



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 08:08 pm GMT

PDB ID : 6EMK
EMDB ID : EMD-3896
Title : Cryo-EM Structure of Saccharomyces cerevisiae Target of Rapamycin Complex 2
Authors : Karuppasamy, M.; Kusmider, B.; Oliveira, T.M.; Gaubitz, C.; Prouteau, M.; Loewith, R.; Schaffitzel, C.
Deposited on : 2017-10-02
Resolution : 8.00 Å (reported)
Based on initial model : 5FVM

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

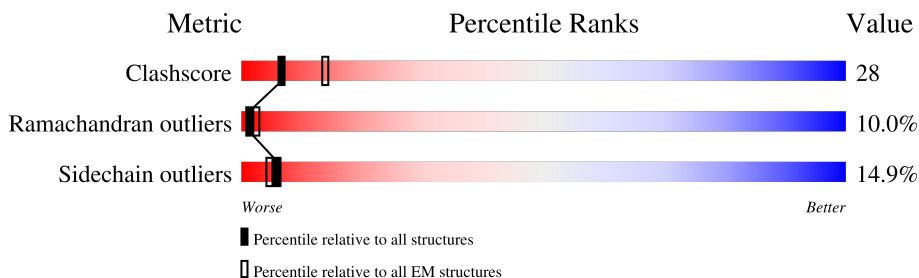
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2474	38% 42% 10% 9%
1	C	2474	38% 43% 9% 9%
2	B	303	41% 47% 10% ..
2	D	303	44% 44% 9% ..
3	E	303	91% 9%
3	F	303	88% 12%
4	G	426	33% 64%
4	H	426	30% 5% 64%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	I	1176	 6% 5% • 88%
5	J	1176	 6% 5% •• 88%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 48012 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Serine/threonine-protein kinase TOR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2262	Total	C	N	O	S	0	0
			18186	11650	3110	3345	81		
1	C	2262	Total	C	N	O	S	0	0
			18186	11650	3110	3345	81		

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	300	Total	C	N	O	S	0	0
			2372	1468	433	460	11		
2	D	300	Total	C	N	O	S	0	0
			2372	1468	433	460	11		

- Molecule 3 is a protein called Target of rapamycin complex 2 subunit TSC11.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	E	303	Total	C	N	O	0	0
			1515	909	303	303		
3	F	303	Total	C	N	O	0	0
			1515	909	303	303		

- Molecule 4 is a protein called Target of rapamycin complex 2 subunit AVO2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	G	155	Total	C	N	O	0	0
			762	452	155	155		
4	H	155	Total	C	N	O	0	0
			762	452	155	155		

- Molecule 5 is a protein called Target of rapamycin complex 2 subunit AVO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	146	1171	739	187	242	3	0	0
5	J	146	1171	739	187	242	3	0	0

GLU	S1742	K1670	A1520	E1428	A1348	F1280	K1205	I1128	Q984	ASP	I861	V774
VAL	Y1743	Q1671	L1523	Y1429	L1351	S1281	R1206	L1129	L985	E914	L862	A775
HIS	L1744	L1672	L1524	M1430	H1352	S1282	Y1207	M1130	G986	E915	K853	S776
TYR	L1745	F1675	L1525	K1433	H1353	C1283	E1208	R1134	I1062	Y916	T854	T777
S1811	D1750	F1675	T1526	K1434	K1354	W1284	D1209	R1135	Y992	P917	L778	A779
M1813	M1751	E1527	E1527	R1435	E1355	E1286	Q1242	E1136	K993	T918	E855	L779
L1814	L1752	L1528	L1528	S1436	V1356	L1287	V1213	T1137	Q994	W919	K760	K760
I1815	W1753	D1682	L1683	L1437	E1357	Q1288	V1214	R997	I860	V920	V761	V761
H1816	K1754	L1683	L1683	Y1438	E1358	T1289	K1215	P998	R861	R921	R861	R861
V1819	K1755	GLY	GLY	A1439	L1359	S1290	L1216	P999	R862	H922	R862	E784
P1820	A1756	ASP	ASP	L1440	L1359	L1291	P1217	E1001	T864	T923	T864	V768
P1821	H1757	PRO	PRO	K1603	P1362	Q1292	Q1220	E1001	V665	I927	V665	V665
A1822	M1758	ASN	ASN	L1446	T1366	E1293	Q1220	K1002	R866	L928	R866	K791
I1823	M1759	ASN	ASN	S1447	T1366	D1294	M1221	I1003	R867	R929	R867	E792
K1824	A1762	ASN	ASN	Q1607	I1367	LEU	I1222	Y1004	I868	D930	I868	W793
G1825	L1763	MET	MET	L1449	E1368	ILE	L1223	E1076	G869	W931	G869	T794
F1826	M1764	ALA	ALA	E1452	A1369	GLN	K1224	D1077	ILE	S932	S932	R795
F1827	M1764	ALA	ALA	K1453	L1370	ALA	L1149	Y1078	LEU	L933	L933	Y796
H1828	V1767	GLN	GLN	K1453	I1371	LEU	W1227	S1079	GLY	H937	L933	L797
S1829	I1768	SER	SER	E1456	S1372	CYS	Y1228	E1009	ALA	K798	K798	K798
I1830	VAL	VAL	VAL	T1456	I1373	ALA	C1229	F1010	GLY	E799	E799	E799
S1831	MET	PRO	PRO	A1457	L1373	ALA	S1230	F1010	ASP	W938	W938	W938
L1832	LEU	GLN	GLN	L1458	L1377	LEU	Q1231	I1084	PRO	A939	A939	L800
S1835	THR	SER	SER	P1459	H1378	SER	Q1232	I1014	TYR	Q942	Q942	M801
S1836	SER	LYS	LYS	M1465	T1380	SER	K1233	K1015	LYS	A943	A943	I804
S1837	VAL	ARG	ARG	L1468	A1383	GLU	E1236	I1016	HIS	I944	I944	N806
L1838	SER	VAL	VAL	L1468	I1384	ASN	D1237	K1098	ARG	C955	C955	N806
Q1839	LYS	PRO	PRO	A1469	A1385	PRO	W1238	K1099	GLU	V956	V956	F815
L1840	LYS	ARG	ARG	L1476	G1385	PRO	W1238	I1170	ILE	S957	S957	K816
A1841	GLN	HIS	HIS	E1477	L1386	GLU	L1241	Q1172	SER	F958	F958	R817
S1842	SER	V1706	P1562	E1477	L1387	ILE	I1242	H1173	SER	L959	L959	D818
S1843	GLY	K1711	Q1563	D1480	K1388	TYR	R1243	S1174	VAL	D960	D960	L821
L1844	GLY	L1712	Q1563	M1489	H1389	GLN	R1244	V1175	GLN	Q961	Q961	L821
W1848	ASP	L1713	D1566	K1490	A1390	MET	L1245	E1105	GLN	I962	I962	L824
F1849	ALA	A1714	K1567	S1491	Q1391	LEU	S1246	G1033	ASN	P963	P963	L824
G1852	SER	R1715	L1569	Q1492	L1396	LEU	I1247	E1034	ALA	P964	P964	L827
E1855	VAL	C1716	T1570	S1493	L1396	ASN	Q1248	F1035	PRO	G965	G965	L827
A1857	THR	K1719	M1571	K1496	W1402	V1320	E1252	V1039	SER	I966	I966	V835
T1858	ASP	W1723	E1572	E1497	Y1403	D1326	S1253	P1040	ILE	I967	I967	V835
M1861	GLU	R1724	T1574	F1498	K1405	D1327	L1258	E1041	ASP	L968	L968	L838
H1862	PHE	V1725	W1576	Y1499	L1406	K1328	R1259	T1042	ILE	V969	V969	L838
I1863	ASP	Q1728	T1577	L1502	Q1407	P1329	R1259	L1043	ALA	M970	M970	Y841
Q1869	ASP	P1729	R1578	L1503	R1408	P1331	R1259	T1044	LEU	R971	R971	P842
I1870	GLY	K1730	L1580	C1504	A1412	P1332	S1263	F1045	LEU	P974	P974	E843
G1871	MET	W1831	G1581	F1510	A1415	L1334	V1267	L1049	VAL	Q977	Q977	L844
L1872	ILE	R1732	C1582	R1511	E1418	K1339	A1272	L1050	GLY	I978	I978	G846
W1873	GLY	L1733	K1583	K1512	K1419	Y1340	R1273	F1046	PRO	D979	D979	L847
L1874	VAL	S1734	K1584	A1513	K1419	L1330	M1192	F1046	PRO	F982	F982	L848
L1875	ASN	M1735	M1585	V1514	G1423	A1341	E1274	L1121	ASN	Q983	Q983	N850
E1875	THR	P1736	L1586	H1516	E1424	Q1342	F1276	W1201	ASN	K1057	K1057	N850
V1876	PHE	D1588	D1588	H1516	E1424	K1343	F1276	P1202	ASN	Q1054	Q1054	N850
L1877	ASP	W1589	W1589	F1517	D1425	C1344	M1277	E1203	ASN	F982	F982	N850
P1878	ALA	L1740	L1740	F1518	S1426	H1345	A1278	R1204	ASN	Q983	Q983	N850
P1878	LYS	G1741	Q1590	M1519	V1427	H1345	S1279	E1204	ASN	Q983	Q983	N850

Q1879	V1950	L2035	R2107	W2178	E2254	E2327	V2404	P2470
L1880	S1951	N2036	P2108	M2181	R2256	V2328	Q2405	F2471
S1882	H1952	Q2037	R2109	S2182	T2257	L2331	E2406	W2472
L1954	E1953	A2038	K2110	T2183	T2258	E2332	V2407	
I1884	L1954	D2039	F2111	T2184	Y2259	G2333	E2408	
H1885	I1955	W2040	C2112	F2185	T2260	S2334	H2411	
Q1886	R1956	Y2043	L2113	F2186	R2261	E2335	A2414	
	A1957	N2044	G2115	W2187	S2262	R2336	L2415	
	A1958	M2044	S2116	H2188	L2263	F2337	R2416	
	W1961	R2047	D2117	L2189	A2264	C2338	R2419	
	H1962	K2048	D2120	E2190	V2265	C2339		
	E1963	L2049	Y2121	H2192	M2266	E2340		
	Q1964	Q2052	K2122	R2193	S2267	W2341		
	W1965	L2053	L2123	E2194	T2268	V2342		
	E1967	D1901	Y2124	E2199	L2272	V2345		
	G1968	G1903	L2125	W2201	L2275	L2346		
	L1904	Q2057	K2126	L2202	L2276	R2347		
	A1905	T2058	G2127	E2203	R2278	M2348		
	H1906	E2060	H2128	H2204	H2279	L2349		
	P1907	L2061	D2130	W2205	H2279	L2353		
	Q1908	Q2062	L2131	P2280	P2280	W2354		
	L1910	H2063	R2132	W2207	S2281	L2357		
	V1911		Q2133	L2208	M2282	L2387		
	Y1912	P2066	D2134	A2211	L2283	F2380		
	F1977	K2067	S2135	M2284	M2284	L2435		
	G1978	L2068	L2136	P2212	L2285	L2436		
	E1979	H1980	V2137	D2286	D2286	R2437		
	M1915	L2069	L2140	R2287	L2288	P2364		
	L1916	S2070	L2143	L2219	K2291	E2438		
	A1917	E2075	L2147	L2220	V2292	M2440		
	I1918	A2077	L2148	V2223	L2293	D2441		
	S1920	V2078	L2151	E2224	H2294	D2442		
	E1921	P2079	D2152	E2235	H2294	D2443		
	S1922	G2080	R2155	L2295	L2295	P2445		
			R2156	D2230	G2298	E2446		
			R1998	L2231	D2298	Q2447		
			R2004	M2231	D2299	V2448		
			E2005	N2232	C2300	D2449		
			I2006	T2233	F2301	K2450		
			G2013	E2234	E2234	L2451		
			R2014	L2242	F2301	S2452		
			N2017	K2244	A2304	Q2452		
			D2018	E2096	L2305	Q2453		
			V1942	E2096	L2306	Q2454		
			L1943	P2097	R2307	T2455		
			L1944	P2097	K2308	T2456		
			V1944	F2099	F2310	V2457		
			D1945	K2094	D2237	E2458		
			D1946	F2099	L2238	E2459		
			Q1947	S2103	L2239	G2462		
			A1947	S2104	Y2239			
			E1948	S2104	L2242	V2465		
			N2033	S2104	W2243	L2466		
			N2034	S2104	L2244	W2468		
				Q2106	E2250	C2469		
					W2251			
					L2253			

• Molecule 1: Serine/threonine-protein kinase TOR2



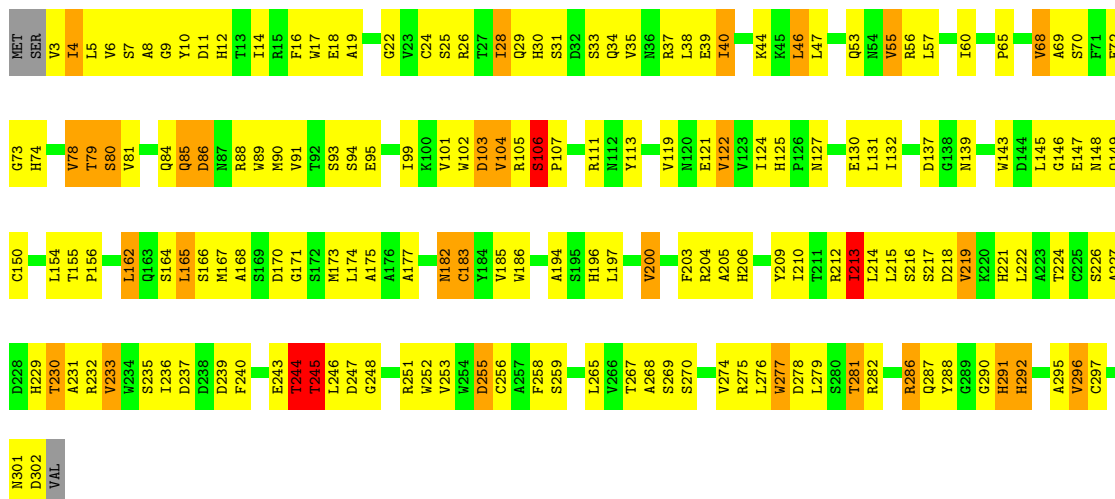
MET	VAL	L137	F213	G276
ASN	ILE	I138	E214	L277
LYR	THR	H139	V215	I278
TYR	GLY	G140	W216	L279
ILE	SER	R141	R217	R280
ASN	ALA	S143	T218	L281
LYS	GLY	S144	C218	D282
THR	HIS	E145	I219	A283
THR	ILE	K146	D220	A284
THR	GLY	I150	W221	V285
PRO	LYS	L151	L222	A286
PRO	ASN	L152	T223	L287
LEU	PHE	V153	L224	G288
LEU	VAL	L156	T225	K289
SER	ASP	I157	M228	G290
LEU	GLU	S161	N229	L291
ARG	SER	L162	S230	L294
ARG	GLN	L163	S231	R297
ALA	ASP	S164	S232	D298
ALA	THR	T163	S233	R299
GLY	THR	L166	S234	P299
GLY	GLU	P167	K235	F306
LYS	ALA	M168	L236	A300
HIS	LYS	R172	E237	L301
ARG	ARG	L177	G237	G302
THR	THR	R178	R238	R303
HIS	THR	F188	H240	Q304
LYS	ARG	F89	H241	R309
LYS	LYS	D90	A241	V305
LEU	LYS	K91	A242	F306
LEU	LEU	Y176	L243	Q307
THR	THR	L177	L244	R308
HIS	HIS	R177	L245	L309
ASP	ASP	F97	L246	F310
ASP	GLU	Q98	K247	Q311
ASP	GLU	E99	L248	L314
ASP	THR	R100	A248	H315
ASP	THR	A101	L249	H315
ASP	THR	T110	M250	G316
ASP	THR	L111	M252	L317
ASP	GLU	L112		N320
GLU	GLU	S113	L257	T321
MET	THR	L114	V258	N322
SER	SER	A115	P259	D323
THR	THR	R190	Y260	S324
THR	THR	L191	V261	H325
THR	SER	A192	N262	H326
ASP	ASN	N194	S263	A327
THR	THR	L195	I264	T328
ASP	ASP	L196	L265	L329
ASN	ASN	G197	D266	L330
HIS	HIS	R198	M267	V331
ASN	ASN	G203	L268	F332
GLY	GLY	G203	W269	R333
PRO	PRO	L206	V270	E334
ASN	ASN	T207	P271	L335
ASP	ASP	L272	L272	L336
SER	SER	R273	R273	S337
GLY	GLY	D274	D274	L338
ARG	ARG	A275	A275	K339

B1383	S1384	A1385	I1386	G1387	I1388	L1389	K1390	H1391	L1398	I1399	L1400	K1401	T1402	E1406	K1407	V1322	E1323	Q1408	Q1409	W1410	W1411	D1412	D1413	A1414	K1421	K1422	K1423	K1424	K1425	F1426	D1427	S1428	H1429	V1430	V1431	M1432	K1435	L1436	R1437	S1438	L1439	Y1440	A1441	G1442	G1443	E1444	W1445	L1448	L1451	A1452	S1453	L1454	K1455	T1458	A1459																																																																											
L1066	K1067	S1068	L1069	V1070	P1074	M1075	Y1079	R1080	H1081	L1082	I1083	M1084	P1085	I1086	V1087	V1088	R1089	M1090	Y1093	S1094	S1097	L1098	K1099	K1100	I1101	S1102	L1103	I1104	T1105	L1106	G1107	R1108	L1109	A1110	K1111	M1112	I1113	M1114	E1117	M1118	S1119	S1120	R1121	Q1124	A1125	L1126	V1127	R1128	I1129	L1130	D1134	R1135																																																																														
E1136	L1137	K1138	K1139	A1140	T1141	M1142	M1143	L1144	L1145	L1148	L1149	L1150	Q1151	L1152	G1153	T1154	P1161	V1162	K1165	A1166	L1167	R1171	I1172	Q1173	H1174	S1175	V1176	Y1177	D1178	M1182	K1183	L1184	L1185	C1189	T1192	M1193	I1194	F1196	L1198	D1197	P1203	E1204	R1205	LEU	I1208	ILE	GLN	ALA	LEU	CYS	LYS																																																																															
P1218	V1219	M1220	Q1221	M1222	K1225	M1226	C1230	S1231	D1238	W1239	Q1240	E1241	V1242	R1244	R1245	R1246	S1247	I1248	Q1249	L1259	R1260	S1261	C1262	S1263	S1264	V1268	Y1269	A1273	R1274	E1275	L1276	F1281	C1284	W1285	V1286	L1287	L1288	S1291	V1292	Q1293	E1294	D1295	LEU	ILE	GLN	ALA	LEU	CYS	LYS																																																																																	
ALA	LEU	SER	SER	SER	GLU	ASN	PRO	PRO	GLU	ILE	TVR	GLN	MET	LEU	ASN	V1322	E1323	F1324	E1325	H1327	L1332	F1333	I1334	G1340	K1341	L1342	A1343	Q1344	H1347	A1348	F1349	A1350	K1351	Y1355	K1356	K1357	V1358	E1359	F1360	P1364	K1365	T1368	I1369	E1370	A1371	L1372	S1373	S1374	I1375	T1382																																																																																
A340	P341	Y342	L343	R344	D345	K346	Y347	D348	D349	I350	Y351	K352	S353	T354	M355	K356	G357	G358	E359	Y360	K361	F362	D363	V364	L365	R366	R367	E368	V369	Y370	A371	I372	L373	L376	A377	A378	F379	D380	P381	A382	I383	T385	K386	K387	Y388	L389	D390	R391	I392	M393	V394	H395	Y396	L397	R398	Y399	L400																																																																									
K401	M402	I403	D404	M409	M410	S411	D412	K413	P414	I350	F415	M501	L416	L417	V418	S419	I420	G421	K422	L423	A424	F425	L437	L438	L439	D440	N441	I442	R443	E444	G445	L446	R447	L448	K449	F450	R453	K454	Q455	F456	E457	K458	D459	L460	F461	Y462	L467	A468	C469	A470	L471	G472	P473	A474	F475	A476	K477																																																																									
L483	C490	L573	M492	S493	D494	E498	T499	Q501	L502	L503	M504	E505	K506	I507	P508	M515	S516	R517	I518	L519	M520	L521	L522	S523	L526	S527	G528	E529	L530	L533	S534	M535	K622	D623	Y537	M541	Q542	P543	S544	I545	V631	H632	E546	R549	T560	A470	G561	L471	S638	E562	D566	I567	T568	L641	S642	A476	D569																																																																									
A570	Q571	I572	L573	I574	M575	C576	F577	L644	L645	M646	D661	P652	W653	A654	E655	L660	L661	Q662	H663	L664	G665	P670	Q671	L672	A673	Q674	P675	D676	M677	Y600	L678	R679	L680	L681	P682	M683	A684	L685	D687	E688	T689	F690	D623	G691	C626	K627	Q628	T629	S630	V631	H632	A633	R549	T634	H635	S636	L703	G561	L471	S638	E562	D566	I567	T568	L641	S642	A476	D569																																																														
P713	S714	L715	T718	L719	L720	E721	L722	F809	L723	Q810	T724	L725	L726	K727	F728	H885	Q886	F887	G888	H889	I890	L891	Q892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999
K799	E800	M801	M802	P803	L804	L805	L806	F809	L723	Q810	T724	L725	L726	K727	F728	H885	Q886	F887	G888	H889	I890	L891	Q892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999
V866	R867	T868	L869	G870	LEU	GLY	ALA	ASP	PRO	TVR	LYS	HIS	ARG	GLU	ILE	GLU	VAL	THR	SER	ASN	SER	VAL	GLU	GLN	ASN	ALA	PRO	SER	ILE	ASP	ILE	ALA	LEU	LEU	MET	L846	G847	L848	L849	L850	M851	L852	L853	K854	ASP	E915	Y916	Y917	P918	P919	P920	P921	P922	H923	H924	G925	P926																																																																									
L929	L934	H938	T939	Q943	M946	H947	F948	Q950	N951	P952	Q953	G954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999																																																																									
H1000	V1001	K1002	E1003	I1004	Y1005	G1006	V1007	L1008	R1009	E1010	F1011	F1012	P1013	I1014	I1015	K1016	L1017	Q1018	I1019	T1020	I1021	I1022	I1023	S1024	S1025	L1026	L1027	L1028	L1029	A1031	L1032	E1033	G1034	E1035	R1038	E1042	T1043	L1044	T1045	F1046	F1047	L1048	D1049	I1050	M1053	S1056	N1057	K1058	R1059	L1060	V1061	P1062	L1063	R1064	I1065																																																																											

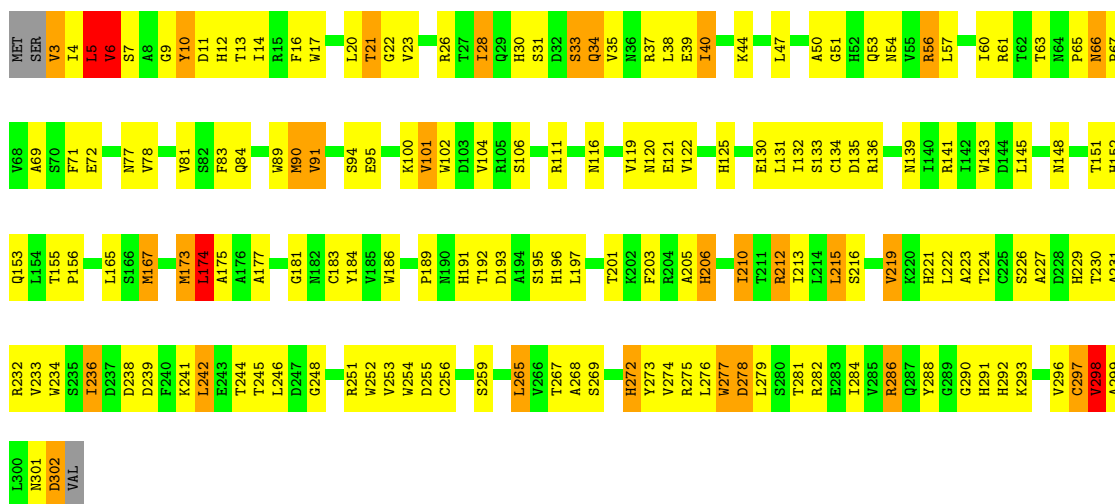
K1460	S1531	V1597	M1681	G1743	PHE	V1878	I1957	S2031	Q2108	V2181	A2266	T2340	V2409
P1461	A1532	R1598	M1682	S1744	ASP	V1879	A1960	K2032	R2109	S2184	V2267	C2341	E2410
L1462	L1533	S1599	H1683	Y1745	ALA	P1880	V1961	N2038	R2110	S2185	M2268	E2342	M2411
V1463	V1534	L1600	D1684	L1746	LYS	Q1881	Q1960	W2039	R2111	R2186	S2269	N2343	E2412
K1465	M1535	V1601	L1685	L1747	GLU	L1882	W1963	A2040	K2112	T2187	M2270	V2344	H2413
A1466	E1536	L1602	L1685	L1748	VAL	L1883	H1964	W2041	F2113	H2188	T2271	M2345	K2414
M1467	S1537	K1603	GLY	T1749	HIS	I1883	E1965	H2041	C2114	V2189	G2272	K2346	N2415
A1468	R1540	P1604	LEU	H1750	TYR	H1887	Q1966	Y2045	I2115	L2190	L2273	V2347	A2416
P1469	ASP	F1606	ASP	F1751	SER	H1887	E1966	Y2045	K2116	L2191	L2274	L2348	L2417
M1542	M1541	E1606	PRO	D1752	S1814	V1893	W1967	N2047	G2120	R2192	D2279	R2349	R2418
L1470	Y1542	ASN	ASN	M1753	M1815	V1893	L1971	F2048	K2121	E2193	R2280	N2351	A2420
M1543	M1543	ASN	ASN	M1543	L1816	S1896	L1971	R2049	D2122	H2194	R2280	K2352	R2421
V1546	V1546	Q1609	MET	K1757	H1818	S1896	A1974	K2050	Y2123	R2195	N2284	G2355	L2424
R1547	R1547	R1611	ILE	A1758	H1819	L1900	S1975	K2050	K2124	R2196	L2285	S2354	L2425
M1548	M1548	L1612	ALA	A1758	R1820	L1901	F1978	Q2054	Y2125	A2197	M2286	L2355	V2425
Q1549	Q1549	F1614	GLN	H1760	H1821	L1901	F1979	Q2054	V2126	K2198	L2287	M2356	M2426
L1477	L1477	SER	SER	M1761	V1822	S1902	F1979	H2065	L2127	R2288	D2288	M2357	R2428
M1550	M1550	VAL	VAL	W1762	I1822	D1903	G1980	V2066	K2128	R2289	R2289	L2358	L2429
E1478	E1478	L1615	PRO	A1763	I1825	G1985	E1981	L2061	G2129	N2203	L2290	L2359	T2430
E1479	E1479	R1619	GLN	L1764	K1826	K1906	H1982	L2062	H2130	H2206	L2290	L2360	T2431
E1483	E1483	R1623	GLN	A1765	K1827	K1906	H1982	E2062	E2131	W2207	K2293	L2361	D2432
I1484	I1484	M1624	SER	M1766	F1828	L1916	T1983	Q2063	D2132	W2208	A2361	A2361	L2433
A1485	A1485	L1624	LYS	F1767	F1828	M1917	T1984	Q2064	L2133	V2209	V2294	F2362	L2433
Q1486	Q1486	M1625	ARG	E1768	F1828	M1918	E1985	H2065	I2133	M2209	L2295	A2363	T2434
Y1487	Y1487	L1626	VAL	E1769	F1828	M1919	K1986	V2066	R2134	L2210	H2296	F2364	G2435
M1491	M1491	A1627	PRO	L1770	S1831	L1912	M1987	S2067	G2135	L2210	L2297	D2365	G2435
K1492	K1492	L1627	ARG	S1771	I1832	V1914	M1987	P2068	D2136	T2220	L2307	L2365	M2436
L1493	L1493	K1628	ARG	MET	S1833	P1915	A1990	P2068	S2137	L2221	G2300	L2366	D2437
Q1494	Q1494	M1629	LEU	LEU	L1834	P1915	L1991	L2071	L2138	L2222	D2301	M2369	L2438
P1496	P1496	L1631	SER	THR	E1708	M1917	L1991	L2071	V2139	L2222	C2302	N2370	R2439
D1497	D1497	S1633	VAL	SER	V1710	M1918	L1994	L2076	Q2141	V2225	F2303	G2371	D2443
R1498	R1498	L1634	VAL	VAL	D1711	M1919	Y1995	E2077	Q2141	E2286	E2304	F2372	L2444
E1499	E1499	L1636	THR	SER	T1712	I1920	E1996	R2077	L2142	V2227	L2307	D2373	D2445
F1500	F1500	E1636	LYS	LYS	T1712	I1920	M1997	A2079	L2142	F2228	L2307	L2374	V2446
I1504	I1504	S1650	LYS	LYS	L1844	E1923	M1997	V2080	L2145	D2239	L2308	P2375	P2447
L1506	L1506	V1653	GLY	GLY	R1845	S1924	M1997	V2080	V2146	L2240	L2309	T2375	P2448
L1507	L1507	Y1654	GLY	GLY	R1845	S1924	M1997	V2080	N2147	L2241	R2309	K2377	E2448
L1508	L1508	Y1655	ASP	ASP	L1847	S1929	M1997	G2082	L2150	K2242	F2312	K2378	Q2449
H1508	H1508	Y1657	ALA	ALA	T1848	Q1928	M1997	G2082	D2153	L2244	P2317	L2379	V2450
R1509	R1509	A1656	ALA	ALA	L1849	K1929	M1997	G2082	A2154	L2244	F2318	E2380	P2451
W1591	W1591	Q1657	SER	SER	W1850	A1930	M1997	K2089	E2155	W2245	R2319	E2382	L2453
W1580	W1580	L1658	GLY	GLY	W1850	A1931	M1997	P2090	C2156	L2246	M2323	T2383	S2459
L1581	L1581	K1659	VAL	VAL	F1853	L1932	M1997	L2091	F2157	S2246	L2324	Q2386	V2460
F1512	F1512	Y1660	THR	THR	W1725	I1932	M1997	V2092	H2160	R2249	Y2326	L2387	E2461
G1583	G1583	L1661	ASP	ASP	E1857	I1935	M1997	K2093	L2161	T2253	Y2326	E2394	M2462
C1584	C1584	W1662	ILE	ILE	E1858	I1935	M1997	K2093	L2161	A2327	M2328	E2394	L2468
A1515	A1515	A1663	ASN	ASN	A1859	E1936	M1997	L2094	L2161	W2254	G2469	N2398	G2469
E1516	E1516	L1663	GLU	GLU	T1860	K1937	M1997	S2095	I2169	L2255	E2329	G2399	V2470
M1587	M1587	L1666	PHE	PHE	M1863	M1938	M1997	K2096	P2170	E2256	V2330	G2399	G2471
I1588	I1588	Q1667	ASP	ASP	H1864	S1942	M1997	F2097	L2171	R2257	S2331	A2400	P2472
D1589	D1589	Q1668	ASN	ASN	E1865	S1942	M1997	P2099	S2172	K2257	G2332	I2401	F2473
F1520	F1520	E1669	GLY	GLY	G1866	V1946	M1997	V2100	P2173	R2258	I2333	T2402	F2473
W1591	W1591	A1670	MET	MET	G1866	V1946	M1997	W2024	F2101	P2173	I2333	T2402	F2473
Q1592	Q1592	L1671	ILE	ILE	L1869	V1952	M1997	S2102	S2175	L2261	G2335	E2403	W2474
R1593	R1593	L1674	GLY	GLY	I1870	S1953	M1997	M2026	V2103	T2282	S2336	E2404	
L1594	L1594	L1674	VAL	VAL	Q1871	S1953	M1997	W2026	V2103	T2282	S2336	E2405	
L1596	L1596	L1674	ASN	ASN	I1872	H1954	M1997	W2026	L2104	R2263	F2337	Q2407	
L1596	L1596	T1678	THR	THR	G1873	L1956	M1997	W2028	S2105	L2285	L2339	R2408	

● Molecule 2: Target of rapamycin complex subunit LST8

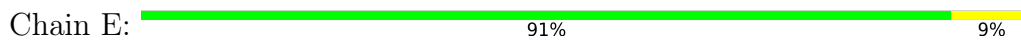




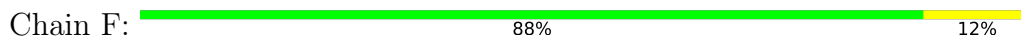
• Molecule 2: Target of rapamycin complex subunit LST8



