL	7.0
2	C	273	ASN	7.0
2	B	191	ARG	7.0
2	B	349	GLN	7.0
2	B	602	LEU	7.0
2	C	404	LEU	7.0
2	C	55	LEU	7.0
1	a	143	SER	7.0
2	B	203	ASN	7.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	34	ILE	7.0
2	C	499	LEU	7.0
2	A	502	MET	7.0
2	C	56	GLY	7.0
2	C	536	ARG	7.0
2	A	64	VAL	7.0
2	A	319	GLU	7.0
2	A	241	THR	7.0
2	B	368	ASP	6.9
2	C	236	ASP	6.9
2	B	65	GLU	6.9
2	B	189	ILE	6.9
2	B	114	ARG	6.9
2	B	391	ALA	6.9
1	c	201	LYS	6.9
2	C	635	GLU	6.9
2	B	375	VAL	6.9
2	C	277	PHE	6.9
2	A	28	ASN	6.9
2	A	108	ILE	6.9
1	c	145	LEU	6.9
2	B	576	GLU	6.9
2	C	20	GLU	6.9
2	C	193	ILE	6.8
2	C	371	ILE	6.8
2	B	91	SER	6.8
2	A	797	GLU	6.8
2	A	76	GLN	6.8
2	C	210	PRO	6.8
2	A	581	HIS	6.8
2	A	730	LEU	6.8
2	C	239	VAL	6.8
2	C	113	ILE	6.8
2	A	524	VAL	6.8
2	C	68	ILE	6.8
2	C	84	ALA	6.8
2	A	358	TYR	6.8
2	B	389	ASP	6.8
2	B	233	ILE	6.7
2	A	521	ALA	6.7
2	C	352	GLN	6.7
2	B	303	SER	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	202	ASN	6.7
2	A	408	THR	6.7
2	A	429	ALA	6.7
2	A	652	THR	6.7
2	C	640	THR	6.7
2	A	459	SER	6.7
2	C	613	VAL	6.7
2	C	702	ILE	6.7
2	B	807	ALA	6.7
1	a	147	VAL	6.7
2	B	690	MET	6.7
2	B	373	ALA	6.7
2	C	244	MET	6.7
2	A	213	GLY	6.7
2	B	784	GLY	6.7
2	C	181	PRO	6.7
2	C	624	PRO	6.7
2	A	510	VAL	6.7
2	B	475	ASP	6.7
2	A	704	ARG	6.7
2	B	570	ILE	6.7
2	A	405	ARG	6.7
2	A	328	ALA	6.7
2	C	89	GLU	6.6
2	A	526	ARG	6.6
1	c	190	SER	6.6
2	B	279	ASP	6.6
2	A	727	SER	6.6
2	A	366	ILE	6.6
2	A	139	LEU	6.6
2	C	417	GLU	6.6
2	C	582	SER	6.6
2	A	14	LEU	6.6
2	A	341	GLN	6.6
2	A	331	GLU	6.6
1	c	131	LEU	6.6
2	A	608	ARG	6.6
2	C	434	GLN	6.6
2	C	28	ASN	6.6
1	c	179	LEU	6.6
2	A	387	LEU	6.6
2	B	376	LYS	6.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	766	ARG	6.5
2	C	369	ASP	6.5
2	C	381	TYR	6.5
2	C	182	VAL	6.5
2	B	53	LEU	6.5
2	B	190	GLN	6.5
2	A	376	LYS	6.5
2	A	403	ARG	6.5
2	C	450	ARG	6.5
2	B	305	ALA	6.5
2	C	691	GLY	6.5
2	B	431	VAL	6.5
2	A	109	LEU	6.5
2	B	743	LEU	6.5
2	C	110	LEU	6.5
2	A	218	ALA	6.5
2	B	806	THR	6.5
2	C	654	LEU	6.5
2	A	312	ILE	6.5
2	C	804	LYS	6.5
2	C	197	SER	6.5
2	A	563	PHE	6.5
2	C	545	GLY	6.5
2	C	217	ILE	6.5
2	A	800	GLU	6.4
2	B	467	GLU	6.4
2	C	42	GLY	6.4
2	A	363	ARG	6.4
2	B	631	LEU	6.4
2	C	558	LEU	6.4
2	A	143	GLY	6.4
2	A	372	GLU	6.4
2	B	221	LEU	6.4
2	B	377	LEU	6.4
2	C	35	LEU	6.4
1	a	175	VAL	6.4
2	B	686	LYS	6.4
2	C	349	GLN	6.4
2	C	632	GLN	6.4
2	C	396	ASP	6.4
2	B	423	VAL	6.4
2	B	518	VAL	6.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	760	TYR	6.4
2	C	611	TYR	6.4
2	B	724	SER	6.4
2	A	689	VAL	6.3
2	A	211	GLY	6.3
2	C	14	LEU	6.3
2	B	372	GLU	6.3
1	b	154	LEU	6.3
2	A	215	THR	6.3
2	A	603	THR	6.3
2	C	72	GLN	6.3
1	b	173	GLU	6.3
2	B	232	GLU	6.3
2	C	302	PRO	6.3
2	A	767	ARG	6.3
2	A	720	THR	6.3
2	C	569	MET	6.3
2	A	539	GLY	6.3
2	A	34	ILE	6.3
2	C	574	MET	6.3
1	b	163	LEU	6.3
2	B	67	LEU	6.3
2	B	786	ILE	6.3
2	C	460	TRP	6.3
2	B	506	LEU	6.3
2	B	399	GLY	6.2
2	C	724	SER	6.2
2	B	210	PRO	6.2
2	A	509	ARG	6.2
1	a	181	ILE	6.2
2	A	205	VAL	6.2
2	A	216	ALA	6.2
2	C	119	VAL	6.2
2	B	14	LEU	6.2
2	B	693	LEU	6.2
2	A	792	ILE	6.2
2	B	502	MET	6.2
2	A	349	GLN	6.2
2	A	311	CYS	6.2
2	A	565	ASP	6.2
2	B	417	GLU	6.2
2	C	158	ALA	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	771	LYS	6.2
1	c	158	GLU	6.2
2	B	258	GLU	6.2
2	B	509	ARG	6.2
2	C	388	PRO	6.2
1	c	204	ILE	6.2
2	B	453	VAL	6.2
2	C	392	ILE	6.2
2	A	474	ASP	6.2
2	A	401	LYS	6.2
1	a	195	ARG	6.1
2	A	431	VAL	6.1
2	B	231	PRO	6.1
2	B	166	LEU	6.1
2	A	770	GLN	6.1
2	B	63	GLU	6.1
2	B	267	GLU	6.1
2	B	331	GLU	6.1
2	B	766	ARG	6.1
2	B	749	ALA	6.1
2	A	417	GLU	6.1
2	A	741	ILE	6.1
2	B	278	ILE	6.1
2	A	752	ALA	6.1
2	C	303	SER	6.1
2	A	620	GLU	6.1
2	C	332	ARG	6.1
1	b	196	LEU	6.1
2	C	162	THR	6.1
2	A	554	LEU	6.1
1	b	203	ILE	6.1
2	C	614	VAL	6.1
2	B	772	HIS	6.1
2	B	60	ILE	6.0
2	B	207	ILE	6.0
2	C	706	ASP	6.0
2	B	45	ILE	6.0
2	A	369	ASP	6.0
2	A	202	ASN	6.0
2	C	540	SER	6.0
2	B	545	GLY	6.0
2	C	36	LEU	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	b	164	TYR	6.0
2	A	29	ILE	6.0
2	C	338	GLN	6.0
2	C	656	MET	6.0
2	A	200	THR	6.0
2	B	582	SER	6.0
2	A	719	LEU	6.0
2	C	354	LEU	6.0
2	A	388	PRO	6.0
2	A	516	ALA	5.9
2	A	749	ALA	5.9
2	B	119	VAL	5.9
2	A	483	TRP	5.9
2	C	163	LEU	5.9
2	C	616	LEU	5.9
2	B	216	ALA	5.9
2	B	392	ILE	5.9
2	C	109	LEU	5.9
1	b	129	PHE	5.9
2	A	625	ASP	5.9
2	C	120	ALA	5.9
2	A	639	LEU	5.9
2	A	804	LYS	5.9
2	A	722	ILE	5.9
2	B	792	ILE	5.9
2	C	213	GLY	5.9
2	B	501	ASN	5.9
2	A	130	SER	5.9
2	C	655	ILE	5.9
1	c	194	HIS	5.9
2	B	508	SER	5.9
1	c	134	GLY	5.9
2	A	453	VAL	5.9
2	C	93	ASP	5.9
1	b	193	ILE	5.9
2	B	741	ILE	5.9
2	B	186	SER	5.9
1	b	131	LEU	5.9
2	A	798	ASP	5.8
2	B	325	GLU	5.8
2	C	533	ASP	5.8
2	C	60	ILE	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	75	SER	5.8
2	B	142	LEU	5.8
2	B	662	ALA	5.8
2	A	525	ARG	5.8
2	B	623	HIS	5.8
2	A	544	LEU	5.8
2	C	99	GLY	5.8
2	C	204	PRO	5.8
1	a	185	TYR	5.8
2	A	196	LEU	5.8
2	A	506	LEU	5.8
2	B	473	VAL	5.8
2	C	245	GLY	5.8
2	B	737	GLN	5.8
2	C	80	TYR	5.8
2	A	503	GLU	5.8
2	B	441	SER	5.8
2	B	312	ILE	5.8
2	C	221	LEU	5.8
1	b	194	HIS	5.8
2	C	266	ASP	5.8
1	a	164	TYR	5.8
2	A	635	GLU	5.8
2	B	742	GLU	5.8
2	C	529	ALA	5.8
2	B	350	ILE	5.8
2	B	270	GLN	5.8
2	C	633	VAL	5.8
2	C	579	GLU	5.7
2	A	472	THR	5.7
2	A	640	THR	5.7
2	B	403	ARG	5.7
2	A	135	ARG	5.7
2	A	189	ILE	5.7
2	A	395	ILE	5.7
2	B	380	ARG	5.7
2	A	481	SER	5.7
1	a	129	PHE	5.7
2	B	196	LEU	5.7
2	A	164	ASP	5.7
2	C	394	LEU	5.7
2	A	649	PHE	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	124	LEU	5.7
2	C	563	PHE	5.7
2	A	78	ILE	5.7
2	C	554	LEU	5.7
2	B	328	ALA	5.7
2	C	443	ARG	5.7
2	B	262	LYS	5.7
2	C	218	ALA	5.7
2	C	617	ASP	5.7
2	C	728	ASP	5.7
2	B	90	LEU	5.6
2	C	190	GLN	5.6
2	A	605	LYS	5.6
1	c	180	SER	5.6
2	B	394	LEU	5.6
2	B	701	PHE	5.6
2	B	788	LYS	5.6
1	a	169	ASN	5.6
2	A	460	TRP	5.6
2	A	699	PRO	5.6
2	C	229	GLU	5.6
2	B	238	ARG	5.6
2	C	15	ALA	5.6
2	C	524	VAL	5.6
2	B	276	LEU	5.6
2	B	474	ASP	5.6
1	b	161	TYR	5.6
2	A	381	TYR	5.6
1	a	215	HIS	5.6
2	A	482	SER	5.6
2	B	220	GLY	5.6
1	a	178	GLN	5.6
2	A	112	LEU	5.6
2	B	224	GLN	5.6
2	C	452	GLN	5.6
1	a	162	TYR	5.6
2	A	350	ILE	5.6
2	B	193	ILE	5.6
2	B	520	VAL	5.6
2	C	47	ALA	5.6
1	a	142	LEU	5.6
2	A	693	LEU	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	632	GLN	5.6
1	c	193	ILE	5.6
2	C	562	ILE	5.6
2	A	694	LYS	5.6
2	C	742	GLU	5.6
1	b	143	SER	5.5
2	A	651	ASN	5.5
2	B	805	THR	5.5
2	C	532	LYS	5.5
2	A	789	GLY	5.5
2	B	728	ASP	5.5
2	B	793	VAL	5.5
2	B	242	LEU	5.5
2	C	196	LEU	5.5
2	C	159	ASN	5.5
2	C	269	ARG	5.5
2	B	472	THR	5.5
2	C	241	THR	5.5
2	A	55	LEU	5.5
2	A	504	ASN	5.5
2	C	653	ILE	5.5
2	A	50	LEU	5.5
2	A	119	VAL	5.5
2	C	346	GLU	5.5
2	A	324	ILE	5.5
2	C	274	ILE	5.5
2	A	123	VAL	5.5
2	B	265	MET	5.5
2	B	200	THR	5.5
2	B	505	ILE	5.5
2	C	175	LYS	5.5
2	A	96	ARG	5.5
2	B	358	TYR	5.5
2	C	27	ASN	5.5
2	A	479	VAL	5.5
2	B	206	LEU	5.5
2	B	628	ASN	5.5
2	B	729	GLN	5.5
2	C	265	MET	5.5
2	A	206	LEU	5.4
2	A	616	LEU	5.4
1	c	126	LYS	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	378	SER	5.4
2	A	724	SER	5.4
2	C	347	SER	5.4
2	A	505	ILE	5.4
2	C	630	LEU	5.4
2	C	192	VAL	5.4
2	B	92	MET	5.4
2	C	760	TYR	5.4
2	A	57	SER	5.4
2	A	630	LEU	5.4
2	B	470	GLU	5.4
2	B	7	THR	5.4
2	B	302	PRO	5.4
2	A	541	PHE	5.4
2	C	543	PHE	5.4
1	b	130	VAL	5.4
2	B	463	LYS	5.4
1	b	138	ASP	5.4
2	A	757	ASP	5.4
2	A	782	LEU	5.4
2	C	341	GLN	5.4
2	C	319	GLU	5.4
2	B	702	ILE	5.4
2	B	548	GLY	5.4
1	c	138	ASP	5.4
2	A	352	GLN	5.4
2	B	696	ALA	5.4
2	C	315	THR	5.3
2	B	169	ASP	5.3
2	B	575	SER	5.3
1	c	148	ASN	5.3
2	A	717	LYS	5.3
2	B	393	ASP	5.3
2	C	299	ILE	5.3
2	A	577	TYR	5.3
2	B	770	GLN	5.3
2	B	268	ILE	5.3
2	C	169	ASP	5.3
1	a	210	GLU	5.3
2	A	785	ASN	5.3
2	C	703	ASN	5.3
1	a	161	TYR	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	b	192	SER	5.3
2	C	325	GLU	5.3
2	C	692	GLU	5.3