• Molecule 3: Target of rapamycin complex 2 subunit TSC11



• Molecule 3: Target of rapamycin complex 2 subunit TSC11



VAL VAL
LEU LEU
VAL VAL
LYS LYS
SER SER
LYS LYS
ARG ARG
VAL VAL
PRO PRO
GLU GLU
HIS HIS
PHE PHE
LYS LYS
ILE ILE
PHE PHE
VAL VAL
ARG ARG
ARG ARG
GLU GLU
GLY GLY
GLN GLN
ASP ASP
ILE ILE
LYS LYS
ARG ARG
TYR TYR
PHE PHE
GLU GLU
ALA ALA
VAL VAL
SER SER
GLY GLY
GLN GLN
GLU GLU
CYS CYS
THR THR
ILE ILE
VAL VAL
THR THR
ARG ARG
LEU LEU
GLN GLN
ASN ASN
LEU LEU
SER SER
ALA ALA
TYR TYR
ARG ARG
MET MET
ASN ASN
HIS HIS
LYS LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT	Depositor
Number of particles used	16190, 10663	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50, 47	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON II (4k x 4k), GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0147	Depositor
Map size (\AA)	441.6, 441.6, 441.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.38, 1.38, 1.38	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.60	0/18019	0.94	52/23495 (0.2%)
1	C	0.60	0/17986	0.93	40/23389 (0.2%)
2	B	0.60	0/2362	0.89	7/3108 (0.2%)
2	D	0.60	0/2353	0.93	4/3080 (0.1%)
4	G	0.48	0/715	0.68	0/918
4	H	0.49	0/718	0.87	2/927 (0.2%)
5	I	1.03	2/1165 (0.2%)	1.09	7/1526 (0.5%)
5	J	0.88	0/1160	1.01	8/1509 (0.5%)
All	All	0.62	2/44478 (0.0%)	0.93	120/57952 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	28
1	C	0	25
2	B	0	4
2	D	0	2
5	I	0	2
5	J	0	2
All	All	1	63

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	713	LEU	N-CA	5.35	1.57	1.46
5	I	714	TYR	N-CA	5.27	1.56	1.46

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1084	MET	C-N-CD	-9.18	100.41	120.60
2	D	174	LEU	CA-CB-CG	8.54	134.94	115.30
1	A	2426	ARG	N-CA-C	7.87	132.25	111.00
2	B	106	SER	C-N-CD	-7.69	103.69	120.60
5	I	713	LEU	CA-CB-CG	7.55	132.67	115.30
1	C	467	LEU	CA-CB-CG	7.49	132.52	115.30
1	A	234	LEU	CA-CB-CG	7.28	132.05	115.30
1	C	822	LEU	CA-CB-CG	7.16	131.77	115.30
1	C	2355	LEU	N-CA-C	7.16	130.33	111.00
1	A	2431	LEU	CA-CB-CG	7.04	131.50	115.30
1	C	233	SER	N-CA-C	7.03	129.97	111.00
1	C	281	LEU	CA-CB-CG	6.98	131.34	115.30
1	C	235	LEU	CA-CB-CG	6.96	131.31	115.30
1	C	2190	LEU	CA-CB-CG	6.95	131.29	115.30
2	B	245	THR	N-CA-C	6.87	129.54	111.00
1	C	175	ASN	C-N-CA	6.81	138.72	121.70
1	C	1185	LEU	CA-CB-CG	6.78	130.90	115.30
1	A	286	LEU	CB-CG-CD1	-6.78	99.48	111.00
1	A	178	VAL	CB-CA-C	6.77	124.26	111.40
1	C	1834	LEU	CA-CB-CG	6.74	130.80	115.30
5	I	728	LEU	CA-CB-CG	6.69	130.69	115.30
5	J	728	LEU	CA-CB-CG	6.67	130.63	115.30
5	I	685	SER	C-N-CA	6.60	138.21	121.70
5	I	659	LEU	CA-CB-CG	6.49	130.24	115.30
1	C	1996	GLU	N-CA-C	6.46	128.43	111.00
5	J	659	LEU	CA-CB-CG	6.37	129.96	115.30
1	A	1731	TRP	C-N-CA	6.35	137.58	121.70
2	D	215	LEU	CA-CB-CG	6.33	129.86	115.30
2	B	104	VAL	N-CA-C	-6.31	93.95	111.00
5	J	701	SER	C-N-CA	6.30	137.45	121.70
1	C	2078	LEU	CA-CB-CG	-6.25	100.91	115.30
1	C	305	TRP	CA-CB-CG	6.20	125.48	113.70
1	A	1083	MET	N-CA-C	6.18	127.70	111.00
2	D	5	LEU	CA-CB-CG	6.18	129.52	115.30
1	A	344	ASP	C-N-CA	6.16	137.09	121.70
1	C	424	ALA	C-N-CA	6.10	136.96	121.70
1	C	2308	LEU	CA-CB-CG	6.10	129.32	115.30
1	C	1286	VAL	C-N-CA	6.08	136.91	121.70
1	C	2155	GLU	N-CA-C	6.08	127.42	111.00
1	A	594	LEU	CA-CB-CG	6.06	129.25	115.30
2	D	265	LEU	CA-CB-CG	6.02	129.14	115.30
5	J	701	SER	N-CA-C	5.97	127.11	111.00
1	A	974	PRO	C-N-CD	-5.96	107.49	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2161	LEU	CA-CB-CG	5.93	128.94	115.30
1	A	347	ASP	C-N-CA	5.93	136.52	121.70
5	J	741	LEU	CA-CB-CG	5.91	128.90	115.30
1	A	742	CYS	C-N-CA	5.90	136.44	121.70
1	C	1981	GLU	N-CA-C	5.89	126.90	111.00
1	C	417	LEU	CA-CB-CG	5.88	128.83	115.30
1	A	1449	LEU	CA-CB-CG	5.87	128.81	115.30
1	C	1971	LEU	CA-CB-CG	5.87	128.80	115.30
1	C	1585	GLN	N-CA-C	5.87	126.85	111.00
1	A	2440	ASN	C-N-CA	5.85	136.31	121.70
1	C	1293	GLN	N-CA-C	5.85	126.78	111.00
1	A	2018	ASP	N-CA-C	5.84	126.77	111.00
1	C	2221	LEU	CA-CB-CG	5.83	128.72	115.30
2	B	165	LEU	CA-CB-CG	5.82	128.69	115.30
1	A	588	LEU	CA-CB-CG	5.77	128.57	115.30
1	A	1090	THR	C-N-CA	5.75	136.07	121.70
1	A	482	LEU	CA-CB-CG	5.74	128.50	115.30
1	C	1372	LEU	CA-CB-CG	5.72	128.46	115.30
1	A	797	LEU	CA-CB-CG	5.71	128.42	115.30
1	C	2244	LEU	CA-CB-CG	5.67	128.34	115.30
2	B	162	LEU	CA-CB-CG	5.66	128.32	115.30
1	A	768	GLN	C-N-CA	5.66	135.84	121.70
1	A	2335	PHE	N-CA-C	-5.63	95.79	111.00
1	A	1584	LYS	N-CA-C	5.59	126.10	111.00
1	A	1396	LEU	CA-CB-CG	5.56	128.10	115.30
1	A	2425	LYS	C-N-CA	5.55	135.57	121.70
1	C	595	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	2018	ASP	C-N-CA	5.49	135.43	121.70
1	A	394	HIS	C-N-CA	5.49	135.42	121.70
1	A	1446	LEU	C-N-CA	5.49	135.41	121.70
5	I	719	LYS	C-N-CD	-5.48	108.55	120.60
1	A	1434	LEU	CA-CB-CG	5.47	127.88	115.30
1	C	2077	GLU	N-CA-C	5.46	125.75	111.00
5	I	758	LEU	CA-CB-CG	5.46	127.85	115.30
5	J	681	TYR	CA-CB-CG	5.46	123.77	113.40
1	C	1996	GLU	C-N-CA	5.45	135.34	121.70
4	H	66	LYS	N-CA-C	5.45	125.72	111.00
1	A	2441	ASP	N-CA-C	5.40	125.59	111.00
1	A	2390	ALA	C-N-CA	5.38	135.14	121.70
1	C	691	GLY	N-CA-C	5.34	126.46	113.10
2	B	46	LEU	CA-CB-CG	5.33	127.57	115.30
1	C	196	LEU	CA-CB-CG	5.33	127.55	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1166	LEU	CA-CB-CG	5.31	127.52	115.30
1	C	503	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	719	LEU	CA-CB-CG	5.30	127.50	115.30
1	A	221	LEU	CA-CB-CG	5.27	127.41	115.30
1	A	644	LEU	CA-CB-CG	5.26	127.41	115.30
1	A	1082	ILE	C-N-CA	5.26	134.84	121.70
4	H	182	ILE	C-N-CA	5.24	134.81	121.70
5	I	741	LEU	CA-CB-CG	5.23	127.33	115.30
5	J	713	LEU	CA-CB-CG	5.21	127.29	115.30
1	C	130	LEU	CA-CB-CG	5.21	127.28	115.30
1	C	1167	LEU	CA-CB-CG	5.20	127.26	115.30
1	A	821	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	725	LEU	CA-CB-CG	5.18	127.21	115.30
2	B	213	ILE	CB-CA-C	5.17	121.93	111.60
1	A	416	LEU	CA-CB-CG	5.17	127.18	115.30
5	J	791	LEU	CA-CB-CG	5.11	127.06	115.30
1	A	1731	TRP	N-CA-C	5.11	124.80	111.00
1	A	1498	PHE	C-N-CA	5.11	134.47	121.70
1	A	649	THR	C-N-CA	5.10	134.46	121.70
1	A	1579	LEU	CA-CB-CG	5.10	127.03	115.30
1	C	347	TYR	C-N-CA	5.10	134.45	121.70
1	C	1293	GLN	C-N-CA	5.09	134.43	121.70
1	A	1341	ALA	C-N-CA	5.08	134.40	121.70
1	A	2436	ILE	N-CA-C	5.08	124.71	111.00
1	C	798	LEU	CA-CB-CG	5.07	126.96	115.30
1	A	1587	ASP	C-N-CA	5.06	134.35	121.70
1	C	232	SER	C-N-CA	5.06	134.35	121.70
1	A	1733	LEU	C-N-CA	5.05	134.33	121.70
1	A	328	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	1476	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	2136	LEU	CA-CB-CG	5.03	126.86	115.30
1	C	720	LEU	CA-CB-CG	5.02	126.84	115.30
1	A	2283	LEU	CA-CB-CG	5.01	126.82	115.30
1	A	740	LEU	CA-CB-CG	5.00	126.81	115.30
1	A	768	GLN	N-CA-C	-5.00	97.50	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	257	TYR	CA

All (63) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1089	MET	Peptide
1	A	1241	TRP	Peptide
1	A	1385	GLY	Peptide
1	A	1523	LEU	Peptide
1	A	1587	ASP	Peptide
1	A	1731	TRP	Peptide
1	A	178	VAL	Peptide
1	A	180	ILE	Peptide
1	A	1976	PHE	Peptide
1	A	2121	TYR	Peptide
1	A	2123	TYR	Peptide
1	A	2334	SER	Peptide
1	A	2367	ASN	Peptide
1	A	2385	LEU	Peptide
1	A	2431	LEU	Peptide
1	A	2436	ILE	Peptide
1	A	256	LEU	Peptide
1	A	257	TYR	Peptide
1	A	347	ASP	Peptide
1	A	394	HIS	Peptide
1	A	400	LYS	Peptide
1	A	401	ASN	Peptide
1	A	402	ILE	Peptide
1	A	488	ASN	Peptide
1	A	489	CYS	Peptide
1	A	604	ASP	Peptide
1	A	649	THR	Peptide
1	A	958	PHE	Peptide
2	B	103	ASP	Peptide
2	B	244	THR	Peptide
2	B	291	HIS	Peptide
2	B	31	SER	Peptide
1	C	1084	MET	Peptide
1	C	1151	GLN	Peptide
1	C	1152	LEU	Peptide
1	C	1286	VAL	Peptide
1	C	131	ASN	Peptide
1	C	1610	VAL	Peptide
1	C	1611	ARG	Peptide
1	C	1636	GLU	Peptide
1	C	1670	ALA	Peptide
1	C	1995	TYR	Peptide
1	C	2027	ASN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	2076	LEU	Peptide
1	C	2077	GLU	Peptide
1	C	2078	LEU	Peptide
1	C	2145	LEU	Peptide
1	C	2155	GLU	Peptide
1	C	2308	LEU	Peptide
1	C	235	LEU	Peptide
1	C	2416	ALA	Peptide
1	C	403	ILE	Peptide
1	C	646	MET	Peptide
1	C	651	ASP	Peptide
1	C	665	GLY	Peptide
1	C	712	VAL	Peptide
1	C	916	TYR	Peptide
2	D	173	MET	Peptide
2	D	34	GLN	Peptide
5	I	682	ILE	Peptide
5	I	697	VAL	Peptide
5	J	736	PRO	Peptide
5	J	760	ARG	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	18186	0	18002	1077	0
1	C	18186	0	17976	1069	0
2	B	2372	0	2199	140	0
2	D	2372	0	2191	145	0
3	E	1515	0	491	15	0
3	F	1515	0	490	23	0
4	G	762	0	290	6	0
4	H	762	0	293	9	0
5	I	1171	0	1119	61	0
5	J	1171	0	1116	54	0
All	All	48012	0	44167	2571	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 28.