2	A	62	LYS	5.3
2	B	744	THR	5.3
2	A	335	GLN	5.3
2	A	397	GLU	5.3
2	B	36	LEU	5.3
2	C	351	LEU	5.3
2	C	615	LEU	5.3
2	A	407	PHE	5.3
2	B	140	GLN	5.3
2	A	647	VAL	5.3
2	B	42	GLY	5.3
2	A	65	GLU	5.3
2	A	478	MET	5.3
2	B	383	SER	5.3
2	A	305	ALA	5.2
2	B	411	PRO	5.2
2	A	32	GLU	5.2
2	B	706	ASP	5.2
2	B	719	LEU	5.2
2	B	386	PHE	5.2
2	C	3	PHE	5.2
2	C	570	ILE	5.2
1	b	171	THR	5.2
2	B	160	THR	5.2
2	C	134	ALA	5.2
2	A	342	PRO	5.2
2	B	573	ASP	5.2
2	C	356	ASP	5.2
2	C	475	ASP	5.2
1	b	141	SER	5.2
2	A	306	ARG	5.2
2	A	433	SER	5.2
2	A	508	SER	5.2
2	B	40	ARG	5.2
2	C	156	SER	5.2
2	B	234	LEU	5.2
2	A	269	ARG	5.2
2	B	571	ARG	5.2
2	A	452	GLN	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	143	GLY	5.2
2	B	624	PRO	5.2
2	A	484	THR	5.2
2	A	20	GLU	5.2
2	C	520	VAL	5.2
2	C	71	GLY	5.2
2	A	81	THR	5.2
1	c	189	SER	5.2
2	A	658	SER	5.2
2	B	202	ASN	5.1
2	C	132	ASN	5.1
2	C	263	LYS	5.1
2	A	731	THR	5.1
2	C	415	GLU	5.1
2	A	523	ALA	5.1
2	B	172	ALA	5.1
2	B	439	ALA	5.1
2	C	208	GLY	5.1
1	c	177	ASN	5.1
1	c	213	LYS	5.1
2	B	390	LYS	5.1
2	B	122	ARG	5.1
2	B	310	GLN	5.1
2	B	89	GLU	5.1
2	C	118	GLY	5.1
1	c	202	LEU	5.1
2	C	242	LEU	5.1
2	C	260	ARG	5.1
2	A	229	GLU	5.1
2	B	748	LYS	5.1
2	B	783	ARG	5.1
1	c	192	SER	5.1
2	A	435	GLU	5.1
2	B	435	GLU	5.1
2	B	652	THR	5.1
2	A	185	ARG	5.1
2	C	693	LEU	5.1
2	B	264	VAL	5.1
2	A	466	GLN	5.1
2	B	3	PHE	5.1
2	A	125	ASN	5.1
2	A	527	ALA	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	116	GLY	5.1
2	C	707	GLU	5.1
2	A	191	ARG	5.1
2	C	517	VAL	5.1
1	b	167	PHE	5.0
2	A	365	SER	5.0
2	A	568	SER	5.0
2	A	709	ILE	5.1
2	A	750	LYS	5.0
2	C	658	SER	5.0
1	b	200	GLY	5.0
2	B	544	LEU	5.0
2	C	194	GLU	5.0
2	C	82	PRO	5.0
2	C	264	VAL	5.0
2	B	447	GLN	5.0
2	C	463	LYS	5.0
2	A	279	ASP	5.0
2	B	433	SER	5.0
2	C	433	SER	5.0
2	C	83	ARG	5.0
2	C	380	ARG	5.0
2	A	8	GLU	5.0
1	c	147	VAL	5.0
2	A	578	MET	5.0
2	A	6	PHE	5.0
2	A	799	GLY	5.0
2	A	753	GLU	5.0
1	b	216	PHE	5.0
2	C	506	LEU	5.0
2	A	111	GLY	5.0
2	B	405	ARG	5.0
2	B	93	ASP	5.0
2	C	358	TYR	5.0
2	C	689	VAL	5.0
2	B	339	VAL	5.0
2	A	612	SER	5.0
2	C	337	ILE	5.0
2	C	422	GLU	5.0
2	C	551	LYS	5.0
1	b	157	PHE	5.0
1	c	211	THR	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	9	ARG	5.0
2	C	571	ARG	5.0
1	b	202	LEU	5.0
2	B	131	LEU	5.0
2	B	553	GLU	5.0
2	A	784	GLY	5.0
2	B	87	VAL	5.0
2	A	131	LEU	4.9
2	B	547	THR	4.9
2	C	271	ALA	4.9
2	A	790	GLN	4.9
2	B	301	LYS	4.9
2	B	348	ILE	4.9
1	b	150	SER	4.9
1	c	186	ALA	4.9
2	A	656	MET	4.9
2	A	338	GLN	4.9
2	C	544	LEU	4.9
2	B	482	SER	4.9
2	C	46	ALA	4.9
2	C	360	ALA	4.9
2	A	42	GLY	4.9
2	A	85	LYS	4.9
2	A	412	ASN	4.9
2	C	464	GLN	4.9
2	A	39	VAL	4.9
2	A	165	SER	4.9
2	A	706	ASP	4.9
2	C	530	GLY	4.9
2	B	408	THR	4.9
2	C	316	THR	4.9
2	C	780	GLU	4.9
1	a	145	LEU	4.9
1	a	150	SER	4.9
2	B	197	SER	4.9
2	B	366	ILE	4.9
2	C	619	ILE	4.9
2	B	614	VAL	4.9
1	a	184	GLU	4.9
1	a	206	GLU	4.9
2	B	261	LEU	4.9
2	A	513	GLN	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	9	ARG	4.9
2	C	97	LYS	4.9
2	B	371	ILE	4.8
2	C	648	ASP	4.8
2	A	155	ASN	4.8
2	A	375	VAL	4.8
2	B	158	ALA	4.8
2	C	243	ASP	4.8
2	C	138	VAL	4.8
2	C	480	VAL	4.8
2	B	478	MET	4.8
1	b	158	GLU	4.8
2	C	372	GLU	4.8
1	b	142	LEU	4.8
2	B	239	VAL	4.8
2	A	268	ILE	4.8
2	C	207	ILE	4.8
2	B	720	THR	4.8
2	B	752	ALA	4.8
2	A	201	LYS	4.8
2	B	124	LEU	4.8
2	B	449	LEU	4.8
2	C	482	SER	4.8
2	C	428	ASP	4.8
2	B	184	GLY	4.8
2	A	124	LEU	4.8
2	C	553	GLU	4.8
2	A	138	VAL	4.8
2	A	344	VAL	4.8
2	A	613	VAL	4.8
1	b	211	THR	4.8
2	A	77	THR	4.8
2	A	602	LEU	4.8
2	C	435	GLU	4.8
2	B	480	VAL	4.8
2	B	540	SER	4.8
2	B	127	LEU	4.8
2	C	546	PRO	4.7
2	B	747	ALA	4.7
1	a	141	SER	4.7
1	c	150	SER	4.7
2	A	48	LYS	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	789	GLY	4.7
2	A	199	ARG	4.7
2	B	241	THR	4.7
2	A	534	PRO	4.7
2	B	48	LYS	4.7
2	A	141	LEU	4.7
2	A	550	GLY	4.7
2	C	500	LEU	4.7
2	B	763	ARG	4.7
2	A	368	ASP	4.7
1	c	187	THR	4.7
2	B	337	ILE	4.7
2	C	712	HIS	4.7
2	B	429	ALA	4.7
2	A	93	ASP	4.7
2	B	217	ILE	4.7
2	B	421	ASP	4.7
2	C	100	HIS	4.7
1	b	217	ALA	4.7
2	C	140	GLN	4.7
2	B	75	SER	4.7
2	B	460	TRP	4.7
1	b	209	LEU	4.7
2	C	234	LEU	4.7
2	A	193	ILE	4.7
2	B	625	ASP	4.7
2	A	707	GLU	4.7
2	A	736	GLU	4.7
2	B	367	THR	4.7
2	C	171	THR	4.7
2	C	216	ALA	4.7
2	C	30	GLY	4.7
2	C	471	VAL	4.7
2	B	425	LYS	4.7
2	B	115	GLU	4.7
2	B	212	VAL	4.6
2	B	364	VAL	4.6
1	a	214	LYS	4.6
2	C	781	LEU	4.6
2	C	496	THR	4.6
1	b	178	GLN	4.6
2	A	323	TYR	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	611	TYR	4.6
1	c	160	ARG	4.6
2	A	15	ALA	4.6
2	A	622	ALA	4.6
1	a	165	VAL	4.6
2	A	382	ILE	4.6
2	A	574	MET	4.6
2	A	3	PHE	4.6
2	C	168	ARG	4.6
2	A	82	PRO	4.6
2	A	364	VAL	4.6
2	A	778	SER	4.6
2	B	353	GLY	4.6
2	B	725	LEU	4.6
2	A	703	ASN	4.6
2	B	335	GLN	4.6
2	C	227	ASN	4.6
2	A	17	ALA	4.6
1	a	207	HIS	4.6
2	A	127	LEU	4.6
2	A	128	GLY	4.6
2	A	522	LYS	4.6
1	a	125	GLN	4.6
2	A	343	SER	4.6
2	B	400	SER	4.6
2	A	162	THR	4.6
1	c	217	ALA	4.6
2	A	686	LYS	4.6
2	B	130	SER	4.6
2	B	663	SER	4.6
1	b	191	ILE	4.5
2	A	519	ALA	4.5
2	B	418	GLN	4.5
1	b	177	ASN	4.5
2	A	181	PRO	4.5
2	C	161	PRO	4.5
1	c	184	GLU	4.5
2	C	114	ARG	4.5
2	B	15	ALA	4.5
2	C	436	PHE	4.5
2	C	272	GLY	4.5
2	B	194	GLU	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	556	ARG	4.5
2	C	561	SER	4.5
2	C	717	LYS	4.5
2	C	379	ASP	4.5
2	A	619	ILE	4.5
2	C	748	LYS	4.5
1	b	162	TYR	4.5
1	b	185	TYR	4.5
1	b	190	SER	4.5
2	C	130	SER	4.5
1	a	138	ASP	4.5
1	a	183	LEU	4.5
2	C	170	LEU	4.5
2	A	540	SER	4.5
1	c	209	LEU	4.5
2	B	227	ASN	4.5
2	B	382	ILE	4.5
2	B	653	ILE	4.5
2	B	307	GLY	4.5
2	B	159	ASN	4.5
2	C	125	ASN	4.5
2	B	320	TYR	4.5
2	C	21	ALA	4.5
2	C	521	ALA	4.5
2	A	186	SER	4.5
2	A	740	SER	4.5
2	B	388	PRO	4.4
2	B	764	PRO	4.4
2	A	275	ILE	4.4
2	C	108	ILE	4.4
1	b	208	ALA	4.4
2	B	157	ASN	4.4
2	A	457	LYS	4.4
1	b	180	SER	4.4
2	B	34	ILE	4.4
2	B	164	ASP	4.4
2	B	445	THR	4.4
1	c	146	ASN	4.4
2	B	503	GLU	4.4
2	C	94	GLU	4.4
2	A	110	LEU	4.4
2	A	208	GLY	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	207	ILE	4.4
2	A	498	LYS	4.4
2	A	716	LYS	4.4
2	B	126	ASN	4.4
2	B	703	ASN	4.4
2	C	399	GLY	4.4
1	b	212	ILE	4.4
2	A	230	VAL	4.4
2	B	577	TYR	4.4
2	A	354	LEU	4.4
2	C	279	ASP	4.4
2	C	393	ASP	4.4
2	C	79	HIS	4.4
2	C	326	LYS	4.4
2	C	534	PRO	4.4
2	C	502	MET	4.4
2	B	10	ALA	4.4
2	C	135	ARG	4.4
2	C	268	ILE	4.4
2	C	123	VAL	4.4
2	B	537	PRO	4.4
2	C	501	ASN	4.4
1	a	163	LEU	4.4
2	B	527	ALA	4.4
2	A	264	VAL	4.4
2	A	795	ASP	4.4
2	B	31	THR	4.4
2	C	317	LEU	4.4
2	C	461	LYS	4.4
2	B	430	ALA	4.3
2	B	612	SER	4.3
2	B	82	PRO	4.3
2	B	229	GLU	4.3
2	B	626	VAL	4.3
2	B	775	ASP	4.3
2	A	420	LEU	4.3
2	A	320	TYR	4.3
2	A	549	VAL	4.3
2	A	106	GLU	4.3
2	A	161	PRO	4.3
2	B	219	GLU	4.3
2	B	304	LEU	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	318	ASP	4.3
2	C	573	ASP	4.3
2	A	280	ALA	4.3
2	B	746	ALA	4.3
2	C	559	ALA	4.3
1	c	191	ILE	4.3
2	C	129	VAL	4.3
2	A	383	SER	4.3
2	B	451	GLU	4.3
2	A	687	ASP	4.3
2	A	738	ASP	4.3
2	B	738	ASP	4.3
2	B	798	ASP	4.3
2	B	9	ARG	4.3
2	C	550	GLY	4.3
1	c	144	LYS	4.3
2	C	201	LYS	4.3
1	c	176	GLU	4.3
2	A	209	GLU	4.3
1	a	152	THR	4.3
2	A	776	ARG	4.3
2	C	278	ILE	4.3
2	C	479	VAL	4.3
2	A	726	MET	4.3
2	C	37	GLY	4.3
2	C	383	SER	4.3
2	C	568	SER	4.3
1	b	137	GLU	4.3
2	C	88	ILE	4.3
2	A	374	ALA	4.3
2	A	518	VAL	4.3
2	C	687	ASP	4.3
1	b	136	PHE	4.3
2	A	631	LEU	4.3
2	B	313	GLY	4.3
2	B	94	GLU	4.2
2	C	620	GLU	4.2
2	B	404	LEU	4.2
2	C	541	PHE	4.2
2	B	204	PRO	4.2
2	B	275	ILE	4.2
2	C	663	SER	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	694	LYS	4.2
1	a	212	ILE	4.2
2	B	28	ASN	4.2
2	A	192	VAL	4.2
2	A	79	HIS	4.2
2	C	53	LEU	4.2
2	A	262	LYS	4.2
1	c	155	TYR	4.2
1	b	149	GLY	4.2
2	B	4	GLY	4.2
2	B	11	GLN	4.2
2	C	61	GLN	4.2
2	A	775	ASP	4.2
2	B	55	LEU	4.2
2	A	569	MET	4.2
1	b	207	HIS	4.2
2	B	789	GLY	4.2
2	A	318	ASP	4.2
2	A	384	ASP	4.2