All (2571) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2060:GLU:HB3	1:A:2062:GLN:HG2	1.25	1.18
1:A:841:TYR:HB2	1:A:843:GLU:HG2	1.16	1.13
1:C:983:PHE:HB3	1:C:1022:ILE:HG12	1.31	1.10
1:A:179:LEU:HD22	1:A:233:LYS:HG3	1.31	1.10
2:D:297:CYS:HA	2:D:298:VAL:HB	1.25	1.09
1:A:1083:MET:HB3	1:A:1084:PRO:HD3	1.34	1.08
1:C:265:LEU:HA	1:C:307:GLN:HB3	1.29	1.07
1:C:2337:PHE:HZ	1:C:2450:VAL:HG13	1.16	1.07
1:C:230:SER:HB3	1:C:233:SER:HB2	1.34	1.07
2:D:4:ILE:HG12	2:D:60:ILE:HG12	1.36	1.05
2:B:4:ILE:HG12	2:B:60:ILE:HG12	1.38	1.05
1:C:1442:LEU:HB3	1:C:1624:MET:HG2	1.36	1.05
1:A:650:ASP:H	1:A:651:PRO:HD3	1.20	1.04
5:J:655:SER:HA	5:J:659:LEU:HB2	1.40	1.02
1:C:2374:LEU:HD11	1:C:2417:ILE:HB	1.39	1.02
1:A:652:VAL:HB	3:F:100:UNK:H2	1.22	1.01
1:A:1151:LEU:CB	1:A:1152:GLY:HA2	1.90	1.01
1:C:1612:ILE:HG23	1:C:1615:ALA:HB3	1.39	1.00
1:C:842:TYR:HB3	1:C:844:GLU:HG2	1.41	1.00
5:J:699:LYS:HE2	5:J:737:ASN:HB2	1.44	0.99
2:D:84:GLN:HB3	2:D:89:TRP:HB2	1.45	0.99
1:A:2121:TYR:HA	1:A:2122:LYS:HB2	1.45	0.96
1:A:1263:SER:HB3	1:A:1268:TYR:HE2	1.30	0.96
1:C:297:ARG:HD2	1:C:339:LYS:HG3	1.48	0.96
1:C:1763:ALA:HB1	1:C:1825:ILE:HA	1.45	0.96
1:C:857:ASN:HB3	1:C:1586:LYS:HA	1.47	0.96
5:I:693:PHE:CE2	5:I:760:ARG:HB3	2.01	0.95
1:A:2126:LYS:HD3	1:A:2131:ILE:HD11	1.48	0.95
1:C:2062:GLU:HA	1:C:2063:LEU:HB2	1.48	0.94
1:A:581:LEU:HA	1:A:583:HIS:N	1.81	0.94
1:C:401:LYS:HA	1:C:403:ILE:HG23	1.49	0.94
2:B:265:LEU:HB2	2:B:279:LEU:HD12	1.46	0.94
1:C:1011:PHE:HD1	1:C:1022:ILE:HG23	1.29	0.94
1:A:801:MET:HA	1:A:804:ILE:HB	1.47	0.94
1:A:280:LEU:HA	1:A:330:VAL:HG22	1.48	0.94
1:A:771:SER:HB2	1:A:774:VAL:HB	1.50	0.94
2:B:4:ILE:HG21	2:B:40:ILE:HD11	1.47	0.93
1:C:1630:VAL:HB	1:C:1634:LEU:HG	1.50	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:LYS:HD3	1:C:350:ILE:HG12	1.51	0.93
1:A:1043:LEU:HD11	1:C:702:ARG:HD3	1.52	0.92
1:A:650:ASP:H	1:A:651:PRO:CD	1.80	0.92
1:C:2045:TYR:HB3	1:C:2049:ARG:HH12	1.33	0.91
1:C:1850:TRP:HZ2	1:C:1859:ALA:HB1	1.36	0.91
1:C:2337:PHE:CZ	1:C:2450:VAL:HG13	2.05	0.91
1:A:281:ASP:HA	1:A:284:VAL:HB	1.52	0.90
1:A:2112:CYS:HB2	1:A:2120:ASP:HB3	1.51	0.90
2:D:229:HIS:HB3	2:D:251:ARG:HB2	1.53	0.90
1:A:636:VAL:HG13	1:A:675:ASP:HB3	1.52	0.89
1:C:2004:THR:HG1	1:C:2008:ILE:N	1.68	0.89
1:A:1371:ILE:HD13	1:A:1387:LEU:HG	1.53	0.89
1:A:2078:VAL:HG13	1:A:2089:ILE:HA	1.53	0.89
1:A:856:ASN:HB2	1:A:1580:LEU:HA	1.54	0.89
1:C:188:VAL:HG21	1:C:233:SER:HB3	1.52	0.89
1:A:704:SER:HB2	1:A:709:TYR:HB2	1.55	0.88
1:A:824:LEU:HD21	1:A:1534:GLU:HB2	1.55	0.88
1:A:1212:GLN:HB2	1:A:1252:GLU:HG3	1.55	0.88
1:A:2337:ILE:HA	1:A:2340:GLU:HG2	1.55	0.87
2:B:9:GLY:HA2	2:B:296:VAL:HG23	1.54	0.87
1:A:1617:ARG:HE	1:A:1657:LYS:HB3	1.39	0.87
1:A:117:VAL:HB	1:A:120:GLU:HA	1.57	0.86
1:A:768:GLN:HB2	1:A:770:ALA:H	1.40	0.86
1:A:849:ILE:HG12	1:A:1548:ILE:HA	1.57	0.86
1:A:1045:PHE:HZ	1:A:1064:ILE:HA	1.40	0.86
1:C:1547:ARG:HA	1:C:1550:ILE:HD12	1.57	0.86
1:C:1850:TRP:CZ2	1:C:1859:ALA:HB1	2.10	0.86
1:A:835:VAL:HG11	1:A:844:LEU:HB2	1.58	0.86
1:A:1820:ILE:H	1:A:1821:PRO:HD3	1.40	0.86
1:C:333:ARG:HB3	1:C:373:LEU:HB2	1.55	0.86
1:A:177:ARG:H	1:A:178:VAL:CG2	1.88	0.86
1:A:581:LEU:HA	1:A:583:HIS:H	1.36	0.85
2:B:210:ILE:HD13	2:B:224:THR:CG2	2.06	0.85
1:C:1011:PHE:CD1	1:C:1022:ILE:HG23	2.11	0.85
1:C:1619:ARG:HA	1:C:1626:LEU:HG	1.58	0.85
2:B:210:ILE:HD13	2:B:224:THR:HG23	1.58	0.85
1:C:2145:LEU:HB3	1:C:2146:VAL:HG13	1.59	0.85
1:A:1151:LEU:HB3	1:A:1152:GLY:HA2	1.58	0.85
2:D:26:ARG:HE	2:D:60:ILE:HD12	1.38	0.84
1:A:1151:LEU:HB2	1:A:1152:GLY:HA2	1.57	0.84
1:A:1589:TRP:HE3	1:A:1612:PHE:HE1	1.23	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2064:GLN:HG3	1:C:2065:HIS:CD2	2.13	0.84
1:A:1216:LEU:HA	1:A:1217:PRO:HA	1.59	0.84
1:C:2247:LYS:HA	1:C:2249:ARG:H	1.41	0.84
2:B:127:ASN:HD21	2:B:130:GLU:HB2	1.41	0.84
1:C:634:LEU:HD22	1:C:675:PRO:HG2	1.58	0.84
1:A:1545:ARG:HA	1:A:1548:ILE:HD12	1.60	0.83
1:A:2259:TYR:HA	1:A:2262:SER:HB2	1.58	0.83
1:A:860:ILE:HG22	1:A:863:GLY:HA3	1.59	0.83
1:C:1615:ALA:HB2	1:C:1629:LYS:HE2	1.60	0.83
2:D:14:ILE:HG22	2:D:38:LEU:HD23	1.60	0.83
4:H:120:ASP:HA	4:H:121:TYR:CB	2.08	0.83
1:A:1116:GLU:O	1:C:664:LEU:HB2	1.77	0.83
1:A:177:ARG:H	1:A:178:VAL:HG23	1.41	0.83
2:B:14:ILE:HG22	2:B:38:LEU:HD23	1.60	0.83
1:A:1587:ASP:N	1:A:1588:VAL:HB	1.94	0.83
5:I:647:LYS:HD3	5:I:649:LYS:HE3	1.61	0.83
1:C:1246:LEU:HA	1:C:1276:LEU:HD23	1.59	0.83
2:D:286:ARG:HB3	2:D:288:TYR:OH	1.79	0.83
1:A:1341:ALA:HB3	1:A:1342:GLN:HB2	1.61	0.82
1:C:113:SER:C	1:C:114:LEU:HA	2.00	0.82
1:A:345:LYS:HE3	1:A:349:ILE:HG12	1.61	0.82
1:C:1491:MET:HG3	1:C:1492:LYS:N	1.93	0.82
1:A:124:ARG:HG3	1:A:155:LEU:HD11	1.59	0.82
1:A:331:PHE:HE2	1:A:349:ILE:HG21	1.44	0.82
1:A:2200:LEU:HG	1:A:2471:PHE:HZ	1.45	0.82
1:A:124:ARG:HH21	1:A:170:SER:HB3	1.44	0.82
3:F:507:UNK:C	3:F:508:UNK:HA	2.10	0.81
1:C:721:GLU:HB3	1:C:722:LEU:HB2	1.62	0.81
1:C:1722:GLN:HG2	1:C:1748:ALA:HB1	1.60	0.81
1:A:722:LEU:HA	1:A:760:LEU:HD13	1.63	0.81
1:A:652:VAL:HB	3:F:100:UNK:N	1.95	0.81
2:B:90:MET:N	2:B:104:VAL:HG22	1.95	0.81
1:C:335:LEU:HD23	1:C:338:LEU:HD22	1.63	0.81
1:C:189:MET:HA	1:C:193:ALA:HB3	1.63	0.81
1:A:138:HIS:NE2	1:A:178:VAL:HG12	1.97	0.80
1:C:1414:ALA:HB1	1:C:1442:LEU:HD11	1.64	0.80
1:A:2075:GLU:HA	1:A:2091:LYS:HG2	1.62	0.80
1:C:346:LYS:HA	1:C:349:ASP:HB2	1.62	0.80
1:A:1446:LEU:H	1:A:1447:SER:HB2	1.47	0.80
1:A:1263:SER:HB3	1:A:1268:TYR:CE2	2.17	0.80
1:C:346:LYS:HD3	1:C:350:ILE:CG1	2.12	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:726:LEU:HB2	1:C:761:LEU:HB3	1.64	0.80
1:A:366:ARG:HD3	1:A:413:PRO:HB2	1.64	0.80
5:I:757:LYS:HG3	5:I:784:GLN:HG2	1.63	0.80
1:A:1097:LEU:HA	1:A:1100:ILE:HB	1.65	0.79
1:C:2288:ASP:HB3	1:C:2290:ILE:HG13	1.65	0.79
1:A:188:MET:HG3	1:A:236:TYR:HB3	1.63	0.79
2:B:46:LEU:HD22	2:B:68:VAL:HG11	1.64	0.79
1:A:356:TYR:HB3	1:A:365:ARG:HE	1.48	0.79
1:C:569:ASP:HA	1:C:573:LEU:HD12	1.63	0.79
1:A:91:LEU:HD11	1:A:143:SER:HB3	1.64	0.79
1:A:257:TYR:HB3	1:A:258:PRO:C	2.03	0.79
1:C:332:PHE:HZ	1:C:350:ILE:HG12	1.48	0.79
1:A:2426:ARG:O	1:A:2433:GLY:HA2	1.82	0.79
1:C:2061:LEU:O	1:C:2100:VAL:HA	1.82	0.79
1:C:918:PRO:HB3	1:C:1214:VAL:HG21	1.63	0.79
1:A:113:LEU:HB2	1:A:117:VAL:HG22	1.65	0.79
1:A:1814:LEU:HD23	1:A:1819:VAL:HG21	1.65	0.78
1:A:1820:ILE:N	1:A:1821:PRO:HD3	1.97	0.78
1:C:1590:VAL:O	1:C:1594:ILE:HG13	1.83	0.78
1:C:188:VAL:CG1	1:C:234:LYS:HA	2.13	0.78
1:A:2091:LYS:C	1:A:2092:ILE:HA	2.03	0.78
1:C:1454:GLU:O	1:C:1458:THR:HG23	1.84	0.78
1:C:1612:ILE:CG2	1:C:1615:ALA:HB3	2.13	0.78
5:I:785:ASN:HB3	5:I:788:GLU:N	1.98	0.78
1:A:178:VAL:HG11	1:A:190:LEU:HD12	1.65	0.78
1:C:266:ASP:N	1:C:267:ASN:HB2	1.98	0.78
1:C:1496:PRO:HB3	1:C:1525:LEU:HB3	1.64	0.78
1:A:1730:LYS:HB3	1:A:1735:ASN:HB3	1.65	0.78
1:C:337:SER:HB2	1:C:376:LEU:HB2	1.64	0.78
1:A:1588:VAL:O	1:A:1592:ILE:HG12	1.84	0.78
1:A:436:LEU:HA	1:A:439:ASP:HB2	1.65	0.77
1:C:437:LEU:HA	1:C:440:ASP:HB2	1.65	0.77
5:J:699:LYS:HB2	5:J:760:ARG:HB2	1.66	0.77
1:A:1492:GLN:HA	1:A:1493:SER:N	1.99	0.77
1:C:700:ILE:HD12	1:C:718:THR:HG22	1.66	0.77
1:C:983:PHE:HB3	1:C:1022:ILE:CG1	2.12	0.77
1:C:2339:ILE:HA	1:C:2342:GLU:HG2	1.66	0.77
1:A:1083:MET:HB3	1:A:1084:PRO:CD	2.13	0.77
5:I:730:VAL:HG11	5:I:790:PRO:HD2	1.67	0.77
1:C:2007:GLU:HB3	1:C:2065:HIS:HB3	1.65	0.77
1:A:1900:SER:HB3	1:A:1932:ILE:HD12	1.64	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1011:PHE:HD1	1:C:1022:ILE:CG2	1.98	0.77
1:A:270:PRO:HB2	1:A:279:ARG:HB2	1.64	0.77
1:A:2425:LYS:HA	1:A:2434:ASN:HD22	1.49	0.77
1:C:1108:ARG:HA	1:C:1150:LEU:HD11	1.66	0.77
1:A:399:LEU:O	1:A:402:ILE:HG23	1.85	0.76
5:J:710:ALA:HB1	5:J:718:LYS:HG2	1.65	0.76
5:I:700:SER:HA	5:I:731:GLU:HB3	1.67	0.76
1:A:2283:LEU:HD21	1:A:2317:ARG:HD3	1.67	0.76
2:B:8:ALA:HB1	2:B:12:HIS:HA	1.66	0.76
1:C:1952:VAL:HA	1:C:1955:GLU:HB2	1.68	0.76
1:A:234:LEU:HD11	1:A:270:PRO:HG3	1.68	0.76
1:A:1110:LYS:HD3	1:A:1148:LEU:HD21	1.67	0.76
1:C:956:CYS:HG	1:C:957:VAL:N	1.83	0.76
1:C:468:ALA:HA	1:C:469:CYS:HA	1.67	0.76
1:C:992:ILE:N	1:C:993:VAL:HA	2.00	0.76
1:C:98:GLN:HA	1:C:101:ALA:HB3	1.66	0.76
5:J:693:PHE:CZ	5:J:760:ARG:HB3	2.21	0.76
1:A:1601:LYS:HB2	1:A:1602:PRO:HD2	1.68	0.75
1:C:261:VAL:HG11	1:C:303:LYS:HD2	1.68	0.75
1:C:1140:ALA:HB1	1:C:1173:GLN:CB	2.15	0.75
1:C:1557:ILE:HD13	1:C:1577:TRP:CZ2	2.22	0.75
5:J:698:ARG:HG3	5:J:788:GLU:HG2	1.65	0.75
1:A:1969:LEU:HB3	1:A:1970:ASP:HA	1.66	0.75
1:A:1848:TRP:HZ2	1:A:1857:ALA:HB1	1.50	0.75
2:B:122:VAL:HG13	2:B:131:LEU:HD11	1.69	0.75
1:A:1215:LYS:HD2	1:A:1249:LEU:HA	1.68	0.75
1:A:367:GLU:HA	1:A:370:ALA:HB3	1.69	0.75
1:C:2222:LEU:HD21	2:D:227:ALA:HB2	1.69	0.75
1:A:391:ILE:HA	1:A:395:TYR:HD2	1.51	0.75
1:C:240:HIS:HA	1:C:241:ALA:C	2.08	0.75
2:B:79:THR:HG1	2:B:95:GLU:N	1.84	0.75
1:A:2161:ILE:HG12	1:A:2266:MET:HB2	1.67	0.74
1:C:395:HIS:HE1	1:C:438:ILE:HG21	1.52	0.74
1:C:1013:PRO:HA	1:C:1022:ILE:O	1.85	0.74
1:C:1111:LYS:HD2	1:C:1149:LEU:HD21	1.68	0.74
1:C:2104:ILE:HA	1:C:2105:SER:HB2	1.68	0.74
1:C:332:PHE:CZ	1:C:350:ILE:HG12	2.21	0.74
1:A:2266:MET:HB2	1:A:2292:VAL:HG21	1.68	0.74
1:C:1100:LYS:HA	1:C:1103:ILE:HB	1.67	0.74
1:C:2131:GLU:HB3	1:C:2132:ASP:N	2.03	0.74
1:C:2263:ARG:HG2	1:C:2339:ILE:HD13	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1971:LEU:HD13	1:C:1991:LEU:HD21	1.70	0.74
2:B:40:ILE:HG23	2:B:47:LEU:HB3	1.70	0.73
1:C:1430:GLU:HB2	1:C:1431:VAL:N	2.02	0.73
1:A:1734:SER:HB3	1:A:1735:ASN:HB2	1.69	0.73
2:B:33:SER:HG	2:B:34:GLN:N	1.87	0.73
4:H:68:GLU:O	4:H:71:LYS:N	2.21	0.73
2:B:12:HIS:CE1	2:B:35:VAL:H	2.07	0.73
1:C:1058:LYS:HD2	1:C:1060:ILE:HD12	1.69	0.73
1:A:2185:PHE:HA	1:A:2188:LEU:HG	1.70	0.73
1:C:1978:PHE:HA	1:C:1983:ASN:HB2	1.71	0.73
1:A:188:MET:HA	1:A:192:ALA:HB3	1.71	0.73
1:A:677:LEU:HG	1:A:726:LYS:HB3	1.71	0.73
1:A:698:ILE:HG23	1:C:1079:TYR:CE2	2.24	0.73
1:A:1060:VAL:HA	1:A:1063:ARG:HD2	1.71	0.73
1:A:1723:TRP:HE1	1:A:1739:ILE:HG23	1.54	0.73
1:A:2061:LEU:HD12	1:A:2097:PRO:HA	1.69	0.73
1:A:2423:VAL:O	1:A:2426:ARG:HB3	1.89	0.72
1:C:2126:VAL:HG12	1:C:2180:TRP:HE3	1.53	0.72
1:C:674:GLN:OE1	1:C:720:LEU:HD22	1.89	0.72
1:C:315:HIS:CD2	1:C:320:ASN:HD21	2.08	0.72
1:C:1140:ALA:HB1	1:C:1173:GLN:HB2	1.69	0.72
1:C:1026:GLU:HG3	1:C:1030:LYS:HE2	1.69	0.72
1:A:1223:LEU:HD13	1:A:1244:ARG:HH22	1.54	0.72
4:H:100:ARG:C	4:H:101:PHE:HA	2.09	0.72
1:A:303:GLN:HB3	1:A:307:ARG:HB2	1.72	0.72
1:A:1440:LEU:HD22	1:A:1622:MET:HG2	1.71	0.72
1:C:842:TYR:HB3	1:C:844:GLU:CG	2.20	0.72
1:C:518:ILE:HG22	1:C:520:ASN:H	1.54	0.72
1:A:673:GLN:HA	1:A:676:ASN:ND2	2.04	0.72
1:A:2223:VAL:HG22	1:A:2459:GLU:HB3	1.71	0.72
1:C:401:LYS:HG3	1:C:403:ILE:HG12	1.72	0.72
1:C:797:TYR:CE2	1:C:844:GLU:HB3	2.25	0.72
1:C:2096:LYS:HA	1:C:2097:PHE:CG	2.25	0.72
2:B:53:GLN:HE21	2:B:94:SER:HB3	1.55	0.71
5:I:703:ILE:HG13	5:I:703:ILE:O	1.89	0.71
1:A:1027:ILE:HG21	1:A:1071:PHE:HA	1.72	0.71
5:J:690:ARG:HG2	5:J:691:ASN:HB2	1.72	0.71
1:A:2325:ALA:HA	1:A:2326:MET:C	2.11	0.71
1:C:235:LEU:HG	1:C:236:GLU:HA	1.71	0.71
1:A:1849:PHE:HB3	1:A:1886:GLN:HG3	1.72	0.71
1:A:704:SER:OG	1:A:714:LEU:HA	1.89	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:836:VAL:HG21	1:C:845:LEU:HB2	1.73	0.71
1:C:1505:LEU:HB3	1:C:1514:LYS:HG2	1.73	0.71
1:A:284:VAL:HG22	1:A:334:LEU:HD11	1.72	0.71
1:C:947:HIS:HA	1:C:950:GLN:HB2	1.72	0.71
1:A:1630:ASN:HA	1:A:1633:LEU:HD13	1.72	0.70
1:C:674:GLN:HB3	1:C:720:LEU:HB3	1.72	0.70
1:A:856:ASN:HB3	1:A:1584:LYS:HG2	1.73	0.70
1:A:1151:LEU:HB2	1:A:1152:GLY:CA	2.21	0.70
1:C:242:ALA:HA	1:C:245:ILE:HB	1.73	0.70
1:A:845:LEU:HG	1:A:1525:VAL:HG23	1.73	0.70
1:C:2145:LEU:CB	1:C:2146:VAL:HG13	2.22	0.70
1:C:797:TYR:HE2	1:C:844:GLU:HB3	1.55	0.70
1:C:1451:LEU:O	1:C:1455:LYS:N	2.16	0.70
1:C:2077:GLU:HA	1:C:2093:LYS:HG2	1.74	0.70
2:D:201:THR:HB	2:D:203:PHE:HE1	1.54	0.70
1:A:797:LEU:O	1:A:800:LEU:HB2	1.90	0.70
1:C:89:PHE:HA	1:C:101:ALA:HB2	1.71	0.70
1:C:260:TYR:HE1	1:C:300:ALA:HB1	1.56	0.70
1:C:490:CYS:HB3	1:C:491:PRO:HD3	1.74	0.70
1:C:777:SER:HA	1:C:780:LEU:HB3	1.71	0.70
1:A:142:SER:HA	1:A:145:LYS:HE3	1.74	0.70
1:A:2035:LEU:HD21	5:I:648:LYS:HE2	1.72	0.70
1:A:2053:LEU:HG	1:A:2056:LEU:HD22	1.73	0.70
1:C:157:ILE:HG12	1:C:172:ARG:HH22	1.55	0.70
1:C:336:LEU:HD22	1:C:342:TYR:HB3	1.74	0.70
5:J:730:VAL:HG21	5:J:789:THR:HA	1.72	0.70
1:C:1832:ILE:HD13	1:C:1837:SER:HB3	1.72	0.70
1:C:1920:ILE:HD13	1:C:1935:ILE:HD11	1.74	0.70
1:A:702:LEU:HD23	1:A:713:SER:HB3	1.74	0.70
1:C:1409:GLN:H	1:C:1410:ARG:HB3	1.56	0.69
1:A:91:LEU:HD11	1:A:143:SER:CB	2.21	0.69
1:A:841:TYR:CB	1:A:843:GLU:HG2	2.09	0.69
1:C:1983:ASN:HB3	1:C:1986:LYS:HB3	1.73	0.69
2:B:253:VAL:HB	2:B:267:THR:HG23	1.73	0.69
1:C:1097:SER:HG	1:C:1098:LEU:N	1.91	0.69
1:C:1718:CYS:HB2	1:C:1759:TRP:CH2	2.26	0.69
1:A:1503:LEU:HB3	1:A:1512:LYS:HG2	1.73	0.69
1:A:394:HIS:HB2	1:A:395:TYR:CG	2.27	0.69
1:A:1380:THR:HA	1:A:1383:ALA:HB3	1.75	0.69
1:A:1555:ILE:HG13	1:A:1556:ILE:H	1.57	0.69
1:C:329:LEU:HD21	1:C:357:TYR:CD2	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1088:VAL:HA	1:C:1100:LYS:HD2	1.73	0.69
1:C:1818:HIS:HA	1:C:1821:VAL:H	1.58	0.69
1:C:2031:SER:HG	1:C:2032:LYS:N	1.90	0.69
1:A:180:ILE:HG22	1:A:223:LEU:CD1	2.22	0.69
2:D:278:ASP:HB3	2:D:281:THR:HB	1.75	0.69
1:A:187:VAL:HG11	1:A:233:LYS:HA	1.73	0.69
1:C:179:VAL:HG11	1:C:191:LEU:HD13	1.74	0.69
1:C:1070:VAL:HG11	1:C:1109:LEU:HD23	1.74	0.69
2:D:83:PHE:CE1	2:D:104:VAL:HG21	2.27	0.69
1:A:296:ARG:HH11	1:A:338:LYS:HG2	1.58	0.69
1:A:361:PHE:HE1	1:A:414:PHE:CZ	2.10	0.69
1:A:1082:ILE:HG23	1:A:1085:ILE:HG12	1.74	0.69
1:A:1415:ALA:HA	1:A:1418:GLU:HB2	1.74	0.69
1:C:280:ARG:HH12	1:C:328:THR:HB	1.58	0.69
1:C:688:GLU:C	1:C:691:GLY:H	1.97	0.69
5:I:730:VAL:HB	5:I:788:GLU:O	1.92	0.69
1:C:681:LEU:HD11	1:C:724:THR:HG22	1.75	0.69
1:A:1668:ALA:HA	1:A:1671:GLN:HB2	1.74	0.69
1:A:2184:THR:HB	1:A:2284:MET:HB2	1.75	0.69
1:C:1612:ILE:HG23	1:C:1615:ALA:CB	2.22	0.69
1:C:260:TYR:CE1	1:C:300:ALA:HB1	2.28	0.68
1:C:628:GLN:O	1:C:631:VAL:HG22	1.92	0.68
1:C:818:ARG:HD2	1:C:868:LEU:HD13	1.76	0.68
1:C:2193:GLU:HA	1:C:2196:GLU:HB2	1.76	0.68
1:C:2319:ARG:HG2	1:C:2470:TRP:HZ3	1.58	0.68
1:C:378:ALA:HA	1:C:379:PHE:N	2.08	0.68
1:C:334:GLU:HG3	1:C:372:ILE:HD12	1.75	0.68
2:D:120:ASN:HD21	2:D:136:ARG:HA	1.59	0.68
1:A:453:LYS:N	1:A:454:GLN:HA	2.08	0.68
1:A:533:SER:HA	1:A:534:ASN:C	2.14	0.68
2:B:217:SER:HG	2:B:218:ASP:N	1.92	0.68
1:C:1421:LYS:HE2	1:C:1435:LYS:HD2	1.76	0.68
1:C:2186:THR:HA	1:C:2286:MET:HA	1.75	0.68
2:B:53:GLN:HG3	2:B:78:VAL:HG13	1.75	0.68
1:C:783:LEU:H	1:C:784:GLY:HA3	1.57	0.68
1:C:1474:ALA:HA	1:C:1478:LEU:H	1.57	0.68
2:B:12:HIS:HB3	2:B:30:HIS:O	1.93	0.68
1:A:300:LEU:HA	1:A:303:GLN:HB2	1.75	0.68
1:A:841:TYR:HB2	1:A:843:GLU:CG	2.10	0.68
1:A:2411:HIS:HA	1:A:2414:ALA:HB3	1.76	0.68
5:J:694:THR:C	5:J:696:LYS:H	1.97	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ARG:HD3	1:A:453:LYS:HB2	1.76	0.68
1:C:115:ALA:HB1	1:C:161:LEU:HB2	1.76	0.68
1:A:2211:ALA:HB2	1:A:2225:VAL:HG21	1.76	0.68
1:C:1533:LEU:C	1:C:1534:VAL:HA	2.14	0.68
2:D:232:ARG:HG2	2:D:245:THR:HA	1.76	0.68
1:A:1087:VAL:HB	1:A:1102:ILE:HG21	1.76	0.67
1:A:2315:PRO:HB3	1:A:2451:LEU:HB3	1.77	0.67
1:C:1611:ARG:C	1:C:1613:LYS:H	1.96	0.67
1:C:2409:VAL:N	1:C:2410:GLU:HG2	2.09	0.67
1:A:627:GLN:O	1:A:630:VAL:HG12	1.94	0.67
1:A:1516:HIS:HA	1:A:1519:ASN:HB2	1.75	0.67
1:A:1159:VAL:HG21	1:C:622:LYS:HD3	1.75	0.67
1:C:2142:LEU:HD11	1:C:2362:PHE:CE2	2.28	0.67
1:C:2370:TRP:N	1:C:2371:GLY:HA3	2.10	0.67
1:A:314:HIS:HD2	1:A:328:LEU:HD11	1.60	0.67
1:A:1906:HIS:HA	1:A:1908:GLN:HB3	1.76	0.67
5:I:685:SER:HB3	5:I:686:LYS:HB2	1.77	0.67
1:A:1573:GLU:O	1:A:1577:THR:N	2.27	0.67
1:C:1920:ILE:HG12	1:C:1932:LEU:HG	1.74	0.67
2:D:10:TYR:HE2	2:D:293:LYS:HG3	1.60	0.67
1:A:835:VAL:HG13	1:A:1525:VAL:HG11	1.76	0.67
1:C:1542:TYR:H	1:C:1543:ASN:HA	1.58	0.67
2:B:5:LEU:HA	2:B:6:VAL:N	2.10	0.67
1:C:268:ILE:HG23	1:C:311:GLN:HG3	1.77	0.67
1:C:1844:LEU:HB2	1:C:2358:ILE:HG21	1.77	0.67
1:A:396:LEU:HD23	1:A:400:LYS:HG2	1.76	0.67
1:A:1558:TYR:HA	1:A:1562:PRO:HD2	1.77	0.67
1:C:1382:THR:HA	1:C:1385:ALA:HB3	1.77	0.66
1:C:961:ASP:HB3	1:C:965:PRO:HG2	1.77	0.66
1:C:2354:SER:HA	1:C:2356:MET:H	1.60	0.66
1:A:650:ASP:N	1:A:651:PRO:HD3	2.04	0.66
1:A:2363:ASP:HB2	1:A:2367:ASN:O	1.96	0.66
1:A:257:TYR:CG	1:A:286:LEU:HD11	2.31	0.66
2:B:22:GLY:HA3	2:B:286:ARG:HD3	1.76	0.66
2:B:255:ASP:OD1	2:B:297:CYS:HA	1.95	0.66
1:C:188:VAL:HA	1:C:192:ALA:HB3	1.76	0.66
1:A:704:SER:HG	1:A:714:LEU:HA	1.60	0.66
1:A:855:GLU:O	1:A:1588:VAL:HG22	1.94	0.66
1:A:1228:TYR:HE1	1:A:1293:GLU:HB2	1.61	0.66
1:C:271:PRO:HG2	1:C:280:ARG:HB2	1.78	0.66
1:C:418:VAL:HB	1:C:419:SER:N	2.11	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:ALA:HA	1:A:698:ILE:HB	1.76	0.66
1:A:2283:LEU:HD21	1:A:2317:ARG:CD	2.25	0.66
1:C:2374:LEU:HD21	1:C:2417:ILE:HD12	1.78	0.66
1:A:178:VAL:HB	1:A:179:LEU:HG	1.78	0.66
1:A:179:LEU:HD13	1:A:233:LYS:HE3	1.76	0.66
1:A:1020:ILE:HG21	1:A:1024:ILE:HB	1.78	0.66
1:A:1918:ILE:HG12	1:A:1930:LEU:HG	1.78	0.66
2:D:205:ALA:HB3	2:D:206:HIS:HB2	1.78	0.66
2:D:229:HIS:CB	2:D:251:ARG:HB2	2.25	0.66
1:A:664:GLY:HA2	1:A:671:LEU:HG	1.77	0.66
1:A:2251:THR:HA	1:A:2254:GLU:HB3	1.75	0.66
1:C:181:ILE:HG22	1:C:228:ASN:HD21	1.60	0.66
1:C:188:VAL:HG11	1:C:234:LYS:HA	1.76	0.66
1:C:1056:SER:HG	1:C:1057:ASN:N	1.94	0.66
1:C:1440:TYR:HE1	1:C:1473:GLY:HA3	1.61	0.66
1:A:197:ARG:C	1:A:199:THR:HG23	2.16	0.66
1:A:687:GLU:C	1:A:690:GLY:H	1.99	0.66
1:C:268:ILE:CG2	1:C:311:GLN:HG3	2.26	0.66
1:A:835:VAL:HG21	1:A:844:LEU:H	1.61	0.66
1:C:90:ASP:HB3	1:C:91:LYS:HG2	1.77	0.66
1:C:2114:CYS:HB3	1:C:2123:TYR:C	2.17	0.66
1:A:391:ILE:HA	1:A:395:TYR:CD2	2.31	0.65
1:A:1848:TRP:CZ2	1:A:1857:ALA:HB1	2.30	0.65
1:A:1858:THR:HA	1:A:1862:HIS:HB3	1.78	0.65
1:A:2078:VAL:HG22	1:A:2089:ILE:HG23	1.78	0.65
2:D:297:CYS:CA	2:D:298:VAL:HB	2.15	0.65
1:A:2407:VAL:HG13	1:A:2408:GLU:OE1	1.97	0.65
2:B:216:SER:HG	2:B:221:HIS:N	1.95	0.65
1:C:1505:LEU:HB3	1:C:1514:LYS:CG	2.26	0.65
2:B:3:VAL:HG11	2:B:19:ALA:HB3	1.79	0.65
1:C:1284:CYS:SG	1:C:1288:LEU:HB3	2.36	0.65
1:C:2114:CYS:HB2	1:C:2122:ASP:HB3	1.78	0.65
2:D:272:HIS:HA	2:D:293:LYS:O	1.95	0.65
1:A:280:LEU:O	1:A:283:ALA:N	2.30	0.65
1:A:2261:ARG:HG2	1:A:2337:ILE:HD13	1.78	0.65
1:C:572:ILE:HG22	1:C:573:LEU:HG	1.78	0.65
2:D:33:SER:CB	2:D:51:GLY:HA2	2.27	0.65
1:A:259:TYR:CD1	1:A:260:VAL:HG23	2.32	0.65
1:A:632:ALA:HA	1:A:635:SER:HB2	1.77	0.65
1:A:2286:ASP:HB3	1:A:2288:ILE:HG13	1.79	0.65
1:C:1248:ILE:HG12	1:C:1260:ARG:HH12	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:TYR:N	1:A:293:ILE:HA	2.12	0.65
1:A:1723:TRP:NE1	1:A:1739:ILE:HG23	2.11	0.65
1:C:2015:GLY:HA2	1:C:2018:LEU:HG	1.79	0.65
1:A:345:LYS:O	1:A:372:LEU:HD21	1.96	0.65
2:D:101:VAL:HG11	2:D:143:TRP:CH2	2.31	0.65
1:A:682:MET:O	1:A:685:ASN:HB2	1.97	0.64
1:A:2432:THR:H	1:A:2447:GLN:NE2	1.95	0.64
1:C:402:ASN:HA	1:C:414:PRO:HG3	1.80	0.64
1:C:662:GLN:HE22	1:C:677:ASN:HA	1.60	0.64
1:C:1007:VAL:HG13	1:C:1009:ARG:CZ	2.27	0.64
1:C:1575:GLU:O	1:C:1579:THR:N	2.30	0.64
2:D:216:SER:HG	2:D:221:HIS:N	1.94	0.64
1:C:1495:SER:HG	1:C:1498:LYS:N	1.94	0.64
1:C:1954:HIS:HA	1:C:1957:ILE:HG22	1.78	0.64
5:J:694:THR:HG22	5:J:696:LYS:HB2	1.78	0.64