2	B	324	ILE	4.2
2	C	368	ASP	4.2
2	A	21	ALA	4.2
2	C	237	LYS	4.2
2	A	779	GLU	4.2
2	A	197	SER	4.2
2	B	352	GLN	4.2
2	A	377	LEU	4.2
1	c	135	ASP	4.2
2	A	231	PRO	4.2
2	A	386	PHE	4.2
2	A	618	ALA	4.2
2	C	378	SER	4.2
2	A	223	GLN	4.2
2	A	394	LEU	4.2
2	A	733	ARG	4.2
2	A	580	LYS	4.2
2	B	731	THR	4.2
2	A	430	ALA	4.2
2	B	26	HIS	4.1
1	b	197	GLU	4.1
2	A	54	GLY	4.1
2	C	465	GLY	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	317	LEU	4.1
2	C	67	LEU	4.1
2	B	452	GLN	4.1
2	B	523	ALA	4.1
1	a	135	ASP	4.1
2	B	260	ARG	4.1
2	B	192	VAL	4.1
2	B	464	GLN	4.1
2	B	541	PHE	4.1
2	B	370	ALA	4.1
2	C	280	ALA	4.1
2	A	22	LEU	4.1
1	a	144	LYS	4.1
2	B	230	VAL	4.1
2	A	137	GLN	4.1
2	C	101	SER	4.1
1	a	211	THR	4.1
2	A	330	LEU	4.1
2	C	127	LEU	4.1
2	A	728	ASP	4.1
2	C	40	ARG	4.1
2	C	626	VAL	4.1
2	B	84	ALA	4.1
2	A	558	LEU	4.1
2	A	606	VAL	4.1
2	B	176	GLU	4.1
2	C	43	GLU	4.1
2	A	441	SER	4.1
2	C	143	GLY	4.1
2	C	211	GLY	4.1
2	C	660	VAL	4.1
2	A	690	MET	4.1
2	B	188	GLU	4.1
2	A	24	LEU	4.1
2	A	276	LEU	4.1
1	c	156	SER	4.1
2	C	400	SER	4.1
2	C	220	GLY	4.1
2	C	446	GLU	4.0
2	B	733	ARG	4.0
2	A	561	SER	4.0
2	B	689	VAL	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	657	THR	4.0
2	C	772	HIS	4.0
2	C	497	ASP	4.0
2	A	532	LYS	4.0
2	A	203	ASN	4.0
2	C	472	THR	4.0
1	c	198	GLU	4.0
2	B	379	ASP	4.0
2	B	384	ASP	4.0
2	C	503	GLU	4.0
2	C	355	ARG	4.0
2	A	761	GLY	4.0
2	C	478	MET	4.0
2	C	564	GLY	4.0
2	C	612	SER	4.0
2	A	609	LYS	4.0
2	B	401	LYS	4.0
2	B	209	GLU	4.0
2	B	185	ARG	4.0
2	C	318	ASP	4.0
2	B	790	GLN	4.0
2	C	447	GLN	4.0
2	A	615	LEU	4.0
2	B	121	ALA	4.0
2	C	701	PHE	4.0
1	a	154	LEU	4.0
2	B	758	LEU	4.0
2	A	768	ALA	4.0
1	a	198	GLU	4.0
1	b	188	GLU	4.0
2	B	514	ASP	4.0
2	A	538	ILE	4.0
2	B	134	ALA	4.0
2	B	360	ALA	4.0
2	B	129	VAL	4.0
2	C	803	VAL	4.0
1	a	133	PHE	4.0
2	A	543	PHE	4.0
2	A	53	LEU	3.9
2	B	753	GLU	3.9
2	A	88	ILE	3.9
2	A	70	ARG	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	157	ASN	3.9
2	C	424	ARG	3.9
2	C	261	LEU	3.9
2	C	581	HIS	3.9
1	c	206	GLU	3.9
2	B	208	GLY	3.9
2	B	213	GLY	3.9
2	B	804	LYS	3.9
1	a	128	GLN	3.9
2	A	533	ASP	3.9
2	B	745	ASP	3.9
2	A	531	LEU	3.9
2	C	416	LEU	3.9
2	C	537	PRO	3.9
2	B	162	THR	3.9
1	b	140	ILE	3.9
2	A	340	ASP	3.9
2	C	96	ARG	3.9
2	C	527	ALA	3.9
2	A	416	LEU	3.9
2	C	659	ASN	3.9
2	C	63	GLU	3.9
2	A	98	LEU	3.9
2	A	180	ASP	3.9
2	A	734	LEU	3.9
2	A	56	GLY	3.9
2	B	658	SER	3.9
2	C	629	ILE	3.9
2	C	657	THR	3.9
2	C	763	ARG	3.9
2	A	633	VAL	3.9
2	B	330	LEU	3.9
2	C	142	LEU	3.9
2	C	770	GLN	3.9
2	B	345	ASP	3.9
2	B	495	GLU	3.9
2	B	448	ARG	3.9
2	C	603	THR	3.9
2	A	72	GLN	3.9
2	C	224	GLN	3.9
2	A	225	ILE	3.9
2	A	353	GLY	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	507	HIS	3.9
2	A	232	GLU	3.9
2	C	607	ARG	3.9
1	a	151	LYS	3.8
2	B	534	PRO	3.8
2	A	163	LEU	3.8
2	B	38	LEU	3.8
2	A	212	VAL	3.8
2	A	700	GLU	3.8
2	C	167	ALA	3.8
2	A	530	GLY	3.8
2	B	739	LEU	3.8
2	A	711	PHE	3.8
2	B	165	SER	3.8
2	A	443	ARG	3.8
2	A	783	ARG	3.8
2	B	424	ARG	3.8
2	A	692	GLU	3.8
2	B	481	SER	3.8
2	B	54	GLY	3.8
2	A	263	LYS	3.8
2	B	533	ASP	3.8
2	A	33	HIS	3.8
2	B	132	ASN	3.8
2	A	805	THR	3.8
2	B	699	PRO	3.8
2	C	547	THR	3.8
2	B	711	PHE	3.8
2	C	92	MET	3.8
2	B	396	ASP	3.8
2	B	768	ALA	3.8
2	C	58	GLU	3.8
2	C	505	ILE	3.8
2	A	260	ARG	3.8
2	A	302	PRO	3.8
2	A	545	GLY	3.8
2	C	609	LYS	3.8
1	a	166	ASP	3.8
2	A	188	GLU	3.8
1	b	126	LYS	3.7
1	b	156	SER	3.7
1	c	199	TYR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	a	191	ILE	3.7
2	B	499	LEU	3.7
2	C	413	LEU	3.7
2	A	463	LYS	3.7
2	B	776	ARG	3.7
2	C	385	ARG	3.7
2	B	517	VAL	3.7
2	C	411	PRO	3.7
2	C	649	PHE	3.7
2	A	11	GLN	3.7
2	B	651	ASN	3.7
2	A	26	HIS	3.7
2	B	175	LYS	3.7
2	B	661	GLY	3.7
2	B	734	LEU	3.7
2	A	114	ARG	3.7
2	B	432	GLN	3.7
1	c	161	TYR	3.7
2	A	542	ILE	3.7
2	B	381	TYR	3.7
2	C	105	THR	3.7
2	A	40	ARG	3.7
2	C	333	ARG	3.7
2	A	742	GLU	3.7
2	B	422	GLU	3.7
2	C	384	ASP	3.7
2	C	223	GLN	3.7
2	B	201	LYS	3.7
2	C	203	ASN	3.7
1	a	153	THR	3.7
1	c	175	VAL	3.7
2	B	799	GLY	3.7
2	C	548	GLY	3.7
2	A	183	ILE	3.7
2	A	391	ALA	3.7
2	B	237	LYS	3.7
2	A	321	ARG	3.7
2	A	744	THR	3.7
1	a	149	GLY	3.7
2	C	111	GLY	3.7
2	C	754	GLU	3.7
2	A	648	ASP	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	767	ARG	3.6
1	a	177	ASN	3.6
2	B	228	ASN	3.6
2	C	412	ASN	3.6
2	C	578	MET	3.6
2	C	361	HIS	3.6
2	A	49	ALA	3.6
2	C	320	TYR	3.6
2	A	617	ASP	3.6
2	B	428	ASP	3.6
2	A	803	VAL	3.6
2	C	481	SER	3.6
2	C	542	ILE	3.6
2	B	521	ALA	3.6
2	C	773	VAL	3.6
2	A	393	ASP	3.6
2	B	708	ILE	3.6
2	A	31	THR	3.6
2	A	147	THR	3.6
1	b	174	GLU	3.6
2	C	65	GLU	3.6
2	B	269	ARG	3.6
2	A	404	LEU	3.6
2	B	170	LEU	3.6
1	c	166	ASP	3.6
2	A	788	LYS	3.6
2	C	187	LYS	3.6
1	a	189	SER	3.6
2	C	81	THR	3.6
2	B	271	ALA	3.6
2	C	526	ARG	3.6
2	C	322	LYS	3.6
2	B	504	ASN	3.6
2	A	84	ALA	3.6
2	C	518	VAL	3.6
2	C	698	ARG	3.6
2	C	449	LEU	3.6
2	A	562	ILE	3.6
2	A	691	GLY	3.6
2	A	475	ASP	3.6
2	C	363	ARG	3.6
2	C	515	GLU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	a	126	LYS	3.6
2	B	732	LYS	3.6
2	C	565	ASP	3.5
2	B	205	VAL	3.5
2	A	58	GLU	3.5
2	A	359	GLU	3.5
2	C	583	THR	3.5
2	B	69	GLY	3.5
2	C	11	GLN	3.5
2	C	512	GLY	3.5
2	B	112	LEU	3.5
1	a	213	LYS	3.5
2	A	156	SER	3.5
2	C	495	GLU	3.5
2	C	786	ILE	3.5
1	a	187	THR	3.5
2	C	367	THR	3.5
2	C	339	VAL	3.5
2	B	47	ALA	3.5
2	C	438	LYS	3.5
2	A	107	HIS	3.5
2	A	146	GLU	3.5
2	B	454	GLU	3.5
2	A	729	GLN	3.5
2	C	513	GLN	3.5
2	C	262	LYS	3.5
2	B	442	LEU	3.5
2	B	657	THR	3.5
2	B	613	VAL	3.5
2	C	783	ARG	3.5
2	B	532	LYS	3.5
2	C	610	PRO	3.5
2	A	555	ALA	3.5
2	C	477	ALA	3.5
2	C	621	LYS	3.5
2	A	371	ILE	3.5
2	A	760	TYR	3.5
2	B	705	ILE	3.5
2	C	122	ARG	3.5
2	C	606	VAL	3.5
2	A	121	ALA	3.5
1	a	190	SER	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	c	205	SER	3.5
2	A	167	ALA	3.5
2	A	557	ALA	3.5
1	a	155	TYR	3.5
2	A	170	LEU	3.4
1	a	134	GLY	3.4
1	b	135	ASP	3.4
2	A	169	ASP	3.4
2	B	41	GLU	3.4
2	C	575	SER	3.4
1	b	169	ASN	3.4
2	C	374	ALA	3.4
2	C	639	LEU	3.4
2	B	633	VAL	3.4
2	C	390	LYS	3.4
2	C	514	ASP	3.4
2	A	476	ILE	3.4
2	A	136	GLN	3.4
2	A	373	ALA	3.4
2	C	49	ALA	3.4
2	B	556	ARG	3.4
2	C	427	LYS	3.4
2	C	718	HIS	3.4
1	a	172	ASP	3.4
2	B	622	ALA	3.4
2	B	16	LEU	3.4
2	B	338	GLN	3.4
2	B	145	ASN	3.4
1	a	139	VAL	3.4
2	C	605	LYS	3.4
2	C	306	ARG	3.4
2	C	407	PHE	3.4
2	C	769	ILE	3.4
2	A	762	ALA	3.4
2	A	448	ARG	3.4
2	C	650	ARG	3.4
2	B	111	GLY	3.4
2	C	785	ASN	3.4
2	A	572	ILE	3.4
2	A	426	GLU	3.4
2	B	611	TYR	3.4
2	C	376	LYS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	711	PHE	3.4
2	B	574	MET	3.4
1	b	205	SER	3.4
1	a	146	ASN	3.4
1	a	196	LEU	3.4
1	c	208	ALA	3.3
2	C	622	ALA	3.3
2	B	797	GLU	3.3
2	B	306	ARG	3.3
1	c	128	GLN	3.3
2	A	4	GLY	3.3
2	A	309	LEU	3.3
2	B	56	GLY	3.3
2	C	10	ALA	3.3
2	A	715	GLU	3.3
2	B	39	VAL	3.3
2	B	704	ARG	3.3
1	b	168	CYS	3.3
2	C	222	ALA	3.3
2	C	519	ALA	3.3
2	A	159	ASN	3.3
2	A	103	VAL	3.3
2	B	610	PRO	3.3
2	A	240	MET	3.3
1	a	176	GLU	3.3
2	A	437	GLU	3.3
2	B	346	GLU	3.3
2	C	166	LEU	3.3
2	B	740	SER	3.3
2	A	242	LEU	3.3
1	b	144	LYS	3.3
2	B	95	ALA	3.3
2	B	22	LEU	3.3
2	C	107	HIS	3.3
2	B	513	GLN	3.3
2	A	423	VAL	3.3
2	B	756	VAL	3.3
1	a	170	MET	3.3
2	B	98	LEU	3.3
2	C	330	LEU	3.3
2	A	204	PRO	3.3
2	A	445	THR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	81	THR	3.3
2	A	326	LYS	3.2
2	B	779	GLU	3.2
2	B	223	GLN	3.2
2	B	387	LEU	3.2
2	B	560	GLU	3.2
2	B	736	GLU	3.2
1	a	216	PHE	3.2
2	A	52	ALA	3.2
2	A	756	VAL	3.2
2	A	45	ILE	3.2
2	B	259	ASP	3.2
2	A	228	ASN	3.2
2	B	563	PHE	3.2
2	B	413	LEU	3.2
2	C	321	ARG	3.2
2	C	387	LEU	3.2
2	A	755	GLY	3.2
2	B	565	ASP	3.2
2	B	795	ASP	3.2
2	B	568	SER	3.2
2	C	721	GLU	3.2
2	B	52	ALA	3.2
2	C	226	ILE	3.2
2	C	382	ILE	3.2
1	a	130	VAL	3.2
2	B	344	VAL	3.2
2	C	406	SER	3.2
2	C	494	THR	3.2
2	A	41	GLU	3.2
2	A	73	GLU	3.2
2	C	516	ALA	3.2
2	C	560	GLU	3.2