1:A:854:THR:HB	1:A:1579:LEU:HB2	1.80	0.64
1:A:2095:PHE:HB2	1:A:2096:GLU:N	2.11	0.64
1:C:533:GLN:C	1:C:535:ASN:H	2.00	0.64
1:C:1725:TRP:HE1	1:C:1741:ILE:HG22	1.63	0.64
1:A:360:LYS:HE2	1:A:365:ARG:HH22	1.62	0.64
1:A:1627:LYS:O	1:A:1630:ASN:N	2.31	0.64
1:C:601:ILE:HG12	1:C:603:HIS:HB2	1.79	0.64
1:C:1510:ASN:ND2	4:G:73:PHE:HA	2.12	0.64
1:A:1517:ILE:HG12	1:A:1553:GLU:HB3	1.78	0.64
1:A:1559:LYS:N	1:A:1572:ARG:HH22	1.95	0.64
1:A:1041:GLU:HA	1:A:1044:THR:HG22	1.80	0.64
1:A:1453:LYS:HE3	1:A:1465:MET:CE	2.28	0.64
5:I:740:SER:HB2	5:I:768:SER:HA	1.80	0.64
1:A:633:LEU:HA	1:A:636:VAL:HB	1.79	0.64
1:A:742:CYS:HB2	1:A:743:THR:OG1	1.97	0.64
1:C:2374:LEU:HB3	1:C:2375:PRO:HD3	1.79	0.64
2:D:201:THR:HB	2:D:203:PHE:CE1	2.32	0.64
1:A:1963:GLU:HG2	1:A:2056:LEU:HD21	1.80	0.64
1:C:2244:LEU:HD11	1:C:2328:MET:HA	1.79	0.64
1:A:331:PHE:HZ	1:A:345:LYS:HE2	1.63	0.63
1:A:1829:SER:HG	1:A:1830:ILE:N	1.96	0.63
1:C:1725:TRP:NE1	1:C:1741:ILE:HG22	2.13	0.63
1:A:613:LEU:HA	1:A:616:CYS:HB3	1.80	0.63
1:A:856:ASN:HA	1:A:1584:LYS:HA	1.80	0.63
1:A:124:ARG:NH2	1:A:170:SER:HB3	2.12	0.63
1:A:1291:TYR:HE1	1:A:1340:TYR:HE2	1.45	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1837:SER:HG	1:A:1839:GLN:N	1.96	0.63
1:C:188:VAL:HG13	1:C:234:LYS:HA	1.79	0.63
1:C:948:ILE:HG13	1:C:952:LEU:HD13	1.81	0.63
5:J:730:VAL:HG11	5:J:790:PRO:HD2	1.81	0.63
1:A:2259:TYR:HA	1:A:2262:SER:CB	2.26	0.63
1:A:1617:ARG:HA	1:A:1624:LEU:HD22	1.81	0.63
1:C:1758:ALA:HA	1:C:1761:ASN:HD22	1.62	0.63
1:A:1969:LEU:HD13	1:A:1989:LEU:HD21	1.80	0.63
1:A:2266:MET:HA	1:A:2269:THR:HB	1.79	0.63
1:C:115:ALA:C	1:C:117:GLU:H	2.02	0.63
1:C:1965:GLU:OE1	1:C:2054:GLN:HG3	1.99	0.63
2:B:55:VAL:HA	2:B:81:VAL:HG21	1.80	0.63
1:C:453:ARG:HD3	1:C:454:LYS:HB2	1.81	0.63
5:I:678:LEU:HD21	5:I:688:TYR:CE2	2.34	0.63
1:C:309:LEU:HA	1:C:346:LYS:HZ1	1.63	0.63
1:C:1978:PHE:HB2	1:C:1987:MET:HB2	1.79	0.62
1:C:1983:ASN:HD22	1:C:1987:MET:HG3	1.64	0.62
1:C:2141:GLN:C	1:C:2142:LEU:HA	2.19	0.62
1:C:2433:LEU:HD22	1:C:2449:GLN:HA	1.81	0.62
3:E:404:UNK:O	3:E:408:UNK:N	2.27	0.62
1:C:825:LEU:HA	1:C:828:LEU:HB2	1.81	0.62
1:C:1119:SER:HG	1:C:1120:SER:N	1.97	0.62
1:C:1440:TYR:HD1	1:C:1445:TRP:HE1	1.45	0.62
3:E:401:UNK:C	3:E:402:UNK:HA	2.29	0.62
5:I:655:SER:HA	5:I:659:LEU:CB	2.29	0.62
5:I:707:ILE:HD13	5:I:728:LEU:HG	1.80	0.62
1:C:379:PHE:HB2	1:C:381:PRO:HD2	1.80	0.62
1:C:849:LEU:HD22	1:C:1549:GLN:HB3	1.82	0.62
1:A:341:TYR:CE2	1:A:345:LYS:HE2	2.35	0.62
1:C:865:THR:HA	1:C:868:LEU:HD12	1.81	0.62
1:A:1555:ILE:HD13	1:A:1575:TRP:CZ2	2.34	0.62
1:A:1566:ASP:HB3	1:A:1568:ARG:HG3	1.81	0.62
2:B:232:ARG:HG2	2:B:245:THR:HA	1.79	0.62
1:C:1429:VAL:HB	1:C:1435:LYS:HZ2	1.64	0.62
5:I:655:SER:HA	5:I:659:LEU:HB2	1.81	0.62
1:A:2059:LEU:HD21	1:A:2099:PHE:HB2	1.81	0.62
1:C:181:ILE:H	1:C:182:PRO:N	1.96	0.62
1:C:305:TRP:HE1	1:C:341:PRO:HG2	1.64	0.62
1:C:670:PRO:HD2	1:C:671:GLN:N	2.14	0.62
1:C:760:ILE:HG13	1:C:761:LEU:HA	1.82	0.62
1:C:1956:LEU:HD21	1:C:2127:LEU:HD22	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:VAL:HG11	1:A:232:SER:O	1.99	0.62
1:A:600:ILE:H	1:A:602:HIS:HB2	1.64	0.62
1:A:2043:TYR:HB3	1:A:2047:ARG:HH12	1.63	0.62
1:A:593:ARG:O	1:A:597:ILE:N	2.33	0.62
1:A:849:ILE:HB	1:A:1551:GLU:N	2.15	0.62
1:A:993:LYS:HA	1:A:994:GLN:HB2	1.80	0.62
1:A:1555:ILE:HG13	1:A:1556:ILE:N	2.15	0.62
1:A:2457:SER:HA	1:A:2458:VAL:HA	1.82	0.62
5:J:701:SER:H	5:J:702:THR:HB	1.65	0.62
1:A:300:LEU:HD13	1:A:303:GLN:HB2	1.81	0.62
1:A:499:LEU:HA	1:A:502:LEU:HB2	1.81	0.62
1:A:845:LEU:HD22	1:A:1547:GLN:HG3	1.80	0.62
1:C:764:ILE:HA	1:C:806:ILE:HG21	1.80	0.62
1:C:1274:ARG:HB2	1:C:1327:HIS:HE1	1.64	0.62
2:D:254:TRP:CD1	2:D:296:VAL:HA	2.35	0.62
1:A:1291:TYR:HE1	1:A:1340:TYR:CE2	2.17	0.62
1:A:1371:ILE:CD1	1:A:1387:LEU:HG	2.28	0.62
1:A:1634:GLU:HG3	1:A:1651:VAL:HG11	1.82	0.62
1:A:1820:ILE:N	1:A:1821:PRO:CD	2.63	0.62
1:A:2078:VAL:N	1:A:2090:VAL:O	2.32	0.62
1:C:221:TRP:HA	1:C:235:LEU:HD13	1.82	0.62
1:C:355:MET:SD	1:C:389:LEU:HD13	2.40	0.62
1:A:1592:ILE:HD12	1:A:1596:ARG:HD3	1.82	0.61
1:A:2301:PHE:N	1:A:2374:THR:HG1	1.98	0.61
1:C:1218:PRO:HB2	1:C:1221:GLN:HB2	1.81	0.61
1:A:517:ILE:HG22	1:A:519:ASN:H	1.65	0.61
1:C:793:GLU:HG3	1:C:795:THR:OG1	2.00	0.61
1:C:1964:HIS:NE2	1:C:2008:ILE:HA	2.15	0.61
1:C:2062:GLU:HG2	1:C:2064:GLN:H	1.64	0.61
1:A:443:GLU:HB3	1:A:446:ARG:HH11	1.64	0.61
1:A:280:LEU:HA	1:A:330:VAL:CG2	2.26	0.61
1:A:776:SER:HA	1:A:779:LEU:HB3	1.81	0.61
1:A:1224:LYS:HB2	1:A:1241:TRP:CE2	2.36	0.61
1:C:203:GLY:HA2	1:C:206:LEU:HB3	1.82	0.61
1:C:351:TYR:HH	1:C:386:LYS:N	1.98	0.61
2:B:210:ILE:HD13	2:B:224:THR:HG22	1.82	0.61
1:C:1557:ILE:CG2	1:C:1577:TRP:HE1	2.13	0.61
1:C:2096:LYS:HA	1:C:2097:PHE:CB	2.30	0.61
2:B:233:VAL:O	2:B:243:GLU:HB3	1.99	0.61
1:C:264:ILE:O	1:C:268:ILE:HB	2.00	0.61
1:C:938:HIS:HE1	1:C:978:GLN:HA	1.65	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1295:ASP:CG	1:C:1342:TYR:OH	2.38	0.61
5:J:730:VAL:HG21	5:J:790:PRO:HD2	1.81	0.61
1:A:1592:ILE:HB	1:A:1596:ARG:HB3	1.82	0.61
1:C:2185:ASP:O	1:C:2287:LEU:HG	2.01	0.61
1:C:2354:SER:HA	1:C:2356:MET:N	2.15	0.61
1:A:331:PHE:HZ	1:A:345:LYS:CE	2.13	0.61
1:A:1084:PRO:HG2	1:A:1117:MET:SD	2.41	0.61
2:B:127:ASN:ND2	2:B:130:GLU:HB2	2.14	0.61
1:C:1074:PRO:HA	1:C:1075:ASN:HB2	1.81	0.61
1:C:1151:GLN:HA	1:C:1151:GLN:NE2	2.15	0.61
1:C:1391:HIS:HB2	1:C:2334:GLU:HG2	1.81	0.61
1:A:345:LYS:HG3	1:A:349:ILE:CG1	2.31	0.61
1:C:213:PHE:O	1:C:217:THR:N	2.33	0.61
1:C:265:LEU:CA	1:C:307:GLN:HB3	2.20	0.61
1:C:630:SER:O	1:C:634:LEU:HG	2.01	0.61
1:A:346:TYR:OH	1:A:382:ILE:HG13	2.00	0.61
1:A:360:LYS:HE2	1:A:365:ARG:NH2	2.16	0.61
1:C:1591:TRP:HE3	1:C:1614:PHE:HE1	1.49	0.61
1:C:1906:LYS:C	1:C:1909:PRO:HD3	2.21	0.61
1:C:2268:MET:HA	1:C:2271:THR:HB	1.81	0.61
2:D:183:CYS:SG	2:D:213:ILE:HG21	2.41	0.61
1:A:835:VAL:HB	1:A:844:LEU:HD23	1.83	0.60
2:D:9:GLY:O	2:D:12:HIS:CE1	2.54	0.60
3:E:408:UNK:C	3:E:410:UNK:H	2.13	0.60
1:C:766:PRO:HG3	1:C:809:PHE:HB3	1.83	0.60
1:C:1140:ALA:HB1	1:C:1173:GLN:HB3	1.83	0.60
1:C:1938:MET:HB3	1:C:1946:VAL:HG11	1.82	0.60
1:A:182:SER:HB3	1:A:187:VAL:HG23	1.81	0.60
1:A:324:VAL:HG22	1:A:327:THR:CG2	2.31	0.60
2:B:182:ASN:HA	2:B:183:CYS:HB2	1.82	0.60
1:C:681:LEU:HD22	1:C:728:PHE:HD1	1.66	0.60
1:C:1661:LEU:HG	1:C:1666:LEU:HB2	1.83	0.60
5:I:759:ASP:HB2	5:I:761:LYS:H	1.66	0.60
1:A:1679:MET:HA	1:A:1682:ASP:HB2	1.84	0.60
1:C:173:LEU:HD21	1:C:209:ASP:HA	1.81	0.60
3:E:214:UNK:C	3:E:215:UNK:H2	2.13	0.60
5:J:699:LYS:HD3	5:J:760:ARG:HD2	1.84	0.60
1:A:699:ILE:HG23	1:A:717:THR:HG22	1.82	0.60
1:A:1716:CYS:HB2	1:A:1757:TRP:CH2	2.37	0.60
1:C:235:LEU:CG	1:C:236:GLU:HA	2.31	0.60
1:C:1389:LEU:HD11	1:C:1403:THR:HA	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1625:ALA:O	1:C:1626:LEU:N	2.34	0.60
1:C:2026:MET:HG3	1:C:2027:ASN:H	1.66	0.60
2:D:206:HIS:CD2	2:D:224:THR:HG22	2.36	0.60
1:A:381:ALA:HB1	1:A:385:LYS:HD3	1.84	0.60
1:A:2132:ARG:HA	1:A:2135:SER:HB2	1.83	0.60
2:B:99:ILE:HD13	2:B:122:VAL:HG21	1.82	0.60
1:C:285:VAL:HG22	1:C:335:LEU:CD1	2.31	0.60
1:C:1025:ILE:HA	1:C:1028:ILE:HG12	1.82	0.60
1:A:1885:HIS:HA	1:A:1886:GLN:N	2.17	0.60
1:A:2336:ARG:HA	1:A:2339:CYS:HB2	1.83	0.60
2:B:246:LEU:HD11	2:B:282:ARG:O	2.02	0.60
1:C:181:ILE:HG22	1:C:224:LEU:HD13	1.82	0.60
1:C:767:LYS:HB3	1:C:772:SER:HA	1.83	0.60
2:D:100:LYS:HA	2:D:101:VAL:HG12	1.83	0.60
1:C:1881:GLN:HG2	1:C:2134:ARG:HH21	1.65	0.60
2:D:37:ARG:HH22	2:D:212:ARG:HH22	1.48	0.60
1:A:1139:ALA:HB1	1:A:1172:GLN:OE1	2.02	0.60
2:B:206:HIS:CE1	2:B:226:SER:HB2	2.37	0.60
1:C:2063:LEU:H	1:C:2066:VAL:H	1.50	0.60
1:C:2407:GLN:O	1:C:2409:VAL:N	2.34	0.60
5:J:730:VAL:CG2	5:J:789:THR:HA	2.32	0.60
1:A:2238:LEU:HB3	1:A:2326:MET:H	1.67	0.60
1:C:997:ILE:HA	1:C:1000:HIS:HD2	1.67	0.60
1:A:683:ALA:HA	1:A:688:ILE:HD13	1.84	0.59
1:A:1283:CYS:HA	1:A:1287:LEU:N	2.17	0.59
1:A:2187:VAL:HA	1:A:2190:ARG:HG2	1.84	0.59
1:A:2266:MET:CB	1:A:2292:VAL:HG21	2.32	0.59
1:C:1541:ALA:CB	1:C:1542:TYR:HA	2.32	0.59
1:C:2062:GLU:CA	1:C:2063:LEU:HB2	2.28	0.59
3:E:607:UNK:HA	3:E:608:UNK:C	2.32	0.59
1:A:233:LYS:HE2	1:A:237:ARG:HG2	1.83	0.59
1:A:314:HIS:HB2	1:A:328:LEU:HD21	1.85	0.59
1:A:347:ASP:N	1:A:348:ASP:HB2	2.17	0.59
1:A:1600:ILE:HG13	1:A:1601:LYS:H	1.65	0.59
1:C:1578:ASN:C	1:C:1579:THR:N	2.55	0.59
1:C:1612:ILE:HG21	1:C:1656:ALA:HB1	1.83	0.59
1:C:176:TYR:CE1	1:C:191:LEU:HD22	2.37	0.59
1:A:569:ALA:O	1:A:573:ILE:HG13	2.03	0.59
1:A:1945:ASP:HA	1:A:1948:GLU:HB2	1.85	0.59
1:C:280:ARG:HH22	1:C:328:THR:HB	1.68	0.59
1:C:801:LEU:HD23	1:C:805:ILE:HD11	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1474:ALA:HB1	1:C:1478:LEU:HD23	1.84	0.59
1:C:1661:LEU:O	1:C:1666:LEU:N	2.35	0.59
1:A:824:LEU:CD2	1:A:1534:GLU:HB2	2.31	0.59
2:B:276:LEU:O	2:B:286:ARG:N	2.35	0.59
1:C:2064:GLN:HG3	1:C:2065:HIS:HD2	1.64	0.59
1:C:2247:LYS:HA	1:C:2249:ARG:N	2.16	0.59
5:J:674:GLU:HB2	5:J:693:PHE:CE2	2.37	0.59
1:A:818:ASP:HA	1:A:821:LEU:HB3	1.83	0.59
1:A:864:THR:HG23	1:A:867:LEU:HD12	1.84	0.59
1:A:1320:VAL:HG22	1:A:1345:HIS:CE1	2.38	0.59
1:A:1423:GLY:HA3	1:A:1424:GLU:HG3	1.84	0.59
1:C:1674:LEU:O	1:C:1678:THR:N	2.36	0.59
1:C:1844:LEU:HD11	1:C:1878:VAL:HG11	1.84	0.59
1:C:2024:TRP:HB2	1:C:2039:GLN:HG2	1.85	0.59
2:D:17:TRP:HZ2	2:D:290:GLY:HA3	1.67	0.59
1:A:211:GLU:HG3	1:A:211:GLU:O	2.01	0.59
1:A:300:LEU:HD12	1:A:339:ALA:HB2	1.85	0.59
1:A:419:ILE:HG21	1:A:462:CYS:HB3	1.85	0.59
1:A:732:LYS:HB3	1:A:735:GLU:HB2	1.84	0.59
1:A:2079:PRO:HD3	1:A:2090:VAL:HG13	1.83	0.59
1:A:2394:LEU:HD21	1:A:2404:VAL:HG13	1.83	0.59
1:C:1757:LYS:HA	1:C:1832:ILE:HG21	1.85	0.59
1:C:2080:VAL:HA	1:C:2092:VAL:HG12	1.84	0.59
1:A:2204:HIS:CE1	1:A:2470:PRO:HD2	2.37	0.59
1:A:2242:LEU:HD11	1:A:2326:MET:HA	1.83	0.59
2:B:229:HIS:HD2	2:B:252:TRP:H	1.50	0.59
1:A:594:LEU:HD23	1:A:597:ILE:HD12	1.84	0.59
1:A:1049:ILE:HD12	1:A:1064:ILE:HG12	1.85	0.59
1:C:188:VAL:CG2	1:C:233:SER:HB3	2.31	0.59
1:C:2062:GLU:O	1:C:2065:HIS:HB2	2.03	0.59
1:A:194:THR:HG22	1:A:197:ARG:HH21	1.68	0.58
1:A:260:VAL:HG22	1:A:303:GLN:HE21	1.68	0.58
1:A:336:SER:HB2	1:A:375:LEU:HB2	1.85	0.58
1:A:688:ILE:HG13	1:A:689:PHE:N	2.18	0.58
1:A:1054:GLN:HE21	1:A:1057:LYS:HG2	1.68	0.58
1:A:1178:GLN:HA	1:A:1181:ASN:HB2	1.83	0.58
1:A:1232:GLN:O	1:A:1233:LYS:HB2	2.03	0.58
1:C:353:SER:HB3	1:C:357:TYR:CE2	2.38	0.58
1:C:2258:ARG:O	1:C:2262:THR:N	2.36	0.58
1:A:515:SER:O	1:A:518:LEU:HG	2.03	0.58
1:C:1294:GLU:HA	1:C:1295:ASP:HA	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1494:GLN:HA	1:C:1495:SER:N	2.19	0.58
1:A:241:ALA:HA	1:A:244:ILE:HB	1.83	0.58
1:A:554:SER:H	1:A:555:PHE:HB2	1.66	0.58
1:A:2060:GLU:HG2	1:A:2097:PRO:C	2.23	0.58
1:C:116:ARG:NH2	1:C:156:LEU:HD23	2.18	0.58
1:C:260:TYR:H	1:C:260:TYR:HD2	1.50	0.58
1:C:651:ASP:HB3	1:C:652:PRO:HA	1.85	0.58
1:C:1430:GLU:HA	1:C:1458:THR:HG22	1.85	0.58
1:A:353:THR:OG1	1:A:368:VAL:HG12	2.03	0.58
1:A:1273:ARG:HE	1:A:1277:ASN:HD22	1.49	0.58
1:C:857:ASN:HB3	1:C:1586:LYS:CA	2.27	0.58
1:C:2080:VAL:HG12	1:C:2083:THR:HB	1.84	0.58
1:A:445:LEU:HG	1:A:449:PHE:CE2	2.39	0.58
1:A:1574:THR:HG22	1:A:1578:ARG:HB2	1.86	0.58
1:A:2425:LYS:HA	1:A:2434:ASN:ND2	2.16	0.58
1:C:471:LEU:HD13	1:C:475:PHE:HB2	1.84	0.58
1:C:710:TYR:N	1:C:714:SER:HG	2.01	0.58
1:C:1373:ILE:HD13	1:C:1389:LEU:HD23	1.84	0.58
1:C:1384:SER:HB3	1:C:2335:GLY:HA3	1.84	0.58
1:C:1451:LEU:O	1:C:1454:GLU:N	2.37	0.58
1:C:1914:TYR:O	1:C:1918:VAL:HG23	2.03	0.58
1:A:276:LEU:HB3	1:A:279:ARG:HH21	1.68	0.58
1:C:2446:VAL:O	1:C:2450:VAL:HB	2.03	0.58
1:A:187:VAL:HA	1:A:191:ALA:HB3	1.85	0.58
1:A:1870:ILE:HG22	1:A:1873:TRP:N	2.17	0.58
2:B:105:ARG:O	2:B:106:SER:HB2	2.04	0.58
1:C:681:LEU:HD13	1:C:728:PHE:HA	1.85	0.58
1:A:246:LYS:N	1:A:289:CYS:HG	2.01	0.58
1:A:1113:ASN:HB3	1:A:1149:LEU:HB3	1.86	0.58
1:A:1602:PRO:HG2	1:A:1635:GLU:HG2	1.86	0.58
1:C:378:ALA:HB2	1:C:386:LYS:HD2	1.85	0.58
1:C:2268:MET:SD	1:C:2296:HIS:N	2.77	0.58
2:D:16:PHE:HB2	2:D:26:ARG:HB3	1.84	0.58
2:D:233:VAL:HG21	2:D:279:LEU:HD11	1.86	0.58
1:C:213:PHE:CE1	1:C:239:ARG:HA	2.38	0.58
1:C:214:GLU:HA	1:C:217:THR:HG22	1.86	0.58
1:C:1629:LYS:HE3	1:C:1633:THR:HG21	1.86	0.58
1:C:1743:GLY:HA3	1:C:1746:LEU:HB2	1.85	0.58
1:C:1832:ILE:HD13	1:C:1837:SER:CB	2.32	0.58
1:C:2115:ILE:HG13	1:C:2125:TYR:CE2	2.39	0.58
1:A:1049:ILE:HG23	1:A:1064:ILE:HD13	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1446:LEU:N	1:A:1447:SER:HB2	2.17	0.58
1:A:331:PHE:CE2	1:A:349:ILE:HG21	2.34	0.57
1:A:519:ASN:HB3	1:A:520:LEU:HD13	1.85	0.57
1:A:680:LEU:HD13	1:A:727:PHE:HA	1.84	0.57
1:A:1139:ALA:HA	1:A:1172:GLN:HB3	1.84	0.57
1:C:89:PHE:HE2	1:C:131:ASN:ND2	2.01	0.57
1:C:1819:ARG:HE	1:C:1853:PHE:HZ	1.51	0.57
1:A:1061:PRO:HA	1:A:1064:ILE:HD12	1.86	0.57
1:C:213:PHE:HE1	1:C:239:ARG:HA	1.68	0.57
1:C:1009:ARG:HB2	1:C:1011:PHE:CD2	2.40	0.57
1:C:2112:LYS:HD2	1:C:2180:TRP:HZ3	1.69	0.57
1:A:344:ASP:HB2	1:A:345:LYS:HB2	1.86	0.57
1:A:345:LYS:HG3	1:A:349:ILE:HG12	1.86	0.57
1:A:669:PRO:HG2	1:A:719:LEU:HD21	1.86	0.57
1:A:693:LEU:HA	1:A:696:ILE:HD12	1.85	0.57
1:A:1821:PRO:HA	1:A:1824:LYS:HG3	1.86	0.57
2:B:29:GLN:HB3	5:I:682:ILE:HG21	1.84	0.57
1:C:2180:TRP:HA	1:C:2181:VAL:HB	1.84	0.57
2:D:186:TRP:HB3	2:D:197:LEU:HB3	1.86	0.57
1:A:232:SER:HB2	1:A:236:TYR:HE2	1.69	0.57
1:A:848:LEU:H	1:A:1547:GLN:HE22	1.52	0.57
1:A:947:ILE:HG13	1:A:951:LEU:HD13	1.85	0.57
1:A:1010:PHE:HD1	1:A:1021:ILE:HG23	1.70	0.57
1:A:1034:GLU:HA	1:A:1035:PHE:N	2.19	0.57
1:A:1099:LYS:HA	1:A:1102:ILE:HB	1.85	0.57
1:A:1453:LYS:HE3	1:A:1465:MET:HE3	1.87	0.57
1:A:1502:ILE:HB	1:A:1594:ARG:HH22	1.69	0.57
1:A:1596:ARG:C	1:A:1598:LEU:H	2.06	0.57
1:C:135:PHE:HA	1:C:145:GLU:O	2.04	0.57
1:C:694:LEU:HD12	1:C:697:ILE:HD12	1.86	0.57
1:C:2138:LEU:O	1:C:2142:LEU:N	2.37	0.57
1:A:1384:ILE:HD13	1:A:1408:ARG:NH2	2.20	0.57
1:C:359:GLU:HG3	1:C:389:LEU:HD21	1.85	0.57
1:A:1856:GLU:O	1:A:1861:MET:N	2.37	0.57
1:A:1935:LYS:O	1:A:1939:HIS:N	2.37	0.57
1:C:193:ALA:HA	1:C:196:LEU:HB3	1.86	0.57
1:C:689:ILE:HG13	1:C:690:PHE:N	2.20	0.57
1:C:1448:LEU:HD13	1:C:1470:LEU:HA	1.85	0.57
5:I:693:PHE:CZ	5:I:760:ARG:HB3	2.39	0.57
2:B:231:ALA:HB1	2:B:265:LEU:HD21	1.86	0.57
1:C:1443:GLY:HA3	1:C:1628:LYS:HD2	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1771:SER:HB2	1:C:1845:ARG:HH22	1.70	0.57
1:C:2344:VAL:O	1:C:2348:LEU:HG	2.03	0.57
1:A:1039:VAL:HG23	1:A:1040:PRO:HD3	1.85	0.57
2:D:267:THR:HG1	2:D:277:TRP:HE1	1.51	0.57
1:A:768:GLN:HB2	1:A:770:ALA:N	2.16	0.57
1:A:1969:LEU:CB	1:A:1970:ASP:HA	2.35	0.57
2:B:278:ASP:HB3	2:B:281:THR:HB	1.87	0.57
1:C:280:ARG:HH12	1:C:328:THR:CB	2.18	0.57
1:C:347:TYR:OH	1:C:383:ILE:O	2.22	0.57
1:C:700:ILE:HD12	1:C:718:THR:CG2	2.35	0.57
1:C:860:HIS:O	1:C:862:ARG:N	2.34	0.57
1:C:2288:ASP:HB3	1:C:2290:ILE:CG1	2.35	0.57
2:D:231:ALA:HB2	2:D:253:VAL:HG11	1.86	0.57
1:A:259:TYR:HD1	1:A:260:VAL:HG23	1.68	0.57
1:A:471:GLY:C	4:H:187:THR:HA	2.25	0.57
1:A:569:ALA:HA	1:A:591:PHE:HE1	1.69	0.57
1:A:766:LYS:O	1:A:768:GLN:N	2.31	0.57
1:A:1001:GLU:HG2	1:A:1044:THR:HG21	1.86	0.57
1:A:1020:ILE:CG2	1:A:1024:ILE:HB	2.35	0.57
1:A:1103:ILE:HB	1:A:1141:MET:HE2	1.86	0.57
1:A:1406:LEU:HD13	1:A:1412:ALA:HA	1.85	0.57
1:C:450:PHE:HB3	1:C:453:ARG:HD2	1.87	0.57
1:C:2352:LYS:O	1:C:2356:MET:HG2	2.04	0.57
5:J:755:PHE:CE2	5:J:781:GLU:HB3	2.39	0.57
1:A:177:ARG:H	1:A:178:VAL:HG22	1.69	0.56
1:A:1010:PHE:HE1	1:A:1022:SER:HB2	1.69	0.56
1:A:2112:CYS:HB3	1:A:2122:LYS:N	2.20	0.56
1:C:216:ARG:HD2	1:C:234:LYS:NZ	2.20	0.56
1:C:346:LYS:HB3	1:C:350:ILE:HG13	1.87	0.56
1:C:828:LEU:HD11	1:C:848:ILE:HG21	1.87	0.56
1:C:1407:LYS:HD2	1:C:1413:ASP:N	2.20	0.56
2:D:276:LEU:HB3	2:D:286:ARG:HB2	1.87	0.56
1:A:457:LYS:HB3	1:A:485:LEU:HD11	1.87	0.56
1:A:1076:GLU:HB3	1:A:1079:SER:OG	2.05	0.56
1:A:1090:THR:HG23	1:A:1091:GLU:HB2	1.86	0.56
1:A:2453:GLN:O	1:A:2457:SER:N	2.34	0.56
2:B:17:TRP:HZ2	2:B:290:GLY:HA2	1.69	0.56
1:C:234:LYS:HE3	1:C:238:ARG:HG2	1.86	0.56
1:C:804:LEU:HD23	1:C:851:ASN:HB2	1.87	0.56
1:C:862:ARG:HG3	1:C:863:ARG:H	1.70	0.56
1:C:2097:PHE:HD1	1:C:2097:PHE:C	2.09	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2125:TYR:HA	1:C:2179:GLY:HA2	1.86	0.56
1:C:2432:LYS:HE2	1:C:2433:LEU:N	2.20	0.56
1:A:198:LEU:HA	1:A:248:LEU:HG	1.88	0.56
1:A:856:ASN:CB	1:A:1580:LEU:HA	2.31	0.56
1:A:861:ARG:HB3	1:A:1540:TYR:CD2	2.41	0.56
1:A:1510:PHE:CZ	1:A:1514:GLU:HA	2.40	0.56
1:A:2301:PHE:HZ	1:A:2423:VAL:HG22	1.70	0.56
1:C:112:THR:HG22	1:C:114:LEU:HD12	1.85	0.56
1:C:853:LEU:HD12	1:C:1580:ARG:HD3	1.87	0.56
1:C:1349:PHE:HD2	1:C:1351:LYS:N	2.03	0.56
1:C:1594:ILE:HB	1:C:1598:ARG:HB3	1.87	0.56
1:C:1831:SER:HG	1:C:1832:ILE:N	2.01	0.56
1:C:2437:ASP:HB3	1:C:2438:ILE:HG12	1.86	0.56
2:D:10:TYR:CE2	2:D:293:LYS:HG3	2.38	0.56
1:A:1427:VAL:HG23	1:A:1428:GLU:H	1.70	0.56
1:A:1584:LYS:O	1:A:1585:ASN:HB3	2.05	0.56
1:A:1666:ASP:O	1:A:1670:LYS:N	2.38	0.56
1:C:2157:PHE:O	1:C:2160:HIS:HB2	2.05	0.56
1:C:2448:GLU:C	1:C:2449:GLN:N	2.59	0.56
1:A:387:TYR:O	1:A:391:ILE:N	2.38	0.56
1:A:655:ILE:HA	1:A:658:GLU:HB2	1.88	0.56
1:A:2060:GLU:HG3	1:A:2098:VAL:HG23	1.85	0.56
1:C:444:GLU:HA	1:C:447:ARG:HB2	1.88	0.56
1:C:1370:GLU:HA	1:C:1373:ILE:HD12	1.88	0.56
1:C:1584:CYS:O	1:C:1585:GLN:HB2	2.05	0.56
1:A:827:LEU:HD11	1:A:847:ILE:HG21	1.86	0.56
1:A:1243:ARG:HH21	1:A:1259:ARG:HG2	1.71	0.56
1:C:2126:VAL:HG12	1:C:2180:TRP:CE3	2.38	0.56
1:A:1458:LYS:HB3	1:A:1459:PRO:HD3	1.87	0.56
1:C:285:VAL:HG22	1:C:335:LEU:HD11	1.86	0.56
1:C:1421:LYS:HG3	1:C:1435:LYS:HD2	1.87	0.56
1:A:233:LYS:HE2	1:A:237:ARG:CG	2.35	0.56
1:A:1100:ILE:HG23	1:A:1141:MET:SD	2.46	0.56
1:A:1140:THR:HG22	1:A:1172:GLN:NE2	2.21	0.56
1:A:2318:LEU:HD11	1:A:2455:ALA:HB1	1.86	0.56
5:I:693:PHE:HE2	5:I:760:ARG:HH21	1.54	0.56
1:A:1164:LYS:C	1:A:1166:LEU:H	2.09	0.56
1:A:1428:GLU:HA	1:A:1456:THR:HG22	1.87	0.56
1:C:221:TRP:HA	1:C:235:LEU:CD1	2.36	0.56
1:C:1410:ARG:HG3	1:C:1411:TRP:N	2.20	0.56
1:C:2171:LEU:H	1:C:2176:GLY:HA2	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:40:ILE:HG23	2:D:47:LEU:HD23	1.87	0.56
5:J:655:SER:HA	5:J:659:LEU:CB	2.27	0.56
1:C:297:ARG:HD2	1:C:339:LYS:CG	2.31	0.56
1:C:1061:VAL:N	1:C:1062:PRO:CD	2.70	0.56
1:C:1085:PRO:HG3	1:C:1118:MET:SD	2.46	0.56
1:C:1406:GLU:HG3	1:C:1409:GLN:HG3	1.88	0.56
1:C:1761:ASN:HA	1:C:1764:LEU:HD12	1.88	0.56
1:C:281:LEU:CD1	1:C:330:LEU:HB3	2.36	0.55
1:C:515:ASN:HA	1:C:518:ILE:HD12	1.87	0.55
1:C:2323:MET:HA	1:C:2326:TYR:HB3	1.87	0.55
5:I:720:PRO:HD3	5:I:723:PHE:HB2	1.87	0.55
1:A:1252:GLU:HG2	1:A:1253:SER:H	1.70	0.55
1:A:1961:TRP:HB2	1:A:2006:ILE:HG12	1.87	0.55
1:C:146:LYS:HG2	1:C:191:LEU:HD11	1.87	0.55
1:C:195:THR:HG22	1:C:198:ARG:HH21	1.71	0.55
1:C:1594:ILE:HA	1:C:1597:VAL:HB	1.88	0.55
1:C:2374:LEU:HD12	1:C:2421:ARG:HH22	1.70	0.55
1:A:821:LEU:HA	1:A:824:LEU:HB2	1.87	0.55
1:A:1143:THR:HB	1:A:1177:ASP:HB2	1.88	0.55
1:A:1830:ILE:HG22	1:A:1832:LEU:HD22	1.89	0.55
1:A:1952:HIS:HA	1:A:1955:ILE:HG22	1.88	0.55
2:B:236:ILE:HG23	2:B:237:ASP:HB3	1.88	0.55
1:C:2079:ALA:HB2	1:C:2094:ILE:HG12	1.88	0.55
2:D:223:ALA:HB2	2:D:233:VAL:HG23	1.88	0.55
1:A:89:ASP:HB3	1:A:90:LYS:HG2	1.87	0.55
1:A:487:LEU:HD23	1:A:488:ASN:H	1.71	0.55
1:C:329:LEU:HD23	1:C:366:ARG:HD3	1.89	0.55
1:C:1222:ASN:HA	1:C:1225:LYS:HD2	1.89	0.55
1:C:2103:VAL:HA	1:C:2111:ARG:HA	1.88	0.55