2	B	29	ILE	3.2
2	A	322	LYS	3.2
2	B	735	LYS	3.2
2	C	522	LYS	3.2
2	C	784	GLY	3.2
2	A	406	SER	3.2
2	A	117	GLU	3.2
2	A	222	ALA	3.2
2	A	187	LYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	326	LYS	3.2
2	B	716	LYS	3.2
2	C	418	GLN	3.2
1	a	167	PHE	3.2
2	A	450	ARG	3.2
1	a	192	SER	3.1
2	A	390	LYS	3.1
2	A	632	GLN	3.1
2	C	647	VAL	3.1
2	B	519	ALA	3.1
1	a	218	SER	3.1
2	A	780	GLU	3.1
2	C	73	GLU	3.1
2	C	309	LEU	3.1
2	C	651	ASN	3.1
2	A	751	VAL	3.1
2	C	453	VAL	3.1
2	C	539	GLY	3.1
1	b	214	LYS	3.1
2	B	97	LYS	3.1
2	A	325	GLU	3.1
2	B	446	GLU	3.1
1	a	205	SER	3.1
2	C	139	LEU	3.1
2	A	140	GLN	3.1
2	B	181	PRO	3.1
2	A	261	LEU	3.1
2	A	464	GLN	3.1
2	B	61	GLN	3.1
2	B	177	ASP	3.1
2	C	745	ASP	3.1
1	a	140	ILE	3.1
2	A	370	ALA	3.1
2	A	634	LEU	3.1
2	C	377	LEU	3.1
1	b	198	GLU	3.1
2	A	579	GLU	3.1
2	C	8	GLU	3.1
2	C	69	GLY	3.1
2	A	142	LEU	3.1
2	A	234	LEU	3.1
2	B	110	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	422	GLU	3.1
2	B	198	ARG	3.1
2	A	705	ILE	3.1
2	C	78	ILE	3.1
2	A	345	ASP	3.0
2	B	639	LEU	3.0
2	C	345	ASP	3.0
2	A	439	ALA	3.0
2	B	21	ALA	3.0
2	B	438	LYS	3.0
2	C	695	ARG	3.0
2	A	737	GLN	3.0
2	B	163	LEU	3.0
1	b	166	ASP	3.0
2	A	178	SER	3.0
2	B	552	THR	3.0
2	C	343	SER	3.0
2	C	646	THR	3.0
2	A	132	ASN	3.0
2	C	176	GLU	3.0
1	a	136	PHE	3.0
1	a	159	ASN	3.0
2	C	173	ILE	3.0
2	A	566	GLU	3.0
1	b	187	THR	3.0
2	A	763	ARG	3.0
2	B	77	THR	3.0
1	a	193	ILE	3.0
1	c	183	LEU	3.0
2	B	118	GLY	3.0
2	B	415	GLU	3.0
2	B	18	GLN	3.0
2	A	214	LYS	3.0
2	B	605	LYS	3.0
2	C	133	LYS	3.0
2	C	77	THR	3.0
2	C	441	SER	3.0
2	B	654	LEU	3.0
2	B	529	ALA	3.0
2	A	87	VAL	3.0
2	A	357	ARG	3.0
2	A	796	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	536	ARG	3.0
2	A	745	ASP	3.0
2	C	144	SER	3.0
1	b	159	ASN	3.0
2	A	604	GLU	3.0
2	C	232	GLU	3.0
2	C	538	ILE	2.9
1	b	189	SER	2.9
2	A	102	TYR	2.9
1	a	208	ALA	2.9
2	A	47	ALA	2.9
2	B	516	ALA	2.9
1	b	175	VAL	2.9
2	A	451	GLU	2.9
2	A	456	THR	2.9
2	A	758	LEU	2.9
2	A	748	LYS	2.9
2	A	400	SER	2.9
1	a	186	ALA	2.9
2	B	235	ARG	2.9
2	C	141	LEU	2.9
2	C	696	ALA	2.9
2	C	76	GLN	2.9
2	B	272	GLY	2.9
2	A	610	PRO	2.9
1	a	160	ARG	2.9
1	c	195	ARG	2.9
2	A	238	ARG	2.9
2	C	439	ALA	2.9
2	A	346	GLU	2.9
2	C	771	LYS	2.9
2	A	739	LEU	2.9
2	A	355	ARG	2.9
2	B	225	ILE	2.9
2	B	450	ARG	2.9
2	C	198	ARG	2.9
2	C	342	PRO	2.9
2	B	492	ALA	2.9
2	A	347	SER	2.9
2	B	20	GLU	2.9
2	B	168	ARG	2.9
2	A	807	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	c	215	HIS	2.9
2	B	687	ASP	2.9
2	C	798	ASP	2.9
1	c	173	GLU	2.9
2	B	466	GLN	2.9
2	B	649	PHE	2.9
2	B	616	LEU	2.9
2	A	339	VAL	2.8
2	A	698	ARG	2.8
2	B	522	LYS	2.8
2	C	498	LYS	2.8
2	A	177	ASP	2.8
2	C	757	ASP	2.8
2	B	697	PHE	2.8
2	C	188	GLU	2.8
2	B	27	ASN	2.8
2	A	398	ALA	2.8
2	A	97	LYS	2.8
2	A	91	SER	2.8
2	A	266	ASP	2.8
2	B	37	GLY	2.8
2	B	493	GLN	2.8
2	C	792	ILE	2.8
1	b	184	GLU	2.8
2	A	184	GLY	2.8
2	A	735	LYS	2.8
2	A	166	LEU	2.8
2	C	6	PHE	2.8
2	B	13	VAL	2.8
2	B	660	VAL	2.8
2	A	30	GLY	2.8
2	B	44	GLY	2.8
2	A	473	VAL	2.8
2	C	723	VAL	2.8
2	A	99	GLY	2.8
2	A	732	LYS	2.8
2	A	10	ALA	2.8
2	C	17	ALA	2.8
2	C	228	ASN	2.7
1	b	170	MET	2.7
2	A	148	GLY	2.7
2	B	471	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	b	134	GLY	2.7
2	B	530	GLY	2.7
2	C	761	GLY	2.7
2	C	791	HIS	2.7
2	C	567	GLU	2.7
2	B	494	THR	2.7
2	B	802	VAL	2.7
2	C	455	ASP	2.7
2	C	709	ILE	2.7
2	A	46	ALA	2.7
2	A	746	ALA	2.7
1	a	158	GLU	2.7
2	C	779	GLU	2.7
2	B	484	THR	2.7
1	b	172	ASP	2.7
2	A	179	LEU	2.7
2	C	44	GLY	2.7
2	B	5	ARG	2.7
2	C	473	VAL	2.7
2	C	652	THR	2.7
2	A	396	ASP	2.7
1	b	215	HIS	2.7
2	A	627	PHE	2.7
2	C	29	ILE	2.7
2	A	51	GLN	2.7
2	B	721	GLU	2.7
2	A	118	GLY	2.7
2	A	95	ALA	2.7
2	A	536	ARG	2.7
2	C	423	VAL	2.7
2	A	432	GLN	2.7
2	C	778	SER	2.7
2	A	559	ALA	2.6
2	C	636	ASP	2.6
1	c	162	TYR	2.6
2	C	199	ARG	2.6
2	C	766	ARG	2.6
2	A	227	ASN	2.6
1	a	171	THR	2.6
2	B	555	ALA	2.6
2	C	186	SER	2.6
2	B	19	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	348	ILE	2.6
2	B	322	LYS	2.6
2	A	402	VAL	2.6
2	B	102	TYR	2.6
2	B	615	LEU	2.6
2	C	24	LEU	2.6
2	A	334	PHE	2.6
2	C	59	LYS	2.6
2	C	793	VAL	2.6
2	B	136	GLN	2.6
2	A	69	GLY	2.6
2	A	116	GLY	2.6
2	B	17	ALA	2.6
2	B	167	ALA	2.6
2	A	38	LEU	2.6
2	C	103	VAL	2.6
2	C	75	SER	2.6
2	C	340	ASP	2.6
1	a	157	PHE	2.6
2	C	18	GLN	2.6
1	a	148	ASN	2.6
2	A	747	ALA	2.6
2	C	52	ALA	2.6
2	C	608	ARG	2.6
1	a	156	SER	2.6
2	B	343	SER	2.6
2	C	764	PRO	2.6
2	A	461	LYS	2.6
2	B	531	LEU	2.6
2	B	692	GLU	2.6
2	C	777	LEU	2.6
2	C	74	MET	2.6
1	c	133	PHE	2.5
2	A	444	ASP	2.5
2	B	648	ASP	2.5
2	B	222	ALA	2.5
2	C	618	ALA	2.5
2	A	551	LYS	2.5
2	C	86	LYS	2.5
2	A	786	ILE	2.5
2	B	178	SER	2.5
2	B	347	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	332	ARG	2.5
2	B	525	ARG	2.5
2	B	412	ASN	2.5
1	a	127	LEU	2.5
2	A	160	THR	2.5
2	C	722	ILE	2.5
2	C	794	LEU	2.5
2	B	144	SER	2.5
2	C	740	SER	2.5
1	a	174	GLU	2.5
1	c	157	PHE	2.5
2	C	334	PHE	2.5
2	A	104	GLY	2.5
2	A	267	GLU	2.5
2	C	41	GLU	2.5
2	C	739	LEU	2.5
2	A	465	GLY	2.5
2	B	74	MET	2.5
2	A	419	LYS	2.5
2	B	543	PHE	2.5
2	B	634	LEU	2.5
2	A	74	MET	2.5
2	B	25	GLY	2.5
1	b	128	GLN	2.5
2	B	72	GLN	2.5
2	B	759	GLU	2.5
2	C	366	ILE	2.5
2	C	444	ASP	2.5
2	B	796	VAL	2.5
2	C	4	GLY	2.5
2	C	373	ALA	2.4
2	B	542	ILE	2.4
2	C	426	GLU	2.4
1	c	132	ARG	2.4
2	C	185	ARG	2.4
2	B	180	ASP	2.4
2	C	174	ALA	2.4
2	B	76	GLN	2.4
2	B	83	ARG	2.4
2	A	787	HIS	2.4
2	A	695	ARG	2.4
2	C	802	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	b	153	THR	2.4
2	A	12	LYS	2.4
2	B	263	LYS	2.4
2	C	137	GLN	2.4
2	C	451	GLU	2.4
1	c	218	SER	2.4
2	A	701	PHE	2.4
2	B	771	LYS	2.4
2	A	19	GLU	2.4
1	c	200	GLY	2.4
2	B	583	THR	2.4
2	B	618	ALA	2.4
2	A	607	ARG	2.4
1	b	213	LYS	2.4
2	B	51	GLN	2.3
2	B	707	GLU	2.3
1	a	203	ILE	2.3
2	A	13	VAL	2.3
2	A	195	VAL	2.3
2	B	607	ARG	2.3
2	A	428	ASP	2.3
2	C	420	LEU	2.3
1	c	174	GLU	2.3
2	A	399	GLY	2.3
2	B	635	GLU	2.3
2	C	800	GLU	2.3
2	B	456	THR	2.3
2	B	718	HIS	2.3
1	a	204	ILE	2.3
2	A	337	ILE	2.3
2	A	239	VAL	2.3
2	A	806	THR	2.3
2	A	663	SER	2.3
2	A	455	ASP	2.3
2	B	361	HIS	2.3
2	A	173	ILE	2.3
2	A	637	GLY	2.3
2	A	168	ARG	2.3
2	C	535	LYS	2.3
2	C	782	LEU	2.3
2	B	57	SER	2.3
2	B	33	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	226	ILE	2.3
2	C	755	GLY	2.3
1	c	196	LEU	2.3
2	B	357	ARG	2.3
2	C	308	GLU	2.3
1	c	167	PHE	2.3
2	C	225	ILE	2.3
2	B	342	PRO	2.3
2	A	414	LYS	2.3
2	A	438	LYS	2.3
2	C	753	GLU	2.3
2	C	145	ASN	2.3
2	A	570	ILE	2.3
2	A	781	LEU	2.3
1	a	132	ARG	2.3
2	C	462	GLU	2.2
2	B	512	GLY	2.2
2	C	212	VAL	2.2
2	C	730	LEU	2.2
2	A	560	GLU	2.2
2	B	655	ILE	2.2
2	C	476	ILE	2.2
2	A	105	THR	2.2
2	A	301	LYS	2.2
2	C	456	THR	2.2
2	C	631	LEU	2.2
2	C	768	ALA	2.2
2	A	446	GLU	2.2
2	C	604	GLU	2.2
2	B	173	ILE	2.2
1	c	172	ASP	2.2
2	B	30	GLY	2.2
1	c	151	LYS	2.2
2	B	187	LYS	2.2
2	C	177	ASP	2.2
2	A	5	ARG	2.2
2	A	37	GLY	2.2
2	C	307	GLY	2.2
2	A	101	SER	2.2
2	B	801	PHE	2.2
2	A	71	GLY	2.2
2	C	445	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	179	LEU	2.2
2	A	270	GLN	2.2
2	A	94	GLU	2.2
2	B	695	ARG	2.2
2	A	307	GLY	2.1
1	b	151	LYS	2.1
2	C	458	LYS	2.1
2	B	603	THR	2.1
2	C	235	ARG	2.1
2	C	732	LYS	2.1
2	B	496	THR	2.1
2	C	720	THR	2.1
2	C	448	ARG	2.1
2	B	174	ALA	2.1
2	C	440	ALA	2.1
2	B	500	LEU	2.1
2	C	549	VAL	2.1
1	a	199	TYR	2.1
2	A	274	ILE	2.1
1	c	168	CYS	2.1
2	B	497	ASP	2.1
2	B	355	ARG	2.1
2	C	362	HIS	2.1
2	B	133	LYS	2.1
2	B	551	LYS	2.1
2	A	115	GLU	2.1
2	A	233	ILE	2.1
2	A	308	GLU	2.1
2	A	333	ARG	2.1
2	A	421	ASP	2.1
2	B	636	ASP	2.1
2	C	726	MET	2.1
2	A	440	ALA	2.1
2	A	702	ILE	2.1
2	C	429	ALA	2.1
2	B	171	THR	2.1
2	A	664	GLU	2.1
2	B	240	MET	2.0
1	a	168	CYS	2.0
2	B	341	GLN	2.0
2	C	509	ARG	2.0
2	B	617	ASP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	83	ARG	2.0
2	A	172	ALA	2.0
2	B	455	ASP	2.0
2	C	7	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.