1:A:352:SER:HB3	1:A:356:TYR:CE2	2.42	0.55
1:A:1452:GLU:O	1:A:1456:THR:HG23	2.07	0.55
1:A:1821:PRO:HA	1:A:1824:LYS:CG	2.36	0.55
1:A:2436:ILE:HG13	1:A:2438:ARG:H	1.72	0.55
1:A:2442:LEU:O	1:A:2446:GLU:HB2	2.06	0.55
2:D:12:HIS:O	2:D:13:THR:N	2.39	0.55
2:D:14:ILE:HD11	2:D:28:ILE:HD12	1.89	0.55
1:A:1563:GLN:C	1:A:1568:ARG:HD2	2.27	0.55
1:A:2035:LEU:HD21	5:I:648:LYS:HG3	1.89	0.55
1:C:2008:ILE:HD11	1:C:2066:VAL:HG23	1.87	0.55
1:A:187:VAL:CG1	1:A:233:LYS:HA	2.37	0.55
1:A:1183:LEU:HD13	1:A:1189:LEU:HD22	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1502:ILE:HB	1:A:1594:ARG:NH2	2.22	0.55
1:C:2124:LYS:HB3	1:C:2180:TRP:C	2.27	0.55
1:C:2207:TRP:HA	1:C:2210:LEU:HD12	1.88	0.55
5:I:690:ARG:HG2	5:I:691:ASN:HB2	1.88	0.55
5:J:781:GLU:C	5:J:784:GLN:HB3	2.27	0.55
1:A:1020:ILE:C	1:A:1025:GLU:HB2	2.27	0.55
1:A:1215:LYS:HB2	1:A:1249:LEU:HB3	1.89	0.55
1:A:1621:ARG:HG2	1:A:1624:LEU:HD23	1.88	0.55
1:A:1962:HIS:NE2	1:A:2006:ILE:HA	2.22	0.55
2:B:46:LEU:HD13	2:B:57:LEU:HD13	1.89	0.55
5:I:659:LEU:HD21	5:I:690:ARG:HH12	1.72	0.55
1:C:866:VAL:N	1:C:1537:SER:HG	2.03	0.55
1:C:1014:ILE:HG23	1:C:1064:ARG:HE	1.72	0.55
1:C:2222:LEU:HB3	2:D:254:TRP:HZ3	1.72	0.55
1:A:1238:TRP:O	1:A:1241:TRP:N	2.40	0.55
1:A:1291:TYR:CE1	1:A:1340:TYR:HE2	2.24	0.55
1:A:2429:ASP:HB2	1:A:2439:PHE:HB3	1.88	0.55
1:C:282:ASP:HA	1:C:285:VAL:HB	1.89	0.55
1:C:780:LEU:HD11	1:C:816:PHE:HB2	1.89	0.55
3:E:715:UNK:C	3:E:717:UNK:H	2.20	0.55
2:B:7:SER:HB3	2:B:295:ALA:CB	2.36	0.54
1:C:1009:ARG:HB2	1:C:1011:PHE:CE2	2.41	0.54
1:A:954:ARG:NH1	1:A:992:VAL:H	2.06	0.54
1:A:1419:LYS:HG3	1:A:1433:LYS:HD2	1.89	0.54
1:C:1114:ASN:HB3	1:C:1150:LEU:HA	1.88	0.54
1:C:1165:LYS:HE3	1:C:1171:ARG:HG3	1.89	0.54
1:C:2191:ILE:HD12	1:C:2194:HIS:HD2	1.72	0.54
1:A:455:PHE:HB2	1:A:491:MET:HG3	1.89	0.54
1:A:849:ILE:HG23	1:A:853:LYS:N	2.22	0.54
1:A:993:LYS:HA	1:A:994:GLN:CB	2.38	0.54
1:A:1217:PRO:HB2	1:A:1220:GLN:HB2	1.88	0.54
1:A:1291:TYR:CE1	1:A:1340:TYR:CE2	2.95	0.54
1:C:347:TYR:HE2	1:C:383:ILE:HG12	1.72	0.54
1:C:1031:ALA:HB1	1:C:1034:GLY:O	2.07	0.54
1:C:2360:GLU:C	1:C:2361:ALA:HA	2.28	0.54
5:I:699:LYS:HZ1	5:I:702:THR:HG21	1.71	0.54
5:J:698:ARG:C	5:J:700:SER:H	2.09	0.54
5:J:754:ASN:HB3	5:J:760:ARG:HG3	1.89	0.54
2:D:35:VAL:HG22	2:D:38:LEU:HD21	1.89	0.54
3:F:102:UNK:C	3:F:103:UNK:HA	2.36	0.54
1:A:177:ARG:N	1:A:178:VAL:HG23	2.16	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:PRO:HB2	1:C:144:SER:HB3	1.90	0.54
1:C:1504:ILE:HG21	1:C:1596:ARG:HH12	1.72	0.54
1:C:1611:ARG:C	1:C:1613:LYS:N	2.61	0.54
2:D:165:LEU:HD11	2:D:174:LEU:HD23	1.88	0.54
5:J:658:VAL:HG23	5:J:659:LEU:HD12	1.89	0.54
1:A:1010:PHE:HD1	1:A:1021:ILE:CG2	2.21	0.54
2:B:113:TYR:OH	2:B:150:CYS:HA	2.07	0.54
1:C:2147:ASN:HA	1:C:2150:LEU:HB2	1.88	0.54
2:D:259:SER:HB2	2:D:302:ASP:OD2	2.07	0.54
5:I:700:SER:HA	5:I:731:GLU:CB	2.35	0.54
1:A:152:VAL:HA	1:A:155:LEU:HB3	1.89	0.54
1:A:378:PHE:HB2	1:A:380:PRO:HD2	1.89	0.54
1:A:1499:TYR:H	1:A:1594:ARG:NH2	2.05	0.54
1:A:1713:LEU:HA	1:A:1752:THR:HG21	1.89	0.54
1:A:2044:ASN:HA	1:A:2047:ARG:NH1	2.21	0.54
1:C:2038:ASN:HA	1:C:2041:TRP:HB2	1.88	0.54
2:D:54:ASN:HA	2:D:72:GLU:HG2	1.90	0.54
1:A:358:GLU:HG3	1:A:388:LEU:HD21	1.90	0.54
1:A:542:PHE:HB2	1:A:544:ILE:HG23	1.90	0.54
1:A:635:SER:HA	1:A:638:GLU:HB3	1.89	0.54
1:A:699:ILE:HD12	1:A:717:THR:CG2	2.37	0.54
1:C:2308:LEU:HB3	1:C:2309:ARG:HB2	1.90	0.54
1:C:2412:GLU:HA	1:C:2415:ASN:HB2	1.90	0.54
1:A:650:ASP:N	1:A:651:PRO:CD	2.61	0.54
1:A:1876:VAL:O	1:A:1880:LEU:HG	2.08	0.54
1:A:2043:TYR:CE1	5:I:660:GLU:HG3	2.42	0.54
1:C:168:ASN:HD21	1:C:172:ARG:HH21	1.56	0.54
1:C:358:LYS:HD3	1:C:393:MET:HG3	1.90	0.54
1:C:1585:GLN:O	1:C:1586:LYS:HB2	2.08	0.54
1:C:1662:TRP:HZ3	1:C:1726:ARG:CZ	2.20	0.54
1:C:2102:SER:H	1:C:2113:PHE:HE2	1.56	0.54
2:D:215:LEU:HD22	2:D:236:ILE:HD12	1.90	0.54
5:I:730:VAL:HG21	5:I:789:THR:HA	1.89	0.54
1:A:322:ASP:O	1:A:324:VAL:HG23	2.08	0.54
1:A:445:LEU:HA	1:A:448:LYS:HB2	1.89	0.54
1:A:673:GLN:HG2	1:A:719:LEU:HD13	1.88	0.54
1:A:960:ASP:C	1:A:961:GLN:N	2.61	0.54
1:A:1040:PRO:HA	1:A:1043:LEU:HG	1.90	0.54
1:A:1232:GLN:HG3	1:A:1294:ASP:O	2.08	0.54
1:A:1437:LEU:HB3	1:A:1446:LEU:HD21	1.88	0.54
2:B:84:GLN:HB3	2:B:89:TRP:HB2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:VAL:HG22	2:B:99:ILE:HD11	1.90	0.54
2:B:275:ARG:HG3	2:B:287:GLN:HG3	1.90	0.54
1:C:421:GLY:HA2	1:C:424:ALA:HB2	1.90	0.54
1:C:745:LEU:HD22	1:C:782:VAL:HG21	1.90	0.54
1:C:1459:ALA:HA	1:C:1460:LYS:C	2.27	0.54
1:C:2062:GLU:HA	1:C:2063:LEU:CB	2.31	0.54
1:C:2255:LEU:O	1:C:2259:THR:N	2.37	0.54
1:C:2273:TYR:CD1	1:C:2317:PRO:HA	2.43	0.54
1:C:2373:ASP:HB3	1:C:2418:ARG:HH21	1.73	0.54
1:A:235:GLU:HB3	1:A:278:ILE:HB	1.90	0.53
1:A:1588:VAL:HG12	1:A:1612:PHE:CD1	2.43	0.53
1:A:1589:TRP:HE3	1:A:1612:PHE:CE1	2.15	0.53
1:A:1950:VAL:HA	1:A:1953:GLU:HB2	1.89	0.53
1:C:473:PRO:O	1:C:477:LYS:HG2	2.08	0.53
1:C:951:ASN:HB3	1:C:954:LEU:H	1.72	0.53
3:E:109:UNK:C	3:E:110:UNK:HA	2.39	0.53
1:C:763:VAL:HG12	1:C:806:ILE:HB	1.90	0.53
1:C:818:ARG:HD2	1:C:868:LEU:CD1	2.38	0.53
1:C:1982:HIS:HB3	1:C:1984:THR:N	2.22	0.53
1:C:2080:VAL:HB	1:C:2084:ARG:HG3	1.90	0.53
1:C:2109:ARG:N	1:C:2110:PRO:HD3	2.22	0.53
3:F:659:UNK:O	3:F:661:UNK:N	2.41	0.53
1:A:397:ARG:HB3	1:A:399:LEU:HB2	1.91	0.53
1:A:725:LEU:HG	1:A:726:LYS:N	2.23	0.53
1:A:1652:VAL:HG12	1:A:1656:LEU:HB2	1.91	0.53
1:A:1916:VAL:HG11	1:A:2168:PRO:HB2	1.89	0.53
1:A:2032:VAL:HA	1:A:2035:LEU:HD22	1.90	0.53
1:A:2253:LEU:O	1:A:2257:THR:N	2.42	0.53
1:A:2306:LEU:HD12	1:A:2376:LYS:H	1.73	0.53
1:C:542:GLN:C	1:C:543:PHE:N	2.61	0.53
1:C:573:LEU:HD23	1:C:576:CYS:HB2	1.91	0.53
1:C:1340:GLY:HA2	1:C:1343:ALA:H	1.73	0.53
1:C:1655:TYR:HE1	1:C:1720:LEU:HD21	1.73	0.53
1:C:2172:SER:HB3	1:C:2173:PRO:HD2	1.88	0.53
1:C:2445:ASP:O	1:C:2449:GLN:HB2	2.07	0.53
1:A:689:PHE:HZ	1:A:732:LYS:HD3	1.73	0.53
1:A:1046:PHE:HA	1:A:1049:ILE:HG12	1.90	0.53
1:A:1498:PHE:HD2	1:A:1499:TYR:CD2	2.26	0.53
1:A:1928:ALA:O	1:A:1932:ILE:HG12	2.09	0.53
2:B:231:ALA:HB3	2:B:246:LEU:HB3	1.89	0.53
1:C:862:ARG:HB2	1:C:1537:SER:HA	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1581:LEU:HD12	1:C:1582:LEU:HD23	1.91	0.53
2:D:246:LEU:HD11	2:D:282:ARG:HA	1.89	0.53
1:A:770:ALA:HA	1:A:810:ASP:HB2	1.91	0.53
1:A:1089:MET:HB3	1:A:1092:TYR:CD2	2.44	0.53
1:A:2111:PHE:HD1	1:A:2112:CYS:HA	1.74	0.53
2:B:235:SER:HB3	2:B:239:ASP:HB3	1.89	0.53
1:C:395:HIS:CE1	1:C:438:ILE:HG21	2.38	0.53
1:C:852:ILE:HG21	1:C:1584:CYS:HB2	1.90	0.53
2:D:84:GLN:HB2	2:D:145:LEU:HD22	1.90	0.53
1:A:212:PHE:HE1	1:A:238:ARG:HA	1.72	0.53
1:A:1406:LEU:HD21	1:A:1436:SER:HB3	1.90	0.53
1:A:2057:GLN:HE22	1:A:2103:SER:HB2	1.74	0.53
2:B:16:PHE:HB3	2:B:60:ILE:HD13	1.91	0.53
2:B:79:THR:HG23	2:B:95:GLU:HG3	1.91	0.53
2:B:131:LEU:HB3	2:B:143:TRP:O	2.08	0.53
1:C:214:GLU:HG2	1:C:218:CYS:SG	2.48	0.53
1:C:366:ARG:HA	1:C:369:VAL:HB	1.90	0.53
1:C:1962:LEU:HB2	1:C:1965:GLU:N	2.23	0.53
2:D:156:PRO:HB3	2:D:184:TYR:HB2	1.91	0.53
1:A:520:LEU:O	1:A:522:SER:HA	2.08	0.53
1:C:636:SER:HA	1:C:639:GLU:HB3	1.90	0.53
1:C:2097:PHE:C	1:C:2097:PHE:CD1	2.81	0.53
1:A:354:MET:SD	1:A:388:LEU:HD13	2.48	0.53
1:A:1213:VAL:HG22	1:A:1248:GLN:HE21	1.72	0.53
1:A:1352:HIS:NE2	1:A:2250:GLU:HG3	2.24	0.53
1:A:2262:SER:HB3	1:A:2292:VAL:N	2.24	0.53
2:B:143:TRP:HE1	2:B:148:ASN:HA	1.74	0.53
2:B:258:PHE:CE1	2:B:279:LEU:HD13	2.43	0.53
1:C:173:LEU:HD21	1:C:209:ASP:OD1	2.09	0.53
1:C:284:ALA:HB3	1:C:331:VAL:HG11	1.91	0.53
1:C:333:ARG:NH1	1:C:354:THR:HB	2.24	0.53
1:C:1082:LEU:HA	1:C:1085:PRO:HG2	1.90	0.53
1:C:2304:GLU:O	1:C:2308:LEU:HD13	2.09	0.53
2:D:268:ALA:HB2	2:D:298:VAL:HG21	1.90	0.53
1:A:304:TRP:HB2	1:A:341:TYR:CE2	2.44	0.53
1:A:920:VAL:HG12	1:A:923:ASN:HB2	1.91	0.53
1:A:1328:LYS:HB2	1:A:1329:PRO:HD3	1.91	0.53
1:A:1559:LYS:N	1:A:1572:ARG:NH2	2.57	0.53
1:A:1972:ALA:C	1:A:1974:ARG:H	2.12	0.53
1:A:2059:LEU:C	1:A:2098:VAL:HA	2.29	0.53
1:A:2132:ARG:HB3	1:A:2366:ILE:HG21	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:GLU:C	1:C:123:PHE:H	2.12	0.53
1:C:236:GLU:HG2	1:C:279:ILE:HB	1.90	0.53
1:C:332:PHE:CE1	1:C:336:LEU:HD11	2.44	0.53
1:C:862:ARG:HG3	1:C:863:ARG:N	2.24	0.53
1:C:1510:ASN:HD21	4:G:73:PHE:HA	1.72	0.53
1:C:2081:PRO:HB2	1:C:2123:TYR:CE2	2.44	0.53
2:D:12:HIS:HB3	2:D:30:HIS:O	2.09	0.53
2:B:7:SER:HB2	2:B:274:VAL:HB	1.91	0.53
1:C:938:HIS:CE1	1:C:978:GLN:HA	2.44	0.53
1:C:1149:LEU:HD12	1:C:1194:ILE:HG21	1.91	0.53
1:C:1504:ILE:HG12	1:C:1508:HIS:NE2	2.24	0.53
5:I:737:ASN:HB3	5:I:754:ASN:O	2.08	0.53
1:A:273:ASP:HA	1:A:276:LEU:HD11	1.89	0.52
1:A:853:LYS:HG3	1:A:1582:CYS:HB3	1.89	0.52
1:A:2121:TYR:HA	1:A:2122:LYS:CB	2.30	0.52
1:A:2347:ARG:HH22	1:A:2444:VAL:H	1.56	0.52
1:C:705:SER:HB2	1:C:710:TYR:HB3	1.91	0.52
1:C:857:ASN:CB	1:C:1586:LYS:HA	2.29	0.52
1:C:1021:ILE:HG21	1:C:1025:ILE:HB	1.89	0.52
4:G:75:GLY:HA3	4:G:106:GLY:HA2	1.91	0.52
1:A:2345:VAL:HA	1:A:2348:ASP:OD1	2.09	0.52
1:C:443:ARG:O	1:C:447:ARG:N	2.43	0.52
1:A:267:ILE:O	1:A:279:ARG:HD2	2.08	0.52
1:A:283:ALA:O	1:A:307:ARG:NH2	2.41	0.52
1:A:1191:THR:C	1:A:1193:ILE:H	2.13	0.52
1:A:2155:PHE:HA	1:A:2158:HIS:HB2	1.91	0.52
2:B:154:LEU:HD23	2:B:197:LEU:HD12	1.91	0.52
1:C:265:LEU:HA	1:C:307:GLN:CB	2.19	0.52
1:C:1403:THR:HG23	1:C:1407:LYS:HE2	1.91	0.52
1:C:1505:LEU:HD22	1:C:1514:LYS:HE2	1.90	0.52
1:C:1816:LEU:N	1:C:1817:ILE:HA	2.23	0.52
1:C:2097:PHE:HB3	1:C:2115:ILE:HA	1.92	0.52
2:D:56:ARG:HD3	2:D:67:PRO:HD3	1.90	0.52
1:A:176:LEU:HA	1:A:179:LEU:HB2	1.90	0.52
1:A:565:ASP:O	1:A:570:GLN:N	2.42	0.52
1:A:1852:GLY:HA2	1:A:1891:VAL:HG21	1.91	0.52
1:C:842:TYR:O	1:C:844:GLU:N	2.42	0.52
1:C:2369:ASN:O	1:C:2418:ARG:NH2	2.43	0.52
2:D:44:LYS:HE2	2:D:61:ARG:NH2	2.24	0.52
3:F:353:UNK:C	3:F:354:UNK:H	2.22	0.52
4:H:141:ASN:O	4:H:176:LYS:N	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:LEU:HA	1:A:575:CYS:HB2	1.92	0.52
1:A:963:ILE:HG23	1:A:964:PRO:HD3	1.90	0.52
2:B:8:ALA:HB3	2:B:38:LEU:HD21	1.92	0.52
2:B:156:PRO:HA	2:B:186:TRP:HZ2	1.73	0.52
1:C:1050:ILE:HD12	1:C:1065:ILE:HG12	1.91	0.52
1:C:1144:THR:HG22	1:C:1178:ASP:HB2	1.92	0.52
1:A:436:LEU:HD22	1:A:474:PHE:HZ	1.74	0.52
2:B:55:VAL:HG22	2:B:57:LEU:HD21	1.90	0.52
1:C:573:LEU:HB3	1:C:577:PHE:HD2	1.74	0.52
1:C:1388:ILE:HA	1:C:1391:HIS:HB3	1.91	0.52
1:C:2047:VAL:HA	1:C:2050:LYS:HD2	1.90	0.52
1:C:2084:ARG:HH22	1:C:2169:ILE:HG12	1.75	0.52
1:C:2280:ARG:HB3	1:C:2319:ARG:HH11	1.74	0.52
2:D:101:VAL:HG13	2:D:111:ARG:HB2	1.92	0.52
3:E:357:UNK:C	3:E:358:UNK:H	2.22	0.52
1:A:669:PRO:CG	1:A:719:LEU:HD21	2.39	0.52
1:A:1351:LEU:O	1:A:1355:GLU:HB2	2.10	0.52
1:A:1908:GLN:HB2	1:A:1939:HIS:NE2	2.25	0.52
1:A:1962:HIS:NE2	1:A:2005:GLU:O	2.37	0.52
1:C:231:SER:HA	1:C:234:LYS:HB3	1.90	0.52
1:C:490:CYS:HB3	1:C:491:PRO:CD	2.40	0.52
1:C:998:ARG:NE	1:C:1035:GLU:H	2.08	0.52
1:C:2194:HIS:CE1	1:C:2243:VAL:HB	2.45	0.52
1:A:2049:ILE:O	1:A:2052:GLN:HB3	2.10	0.52
1:C:310:PHE:HA	1:C:317:LEU:HD11	1.92	0.52
1:C:855:THR:HA	1:C:1550:ILE:HG21	1.91	0.52
2:B:227:ALA:HA	2:B:252:TRP:HA	1.92	0.52
1:C:446:LEU:HA	1:C:449:LYS:HB2	1.91	0.52
1:C:450:PHE:CD1	1:C:456:PHE:HA	2.45	0.52
1:C:462:TYR:CD2	1:C:498:GLU:HB3	2.45	0.52
1:C:573:LEU:HB3	1:C:577:PHE:CD2	2.45	0.52
2:D:77:ASN:H	2:D:95:GLU:HB2	1.75	0.52
2:D:212:ARG:NH2	2:D:297:CYS:SG	2.83	0.52
2:D:233:VAL:HG12	2:D:244:THR:HB	1.91	0.52
1:A:290:LEU:HA	1:A:293:ILE:HB	1.92	0.52
1:A:1920:SER:HB3	1:A:2171:PRO:HD3	1.91	0.52
1:C:90:ASP:HA	1:C:131:ASN:O	2.10	0.52
1:C:2063:LEU:HB3	1:C:2099:PRO:HA	1.90	0.52
1:C:2261:TYR:HA	1:C:2264:SER:HB2	1.91	0.52
1:A:409:ASN:HB2	1:A:452:ARG:HD2	1.90	0.51
1:A:581:LEU:HA	1:A:582:ILE:C	2.31	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1968:GLY:HA3	1:A:1992:LEU:HD21	1.92	0.51
1:A:2066:PRO:HA	1:A:2069:LEU:HB3	1.92	0.51
1:A:2078:VAL:HG12	1:A:2081:THR:HG22	1.92	0.51
2:B:229:HIS:HA	2:B:251:ARG:HB2	1.91	0.51
2:B:278:ASP:O	2:B:282:ARG:N	2.42	0.51
1:C:264:ILE:HG23	1:C:268:ILE:HD12	1.91	0.51
1:C:1743:GLY:HA2	1:C:1744:SER:C	2.30	0.51
2:D:71:PHE:HB3	2:D:90:MET:HE1	1.92	0.51
1:A:436:LEU:HD12	1:A:439:ASP:HB3	1.91	0.51
1:A:436:LEU:HD13	1:A:474:PHE:CE1	2.45	0.51
1:A:1134:ARG:HG3	1:A:1138:LYS:HB2	1.91	0.51
1:A:1592:ILE:HA	1:A:1595:VAL:HB	1.93	0.51
2:B:229:HIS:CD2	2:B:252:TRP:H	2.29	0.51
2:B:253:VAL:HA	2:B:268:ALA:O	2.10	0.51
1:C:180:LEU:HG	1:C:234:LYS:HD2	1.92	0.51
1:C:424:ALA:HB3	1:C:425:PHE:HB2	1.93	0.51
1:C:919:THR:HA	1:C:922:ILE:HB	1.91	0.51
1:C:1512:PHE:CZ	1:C:1516:GLU:HA	2.46	0.51
1:C:2100:VAL:O	1:C:2101:PHE:N	2.44	0.51
1:C:2187:PHE:N	1:C:2285:LEU:O	2.43	0.51
2:D:12:HIS:HE1	2:D:35:VAL:HB	1.75	0.51
1:A:220:TRP:HA	1:A:270:PRO:HG3	1.92	0.51
1:A:280:LEU:C	1:A:284:VAL:HG23	2.31	0.51
1:A:1045:PHE:CZ	1:A:1064:ILE:HA	2.33	0.51
1:A:1883:ARG:HG2	1:A:2364:PRO:HG2	1.91	0.51
1:A:2282:ASN:HA	1:A:2295:ILE:O	2.09	0.51
2:B:111:ARG:HH12	2:B:146:GLY:HA3	1.75	0.51
1:C:307:GLN:HA	1:C:310:PHE:HB3	1.91	0.51
1:C:983:PHE:HA	1:C:986:LEU:HD22	1.93	0.51
1:C:1570:ARG:HA	1:C:1573:MET:HG2	1.92	0.51
1:C:2139:VAL:O	1:C:2142:LEU:N	2.43	0.51
1:C:2266:ALA:HB1	1:C:2343:ASN:HD21	1.76	0.51
4:H:120:ASP:CA	4:H:121:TYR:CB	2.85	0.51
1:A:324:VAL:HG22	1:A:327:THR:HG22	1.92	0.51
1:A:1368:GLU:HA	1:A:1371:ILE:HD12	1.92	0.51
1:A:1449:LEU:HB3	1:A:1452:GLU:HB2	1.93	0.51
1:A:2239:TYR:HA	1:A:2242:LEU:HD12	1.92	0.51
1:C:260:TYR:HA	1:C:287:LEU:HD11	1.92	0.51
1:C:569:ASP:HB3	1:C:570:ALA:N	2.25	0.51
1:C:992:ILE:HD12	1:C:994:LYS:HB3	1.91	0.51
1:C:1261:SER:HG	1:C:1263:SER:N	2.07	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1500:PHE:CD1	1:C:1551:ILE:HG23	2.46	0.51
1:C:1670:ALA:O	1:C:1674:LEU:N	2.43	0.51
1:C:1901:LEU:HA	1:C:1904:LEU:HB2	1.91	0.51
2:D:212:ARG:HE	2:D:255:ASP:HB3	1.75	0.51
1:A:138:HIS:NE2	1:A:178:VAL:CG1	2.73	0.51
1:A:1978:GLY:O	1:A:1979:GLU:HB2	2.10	0.51
1:A:2124:VAL:HG12	1:A:2178:TRP:HE3	1.75	0.51
1:C:446:LEU:HD12	1:C:449:LYS:HD2	1.92	0.51
1:C:1100:LYS:O	1:C:1104:ILE:HG12	2.11	0.51
1:C:1429:VAL:HG23	1:C:1430:GLU:H	1.76	0.51
1:C:2128:LYS:HD3	1:C:2131:GLU:HG3	1.92	0.51
1:C:2365:ASP:HB3	1:C:2369:ASN:O	2.10	0.51
1:C:2429:ILE:HD13	1:C:2435:GLY:N	2.25	0.51
5:J:736:PRO:HA	5:J:755:PHE:CD1	2.46	0.51
1:A:288:LYS:O	1:A:292:ILE:HG23	2.11	0.51
1:A:304:TRP:HE1	1:A:340:PRO:HG2	1.76	0.51
1:A:1010:PHE:CD1	1:A:1021:ILE:HG23	2.45	0.51
1:A:2411:HIS:O	1:A:2415:ILE:N	2.43	0.51
1:A:2430:LYS:HA	1:A:2450:LYS:HG3	1.93	0.51
2:B:37:ARG:HH21	2:B:80:SER:HA	1.76	0.51
1:C:1002:GLU:HG2	1:C:1042:GLU:HG3	1.93	0.51
1:C:1570:ARG:O	1:C:1574:ARG:HB2	2.10	0.51
3:E:454:UNK:HA	3:E:455:UNK:C	2.41	0.51
1:A:1065:LEU:HD13	1:A:1101:SER:HB3	1.93	0.51
1:C:314:THR:HA	1:C:317:LEU:HB2	1.93	0.51
1:C:1443:GLY:N	1:C:1628:LYS:HZ2	2.09	0.51
1:C:1475:ALA:HB1	1:C:1484:ILE:HG13	1.93	0.51
1:C:1598:ARG:HA	1:C:1600:LEU:HG	1.92	0.51
1:C:2098:GLU:HB3	1:C:2100:VAL:C	2.31	0.51
1:C:2346:LYS:HG3	1:C:2350:ASP:OD2	2.10	0.51
1:A:722:LEU:CA	1:A:760:LEU:HD13	2.38	0.51
1:A:2044:ASN:HA	1:A:2047:ARG:HH11	1.76	0.51
1:A:2191:GLU:HA	1:A:2194:GLU:HB2	1.93	0.51
2:B:14:ILE:HD11	2:B:28:ILE:HD12	1.93	0.51
2:B:121:GLU:OE1	2:B:165:LEU:HB3	2.11	0.51
2:B:186:TRP:HB3	2:B:197:LEU:HB3	1.92	0.51
1:C:183:SER:HB3	1:C:230:SER:O	2.10	0.51
1:C:1547:ARG:HB3	1:C:1593:ARG:HH21	1.75	0.51
3:F:250:UNK:O	3:F:254:UNK:N	2.44	0.51
5:I:699:LYS:HB2	5:I:760:ARG:HB2	1.91	0.51
1:A:590:GLU:HB3	1:A:594:LEU:HB2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:LEU:HD22	1:A:757:ASP:HB3	1.93	0.51
1:A:1524:LEU:HD11	1:A:1549:ILE:HB	1.91	0.51
1:A:2200:LEU:HG	1:A:2471:PHE:CZ	2.35	0.51
1:A:2239:TYR:O	1:A:2243:TRP:N	2.44	0.51
1:C:138:ILE:C	1:C:140:GLY:H	2.14	0.51
1:C:1518:HIS:HA	1:C:1521:ASN:HB2	1.93	0.51
1:C:1554:LEU:HA	1:C:1557:ILE:HG23	1.92	0.51
1:C:1909:PRO:HB2	1:C:1913:VAL:HB	1.92	0.51
1:C:2026:MET:HG3	1:C:2027:ASN:N	2.25	0.51
2:D:83:PHE:HE1	2:D:104:VAL:HG21	1.74	0.51
5:I:699:LYS:HD3	5:I:737:ASN:HD22	1.74	0.51
5:I:709:PHE:CE2	5:I:716:THR:HB	2.46	0.51
1:A:347:ASP:N	1:A:348:ASP:CB	2.74	0.51
1:A:361:PHE:HE1	1:A:414:PHE:CE1	2.29	0.51
1:A:412:LYS:HZ1	1:A:445:LEU:HD22	1.76	0.51
1:A:774:VAL:O	1:A:777:THR:OG1	2.22	0.51
1:A:1069:VAL:CG1	1:A:1105:LEU:HG	2.41	0.51
1:A:1453:LYS:HG2	1:A:1465:MET:HG2	1.93	0.51
1:A:1879:GLN:HG2	1:A:2132:ARG:HH21	1.76	0.51
1:C:1661:LEU:HD21	1:C:1669:GLU:HB3	1.91	0.51
1:C:1822:ILE:HG23	1:C:1826:LYS:HD2	1.92	0.51
2:D:90:MET:HB3	2:D:102:TRP:HB2	1.92	0.51
2:D:265:LEU:HA	2:D:279:LEU:HD12	1.92	0.51
5:I:664:PHE:HE1	5:I:691:ASN:HD22	1.57	0.51
1:A:120:GLU:HG2	1:A:123:GLN:HB3	1.93	0.50
1:A:341:TYR:CG	1:A:345:LYS:HG2	2.46	0.50
1:A:1008:ARG:HB2	1:A:1010:PHE:CE2	2.46	0.50
1:A:1127:ARG:HG2	1:A:1128:ILE:N	2.26	0.50
1:C:674:GLN:HG2	1:C:720:LEU:HD13	1.92	0.50
1:C:1386:ILE:HG12	1:C:1406:GLU:HB3	1.92	0.50
1:C:2346:LYS:O	1:C:2350:ASP:N	2.44	0.50
1:C:2446:VAL:HB	1:C:2447:PRO:HD3	1.92	0.50
1:A:1544:VAL:O	1:A:1548:ILE:HG13	2.11	0.50
2:B:132:ILE:HG21	2:B:174:LEU:HD11	1.93	0.50
1:C:1015:ILE:HD11	1:C:1067:LYS:HE2	1.93	0.50
1:C:1084:MET:SD	1:C:1084:MET:O	2.69	0.50
1:C:2112:LYS:HA	1:C:2126:VAL:HA	1.93	0.50
2:D:13:THR:HG21	2:D:292:HIS:H	1.75	0.50
2:D:44:LYS:HE2	2:D:61:ARG:HH22	1.75	0.50
5:J:661:TYR:CD2	5:J:697:VAL:HG11	2.47	0.50
5:J:730:VAL:HG21	5:J:790:PRO:CD	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:730:VAL:HB	5:J:788:GLU:O	2.12	0.50
1:A:256:LEU:HD22	1:A:259:TYR:CE2	2.47	0.50
1:A:272:ARG:N	1:A:322:ASP:OD1	2.45	0.50
1:A:673:GLN:OE1	1:A:719:LEU:HD22	2.12	0.50
1:A:1609:ARG:C	1:A:1610:ILE:N	2.65	0.50
1:A:1862:HIS:CD2	1:A:1898:LEU:HD23	2.46	0.50
1:A:2192:HIS:CG	1:A:2237:ASP:HB3	2.46	0.50
1:A:1013:ILE:HG23	1:A:1063:ARG:HE	1.76	0.50
1:A:2334:SER:HA	1:A:2337:ILE:HD12	1.92	0.50
2:B:121:GLU:HG3	2:B:165:LEU:N	2.26	0.50
1:C:502:ILE:HA	1:C:505:GLU:HG2	1.94	0.50
1:C:1135:ARG:HB2	1:C:1136:GLU:HA	1.94	0.50
1:C:1900:LEU:O	1:C:1904:LEU:HG	2.11	0.50
1:A:86:LEU:HA	1:A:89:ASP:HB2	1.92	0.50
1:A:215:ARG:HG3	1:A:233:LYS:HZ3	1.76	0.50
1:A:595:ILE:HG13	1:A:599:TYR:HD2	1.76	0.50
1:A:835:VAL:HG13	1:A:1525:VAL:CG1	2.42	0.50
1:A:1419:LYS:HG3	1:A:1433:LYS:HZ3	1.77	0.50
1:A:2092:ILE:HG22	1:A:2114:LYS:O	2.11	0.50
1:A:2121:TYR:CA	1:A:2122:LYS:HB2	2.30	0.50
1:A:2268:MET:HG2	1:A:2342:VAL:HA	1.94	0.50
2:B:99:ILE:CD1	2:B:122:VAL:HG21	2.41	0.50
1:C:1059:ARG:HD2	1:C:1099:LYS:HB3	1.94	0.50
1:C:1483:GLU:HA	1:C:1486:GLN:HE22	1.77	0.50
1:C:1960:ALA:O	1:C:2111:ARG:NH1	2.45	0.50
2:D:3:VAL:C	2:D:4:ILE:HG13	2.31	0.50
1:A:81:PHE:HB3	1:A:107:SER:HA	1.92	0.50
1:A:256:LEU:HD22	1:A:259:TYR:HE2	1.77	0.50
1:A:1527:GLU:O	1:A:1528:LEU:N	2.44	0.50
1:A:1759:ASN:HA	1:A:1762:LEU:HD12	1.93	0.50
1:C:143:SER:CB	1:C:190:ARG:HE	2.25	0.50
1:C:1445:TRP:O	1:C:1448:LEU:N	2.44	0.50
1:C:1598:ARG:C	1:C:1600:LEU:H	2.14	0.50
1:C:2026:MET:CG	1:C:2027:ASN:H	2.24	0.50
1:C:2061:LEU:HG	1:C:2101:PHE:N	2.27	0.50
2:D:242:LEU:HD11	2:D:245:THR:HG23	1.94	0.50
5:I:709:PHE:HE2	5:I:716:THR:HB	1.77	0.50
5:J:698:ARG:C	5:J:700:SER:N	2.65	0.50
1:A:263:ILE:HA	1:A:266:ASN:HB2	1.93	0.50
1:A:781:VAL:O	1:A:784:GLU:HB3	2.12	0.50
1:A:848:LEU:HD22	1:A:1547:GLN:HB3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1004:TYR:O	1:A:1007:ILE:N	2.44	0.50
1:C:166:LEU:HB3	1:C:167:PRO:HD3	1.94	0.50
1:C:757:ILE:O	1:C:761:LEU:HG	2.10	0.50
1:C:1285:TRP:O	1:C:1286:VAL:HB	2.11	0.50
1:C:1844:LEU:HD21	1:C:1878:VAL:HG21	1.94	0.50
1:C:2153:ASP:HB2	1:C:2346:LYS:HG2	1.93	0.50
2:D:83:PHE:CD1	2:D:104:VAL:HG11	2.47	0.50
5:I:698:ARG:HB2	5:I:700:SER:H	1.77	0.50
5:I:730:VAL:CG2	5:I:789:THR:HA	2.41	0.50
1:A:2367:ASN:HB3	1:A:2371:ASP:HB2	1.93	0.50
2:B:274:VAL:HG12	2:B:291:HIS:HE1	1.75	0.50
1:C:458:LYS:HE3	1:C:461:PHE:HD2	1.77	0.50
1:C:982:TYR:HA	1:C:985:GLN:HB2	1.94	0.50
1:C:1127:VAL:HG23	1:C:1167:LEU:HD11	1.94	0.50
1:C:1487:TYR:HE2	1:C:1498:LYS:HE3	1.77	0.50
1:C:2284:ASN:HB3	1:C:2296:HIS:NE2	2.27	0.50
1:A:260:VAL:O	1:A:263:ILE:N	2.45	0.50
1:A:569:ALA:HA	1:A:591:PHE:CE1	2.47	0.50
2:B:26:ARG:HE	2:B:60:ILE:HD12	1.76	0.50
1:C:571:GLN:O	1:C:575:GLN:N	2.44	0.50
1:C:1165:LYS:C	1:C:1167:LEU:H	2.15	0.50
1:A:1245:LEU:HA	1:A:1275:LEU:HD23	1.94	0.49
1:A:2104:SER:HG	1:A:2106:GLN:N	2.10	0.49
2:B:7:SER:CB	2:B:274:VAL:HB	2.42	0.49
1:C:595:LEU:HA	1:C:598:ILE:HB	1.94	0.49
1:C:998:ARG:HE	1:C:1035:GLU:H	1.60	0.49
1:C:1712:THR:HA	1:C:1715:LEU:HG	1.94	0.49
1:C:2288:ASP:OD2	1:C:2293:LYS:HG3	2.12	0.49
2:D:229:HIS:HD2	2:D:252:TRP:H	1.60	0.49
1:A:971:ARG:HD3	1:A:977:GLN:HE21	1.77	0.49
1:A:1606:ALA:O	1:A:1610:ILE:N	2.44	0.49
1:C:822:LEU:HA	1:C:825:LEU:HB2	1.94	0.49
2:D:121:GLU:HG3	2:D:165:LEU:H	1.77	0.49
2:D:125:HIS:HB3	2:D:130:GLU:HB2	1.94	0.49
3:F:704:UNK:O	3:F:708:UNK:N	2.45	0.49
5:I:650:ARG:HG3	5:I:651:THR:HG23	1.93	0.49
1:A:633:LEU:HB3	1:A:674:PRO:HG2	1.94	0.49
1:A:1976:PHE:HB2	1:A:1985:MET:HB2	1.93	0.49
2:B:57:LEU:HD12	2:B:69:ALA:HB3	1.94	0.49
1:C:157:ILE:HG12	1:C:172:ARG:NH2	2.25	0.49
1:C:1839:SER:OG	1:C:1841:GLN:HB3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:VAL:HA	1:A:366:ARG:HG3	1.94	0.49
1:A:438:LEU:O	1:A:442:ARG:N	2.45	0.49
1:A:633:LEU:HD21	1:A:665:SER:HA	1.94	0.49
1:A:849:ILE:HG21	1:A:1548:ILE:HG23	1.95	0.49
1:A:1660:TRP:HZ3	1:A:1724:ARG:CZ	2.25	0.49
1:A:1811:SER:HB2	1:A:1843:ARG:HH22	1.78	0.49
2:B:16:PHE:HB2	2:B:26:ARG:HB3	1.95	0.49
1:C:1425:GLY:HA2	1:C:1429:VAL:HG13	1.94	0.49
1:C:2339:ILE:HA	1:C:2342:GLU:CG	2.41	0.49
2:D:37:ARG:NH2	2:D:212:ARG:HH22	2.10	0.49
2:D:183:CYS:SG	2:D:222:LEU:HD21	2.52	0.49
5:J:789:THR:O	5:J:791:LEU:N	2.45	0.49
1:A:180:ILE:O	1:A:230:SER:OG	2.30	0.49
1:A:954:ARG:H	1:A:955:CYS:N	2.11	0.49
1:A:2390:ALA:HB3	1:A:2391:ASN:HB2	1.94	0.49
2:B:12:HIS:CB	2:B:30:HIS:O	2.61	0.49
1:C:173:LEU:CD2	1:C:209:ASP:HA	2.42	0.49
1:C:366:ARG:HA	1:C:369:VAL:CG2	2.43	0.49
1:C:1118:MET:HG3	1:C:1121:ARG:CG	2.42	0.49
1:A:636:VAL:CG1	1:A:675:ASP:HB3	2.34	0.49
1:C:281:LEU:HD11	1:C:330:LEU:HB3	1.95	0.49
1:C:690:PHE:HD1	1:C:728:PHE:HZ	1.60	0.49
1:C:1444:GLU:C	1:C:1445:TRP:HA	2.33	0.49
1:C:1732:LYS:HA	1:C:1737:ASN:HB2	1.94	0.49
2:D:101:VAL:HG11	2:D:143:TRP:HH2	1.74	0.49
1:A:649:THR:HB	1:A:650:ASP:HB2	1.95	0.49
1:A:1608:VAL:HA	1:A:1611:LYS:HB2	1.94	0.49
1:A:2286:ASP:HB2	1:A:2291:LYS:H	1.77	0.49
1:C:537:TYR:HB2	1:C:543:PHE:CE2	2.48	0.49
1:C:626:CYS:HB2	1:C:629:THR:HG22	1.93	0.49
1:C:826:GLY:HA3	1:C:827:GLN:HG2	1.93	0.49
1:C:939:THR:HG21	1:C:1262:CYS:SG	2.53	0.49
1:C:1429:VAL:HB	1:C:1435:LYS:NZ	2.27	0.49
1:C:2046:ASN:HA	1:C:2049:ARG:HH11	1.78	0.49
1:A:704:SER:HB2	1:A:709:TYR:CB	2.33	0.49
1:A:933:LEU:HD13	1:A:939:ALA:HB2	1.93	0.49
1:A:993:LYS:HZ2	1:A:1029:LYS:HE3	1.77	0.49
1:A:1120:ARG:HA	1:A:1123:GLN:HG2	1.95	0.49
1:A:1155:PHE:CE2	1:C:622:LYS:HB3	2.47	0.49
1:A:1383:ALA:HA	1:A:1386:ILE:HG22	1.95	0.49
1:A:2126:LYS:HD2	1:A:2176:LEU:HG	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2354:MET:SD	1:A:2427:ILE:HG21	2.53	0.49
2:B:244:THR:HG22	2:B:245:THR:O	2.13	0.49
1:C:543:PHE:CD1	1:C:545:ILE:HG23	2.47	0.49
1:C:573:LEU:HD13	1:C:577:PHE:HE2	1.76	0.49
1:C:1887:HIS:HB2	1:C:1927:ARG:HG2	1.95	0.49
2:D:205:ALA:O	2:D:224:THR:HG21	2.12	0.49
1:A:1341:ALA:H	1:A:1342:GLN:HB3	1.77	0.49
1:A:2043:TYR:HE1	5:I:660:GLU:HG3	1.78	0.49
2:B:26:ARG:NH2	2:B:47:LEU:HD21	2.28	0.49
1:C:682:PHE:C	1:C:684:ALA:H	2.15	0.49
1:C:1061:VAL:N	1:C:1062:PRO:HD3	2.27	0.49
1:A:232:SER:HB2	1:A:236:TYR:CE2	2.48	0.49
1:A:264:LEU:HB2	1:A:306:GLN:CD	2.33	0.49
1:A:1177:ASP:O	1:A:1181:ASN:N	2.46	0.49
1:A:1729:PRO:HD2	1:A:1730:LYS:HD2	1.95	0.49
1:A:2111:PHE:HD1	1:A:2112:CYS:CA	2.25	0.49
1:C:424:ALA:N	1:C:425:PHE:HB2	2.28	0.49
1:C:1760:HIS:CD2	1:C:1832:ILE:HG13	2.48	0.49
2:D:231:ALA:H	2:D:246:LEU:C	2.16	0.49
2:D:253:VAL:N	2:D:269:SER:HG	2.10	0.49
1:A:642:LYS:HE2	1:A:646:ILE:HG12	1.94	0.48
1:A:690:GLY:HA2	1:A:693:LEU:H	1.77	0.48
1:A:792:GLU:HB3	1:A:795:ARG:H	1.78	0.48
1:A:964:PRO:HB3	1:A:967:ILE:HB	1.95	0.48
1:A:1440:LEU:HD13	1:A:1622:MET:CE	2.44	0.48
1:A:1458:LYS:HB3	1:A:1459:PRO:CD	2.42	0.48
2:B:40:ILE:HG21	2:B:44:LYS:HA	1.94	0.48
2:B:78:VAL:HA	2:B:94:SER:HA	1.94	0.48
1:C:439:LEU:HA	1:C:442:ILE:HG12	1.95	0.48
1:C:469:CYS:HG	1:C:470:ALA:N	2.10	0.48
1:C:678:LEU:HD23	1:C:727:LYS:HB3	1.94	0.48
1:C:1763:ALA:HB2	1:C:1828:PHE:HB3	1.94	0.48
1:C:1826:LYS:HB2	1:C:1863:MET:SD	2.53	0.48
2:D:12:HIS:NE2	2:D:34:GLN:HG3	2.28	0.48
5:I:698:ARG:HA	5:I:759:ASP:HA	1.93	0.48
5:J:730:VAL:HG21	5:J:789:THR:CA	2.41	0.48
1:A:817:ARG:HD2	1:A:867:LEU:CD1	2.43	0.48
1:A:1440:LEU:HB3	1:A:1622:MET:SD	2.53	0.48
1:C:91:LYS:HD3	1:C:134:ILE:HG21	1.95	0.48
1:C:285:VAL:HA	1:C:335:LEU:HD13	1.95	0.48
1:C:1515:ALA:O	1:C:1518:HIS:N	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2157:PHE:HD1	1:C:2160:HIS:CD2	2.30	0.48
2:D:131:LEU:O	2:D:143:TRP:N	2.46	0.48
2:D:297:CYS:HA	2:D:298:VAL:CB	2.18	0.48
4:G:132:GLY:O	4:G:134:ASP:N	2.46	0.48
1:A:90:LYS:HB3	1:A:133:ILE:HG21	1.95	0.48
1:A:1245:LEU:HD12	1:A:1275:LEU:HD23	1.94	0.48
1:A:1724:ARG:HG3	1:A:1725:VAL:HG13	1.96	0.48
1:C:842:TYR:CB	1:C:844:GLU:HG2	2.30	0.48
1:C:969:LEU:HD13	1:C:985:GLN:HB3	1.95	0.48
1:C:1088:VAL:HG22	1:C:1103:ILE:HG21	1.94	0.48
1:C:1356:LYS:HD2	1:C:1375:ILE:HD13	1.96	0.48
1:C:1857:PRO:C	1:C:1859:ALA:N	2.65	0.48
1:C:2444:LEU:HD13	1:C:2452:LYS:HE3	1.96	0.48
1:A:215:ARG:O	1:A:219:ASP:HB2	2.14	0.48
1:A:335:LEU:HD13	1:A:341:TYR:HB3	1.94	0.48
1:A:546:LYS:O	1:A:550:SER:N	2.45	0.48
1:A:1069:VAL:HG13	1:A:1105:LEU:HG	1.95	0.48
1:A:1130:ASN:HB3	1:A:1166:LEU:HB3	1.96	0.48
1:A:2305:ILE:HB	1:A:2375:LYS:HD3	1.94	0.48
2:B:18:GLU:HG2	2:B:25:SER:HB2	1.95	0.48
1:C:818:ARG:HB2	1:C:818:ARG:HH11	1.77	0.48
1:C:1069:LEU:HD22	1:C:1106:LEU:O	2.13	0.48
1:C:1192:THR:C	1:C:1194:ILE:H	2.17	0.48
1:C:1273:ALA:HB3	1:C:1324:PHE:CE1	2.48	0.48
3:F:507:UNK:C	3:F:508:UNK:CA	2.88	0.48
1:A:357:LYS:HZ3	1:A:366:ARG:HA	1.79	0.48
1:A:1164:LYS:HB3	1:A:1170:ARG:HG3	1.95	0.48
1:A:1586:ILE:C	1:A:1587:ASP:HB2	2.34	0.48
1:A:2147:LEU:HD22	1:A:2353:LEU:HD13	1.96	0.48
1:C:581:GLN:HG3	1:C:589:LEU:HD22	1.95	0.48
1:C:1668:ASP:HA	1:C:1671:LEU:HD12	1.94	0.48
1:C:1902:SER:HB3	1:C:1934:ILE:HD12	1.96	0.48
2:D:39:GLU:HA	2:D:299:ALA:HB2	1.96	0.48
2:D:210:ILE:HD11	2:D:224:THR:HA	1.95	0.48
1:A:698:ILE:HG23	1:C:1079:TYR:HE2	1.73	0.48
1:A:1548:ILE:HG22	1:A:1552:LEU:HD22	1.96	0.48
1:A:1994:GLU:O	1:A:1997:LYS:HB2	2.12	0.48
1:A:2133:GLN:HG3	1:A:2370:PHE:CZ	2.49	0.48
1:C:377:ALA:HB1	1:C:382:ALA:HB1	1.95	0.48
1:C:1460:LYS:HB2	1:C:1461:PRO:HD2	1.95	0.48
1:C:1557:ILE:HG22	1:C:1577:TRP:HE1	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1578:ASN:HA	1:C:1581:LEU:HG	1.95	0.48
1:C:2279:ASP:HA	1:C:2309:ARG:HH22	1.79	0.48
2:D:37:ARG:HG3	2:D:81:VAL:N	2.29	0.48
5:J:693:PHE:CZ	5:J:760:ARG:HD3	2.48	0.48
1:A:594:LEU:O	1:A:595:ILE:HD12	2.14	0.48
1:A:765:PRO:O	1:A:766:LYS:C	2.51	0.48
1:A:1966:TYR:HB2	1:A:2049:ILE:HD12	1.95	0.48
1:A:2459:GLU:HA	1:A:2462:CYS:HB3	1.94	0.48
1:C:601:ILE:HA	1:C:602:GLU:HA	1.72	0.48
1:C:915:GLU:HB3	1:C:917:TYR:HB2	1.94	0.48
1:C:1244:ARG:HG3	1:C:1269:TYR:OH	2.14	0.48
1:C:2062:GLU:CG	1:C:2099:PRO:HB2	2.44	0.48
5:J:698:ARG:HB2	5:J:700:SER:H	1.78	0.48
1:A:280:LEU:HD11	1:A:333:GLU:OE1	2.14	0.48
1:A:731:PRO:HB3	1:A:736:GLU:HB2	1.95	0.48
1:A:1814:LEU:HB2	1:A:1816:HIS:CD2	2.48	0.48
2:B:6:VAL:HG22	2:B:38:LEU:HD22	1.94	0.48
1:C:280:ARG:NH1	1:C:328:THR:HB	2.27	0.48
1:C:640:VAL:HG13	1:C:643:LYS:HB3	1.96	0.48
1:C:1030:LYS:C	1:C:1032:LEU:H	2.17	0.48
1:C:1121:ARG:HA	1:C:1124:GLN:HG2	1.95	0.48
1:C:1344:GLN:CD	1:C:1350:ALA:H	2.17	0.48
1:C:1623:ARG:CZ	1:C:1663:ALA:HB1	2.44	0.48
1:C:1826:LYS:HE3	1:C:1863:MET:HB2	1.95	0.48
2:D:275:ARG:HD3	2:D:284:ILE:HG12	1.95	0.48
3:F:556:UNK:O	3:F:559:UNK:N	2.47	0.48
1:A:468:CYS:SG	1:A:469:ALA:N	2.87	0.48
1:A:590:GLU:C	1:A:594:LEU:H	2.16	0.48
1:A:619:PHE:HA	1:A:622:ASP:HB3	1.94	0.48
1:A:1060:VAL:N	1:A:1061:PRO:HD2	2.29	0.48
1:A:1434:LEU:HD13	1:A:1468:LEU:HD21	1.95	0.48
1:C:508:PRO:HG3	4:G:188:PHE:HA	1.94	0.48
1:C:631:VAL:HA	1:C:634:LEU:HB2	1.95	0.48
1:C:849:LEU:HD21	1:C:1546:VAL:HB	1.96	0.48
1:C:1014:ILE:HD11	1:C:1022:ILE:HD12	1.96	0.48
1:C:1195:ILE:O	1:C:1195:ILE:HG22	2.14	0.48
1:C:2138:LEU:HD11	1:C:2362:PHE:CZ	2.49	0.48
5:J:707:ILE:HD13	5:J:728:LEU:HD22	1.95	0.48
1:A:323:SER:HB2	1:A:325:HIS:CD2	2.49	0.48
1:A:1489:MET:SD	1:A:1490:LYS:HG2	2.54	0.48
1:A:1556:ILE:O	1:A:1559:LYS:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1823:ILE:HG23	1:A:1824:LYS:H	1.79	0.48
1:C:1050:ILE:CD1	1:C:1065:ILE:HG12	2.43	0.48
1:C:1496:PRO:HA	1:C:1525:LEU:HD22	1.95	0.48
1:C:1591:TRP:HB3	1:C:1614:PHE:HZ	1.79	0.48
1:C:1612:ILE:HG21	1:C:1656:ALA:CB	2.43	0.48
1:C:1745:TYR:O	1:C:1762:TRP:NE1	2.47	0.48
1:C:1866:GLY:HA2	1:C:1869:LEU:HG	1.95	0.48
1:C:1918:VAL:HG22	1:C:2170:PRO:O	2.14	0.48
3:F:554:UNK:C	3:F:556:UNK:N	2.73	0.48
1:A:284:VAL:HG13	1:A:334:LEU:HD21	1.96	0.47
1:A:367:GLU:HA	1:A:370:ALA:CB	2.43	0.47
1:A:1922:SER:HB2	1:A:1926:GLN:HB3	1.96	0.47
1:C:2255:LEU:HG	1:C:2259:THR:HB	1.96	0.47
5:I:699:LYS:NZ	5:I:702:THR:HG21	2.29	0.47
1:A:461:TYR:CD2	1:A:497:GLU:HB3	2.48	0.47
1:A:1736:PRO:HA	1:A:1739:ILE:HB	1.95	0.47
1:A:1972:ALA:HB1	1:A:1988:ALA:CB	2.44	0.47
1:A:2265:VAL:HG23	1:A:2266:MET:H	1.78	0.47
2:B:9:GLY:O	2:B:12:HIS:CE1	2.67	0.47
1:C:401:LYS:O	1:C:414:PRO:HG3	2.14	0.47
1:C:948:ILE:HA	1:C:952:LEU:HB2	1.95	0.47
1:C:1244:ARG:NH2	1:C:1260:ARG:HD3	2.29	0.47
1:C:1601:VAL:O	1:C:1602:ILE:HB	2.14	0.47
1:C:1626:LEU:O	1:C:1630:VAL:HG22	2.13	0.47
1:C:2279:ASP:HB3	1:C:2284:ASN:ND2	2.29	0.47
1:C:2421:ARG:HA	1:C:2424:LEU:HB3	1.94	0.47
3:E:602:UNK:O	3:E:606:UNK:N	2.47	0.47
1:A:453:LYS:H	1:A:454:GLN:HA	1.76	0.47
1:A:1558:TYR:HB2	1:A:1572:ARG:HE	1.80	0.47
1:A:1601:LYS:O	1:A:1603:LYS:N	2.46	0.47
2:B:68:VAL:HG12	2:B:69:ALA:N	2.29	0.47
1:C:347:TYR:O	1:C:351:TYR:HB3	2.15	0.47
1:C:1448:LEU:HD23	1:C:1451:LEU:HD13	1.95	0.47
1:C:2194:HIS:O	1:C:2198:LYS:HD3	2.14	0.47
1:C:2432:LYS:O	1:C:2449:GLN:HG2	2.14	0.47
2:D:10:TYR:O	2:D:12:HIS:CD2	2.67	0.47
1:A:89:ASP:HB3	1:A:90:LYS:H	1.29	0.47
1:A:759:ILE:O	1:A:763:ILE:N	2.47	0.47
1:A:862:ARG:HB3	1:A:2156:ARG:HA	1.96	0.47
1:A:1449:LEU:O	1:A:1453:LYS:N	2.32	0.47
1:A:2061:LEU:H	1:A:2097:PRO:C	2.16	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2107:ARG:N	1:A:2108:PRO:CD	2.77	0.47
1:C:368:GLU:HA	1:C:371:ALA:HB2	1.96	0.47
1:C:2337:PHE:O	1:C:2341:CYS:N	2.47	0.47
2:D:40:ILE:HD13	2:D:301:ASN:HB2	1.95	0.47
2:D:84:GLN:CB	2:D:89:TRP:HB2	2.33	0.47
2:D:246:LEU:HD22	2:D:277:TRP:CZ3	2.49	0.47
3:E:756:UNK:HA	3:E:759:UNK:H2	1.79	0.47
1:A:272:ARG:HG2	1:A:273:ASP:H	1.79	0.47
1:A:400:LYS:HG3	1:A:402:ILE:HG12	1.95	0.47
1:A:673:GLN:HA	1:A:676:ASN:HD21	1.76	0.47
1:A:710:VAL:HG12	1:A:711:VAL:HA	1.96	0.47
1:A:1027:ILE:HB	1:A:1070:THR:HB	1.96	0.47
1:A:2075:GLU:O	1:A:2091:LYS:HA	2.15	0.47
1:C:235:LEU:CB	1:C:236:GLU:HA	2.44	0.47
1:C:260:TYR:HD2	1:C:260:TYR:N	2.12	0.47
1:C:301:LEU:HG	1:C:340:ALA:HA	1.96	0.47
1:C:506:LYS:HD3	1:C:508:PRO:O	2.14	0.47
1:C:690:PHE:CE1	1:C:731:MET:HB3	2.50	0.47
1:C:793:GLU:HG2	1:C:796:ARG:HG3	1.97	0.47
5:I:698:ARG:HG3	5:I:788:GLU:HG2	1.95	0.47
1:A:180:ILE:HG22	1:A:223:LEU:HD13	1.93	0.47
1:A:937:HIS:HE1	1:A:977:GLN:HA	1.79	0.47
1:A:1073:PRO:HB3	1:A:1110:LYS:H	1.79	0.47
1:A:1427:VAL:O	1:A:1433:LYS:HE2	2.13	0.47
1:A:2082:ARG:HH12	1:A:2167:ILE:HD13	1.79	0.47
1:A:2189:ILE:O	1:A:2193:ARG:HG3	2.15	0.47
1:C:634:LEU:HA	1:C:637:VAL:HB	1.96	0.47
1:C:651:ASP:CB	1:C:652:PRO:HA	2.44	0.47
1:C:1655:TYR:HA	1:C:1658:LEU:HB2	1.96	0.47
2:D:11:ASP:HB3	2:D:293:LYS:H	1.80	0.47
2:D:213:ILE:HG22	2:D:224:THR:HG23	1.97	0.47
5:I:693:PHE:O	5:I:694:THR:N	2.48	0.47
1:A:115:ARG:HB2	1:A:159:TYR:HB3	1.97	0.47
1:A:125:PHE:O	1:A:129:LEU:HB3	2.14	0.47
1:A:259:TYR:HB3	1:A:293:ILE:HD13	1.95	0.47
1:A:300:LEU:HD22	1:A:303:GLN:HG3	1.95	0.47
1:A:796:TYR:HE2	1:A:843:GLU:HB3	1.79	0.47
1:A:841:TYR:O	1:A:843:GLU:N	2.47	0.47
1:A:848:LEU:H	1:A:1547:GLN:NE2	2.13	0.47
1:A:1516:HIS:O	1:A:1520:ALA:N	2.47	0.47
1:A:1613:ALA:O	1:A:1617:ARG:HG2	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1870:ILE:HG12	1:A:1902:LEU:HA	1.96	0.47
1:A:2245:LYS:HE3	1:A:2287:ARG:HH11	1.78	0.47
1:A:2275:LEU:HG	1:A:2299:ASP:C	2.35	0.47
1:A:2449:ASP:O	1:A:2453:GLN:HB2	2.15	0.47
2:B:91:VAL:HB	2:B:145:LEU:HD21	1.97	0.47
1:C:112:THR:O	1:C:114:LEU:HG	2.15	0.47
1:C:157:ILE:O	1:C:163:THR:HG21	2.15	0.47
1:C:260:TYR:N	1:C:260:TYR:CD2	2.80	0.47
1:C:500:LEU:HD12	1:C:503:LEU:HD12	1.96	0.47
1:C:573:LEU:O	1:C:577:PHE:HB2	2.14	0.47
1:C:620:PHE:HD1	1:C:623:ASP:HB3	1.78	0.47
1:C:712:VAL:HB	1:C:713:PRO:CD	2.45	0.47
1:C:926:MET:HA	1:C:929:LEU:HD23	1.95	0.47
1:C:1541:ALA:HB1	1:C:1542:TYR:HA	1.97	0.47
1:C:1561:LYS:HA	1:C:1570:ARG:HH21	1.78	0.47
1:C:1893:VAL:O	1:C:1896:SER:HB2	2.15	0.47
1:C:1916:LEU:HA	1:C:1919:ALA:HB2	1.96	0.47
2:D:83:PHE:HD1	2:D:104:VAL:HG11	1.78	0.47
2:D:173:MET:HB3	2:D:174:LEU:CA	2.44	0.47
5:J:703:ILE:HG21	5:J:732:ASP:CG	2.34	0.47
1:A:324:VAL:HA	1:A:325:HIS:N	2.30	0.47
1:A:2220:LEU:HD13	2:B:209:TYR:HD2	1.79	0.47
2:B:7:SER:OG	2:B:274:VAL:HB	2.14	0.47
2:B:233:VAL:HG11	2:B:279:LEU:HD21	1.97	0.47
1:C:818:ARG:O	1:C:822:LEU:HB3	2.15	0.47
1:C:1239:TRP:O	1:C:1243:ILE:HG12	2.15	0.47
2:D:4:ILE:O	2:D:5:LEU:HB3	2.14	0.47
5:J:681:TYR:O	5:J:681:TYR:CD1	2.68	0.47
1:A:259:TYR:HB2	1:A:290:LEU:CD1	2.45	0.47
1:A:1126:VAL:HG23	1:A:1166:LEU:HD11	1.97	0.47
1:A:2113:ILE:HG13	1:A:2123:TYR:CE2	2.49	0.47
1:C:260:TYR:HE1	1:C:300:ALA:CB	2.27	0.47
1:C:410:ASN:O	1:C:450:PHE:HD2	1.97	0.47
1:C:417:LEU:HD13	1:C:460:LEU:HD11	1.97	0.47
1:C:1513:LYS:HA	1:C:1516:GLU:HB3	1.97	0.47
1:C:1587:ASN:O	1:C:1590:VAL:HG23	2.14	0.47
1:C:2432:LYS:HD3	1:C:2437:ASP:HB2	1.97	0.47
2:D:221:HIS:HB3	2:D:233:VAL:HG22	1.97	0.47
4:G:136:TRP:HA	4:G:137:VAL:O	2.15	0.47
5:I:737:ASN:OD1	5:I:768:SER:HB2	2.15	0.47
1:A:328:LEU:O	1:A:368:VAL:HG13	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:TYR:CG	1:A:441:ILE:HB	2.50	0.47
1:A:620:ILE:HA	1:A:660:LEU:HD21	1.97	0.47
1:A:947:ILE:HA	1:A:951:LEU:HD13	1.96	0.47
1:A:1087:VAL:HA	1:A:1099:LYS:HD2	1.97	0.47
1:A:1227:TRP:CH2	1:A:1238:TRP:HE3	2.33	0.47
1:C:382:ALA:C	1:C:386:LYS:HD3	2.35	0.47
1:C:721:GLU:CB	1:C:722:LEU:HB2	2.40	0.47
1:C:836:VAL:CG2	1:C:845:LEU:HD12	2.45	0.47
1:C:1070:VAL:CG2	1:C:1106:LEU:HG	2.45	0.47
1:C:1521:ASN:HB3	1:C:1525:LEU:HD21	1.95	0.47
1:C:1636:GLU:HG2	1:C:1653:VAL:HG21	1.96	0.47
1:A:145:LYS:HD3	1:A:186:GLU:HG3	1.97	0.46
1:A:399:LEU:HB3	1:A:405:ASN:O	2.15	0.46
1:A:1555:ILE:HG21	1:A:1575:TRP:NE1	2.30	0.46
2:B:125:HIS:HA	2:B:167:MET:HE1	1.96	0.46
2:B:221:HIS:CE1	2:B:279:LEU:HD22	2.49	0.46
1:C:1757:LYS:HD2	1:C:1832:ILE:HG21	1.97	0.46
1:A:676:ASN:HB3	1:A:723:THR:HA	1.96	0.46
1:A:788:VAL:HB	1:A:795:ARG:HH11	1.80	0.46
1:A:1820:ILE:HG23	1:A:1824:LYS:HG2	1.97	0.46
1:A:1877:LEU:HD23	1:A:1913:PRO:HD2	1.96	0.46
2:B:40:ILE:HG23	2:B:47:LEU:HD23	1.96	0.46
2:B:105:ARG:O	2:B:106:SER:CB	2.62	0.46
2:B:168:ALA:HB3	2:B:171:GLY:H	1.80	0.46
1:C:1044:LEU:O	1:C:1048:LEU:HB2	2.15	0.46
1:C:2192:ARG:O	1:C:2196:GLU:N	2.46	0.46
1:A:91:LEU:HD13	1:A:144:GLU:HG3	1.97	0.46
1:A:698:ILE:O	1:C:1079:TYR:HE2	1.98	0.46
1:A:1504:CYS:SG	1:A:1510:PHE:HA	2.55	0.46
1:A:2182:SER:HA	1:A:2287:ARG:H	1.81	0.46
2:B:91:VAL:HG11	2:B:131:LEU:HD13	1.97	0.46
2:B:233:VAL:HG21	2:B:279:LEU:HG	1.96	0.46
1:C:269:TRP:HB2	1:C:310:PHE:HE2	1.80	0.46
1:C:601:ILE:HA	1:C:603:HIS:HB2	1.98	0.46
1:C:703:LEU:HD13	1:C:714:SER:HB3	1.96	0.46
1:C:1295:ASP:CG	1:C:1342:TYR:HH	2.18	0.46
1:C:1369:ILE:HA	1:C:1372:LEU:HD23	1.97	0.46
1:C:1432:MET:O	1:C:1435:LYS:HG3	2.14	0.46
1:C:1627:ALA:O	1:C:1631:LEU:HG	2.16	0.46
1:C:2133:ILE:CD1	1:C:2176:GLY:HA3	2.45	0.46
1:C:2194:HIS:CE1	1:C:2239:ASP:HB3	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:GLY:HA2	1:A:304:TRP:NE1	2.31	0.46
1:A:644:LEU:HA	1:A:647:ALA:HB3	1.98	0.46
1:A:689:PHE:CZ	1:A:732:LYS:HD3	2.51	0.46
1:A:1555:ILE:HG13	1:A:1556:ILE:HG13	1.98	0.46
1:A:1730:LYS:HB3	1:A:1735:ASN:CB	2.41	0.46
1:C:2253:THR:HG22	1:C:2257:ARG:HD2	1.97	0.46
2:D:6:VAL:HG13	2:D:7:SER:HB3	1.97	0.46
1:A:328:LEU:HB3	1:A:368:VAL:HG13	1.98	0.46
1:A:1351:LEU:HD22	1:A:1377:LEU:HD22	1.97	0.46
2:B:60:ILE:O	2:B:60:ILE:HG13	2.15	0.46
2:B:175:ALA:C	2:B:222:LEU:HD21	2.36	0.46
1:C:1445:TRP:HB2	1:C:1478:LEU:HB3	1.97	0.46
1:C:1760:HIS:CG	1:C:1832:ILE:HG13	2.50	0.46
2:D:16:PHE:O	2:D:26:ARG:N	2.48	0.46
2:D:181:GLY:HA2	2:D:210:ILE:HB	1.96	0.46
1:A:763:ILE:HG23	1:A:805:ILE:HD12	1.98	0.46
1:A:1084:PRO:HA	1:A:1087:VAL:HG13	1.98	0.46
1:A:1628:VAL:HB	1:A:1632:LEU:HD12	1.98	0.46
1:A:1884:ILE:HB	1:A:1925:ARG:HD2	1.97	0.46
1:A:2134:ASP:HA	1:A:2137:VAL:HB	1.97	0.46
1:A:2211:ALA:HB1	1:A:2213:ASP:C	2.36	0.46
1:A:2246:SER:O	1:A:2248:SER:N	2.49	0.46
1:C:640:VAL:HB	1:C:679:ARG:HH22	1.79	0.46
1:C:715:LEU:O	1:C:719:LEU:HB3	2.15	0.46
1:C:850:ILE:HG12	1:C:1550:ILE:HA	1.96	0.46
1:C:998:ARG:C	1:C:999:PRO:N	2.68	0.46
1:C:1655:TYR:CE1	1:C:1720:LEU:HD21	2.51	0.46
1:C:2128:LYS:HD2	1:C:2133:ILE:HD11	1.98	0.46
1:C:2222:LEU:HG	2:D:252:TRP:CZ3	2.50	0.46
5:J:701:SER:N	5:J:702:THR:HB	2.29	0.46
1:A:774:VAL:N	1:A:775:ALA:HB2	2.31	0.46
1:A:1610:ILE:HG23	1:A:1654:ALA:HB2	1.98	0.46
1:A:2185:PHE:HB3	1:A:2280:PRO:HA	1.96	0.46
1:A:2368:TRP:HA	1:A:2416:ARG:HH22	1.79	0.46
1:C:89:PHE:HD1	1:C:101:ALA:HB1	1.81	0.46
1:C:533:GLN:C	1:C:535:ASN:N	2.68	0.46
1:C:1090:MET:HB3	1:C:1093:TYR:CD2	2.50	0.46
1:C:1871:GLN:HE21	1:C:1873:GLY:HA3	1.81	0.46
4:H:111:ALA:O	4:H:114:HIS:N	2.49	0.46
5:J:725:GLU:HG3	5:J:726:ASP:H	1.80	0.46
1:A:227:ASN:O	1:A:230:SER:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ARG:HD2	1:A:368:VAL:HG21	1.98	0.46
1:A:449:PHE:HB3	1:A:452:ARG:HD2	1.97	0.46
1:A:636:VAL:HG13	1:A:675:ASP:CB	2.37	0.46
1:A:773:ALA:N	1:A:775:ALA:HB2	2.30	0.46
1:A:1280:PHE:HA	1:A:1281:SER:HA	1.76	0.46
1:A:1587:ASP:N	1:A:1588:VAL:CB	2.75	0.46
1:A:1588:VAL:HG11	1:A:1615:LEU:CD2	2.46	0.46
1:A:1601:LYS:HD2	1:A:1635:GLU:HG3	1.98	0.46
1:A:2099:PHE:HA	1:A:2111:PHE:HE2	1.79	0.46
2:B:230:THR:HG22	2:B:246:LEU:H	1.81	0.46
1:C:346:LYS:HD3	1:C:350:ILE:HG13	1.97	0.46
1:C:1734:ARG:HH12	1:C:1771:SER:HB3	1.80	0.46
1:C:2082:GLY:HA3	1:C:2123:TYR:CE1	2.50	0.46
2:D:53:GLN:HE21	2:D:94:SER:HB3	1.80	0.46
5:I:730:VAL:HG21	5:I:790:PRO:N	2.31	0.46
1:A:361:PHE:CE1	1:A:414:PHE:CZ	2.99	0.46
1:A:1599:VAL:HA	1:A:1600:ILE:HA	1.70	0.46
1:A:1622:MET:O	1:A:1626:LYS:HD3	2.15	0.46
1:A:1911:VAL:O	1:A:1915:MET:N	2.49	0.46
1:A:2109:ARG:HG3	1:A:2125:LEU:HD13	1.98	0.46
1:A:2112:CYS:HB3	1:A:2122:LYS:H	1.79	0.46
1:A:2190:ARG:O	1:A:2194:GLU:N	2.43	0.46
2:B:74:HIS:HE1	2:B:102:TRP:HE1	1.64	0.46
1:C:1526:LEU:HD22	1:C:1548:ALA:HB1	1.98	0.46
1:C:2061:LEU:HD21	1:C:2101:PHE:HB2	1.97	0.46
1:C:2080:VAL:HA	1:C:2092:VAL:CG1	2.46	0.46
1:C:2404:GLU:HB3	1:C:2405:GLU:N	2.30	0.46
1:A:145:LYS:HB3	1:A:189:ARG:HB3	1.98	0.46
1:A:1384:ILE:HD13	1:A:1408:ARG:HH21	1.80	0.46
1:A:1740:LEU:O	1:A:1744:LEU:HG	2.16	0.46
1:A:2030:LYS:HD2	1:A:2033:SER:HB2	1.98	0.46
1:A:2368:TRP:HA	1:A:2416:ARG:NH2	2.31	0.46
1:A:2423:VAL:C	1:A:2426:ARG:HB3	2.36	0.46
2:B:147:GLU:HG2	2:B:149:GLN:HB3	1.98	0.46
2:B:156:PRO:HB3	2:B:186:TRP:HE1	1.81	0.46
1:C:289:LYS:HG3	1:C:338:LEU:HD21	1.98	0.46
1:C:462:TYR:OH	1:C:501:MET:HB2	2.15	0.46
2:D:4:ILE:O	2:D:5:LEU:CB	2.64	0.46
4:H:111:ALA:C	4:H:113:ILE:H	2.18	0.46
5:I:675:SER:HB3	5:I:687:LYS:HD3	1.97	0.46
5:I:698:ARG:HA	5:I:759:ASP:N	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:LYS:HE2	1:A:237:ARG:CD	2.46	0.45
1:A:305:PHE:HD2	1:A:306:GLN:HE21	1.64	0.45
1:A:412:LYS:HZ1	1:A:442:ARG:HD3	1.81	0.45
1:A:725:LEU:HB3	1:A:760:LEU:HB3	1.97	0.45
1:A:1216:LEU:HA	1:A:1217:PRO:CA	2.39	0.45
1:A:2004:ARG:HB3	1:A:2063:HIS:CD2	2.52	0.45
1:A:2377:ILE:HD11	1:A:2415:ILE:HD13	1.98	0.45
1:C:163:THR:O	1:C:168:ASN:HB3	2.16	0.45
1:C:245:ILE:HG12	1:C:249:LEU:HD12	1.97	0.45
1:C:265:LEU:HD13	1:C:307:GLN:HE21	1.82	0.45
1:C:682:PHE:O	1:C:684:ALA:N	2.46	0.45
1:C:747:ASN:C	1:C:749:SER:H	2.20	0.45
1:C:1559:LYS:HG2	1:C:1563:LEU:HD13	1.98	0.45
2:D:4:ILE:HG23	2:D:60:ILE:HD13	1.97	0.45
2:D:6:VAL:O	2:D:274:VAL:HG21	2.16	0.45
3:E:651:UNK:O	3:E:653:UNK:N	2.49	0.45
1:A:357:LYS:HZ2	1:A:414:PHE:HD1	1.62	0.45
1:A:1286:GLU:HA	1:A:1289:THR:HG22	1.97	0.45
1:A:1838:LEU:HA	1:A:1841:ALA:HB3	1.98	0.45
2:B:11:ASP:HB2	2:B:292:HIS:HB2	1.98	0.45
2:B:185:VAL:HG11	2:B:240:PHE:CZ	2.52	0.45
1:C:596:ILE:CD1	1:C:600:TYR:HD2	2.29	0.45
2:D:156:PRO:HA	2:D:186:TRP:HZ2	1.81	0.45
3:F:756:UNK:C	3:F:757:UNK:HA	2.45	0.45
1:A:220:TRP:N	1:A:234:LEU:HD13	2.32	0.45
1:A:354:MET:HG3	1:A:388:LEU:HD22	1.98	0.45
1:A:574:GLN:O	1:A:578:MET:HG2	2.16	0.45
1:A:1555:ILE:O	1:A:1572:ARG:NH2	2.50	0.45
1:A:1758:HIS:CG	1:A:1830:ILE:HD11	2.51	0.45
1:A:2278:ARG:O	1:A:2317:ARG:HD2	2.17	0.45
1:A:2446:GLU:O	1:A:2450:LYS:N	2.43	0.45
2:B:8:ALA:HB3	2:B:35:VAL:HG21	1.97	0.45
2:B:164:SER:CB	2:B:212:ARG:HA	2.46	0.45
2:B:248:GLY:HA3	2:B:251:ARG:NE	2.31	0.45
1:C:329:LEU:O	1:C:369:VAL:HG13	2.16	0.45
1:C:361:LYS:HE3	1:C:366:ARG:NH2	2.31	0.45
1:C:397:LEU:HD23	1:C:401:LYS:HG2	1.99	0.45
1:C:1430:GLU:HA	1:C:1458:THR:CG2	2.45	0.45
1:C:1556:GLU:HA	1:C:1559:LYS:HE3	1.98	0.45
1:C:2258:ARG:O	1:C:2261:TYR:N	2.50	0.45
1:A:115:ARG:HE	1:A:166:PRO:HB2	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:PHE:HB3	1:A:818:ASP:C	2.36	0.45
1:A:1142:ASN:HA	1:A:1145:SER:HB3	1.98	0.45
1:A:1181:ASN:HA	1:A:1184:LEU:HB3	1.97	0.45
1:A:2203:GLU:O	1:A:2207:MET:N	2.49	0.45
1:C:176:TYR:HA	1:C:179:VAL:HG22	1.98	0.45
1:C:715:LEU:HD21	1:C:754:LYS:HG3	1.99	0.45
1:C:799:LYS:C	1:C:800:GLU:N	2.70	0.45
1:C:923:HIS:O	1:C:923:HIS:CG	2.69	0.45
1:C:1860:THR:HA	1:C:1864:HIS:HB3	1.97	0.45
1:C:1880:PRO:HA	1:C:1883:ILE:HG12	1.97	0.45
1:C:2157:PHE:HD1	1:C:2160:HIS:CG	2.34	0.45
1:C:2189:VAL:HA	1:C:2192:ARG:HG2	1.98	0.45
1:A:482:LEU:HD11	1:A:498:THR:HG21	1.98	0.45
1:A:768:GLN:HG3	1:A:770:ALA:O	2.16	0.45
1:A:918:THR:HA	1:A:921:ILE:HB	1.99	0.45
1:A:1453:LYS:HG2	1:A:1465:MET:HE3	1.99	0.45
1:A:1634:GLU:HB3	1:A:1636:THR:H	1.81	0.45
1:A:1675:PHE:HB3	1:A:1715:ARG:CZ	2.46	0.45
1:A:2128:HIS:HA	1:A:2172:LYS:HG3	1.97	0.45
1:A:2130:ASP:HB2	1:A:2366:ILE:HG23	1.97	0.45
1:A:2282:ASN:HB3	1:A:2294:HIS:CD2	2.51	0.45
1:A:2377:ILE:HD12	1:A:2415:ILE:HG21	1.99	0.45
2:B:137:ASP:HB3	2:B:139:ASN:N	2.30	0.45
1:C:271:PRO:CG	1:C:280:ARG:HB2	2.47	0.45
1:C:801:LEU:HB3	1:C:805:ILE:HG13	1.98	0.45
1:C:1007:VAL:H	1:C:1008:ILE:HG12	1.82	0.45
1:C:1924:SER:HB3	1:C:1927:ARG:HD2	1.97	0.45
5:J:707:ILE:HD13	5:J:728:LEU:CD2	2.47	0.45
1:A:1155:PHE:HE2	1:C:622:LYS:HB3	1.82	0.45
1:A:1953:GLU:O	1:A:1957:MET:N	2.50	0.45
2:B:85:GLN:H	2:B:124:ILE:HD13	1.82	0.45
2:B:230:THR:HA	2:B:247:ASP:HA	1.99	0.45
1:C:275:ALA:O	1:C:277:LEU:N	2.50	0.45
1:C:856:GLU:HG3	1:C:1590:VAL:HG13	1.98	0.45
1:C:952:LEU:HD21	1:C:988:SER:O	2.16	0.45
1:C:1734:ARG:NH2	1:C:1771:SER:O	2.49	0.45
1:C:2109:ARG:N	1:C:2110:PRO:CD	2.80	0.45
1:C:2269:SER:HB3	1:C:2318:PHE:CE2	2.51	0.45
2:D:65:PRO:HB2	2:D:66:ASN:C	2.37	0.45
2:D:275:ARG:HB3	2:D:284:ILE:HG23	1.99	0.45
5:J:676:MET:CE	5:J:699:LYS:HE3	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ALA:HA	1:A:106:LEU:HB2	1.98	0.45
1:A:179:LEU:CD2	1:A:233:LYS:HG3	2.23	0.45
1:A:366:ARG:HD3	1:A:413:PRO:CB	2.41	0.45
1:A:623:ASP:N	1:A:629:SER:HG	2.15	0.45
1:A:663:LEU:N	1:C:1117:GLU:HB2	2.31	0.45
1:A:999:HIS:HA	1:A:1002:LYS:HB2	1.98	0.45
1:A:1419:LYS:HE2	1:A:1433:LYS:NZ	2.32	0.45
1:A:1672:LEU:HD11	1:A:1719:LYS:HG3	1.99	0.45
1:A:2082:ARG:NH1	1:A:2167:ILE:HG21	2.31	0.45
1:A:2155:PHE:HD1	1:A:2158:HIS:CG	2.35	0.45
2:B:93:SER:HB2	2:B:119:VAL:HG22	1.99	0.45
2:B:182:ASN:CG	2:B:204:ARG:HE	2.20	0.45
1:C:138:ILE:HG22	1:C:140:GLY:H	1.82	0.45
1:C:763:VAL:HG11	1:C:803:PRO:HA	1.97	0.45
1:C:857:ASN:O	1:C:1585:GLN:N	2.49	0.45
1:C:1173:GLN:O	1:C:1177:TYR:HB2	2.17	0.45
1:C:1504:ILE:HB	1:C:1596:ARG:HH22	1.82	0.45
5:I:703:ILE:HD12	5:I:706:VAL:HG21	1.98	0.45
5:J:709:PHE:HE2	5:J:716:THR:HG1	1.61	0.45
1:A:162:THR:HG1	1:A:167:ASN:N	2.15	0.45
1:A:234:LEU:HD11	1:A:270:PRO:CG	2.41	0.45
1:A:765:PRO:HG3	1:A:805:ILE:HG22	1.99	0.45
1:A:1279:SER:O	1:A:1282:SER:N	2.50	0.45
1:A:2279:HIS:HA	1:A:2467:GLY:O	2.17	0.45
2:B:44:LYS:HD2	2:B:301:ASN:HB3	1.98	0.45
1:C:174:ALA:HB1	1:C:178:ARG:CZ	2.47	0.45
1:C:269:TRP:HB2	1:C:310:PHE:CE2	2.52	0.45
1:C:281:LEU:O	1:C:285:VAL:N	2.50	0.45
1:C:291:LEU:HA	1:C:294:ILE:HD12	1.97	0.45
1:C:690:PHE:CD1	1:C:728:PHE:HZ	2.34	0.45
1:C:2063:LEU:HD12	1:C:2099:PRO:HA	1.99	0.45
1:C:2133:ILE:HD13	1:C:2176:GLY:HA3	1.99	0.45
1:C:2264:SER:O	1:C:2267:VAL:HG12	2.16	0.45
1:C:2280:ARG:HB3	1:C:2319:ARG:HD2	1.98	0.45
1:C:2407:GLN:O	1:C:2409:VAL:CA	2.65	0.45
2:D:13:THR:OG1	2:D:291:HIS:HA	2.16	0.45
3:F:651:UNK:O	3:F:653:UNK:N	2.50	0.45
1:A:1065:LEU:HA	1:A:1068:LEU:HB2	1.98	0.45
1:A:1077:ASP:HB2	1:C:699:ILE:HG12	1.97	0.45
2:B:44:LYS:HB3	2:B:301:ASN:HB3	1.98	0.45
1:C:731:MET:HA	1:C:732:PRO:HD2	1.85	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:969:LEU:HD22	1:C:985:GLN:HG3	1.98	0.45
1:C:1104:ILE:HB	1:C:1142:MET:HB3	1.99	0.45
1:C:1619:ARG:CA	1:C:1626:LEU:HG	2.37	0.45
1:C:1974:ALA:HB1	1:C:1990:ALA:HB3	1.98	0.45
1:C:2017:ASP:O	1:C:2020:ASP:N	2.50	0.45
3:F:606:UNK:HA	3:F:607:UNK:C	2.47	0.45
5:I:736:PRO:HA	5:I:755:PHE:HE1	1.81	0.45
5:J:736:PRO:HA	5:J:755:PHE:HD1	1.80	0.45
1:A:303:GLN:HB3	1:A:307:ARG:CB	2.46	0.45
1:A:449:PHE:CD1	1:A:455:PHE:HA	2.52	0.45
1:A:721:LEU:O	1:A:760:LEU:HB2	2.16	0.45
1:A:964:PRO:HA	1:A:965:GLY:HA3	1.72	0.45
1:A:2043:TYR:HB3	1:A:2047:ARG:HH22	1.81	0.45
1:A:2060:GLU:CB	1:A:2062:GLN:HG2	2.18	0.45
1:A:2205:TRP:HA	1:A:2208:LEU:HB2	1.98	0.45
2:B:229:HIS:CB	2:B:251:ARG:HB2	2.47	0.45
1:C:1531:SER:C	1:C:1532:ALA:HA	2.37	0.45
5:I:647:LYS:HZ2	5:I:649:LYS:HZ1	1.65	0.45
1:A:244:ILE:HA	1:A:248:LEU:HB2	2.00	0.44
1:A:381:ALA:CB	1:A:385:LYS:HD3	2.46	0.44
1:A:1258:LEU:HD23	1:A:1258:LEU:HA	1.92	0.44
1:A:1586:ILE:N	1:A:1615:LEU:HD21	2.32	0.44
1:C:917:TYR:N	1:C:918:PRO:CD	2.79	0.44
1:C:1214:VAL:HG22	1:C:1249:GLN:HE21	1.81	0.44
1:C:1465:LYS:HG3	1:C:1492:LYS:HZ1	1.83	0.44
1:C:1732:LYS:CA	1:C:1737:ASN:HB2	2.47	0.44
1:C:2409:VAL:HA	1:C:2410:GLU:C	2.37	0.44
2:D:205:ALA:N	2:D:206:HIS:O	2.50	0.44
2:D:274:VAL:N	2:D:288:TYR:O	2.50	0.44
1:A:87:ILE:HG12	1:A:99:ARG:HH21	1.83	0.44
1:A:914:GLU:O	1:A:915:TYR:N	2.50	0.44
1:A:1117:MET:HG3	1:A:1120:ARG:HG3	1.99	0.44
2:B:70:SER:HB3	2:B:72:GLU:HG3	1.98	0.44
1:C:632:HIS:O	1:C:636:SER:N	2.51	0.44
1:C:805:ILE:HG12	1:C:851:ASN:CG	2.36	0.44
1:C:1578:ASN:C	1:C:1581:LEU:HG	2.36	0.44
2:D:143:TRP:HE1	2:D:148:ASN:HA	1.81	0.44
1:A:1354:LYS:HE3	1:A:1373:ILE:HD13	1.98	0.44
1:C:177:LEU:HD12	1:C:238:ARG:NH2	2.33	0.44
1:C:288:GLY:O	1:C:338:LEU:HD23	2.17	0.44
1:C:444:GLU:HB3	1:C:447:ARG:HH11	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1000:HIS:HA	1:C:1003:LYS:HB2	1.98	0.44
1:C:1216:LYS:HB3	1:C:1249:GLN:O	2.18	0.44
1:C:1602:ILE:HG22	1:C:1606:GLU:HB2	2.00	0.44
1:C:1749:THR:HB	1:C:1762:TRP:CE3	2.53	0.44
1:A:314:HIS:NE2	1:A:319:ASN:OD1	2.51	0.44
1:A:534:ASN:C	1:A:535:GLN:N	2.71	0.44
1:A:600:ILE:N	1:A:602:HIS:HB2	2.32	0.44
1:C:143:SER:HB3	1:C:190:ARG:HE	1.83	0.44
1:C:220:ASP:O	1:C:235:LEU:HD22	2.18	0.44
1:C:560:THR:O	1:C:562:GLU:N	2.51	0.44
1:C:850:ILE:CD1	1:C:1553:GLU:HB2	2.46	0.44
1:C:1185:LEU:HD13	1:C:1189:CYS:HA	2.00	0.44
2:D:254:TRP:HD1	2:D:296:VAL:HA	1.80	0.44
3:F:252:UNK:O	3:F:253:UNK:N	2.47	0.44
5:J:680:ILE:C	5:J:682:ILE:H	2.21	0.44
5:J:737:ASN:HB3	5:J:754:ASN:HB2	1.98	0.44
1:A:370:ALA:CB	1:A:417:VAL:HA	2.48	0.44
1:A:1567:LYS:O	1:A:1568:ARG:N	2.50	0.44
1:A:2111:PHE:CD1	1:A:2123:TYR:HE2	2.36	0.44
1:A:2116:SER:C	1:A:2117:ASP:HA	2.37	0.44
1:A:2148:LEU:O	1:A:2158:HIS:NE2	2.50	0.44
1:A:2260:THR:HA	1:A:2327:GLU:OE1	2.18	0.44
1:A:2430:LYS:N	1:A:2442:LEU:HD12	2.33	0.44
1:C:297:ARG:HH21	1:C:341:PRO:HA	1.81	0.44
1:C:359:GLU:HG2	1:C:393:MET:HG2	2.00	0.44
1:C:660:ILE:HA	1:C:663:HIS:HB3	1.98	0.44
1:C:1749:THR:HG23	1:C:1759:TRP:HE3	1.82	0.44
1:C:1752:ASP:HA	1:C:1759:TRP:CZ3	2.52	0.44
1:C:2309:ARG:C	1:C:2380:GLU:OE2	2.55	0.44
2:D:4:ILE:HG23	2:D:16:PHE:CD1	2.52	0.44
2:D:12:HIS:CE1	2:D:35:VAL:HB	2.52	0.44
1:A:172:LEU:HD23	1:A:176:LEU:HD13	1.99	0.44
1:A:554:SER:N	1:A:555:PHE:HB2	2.31	0.44
1:A:1589:TRP:O	1:A:1593:LEU:N	2.49	0.44
1:A:1621:ARG:HA	1:A:1624:LEU:HB3	1.99	0.44
1:A:1732:ARG:NH2	1:A:1733:LEU:HG	2.32	0.44
1:A:2181:ASN:HA	1:A:2182:SER:N	2.32	0.44
2:B:86:ASP:HB3	2:B:88:ARG:H	1.81	0.44
1:C:176:TYR:H	1:C:179:VAL:HG22	1.82	0.44
1:C:827:GLN:H	1:C:830:ALA:HB1	1.83	0.44
1:C:1561:LYS:HE3	1:C:1601:VAL:HB	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:TYR:CE1	1:A:498:THR:HA	2.52	0.44
1:A:466:LEU:O	1:A:467:ALA:HB3	2.17	0.44
1:A:507:PRO:HB2	1:A:509:LEU:HD23	1.99	0.44
1:A:675:ASP:N	1:A:675:ASP:OD1	2.50	0.44
1:A:699:ILE:HD13	1:A:699:ILE:HA	1.89	0.44
1:A:796:TYR:OH	1:A:844:LEU:HD22	2.18	0.44
1:A:1025:GLU:HG3	1:A:1029:LYS:HE2	1.98	0.44
1:A:1088:ARG:NH2	1:A:1120:ARG:HB2	2.32	0.44
1:A:1389:HIS:HB2	1:A:2332:GLU:HG2	1.98	0.44
1:A:1725:VAL:HA	1:A:1728:GLN:HB3	1.99	0.44
1:C:216:ARG:HD2	1:C:234:LYS:HZ1	1.82	0.44
1:C:249:LEU:HA	1:C:252:ASN:HB3	2.00	0.44
1:C:355:MET:HB2	1:C:389:LEU:HD22	1.99	0.44
1:C:688:GLU:HB3	1:C:692:ILE:HG13	2.00	0.44
1:C:700:ILE:HG13	1:C:721:GLU:CD	2.38	0.44
1:C:771:ALA:HA	1:C:811:ASP:HB2	1.99	0.44
1:C:1238:ASP:HA	1:C:1241:GLU:HB2	1.98	0.44
1:C:1554:LEU:HA	1:C:1557:ILE:CG2	2.47	0.44
1:C:2116:LYS:HA	1:C:2122:ASP:HA	1.99	0.44
2:D:131:LEU:HB3	2:D:143:TRP:O	2.18	0.44
1:A:328:LEU:HD12	1:A:365:ARG:HD2	1.99	0.44
1:A:676:ASN:HB3	1:A:726:LYS:HE2	2.00	0.44
1:A:861:ARG:NH1	1:A:1540:TYR:HB3	2.33	0.44
1:A:1112:ILE:HG22	1:A:1112:ILE:O	2.18	0.44
1:A:1755:LYS:C	1:A:1758:HIS:HB3	2.38	0.44
1:A:2110:LYS:HD2	1:A:2178:TRP:HZ3	1.83	0.44
1:A:2465:TYR:HA	1:A:2468:TRP:HB3	2.00	0.44
1:C:181:ILE:CG2	1:C:224:LEU:HD13	2.47	0.44
1:C:655:GLU:CG	1:C:658:LEU:HB3	2.48	0.44
1:C:856:GLU:O	1:C:1590:VAL:HA	2.18	0.44
1:C:1344:GLN:HE22	1:C:1351:LYS:N	2.16	0.44
1:C:1504:ILE:HB	1:C:1596:ARG:NH2	2.33	0.44
1:C:2227:VAL:C	1:C:2228:PHE:N	2.71	0.44
1:C:2264:SER:HB3	1:C:2294:VAL:H	1.82	0.44
1:C:2265:LEU:CD1	1:C:2333:ILE:HG22	2.48	0.44
1:C:2317:PRO:HB3	1:C:2453:LEU:HD13	2.00	0.44
1:A:142:SER:HB3	1:A:189:ARG:NE	2.33	0.44
1:A:220:TRP:HH2	1:A:262:SER:HG	1.65	0.44
1:A:256:LEU:HB3	1:A:258:PRO:HA	1.99	0.44
1:A:1060:VAL:N	1:A:1061:PRO:CD	2.81	0.44
1:A:2335:PHE:O	1:A:2339:CYS:N	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2446:GLU:O	1:A:2450:LYS:HG2	2.18	0.44
1:C:332:PHE:C	1:C:333:ARG:HA	2.38	0.44
1:C:399:TYR:CZ	1:C:442:ILE:HG21	2.53	0.44
1:C:819:ASP:O	1:C:823:THR:N	2.51	0.44
1:C:1007:VAL:N	1:C:1008:ILE:HG12	2.32	0.44
1:C:1996:GLU:O	1:C:1999:LYS:HB3	2.18	0.44
1:C:2346:LYS:HD2	1:C:2346:LYS:HA	1.87	0.44
2:D:57:LEU:HD12	2:D:69:ALA:HB3	1.98	0.44
1:A:113:LEU:HD13	1:A:117:VAL:HG13	1.98	0.43
1:A:807:THR:HA	1:A:1578:ARG:CZ	2.47	0.43
1:A:1134:ARG:HG2	1:A:1138:LYS:HE2	1.99	0.43
1:C:239:ARG:NH1	1:C:271:PRO:HG2	2.33	0.43
1:C:583:ILE:HA	1:C:584:HIS:HA	1.76	0.43
1:C:586:GLN:HB3	1:C:629:THR:OG1	2.18	0.43
1:C:950:GLN:O	1:C:953:GLY:N	2.51	0.43
1:C:963:ILE:HG13	1:C:964:ILE:N	2.33	0.43
1:C:965:PRO:O	1:C:969:LEU:HG	2.18	0.43
1:C:1322:VAL:HG22	1:C:1347:HIS:CE1	2.53	0.43
1:C:1421:LYS:NZ	1:C:1451:LEU:HD11	2.33	0.43
1:C:1923:GLU:HB2	1:C:1925:LEU:HG	1.98	0.43
1:C:1975:SER:HA	1:C:1978:PHE:HB3	1.99	0.43
2:D:125:HIS:HB2	2:D:167:MET:SD	2.58	0.43
3:F:367:UNK:C	3:F:369:UNK:N	2.80	0.43
5:J:676:MET:HB3	5:J:688:TYR:HD2	1.82	0.43
1:A:568:ASP:HA	1:A:572:LEU:HD22	2.00	0.43
1:A:1138:LYS:HA	1:A:1141:MET:HB2	2.00	0.43
1:A:1653:TYR:HA	1:A:1656:LEU:HB3	2.00	0.43
1:A:1904:LYS:HA	1:A:1907:PRO:HG3	2.00	0.43
1:A:1946:GLN:C	1:A:1949:LEU:HB2	2.38	0.43
2:B:253:VAL:N	2:B:269:SER:HG	2.16	0.43
1:C:346:LYS:HB3	1:C:350:ILE:CG1	2.48	0.43
1:C:783:LEU:HG	1:C:800:GLU:HG2	1.99	0.43
1:C:846:LEU:HD22	1:C:1549:GLN:HG3	1.99	0.43
1:C:1046:PHE:O	1:C:1050:ILE:HG12	2.18	0.43
2:D:37:ARG:O	2:D:50:ALA:N	2.51	0.43
2:D:151:THR:HA	2:D:152:HIS:HA	2.00	0.43
3:F:659:UNK:C	3:F:661:UNK:N	2.82	0.43
1:A:329:LEU:HD11	1:A:367:GLU:HB2	2.01	0.43
1:A:754:PRO:C	1:A:755:TYR:HA	2.39	0.43
1:A:1391:GLN:NE2	1:A:1405:LYS:HE2	2.34	0.43
1:A:1830:ILE:HD13	1:A:1835:SER:CB	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2154:CYS:SG	1:A:2340:GLU:HB3	2.58	0.43
1:C:291:LEU:HD22	1:C:301:LEU:HD22	2.00	0.43
1:C:362:PHE:CE1	1:C:393:MET:HE3	2.53	0.43
1:C:456:PHE:N	1:C:492:MET:HG3	2.32	0.43
1:C:1070:VAL:HG13	1:C:1106:LEU:HA	2.00	0.43
1:C:1492:LYS:O	1:C:1498:LYS:HB2	2.19	0.43
1:C:2400:ALA:O	1:C:2401:ILE:HG13	2.19	0.43
2:D:12:HIS:CE1	2:D:34:GLN:HG3	2.54	0.43
2:D:134:CYS:SG	2:D:165:LEU:HD13	2.58	0.43
2:D:206:HIS:CD2	2:D:226:SER:HB2	2.53	0.43
1:A:151:ALA:O	1:A:155:LEU:HB2	2.18	0.43
1:A:373:PRO:O	1:A:377:ALA:HB2	2.17	0.43
1:A:502:LEU:HB3	1:A:511:SER:OG	2.18	0.43
1:A:796:TYR:CE2	1:A:843:GLU:HB3	2.53	0.43
1:A:805:ILE:O	1:A:808:PHE:HB3	2.19	0.43
1:A:2140:LEU:HD21	1:A:2360:PHE:HE2	1.83	0.43
1:C:461:PHE:HE2	1:C:483:LEU:HD13	1.82	0.43
1:C:994:LYS:HA	1:C:995:GLN:HB2	1.99	0.43
1:C:1476:TRP:HE1	1:C:1599:SER:HG	1.63	0.43
1:C:2064:GLN:CG	1:C:2065:HIS:CD2	2.93	0.43
1:C:2104:ILE:HD12	1:C:2110:PRO:HD2	2.01	0.43
1:C:2104:ILE:HG12	1:C:2112:LYS:HD3	2.00	0.43
1:A:235:GLU:OE1	1:A:275:LYS:HB2	2.19	0.43
1:A:280:LEU:CD1	1:A:329:LEU:HB3	2.48	0.43
1:A:370:ALA:HB1	1:A:417:VAL:HA	2.01	0.43
1:A:634:HIS:HA	1:A:637:SER:HB2	2.00	0.43
1:A:1156:VAL:HG13	1:A:1157:VAL:HG13	2.01	0.43
1:A:1167:LEU:HG	1:A:1167:LEU:O	2.18	0.43
1:A:1258:LEU:HD22	1:A:1268:TYR:CE2	2.53	0.43
1:A:1436:SER:HB2	1:A:1440:LEU:CD1	2.49	0.43
1:A:2205:TRP:CA	1:A:2208:LEU:HB2	2.48	0.43
1:A:2430:LYS:O	1:A:2447:GLN:HG2	2.19	0.43
2:B:185:VAL:C	2:B:200:VAL:H	2.21	0.43
1:C:257:LEU:HD22	1:C:260:TYR:CG	2.53	0.43
1:C:389:LEU:HA	1:C:392:ILE:HB	1.99	0.43
1:C:857:ASN:CG	1:C:1586:LYS:HG2	2.39	0.43
1:C:1178:ASP:C	1:C:1182:ASN:H	2.22	0.43
1:C:1930:ALA:O	1:C:1934:ILE:HG12	2.18	0.43
1:C:2286:MET:HB3	1:C:2295:ILE:HB	2.00	0.43
1:C:2333:ILE:O	1:C:2333:ILE:HG13	2.18	0.43
2:D:4:ILE:HG23	2:D:16:PHE:HD1	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:720:PRO:CD	5:I:723:PHE:HB2	2.49	0.43
1:A:345:LYS:HD2	1:A:348:ASP:OD2	2.18	0.43
1:A:852:LEU:HD13	1:A:1575:TRP:HA	1.99	0.43
1:A:1898:LEU:O	1:A:1902:LEU:HG	2.19	0.43
1:A:2037:GLN:NE2	1:A:2040:ASP:HB3	2.34	0.43
2:B:269:SER:N	2:B:295:ALA:HB3	2.34	0.43
1:C:1063:ILE:HG22	1:C:1064:ARG:N	2.32	0.43
1:C:1654:VAL:O	1:C:1658:LEU:N	2.50	0.43
1:C:1767:PHE:HD1	1:C:1825:ILE:HG21	1.84	0.43
1:C:2062:GLU:HG2	1:C:2064:GLN:N	2.32	0.43
2:D:6:VAL:HG22	2:D:7:SER:HA	2.00	0.43
2:D:291:HIS:HB3	2:D:293:LYS:O	2.19	0.43
1:A:88:PHE:HD1	1:A:100:ALA:HB1	1.83	0.43
1:A:257:TYR:CD1	1:A:286:LEU:HD11	2.53	0.43
1:A:715:ARG:O	1:A:719:LEU:N	2.52	0.43
1:A:1088:ARG:HH22	1:A:1120:ARG:HB2	1.84	0.43
1:A:1097:LEU:HD23	1:A:1100:ILE:HG21	2.00	0.43
1:A:2268:MET:SD	1:A:2342:VAL:HG23	2.59	0.43
2:B:274:VAL:HG13	2:B:288:TYR:HB2	2.01	0.43
1:C:188:VAL:HB	1:C:237:TYR:CD2	2.54	0.43
1:C:763:VAL:HG12	1:C:763:VAL:O	2.19	0.43
1:C:1841:GLN:O	1:C:1844:LEU:N	2.51	0.43
2:D:26:ARG:HH22	2:D:47:LEU:HD11	1.83	0.43
2:D:248:GLY:HA3	2:D:251:ARG:CZ	2.48	0.43
5:J:676:MET:O	5:J:688:TYR:N	2.51	0.43
1:A:234:LEU:HD21	1:A:270:PRO:HB3	2.01	0.43
1:A:699:ILE:HD12	1:A:717:THR:HG23	1.99	0.43
1:A:701:ARG:O	1:C:1044:LEU:HD11	2.18	0.43
1:A:1073:PRO:HB3	1:A:1110:LYS:N	2.34	0.43
1:A:1241:TRP:N	1:A:1243:ARG:H	2.16	0.43
1:A:2053:LEU:HA	1:A:2056:LEU:HD13	2.00	0.43
1:A:2306:LEU:HG	1:A:2376:LYS:HB2	2.00	0.43
1:C:1407:LYS:HB3	1:C:1412:GLU:HB3	2.00	0.43
1:C:1421:LYS:HZ2	1:C:1451:LEU:HD11	1.84	0.43
1:C:1435:LYS:HE3	1:C:1436:LEU:HG	2.01	0.43
1:C:1749:THR:HB	1:C:1762:TRP:CD2	2.54	0.43
1:A:268:TRP:CZ3	1:A:316:LEU:HD23	2.54	0.43
1:A:331:PHE:HZ	1:A:345:LYS:HE3	1.84	0.43
1:A:409:ASN:O	1:A:449:PHE:HD2	2.01	0.43
1:A:954:ARG:NH1	1:A:958:PHE:HE2	2.16	0.43
1:A:1953:GLU:HB3	1:A:2068:LEU:HG	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2036:ASN:HA	1:A:2039:TRP:CB	2.49	0.43
1:A:2314:VAL:HB	1:A:2315:PRO:HD2	2.01	0.43
1:C:326:HIS:HB3	1:C:365:ILE:HB	2.01	0.43
1:C:388:TYR:O	1:C:392:ILE:N	2.52	0.43
1:C:389:LEU:O	1:C:393:MET:N	2.52	0.43
1:C:414:PRO:C	1:C:417:LEU:HB3	2.39	0.43
1:C:537:TYR:OH	1:C:545:ILE:HD13	2.19	0.43
1:C:700:ILE:HD13	1:C:703:LEU:HD12	2.01	0.43
1:C:840:LEU:O	1:C:842:TYR:N	2.51	0.43
1:C:1615:ALA:HB2	1:C:1629:LYS:HG2	2.00	0.43
1:C:2007:GLU:HG2	1:C:2066:VAL:HB	2.00	0.43
1:C:2063:LEU:O	1:C:2068:PRO:HA	2.19	0.43
1:A:442:ARG:O	1:A:446:ARG:N	2.49	0.43
1:A:714:LEU:HD13	1:A:753:LYS:HE2	2.01	0.43
1:A:771:SER:O	1:A:773:ALA:N	2.52	0.43
1:A:1339:LYS:C	1:A:1343:LYS:HG2	2.38	0.43
1:A:1617:ARG:HD2	1:A:1624:LEU:CD2	2.48	0.43
1:A:2109:ARG:H	1:A:2109:ARG:HG2	1.58	0.43
2:B:30:HIS:CE1	2:B:35:VAL:HG23	2.53	0.43
1:C:121:GLU:OE2	1:C:124:GLN:N	2.52	0.43
1:C:246:ILE:CD1	1:C:258:TYR:N	2.81	0.43
1:C:333:ARG:HG2	1:C:350:ILE:HD13	2.01	0.43
1:C:378:ALA:O	1:C:379:PHE:N	2.52	0.43
1:C:454:LYS:C	1:C:455:GLN:HA	2.38	0.43
1:C:705:SER:HA	1:C:706:VAL:C	2.38	0.43
1:C:1878:VAL:O	1:C:1878:VAL:HG12	2.18	0.43
1:C:1974:ALA:HB1	1:C:1990:ALA:CB	2.49	0.43
1:C:2340:THR:O	1:C:2344:VAL:HG12	2.19	0.43
2:D:21:THR:O	2:D:286:ARG:CZ	2.67	0.43
2:D:177:ALA:HB2	2:D:183:CYS:HA	2.01	0.43
2:D:232:ARG:HA	2:D:244:THR:HG22	2.01	0.43
5:J:729:THR:HB	5:J:730:VAL:HG22	2.00	0.43
5:J:734:SER:HB3	5:J:773:VAL:HB	2.01	0.43
1:A:115:ARG:HH12	1:A:124:ARG:HG3	1.84	0.42
1:A:422:ILE:HG23	1:A:466:LEU:HB2	2.01	0.42
1:A:1904:LYS:HG3	1:A:1939:HIS:HB2	2.00	0.42
1:A:2062:GLN:HG3	1:A:2063:HIS:N	2.34	0.42
1:C:570:ALA:HA	1:C:596:ILE:CD1	2.49	0.42
1:C:814:ASN:C	1:C:818:ARG:HG3	2.39	0.42
1:C:1108:ARG:HD2	1:C:1145:LEU:HB3	1.99	0.42
1:C:1138:THR:HG22	1:C:1142:MET:HG2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1148:LEU:O	1:C:1151:GLN:HB2	2.18	0.42
1:C:1574:ARG:C	1:C:1575:GLU:N	2.73	0.42
2:D:78:VAL:HG21	2:D:81:VAL:HG13	2.01	0.42
2:D:248:GLY:HA3	2:D:251:ARG:NE	2.34	0.42
1:A:171:ARG:O	1:A:171:ARG:HG2	2.19	0.42
1:A:280:LEU:HD13	1:A:329:LEU:HB3	2.02	0.42
1:A:388:LEU:HA	1:A:391:ILE:HB	2.01	0.42
1:A:390:ARG:HA	1:A:393:VAL:HB	2.00	0.42
1:A:413:PRO:HA	1:A:416:LEU:HB3	2.02	0.42
1:A:676:ASN:CB	1:A:726:LYS:HE2	2.49	0.42
1:A:861:ARG:O	1:A:865:VAL:HG23	2.19	0.42
1:A:862:ARG:NH1	1:A:2152:ALA:O	2.51	0.42
1:A:1126:VAL:HG23	1:A:1166:LEU:HD21	2.01	0.42
1:A:1371:ILE:HG21	1:A:1387:LEU:CD1	2.49	0.42
1:A:1430:MET:O	1:A:1433:LYS:HE3	2.17	0.42
1:A:1950:VAL:HG13	1:A:2068:LEU:HD21	2.01	0.42
1:A:2342:VAL:O	1:A:2346:LEU:HG	2.19	0.42
1:C:724:THR:O	1:C:728:PHE:N	2.53	0.42
1:C:1005:TYR:C	1:C:1007:VAL:N	2.72	0.42
1:C:1355:TYR:HA	1:C:1358:VAL:HG12	1.99	0.42
1:C:2104:ILE:O	1:C:2109:ARG:HA	2.20	0.42
5:I:647:LYS:NZ	5:I:649:LYS:NZ	2.67	0.42
5:I:676:MET:HB2	5:I:702:THR:CG2	2.49	0.42
1:A:443:GLU:HA	1:A:446:ARG:HB2	2.01	0.42
1:A:461:TYR:C	1:A:462:CYS:N	2.72	0.42
1:A:482:LEU:HA	1:A:485:LEU:HB2	1.99	0.42
1:A:489:CYS:HA	1:A:539:ASN:HD22	1.84	0.42
1:A:916:TYR:N	1:A:917:PRO:CD	2.82	0.42
1:A:1013:ILE:HD11	1:A:1021:ILE:HD12	2.01	0.42
1:A:1244:ARG:HA	1:A:1247:ILE:HD12	2.01	0.42
1:A:1607:GLN:HA	1:A:1610:ILE:HD12	2.01	0.42
1:A:1943:LEU:HB3	1:A:2076:LEU:HD22	2.01	0.42
1:A:2349:ASN:O	1:A:2353:LEU:N	2.52	0.42
1:C:124:GLN:OE1	1:C:124:GLN:HA	2.17	0.42
1:C:521:LEU:HD23	1:C:537:TYR:HD1	1.84	0.42
1:C:990:ILE:HD11	1:C:1208:TYR:HE2	1.84	0.42
5:I:676:MET:HB3	5:I:688:TYR:HB2	2.00	0.42
1:A:212:PHE:O	1:A:216:THR:HG22	2.19	0.42
1:A:673:GLN:HB3	1:A:719:LEU:HB3	2.01	0.42
1:A:730:MET:HA	1:A:731:PRO:HD2	1.75	0.42
1:A:824:LEU:HA	1:A:827:LEU:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:944:ILE:O	1:A:947:ILE:HB	2.19	0.42
1:A:1117:MET:HG2	1:A:1121:ILE:HG13	2.01	0.42
1:A:1525:VAL:O	1:A:1528:LEU:HD23	2.19	0.42
1:A:1567:LYS:O	1:A:1570:THR:N	2.52	0.42
2:B:40:ILE:CG2	2:B:44:LYS:HA	2.49	0.42
1:C:333:ARG:HH11	1:C:354:THR:HB	1.84	0.42
1:C:377:ALA:O	1:C:382:ALA:HB3	2.20	0.42
1:C:458:LYS:HE3	1:C:461:PHE:CD2	2.54	0.42
1:C:688:GLU:C	1:C:690:PHE:N	2.72	0.42
1:C:1430:GLU:O	1:C:1436:LEU:HD11	2.20	0.42
1:C:1681:MET:HA	1:C:1684:ASP:HB3	2.00	0.42
1:C:1766:ASN:O	1:C:1769:VAL:HB	2.19	0.42
1:C:2116:LYS:HZ3	1:C:2120:GLY:N	2.17	0.42
5:I:736:PRO:HA	5:I:755:PHE:CE1	2.54	0.42
1:A:583:HIS:HB3	1:A:584:HIS:H	1.61	0.42
1:A:865:VAL:HG22	1:A:1535:SER:HB3	2.01	0.42
1:A:1242:ILE:HD12	1:A:1272:ALA:HB1	2.02	0.42
1:A:1586:ILE:HA	1:A:1587:ASP:N	2.34	0.42
1:A:1981:ASN:HB3	1:A:1984:LYS:HB3	2.01	0.42
1:C:1452:ALA:HA	1:C:1455:LYS:HE2	2.00	0.42
1:C:2225:VAL:HG22	1:C:2461:GLU:HB2	2.02	0.42
2:D:222:LEU:HB3	2:D:234:TRP:HB2	2.01	0.42
5:I:668:ASP:HA	5:I:669:LYS:HA	1.93	0.42
1:A:928:LEU:HD21	1:A:942:GLN:CB	2.48	0.42
1:A:1287:LEU:HA	1:A:1290:SER:OG	2.20	0.42
1:A:1435:ARG:O	1:A:1439:ALA:N	2.52	0.42
1:A:2299:ASP:O	1:A:2301:PHE:N	2.53	0.42
1:A:2331:ILE:HA	1:A:2334:SER:HB2	2.02	0.42
2:B:246:LEU:HG	2:B:277:TRP:CZ3	2.55	0.42
1:C:247:LYS:O	1:C:251:ASP:N	2.53	0.42
1:C:654:ALA:HA	1:C:657:ARG:HB2	2.02	0.42
1:C:827:GLN:H	1:C:830:ALA:CB	2.32	0.42
1:C:1161:PRO:HB2	1:C:1162:VAL:N	2.34	0.42
1:C:1610:VAL:C	1:C:1611:ARG:O	2.58	0.42
1:C:1674:LEU:HD11	1:C:1721:LYS:HG3	2.02	0.42
1:C:1980:GLY:HA2	5:J:648:LYS:NZ	2.34	0.42
1:C:2062:GLU:CD	1:C:2064:GLN:HG2	2.39	0.42
2:D:213:ILE:HD12	2:D:222:LEU:HD11	2.02	0.42
4:H:100:ARG:O	4:H:101:PHE:HA	2.19	0.42
5:J:782:LYS:HA	5:J:785:ASN:O	2.20	0.42
1:A:235:GLU:CD	1:A:275:LYS:HB2	2.39	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:PHE:CZ	1:A:345:LYS:HE3	2.54	0.42
1:A:556:MET:HA	1:A:590:GLU:CD	2.40	0.42
1:A:577:LYS:HE3	1:A:618:LEU:HD13	2.02	0.42
1:A:1490:LYS:O	1:A:1496:LYS:HB3	2.20	0.42
1:A:1617:ARG:HD2	1:A:1624:LEU:HD21	2.02	0.42
1:A:1666:ASP:HA	1:A:1669:LEU:HB2	2.01	0.42
1:A:2114:LYS:HA	1:A:2120:ASP:HA	2.01	0.42
1:A:2151:ASP:C	1:A:2155:PHE:HB2	2.40	0.42
1:C:146:LYS:HD2	1:C:190:ARG:HG3	2.01	0.42
1:C:189:MET:HG3	1:C:237:TYR:HB3	2.02	0.42
1:C:213:PHE:CE1	1:C:217:THR:HB	2.55	0.42
1:C:268:ILE:HG21	1:C:311:GLN:HG3	2.00	0.42
1:C:801:LEU:O	1:C:805:ILE:N	2.52	0.42
1:C:917:TYR:N	1:C:918:PRO:HD2	2.35	0.42
5:I:655:SER:HA	5:I:659:LEU:HB3	1.99	0.42
5:I:699:LYS:HG2	5:I:755:PHE:HA	2.01	0.42
5:J:710:ALA:HB1	5:J:718:LYS:CG	2.43	0.42
1:A:259:TYR:HB2	1:A:290:LEU:HD11	2.01	0.42
1:A:300:LEU:HD13	1:A:303:GLN:CB	2.49	0.42
1:A:807:THR:HA	1:A:1578:ARG:NE	2.35	0.42
1:A:969:VAL:HG22	1:A:1003:ILE:HD11	2.00	0.42
1:A:2094:LYS:HD2	1:A:2095:PHE:CZ	2.55	0.42
1:C:398:ARG:O	1:C:401:LYS:HB2	2.19	0.42
1:C:500:LEU:O	1:C:503:LEU:HB2	2.20	0.42
1:C:955:ARG:HH11	1:C:959:PHE:HE2	1.67	0.42
1:C:1098:LEU:N	1:C:1101:ILE:HD12	2.35	0.42
1:C:1952:VAL:O	1:C:1956:LEU:N	2.53	0.42
1:C:2045:TYR:HB3	1:C:2049:ARG:NH1	2.16	0.42
1:C:2362:PHE:N	1:C:2362:PHE:CD1	2.86	0.42
1:A:759:ILE:HG21	1:A:798:LYS:C	2.40	0.42
1:A:930:ASP:HA	1:A:931:PRO:HD3	1.92	0.42
1:A:946:HIS:C	1:A:947:ILE:N	2.73	0.42
1:A:1006:VAL:O	1:A:1007:ILE:N	2.53	0.42
1:A:1580:LEU:HB3	1:A:1584:LYS:HZ1	1.85	0.42
1:A:2304:ALA:C	1:A:2306:LEU:H	2.22	0.42
2:B:84:GLN:OE1	2:B:89:TRP:HB2	2.20	0.42
1:C:146:LYS:HD3	1:C:187:GLU:HG2	2.01	0.42
1:C:781:LYS:O	1:C:785:GLU:N	2.50	0.42
1:C:1504:ILE:HD13	1:C:1596:ARG:CZ	2.50	0.42
1:C:1925:LEU:N	1:C:1928:GLN:HG2	2.34	0.42
1:C:2303:PHE:HB3	1:C:2377:LYS:HG3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2317:PRO:HB2	1:C:2318:PHE:CD2	2.55	0.42
2:D:239:ASP:C	2:D:241:LYS:N	2.73	0.42
1:A:248:LEU:O	1:A:251:ASN:HB3	2.20	0.42
1:A:415:ILE:HG12	1:A:438:LEU:HD13	2.02	0.42
1:A:486:MET:HG3	1:A:494:HIS:HB2	2.02	0.42
1:A:661:GLN:HE21	1:A:672:ALA:HB1	1.84	0.42
1:A:1600:ILE:HG13	1:A:1601:LYS:N	2.33	0.42
1:A:1732:ARG:O	1:A:1734:SER:HB2	2.20	0.42
1:A:1754:TYR:HD1	1:A:1826:PHE:CZ	2.38	0.42
1:A:2334:SER:HB3	1:A:2335:PHE:HA	2.02	0.42
1:A:2398:ALA:HB1	1:A:2399:ILE:HG13	2.02	0.42
1:A:2405:GLN:C	1:A:2407:VAL:H	2.22	0.42
1:A:2436:ILE:HG13	1:A:2438:ARG:N	2.35	0.42
2:B:91:VAL:HA	2:B:101:VAL:HA	2.01	0.42
1:C:136:GLU:HA	1:C:179:VAL:HA	2.01	0.42
1:C:661:LEU:C	1:C:664:LEU:HB3	2.39	0.42
1:C:2203:ASN:O	1:C:2207:TRP:N	2.48	0.42
2:D:7:SER:HB2	2:D:38:LEU:HB2	2.02	0.42
2:D:14:ILE:HD12	2:D:16:PHE:HE2	1.85	0.42
2:D:173:MET:HB3	2:D:174:LEU:HA	2.02	0.42
5:I:698:ARG:HA	5:I:759:ASP:CA	2.50	0.42
5:I:698:ARG:O	5:I:701:SER:N	2.53	0.42
5:J:725:GLU:HG3	5:J:726:ASP:N	2.35	0.42
1:A:212:PHE:CE1	1:A:238:ARG:HA	2.53	0.41
1:A:577:LYS:HZ3	1:A:615:SER:HA	1.85	0.41
1:A:660:LEU:HA	1:A:663:LEU:HB3	2.01	0.41
1:A:843:GLU:C	1:A:845:LEU:H	2.23	0.41
1:A:1954:LEU:O	1:A:1958:ALA:N	2.53	0.41
1:A:1962:HIS:HE2	1:A:2006:ILE:HA	1.85	0.41
1:A:2140:LEU:HD21	1:A:2360:PHE:CE2	2.55	0.41
1:A:2232:ASN:OD1	1:A:2233:THR:N	2.53	0.41
1:A:2436:ILE:HD11	1:A:2438:ARG:HB2	2.02	0.41
2:B:267:THR:HB	2:B:277:TRP:HE1	1.84	0.41
1:C:236:GLU:OE2	1:C:271:PRO:HB3	2.19	0.41
1:C:315:HIS:CD2	1:C:320:ASN:ND2	2.83	0.41
1:C:315:HIS:NE2	1:C:320:ASN:OD1	2.53	0.41
1:C:333:ARG:HG2	1:C:373:LEU:HD13	2.02	0.41
1:C:474:ALA:HA	1:C:477:LYS:NZ	2.35	0.41
1:C:836:VAL:HG22	1:C:845:LEU:HD12	2.02	0.41
1:C:1365:LYS:H	1:C:1368:THR:HG22	1.84	0.41
1:C:1435:LYS:HZ1	1:C:1436:LEU:HG	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1478:LEU:C	1:C:1479:GLU:N	2.73	0.41
1:C:1609:GLN:C	1:C:1611:ARG:O	2.59	0.41
1:C:2112:LYS:C	1:C:2113:PHE:N	2.73	0.41
1:C:2340:THR:HA	1:C:2343:ASN:ND2	2.35	0.41
2:D:26:ARG:HD2	2:D:63:THR:HA	2.02	0.41
2:D:191:HIS:CG	2:D:192:THR:H	2.38	0.41
1:A:335:LEU:HD22	1:A:341:TYR:HB2	2.02	0.41
1:A:350:TYR:OH	1:A:385:LYS:HA	2.19	0.41
1:A:493:ASP:HA	1:A:496:GLN:HG2	2.02	0.41
1:A:675:ASP:O	1:A:679:LEU:N	2.53	0.41
1:A:709:TYR:HA	1:A:713:SER:HB2	2.02	0.41
1:A:742:CYS:HB2	1:A:743:THR:HG1	1.85	0.41
1:A:1060:VAL:O	1:A:1063:ARG:HB2	2.21	0.41
1:A:1351:LEU:HD23	1:A:1373:ILE:HD12	2.02	0.41
1:A:1408:ARG:CZ	1:A:1408:ARG:HB2	2.50	0.41
1:A:1763:ALA:O	1:A:1767:VAL:HG13	2.19	0.41
1:A:2107:ARG:N	1:A:2108:PRO:HD3	2.35	0.41
2:B:183:CYS:SG	2:B:205:ALA:HB2	2.60	0.41
1:C:1061:VAL:HA	1:C:1064:ARG:HB2	2.02	0.41
1:C:1274:ARG:HB2	1:C:1327:HIS:CE1	2.50	0.41
1:C:1281:PHE:CD2	1:C:1332:LEU:HD22	2.56	0.41
1:C:1408:LEU:HD21	1:C:1438:SER:HB3	2.01	0.41
1:C:2307:ILE:HB	1:C:2377:LYS:HD3	2.01	0.41
1:C:2317:PRO:HB3	1:C:2453:LEU:HD22	2.01	0.41
2:D:91:VAL:HG23	2:D:101:VAL:HB	2.01	0.41
2:D:174:LEU:HB3	2:D:175:ALA:H	1.75	0.41
5:J:741:LEU:HB3	5:J:742:LYS:H	1.66	0.41
1:A:281:ASP:CA	1:A:284:VAL:HB	2.35	0.41
1:A:506:ILE:N	1:A:507:PRO:HD2	2.35	0.41
1:A:547:ALA:HA	1:A:550:SER:OG	2.19	0.41
1:A:567:THR:HA	1:A:571:ILE:HG13	2.02	0.41
1:A:769:ASP:HA	1:A:809:GLN:HB2	2.02	0.41
1:A:804:ILE:HG22	1:A:805:ILE:HD13	2.01	0.41
1:A:923:ASN:HD22	1:A:923:ASN:N	2.18	0.41
1:A:1384:ILE:HA	1:A:1385:GLY:HA2	1.74	0.41
1:A:1824:LYS:O	1:A:1827:PHE:HB3	2.20	0.41
1:A:1881:ILE:HG21	1:A:1913:PRO:O	2.20	0.41
1:A:2247:ARG:O	1:A:2248:SER:HB3	2.20	0.41
1:A:2407:VAL:HA	1:A:2411:HIS:HB2	2.01	0.41
1:C:136:GLU:HA	1:C:179:VAL:HG12	2.01	0.41
1:C:153:VAL:HB	1:C:176:TYR:HE2	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:VAL:HG22	1:C:335:LEU:HD13	2.02	0.41
1:C:929:LEU:HD21	1:C:943:GLN:HB2	2.02	0.41
1:C:998:ARG:HG2	1:C:1038:ARG:HG2	2.02	0.41
1:C:1589:ASP:HA	1:C:1591:TRP:CE2	2.55	0.41
1:C:1846:LEU:O	1:C:1847:LEU:HA	2.21	0.41
1:C:1984:THR:O	1:C:1986:LYS:N	2.53	0.41
1:C:2206:HIS:NE2	1:C:2472:PRO:HD2	2.35	0.41
1:C:2274:ILE:HD13	1:C:2274:ILE:HA	1.98	0.41
1:C:2459:SER:HA	1:C:2460:VAL:HA	1.47	0.41
2:D:132:ILE:HG21	2:D:174:LEU:HD11	2.00	0.41
1:A:175:TYR:HD1	1:A:190:LEU:HD13	1.85	0.41
1:A:196:GLY:HA2	1:A:198:LEU:HD12	2.01	0.41
1:A:800:LEU:HB3	1:A:804:ILE:HD12	2.02	0.41
1:A:1593:LEU:HD23	1:A:1596:ARG:HH21	1.85	0.41
1:A:2267:SER:HB3	1:A:2316:PHE:CE2	2.54	0.41
1:C:180:LEU:HD21	1:C:192:ALA:HB2	2.01	0.41
1:C:219:ILE:O	1:C:219:ILE:CG2	2.68	0.41
1:C:257:LEU:HD21	1:C:294:ILE:HG21	2.03	0.41
1:C:798:LEU:O	1:C:801:LEU:HB2	2.21	0.41
1:C:849:LEU:HD21	1:C:1546:VAL:CG2	2.51	0.41
1:C:1033:GLU:OE1	1:C:1075:ASN:ND2	2.53	0.41
1:C:1455:LYS:HE3	1:C:1467:MET:CE	2.49	0.41
1:C:1569:LYS:O	1:C:1573:MET:N	2.44	0.41
1:C:1766:ASN:O	1:C:1767:PHE:N	2.53	0.41
1:C:2174:LYS:O	1:C:2175:SER:HB2	2.20	0.41
1:A:271:LEU:O	1:A:272:ARG:HB2	2.21	0.41
1:A:332:ARG:HA	1:A:372:LEU:HD13	2.02	0.41
1:A:928:LEU:HD21	1:A:942:GLN:HB3	2.02	0.41
1:A:1629:LEU:O	1:A:1630:ASN:N	2.53	0.41
1:C:631:VAL:HA	1:C:634:LEU:HD12	2.01	0.41
1:C:854:LYS:HG3	1:C:1584:CYS:HB2	2.02	0.41
1:C:1113:ILE:N	1:C:1150:LEU:HD22	2.36	0.41
1:C:1817:ILE:O	1:C:1821:VAL:HG23	2.21	0.41
1:C:2157:PHE:CD1	1:C:2160:HIS:CG	3.09	0.41
2:D:84:GLN:HB3	2:D:89:TRP:CB	2.32	0.41
3:F:107:UNK:C	3:F:108:UNK:HA	2.50	0.41
1:A:87:ILE:HG23	1:A:99:ARG:HE	1.86	0.41
1:A:971:ARG:HH22	1:A:984:GLN:HG3	1.84	0.41
1:A:1626:LYS:HB2	1:A:1629:LEU:HG	2.01	0.41
1:A:2419:ARG:HA	1:A:2422:LEU:HB3	2.02	0.41
2:B:166:SER:HG	2:B:215:LEU:N	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:MET:HB2	2:B:215:LEU:HD11	2.01	0.41
1:C:1249:GLN:NE2	1:C:1275:GLU:HG2	2.36	0.41
1:C:1430:GLU:CB	1:C:1431:VAL:N	2.81	0.41
1:C:1857:PRO:C	1:C:1859:ALA:H	2.24	0.41
1:C:1909:PRO:HA	1:C:1912:LEU:N	2.35	0.41
1:C:2113:PHE:N	1:C:2125:TYR:O	2.53	0.41
2:D:189:PRO:HG2	2:D:196:HIS:H	1.86	0.41
3:F:711:UNK:O	3:F:713:UNK:N	2.53	0.41
5:I:703:ILE:HA	5:I:706:VAL:HG23	2.01	0.41
5:I:719:LYS:HA	5:I:720:PRO:HA	1.91	0.41
5:J:705:GLU:O	5:J:709:PHE:N	2.53	0.41
1:A:88:PHE:HZ	1:A:151:ALA:HB2	1.85	0.41
1:A:305:PHE:O	1:A:309:PHE:HB2	2.20	0.41
1:A:854:THR:HG22	1:A:855:GLU:N	2.35	0.41
1:A:1280:PHE:CZ	1:A:1330:LEU:HD13	2.55	0.41
1:A:1386:ILE:HA	1:A:1389:HIS:HB3	2.02	0.41
1:A:2219:LEU:O	1:A:2223:VAL:HG23	2.20	0.41
2:B:17:TRP:CE2	2:B:288:TYR:HB3	2.56	0.41
1:C:131:ASN:HB3	1:C:135:PHE:CE2	2.55	0.41
1:C:153:VAL:HG11	1:C:172:ARG:HG3	2.03	0.41
1:C:653:VAL:CG2	3:E:100:UNK:HA	2.51	0.41
1:C:766:PRO:HD3	1:C:806:ILE:HG22	2.03	0.41
1:C:1720:LEU:O	1:C:1724:GLU:HB3	2.21	0.41
1:C:2080:VAL:HG13	1:C:2091:ILE:HA	2.01	0.41
1:A:291:THR:HG22	1:A:296:ARG:HB3	2.03	0.41
1:A:472:PRO:HG2	1:A:476:LYS:HB3	2.03	0.41
1:A:687:GLU:O	1:A:689:PHE:N	2.53	0.41
1:A:784:GLU:O	1:A:788:VAL:HG22	2.21	0.41
1:A:792:GLU:HG3	1:A:794:THR:OG1	2.21	0.41
1:A:812:SER:HB2	1:A:851:ILE:HG13	2.02	0.41
1:A:1222:ILE:HG12	1:A:1285:VAL:HG11	2.03	0.41
1:A:1824:LYS:HD2	1:A:1861:MET:HB2	2.01	0.41
1:A:1870:ILE:O	1:A:1872:THR:N	2.54	0.41
1:C:437:LEU:HA	1:C:440:ASP:CB	2.44	0.41
1:C:783:LEU:N	1:C:784:GLY:HA3	2.28	0.41
1:C:862:ARG:HH22	1:C:1542:TYR:HB3	1.85	0.41
1:C:1360:PHE:HB3	1:C:1372:LEU:HD22	2.03	0.41
1:C:1431:VAL:HG22	1:C:1463:VAL:HG13	2.03	0.41
1:C:1512:PHE:O	1:C:1515:ALA:N	2.53	0.41
1:C:1541:ALA:CB	1:C:1542:TYR:CA	2.97	0.41
1:C:1576:THR:O	1:C:1580:ARG:N	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1615:ALA:O	1:C:1619:ARG:N	2.53	0.41
1:C:1714:LEU:HD21	1:C:1751:PHE:O	2.20	0.41
1:C:2187:PHE:HE1	1:C:2324:LEU:HD13	1.85	0.41
1:C:2242:LYS:O	1:C:2243:VAL:N	2.53	0.41
1:C:2414:LYS:HA	1:C:2417:ILE:HG13	2.03	0.41
3:F:704:UNK:O	3:F:707:UNK:N	2.54	0.41
1:A:205:LEU:HA	1:A:209:PHE:HB3	2.03	0.41
1:A:260:VAL:HG22	1:A:303:GLN:HG2	2.03	0.41
1:A:417:VAL:HB	1:A:418:SER:N	2.36	0.41
1:A:422:ILE:HG12	1:A:466:LEU:HD13	2.03	0.41
1:A:422:ILE:CG1	1:A:466:LEU:HD13	2.50	0.41
1:A:817:ARG:HD2	1:A:867:LEU:HD13	2.02	0.41
1:A:979:ASP:HA	1:A:982:PHE:CD2	2.56	0.41
1:A:1366:THR:HA	1:A:1369:ALA:HB3	2.02	0.41
1:A:1499:TYR:H	1:A:1594:ARG:HH21	1.68	0.41
1:A:1630:ASN:O	1:A:1633:LEU:HB2	2.21	0.41
1:A:1669:LEU:O	1:A:1672:LEU:HB3	2.20	0.41
1:A:1715:ARG:HH21	1:A:1719:LYS:HE3	1.85	0.41
1:A:1910:LEU:HB3	1:A:1912:TYR:H	1.85	0.41
1:A:1997:LYS:H	1:A:1998:ARG:N	2.19	0.41
1:A:2124:VAL:HG12	1:A:2178:TRP:CE3	2.54	0.41
1:A:2285:LEU:HB2	1:A:2286:ASP:H	1.78	0.41
1:A:2404:VAL:HB	1:A:2408:GLU:HB2	2.03	0.41
1:A:2424:LEU:C	1:A:2427:ILE:H	2.23	0.41
1:A:2431:LEU:HA	1:A:2447:GLN:CG	2.51	0.41
2:B:55:VAL:HG13	2:B:57:LEU:HG	2.03	0.41
2:B:232:ARG:HA	2:B:244:THR:HB	2.02	0.41
1:C:114:LEU:N	1:C:118:VAL:HG22	2.35	0.41
1:C:143:SER:HA	1:C:146:LYS:HE3	2.02	0.41
1:C:217:THR:O	1:C:221:TRP:CG	2.74	0.41
1:C:234:LYS:NZ	1:C:238:ARG:HE	2.18	0.41
1:C:330:LEU:O	1:C:334:GLU:HB2	2.20	0.41
1:C:362:PHE:CD2	1:C:362:PHE:C	2.94	0.41
1:C:378:ALA:CA	1:C:379:PHE:N	2.80	0.41
1:C:613:ALA:HB1	1:C:643:LYS:NZ	2.36	0.41
1:C:683:MET:O	1:C:686:ASN:HB2	2.21	0.41
1:C:721:GLU:HG3	1:C:722:LEU:HD12	2.03	0.41
1:C:801:LEU:O	1:C:802:MET:N	2.53	0.41
1:C:824:THR:C	1:C:826:GLY:H	2.24	0.41
1:C:1053:ASN:HD21	1:C:1061:VAL:HG21	1.85	0.41
1:C:1066:LEU:HD11	1:C:1103:ILE:HG13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1088:VAL:HG22	1:C:1103:ILE:CG2	2.50	0.41
1:C:1281:PHE:CE1	1:C:1332:LEU:HD13	2.56	0.41
1:C:1421:LYS:HB2	1:C:1435:LYS:HB2	2.01	0.41
1:C:1655:TYR:O	1:C:1659:LYS:N	2.53	0.41
1:C:1726:ARG:HG3	1:C:1727:VAL:H	1.84	0.41
1:C:2134:ARG:HB3	1:C:2368:ILE:HB	2.02	0.41
1:C:2185:ASP:O	1:C:2286:MET:HG3	2.21	0.41
1:C:2258:ARG:HD2	1:C:2329:GLU:HB2	2.03	0.41
2:D:9:GLY:HA2	2:D:296:VAL:HG23	2.03	0.41
2:D:141:ARG:HG2	2:D:153:GLN:HB3	2.02	0.41
1:A:543:SER:O	1:A:544:ILE:HG13	2.21	0.41
1:A:759:ILE:HG13	1:A:760:LEU:N	2.36	0.41
1:A:1049:ILE:HD13	1:A:1049:ILE:N	2.36	0.41
1:A:1756:ALA:O	1:A:1759:ASN:HB2	2.21	0.41
1:C:280:ARG:NH2	1:C:328:THR:HB	2.34	0.41
1:C:500:LEU:HA	1:C:503:LEU:HD12	2.04	0.41
1:C:576:CYS:HB3	1:C:580:LEU:HD22	2.03	0.41
1:C:678:LEU:HB2	1:C:727:LYS:HD2	2.03	0.41
1:C:859:PRO:HG3	1:C:1543:ASN:CG	2.42	0.41
1:C:963:ILE:HG13	1:C:964:ILE:H	1.85	0.41
1:C:968:ILE:HA	1:C:971:MET:HB3	2.01	0.41
1:C:994:LYS:HA	1:C:995:GLN:CB	2.51	0.41
1:C:1093:TYR:O	1:C:1100:LYS:HD3	2.21	0.41
1:C:1967:TRP:CD1	1:C:1994:LEU:O	2.74	0.41
1:C:2068:PRO:HB3	1:C:2071:LEU:HD13	2.02	0.41
1:C:2089:LYS:N	1:C:2090:PRO:CD	2.84	0.41
5:J:757:LYS:HB2	5:J:784:GLN:HG2	2.02	0.41
1:A:180:ILE:H	1:A:180:ILE:HG12	1.78	0.40
1:A:1173:HIS:CD2	1:A:1178:GLN:HB2	2.56	0.40
1:A:1523:LEU:HD12	1:A:1524:LEU:HG	2.03	0.40
1:A:1985:MET:HA	1:A:1988:ALA:HB2	2.02	0.40
1:A:2251:THR:CG2	1:A:2255:ARG:HD2	2.51	0.40
2:B:213:ILE:HB	2:B:214:LEU:CA	2.51	0.40
1:C:1991:LEU:HA	1:C:1994:LEU:HG	2.03	0.40
1:C:2470:TRP:CD1	1:C:2472:PRO:HD3	2.56	0.40
1:A:661:GLN:HG2	1:A:672:ALA:HB1	2.03	0.40
1:A:986:GLY:N	1:A:1019:THR:HG1	2.19	0.40
1:A:1580:LEU:HB3	1:A:1584:LYS:NZ	2.36	0.40
1:A:1764:ASN:C	1:A:1767:VAL:HG22	2.41	0.40
1:A:2431:LEU:HA	1:A:2447:GLN:HG2	2.03	0.40
2:B:25:SER:OG	2:B:60:ILE:HD11	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:ILE:HD12	2:B:301:ASN:HB2	2.03	0.40
2:B:194:ALA:HB1	2:B:196:HIS:NE2	2.36	0.40
1:C:97:PRO:C	1:C:99:GLU:H	2.24	0.40
1:C:857:ASN:HB3	1:C:1586:LYS:N	2.37	0.40
1:C:861:ILE:HG22	1:C:864:GLY:N	2.36	0.40
1:C:976:PRO:HA	1:C:979:LEU:HB2	2.03	0.40
1:C:981:PHE:C	1:C:985:GLN:HG2	2.42	0.40
1:C:2000:ARG:HG3	1:C:2003:GLU:OE1	2.21	0.40
1:C:2108:GLN:HE22	1:C:2130:HIS:HB2	1.86	0.40
1:A:120:GLU:HG3	1:A:159:TYR:CZ	2.56	0.40
1:A:172:LEU:HD21	1:A:208:ASP:OD1	2.21	0.40
1:A:1151:LEU:HD11	1:A:1184:LEU:HD21	2.03	0.40
1:A:2077:ALA:HB2	1:A:2091:LYS:C	2.42	0.40
1:A:2095:PHE:CD2	1:A:2113:ILE:HG12	2.56	0.40
1:A:2140:LEU:HA	1:A:2143:LEU:HB2	2.04	0.40
1:A:2202:ILE:HA	1:A:2205:TRP:HB3	2.03	0.40
1:A:2398:ALA:HA	1:A:2399:ILE:HA	1.82	0.40
1:C:194:ASN:H	1:C:195:THR:N	2.19	0.40
1:C:277:LEU:HD11	1:C:324:SER:HB2	2.02	0.40
1:C:389:LEU:C	1:C:391:ARG:H	2.24	0.40
1:C:439:LEU:O	1:C:443:ARG:HG2	2.20	0.40
1:C:446:LEU:HG	1:C:450:PHE:CE2	2.56	0.40
1:C:546:GLU:HA	1:C:549:ARG:CB	2.52	0.40
1:C:763:VAL:HG21	1:C:803:PRO:HB3	2.02	0.40
1:C:983:PHE:CB	1:C:1022:ILE:HG12	2.23	0.40
1:C:1452:ALA:HA	1:C:1455:LYS:HB3	2.03	0.40
1:C:1723:GLY:HA2	1:C:1726:ARG:HD3	2.03	0.40
3:F:251:UNK:HA	3:F:254:UNK:CB	2.51	0.40
3:F:262:UNK:O	3:F:265:UNK:N	2.53	0.40
5:I:654:ASN:O	5:I:659:LEU:HB2	2.20	0.40
1:A:277:ILE:H	1:A:277:ILE:HG13	1.78	0.40
1:A:416:LEU:HD12	1:A:459:LEU:HD21	2.03	0.40
1:A:654:GLU:O	1:A:658:GLU:N	2.54	0.40
1:A:670:GLN:HE22	1:A:716:LYS:HB2	1.86	0.40
1:A:1024:ILE:O	1:A:1024:ILE:HG22	2.22	0.40
1:A:1033:GLY:HA2	1:A:1034:GLU:HA	1.77	0.40
1:A:1440:LEU:CD2	1:A:1622:MET:HG2	2.47	0.40
1:A:1558:TYR:C	1:A:1572:ARG:HH21	2.25	0.40
1:A:2131:ILE:HD13	1:A:2174:GLY:HA3	2.03	0.40
1:A:2450:LYS:HD3	1:A:2450:LYS:HA	1.89	0.40
1:C:86:ASN:HD21	1:C:124:GLN:HB3	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:ARG:HA	1:C:369:VAL:CB	2.51	0.40
1:C:602:GLU:HA	1:C:603:HIS:O	2.22	0.40
1:C:726:LEU:HD13	1:C:761:LEU:HD23	2.03	0.40
1:C:1151:GLN:HB3	1:C:1152:LEU:H	1.61	0.40
1:C:1226:ASN:HD22	1:C:1286:VAL:HG13	1.86	0.40
1:C:1259:LEU:HD23	1:C:1259:LEU:HA	1.93	0.40
1:C:1541:ALA:HB3	1:C:1542:TYR:HA	2.04	0.40
1:C:2005:LEU:O	1:C:2065:HIS:HA	2.22	0.40
1:C:2432:LYS:HA	1:C:2444:LEU:HD12	2.02	0.40
3:E:500:UNK:CB	3:E:702:UNK:HA	2.51	0.40
3:F:803:UNK:C	3:F:805:UNK:N	2.85	0.40
5:J:730:VAL:HG21	5:J:790:PRO:N	2.36	0.40
1:A:138:HIS:HB3	1:A:145:LYS:HE2	2.03	0.40
1:A:431:SER:C	1:A:433:TYR:H	2.25	0.40
1:A:600:ILE:HA	1:A:602:HIS:HB2	2.03	0.40
1:A:699:ILE:HD12	1:A:717:THR:HG22	2.03	0.40
1:A:1164:LYS:CB	1:A:1170:ARG:HG3	2.52	0.40
1:A:1359:LEU:HA	1:A:1362:PRO:HD3	2.03	0.40
1:A:1910:LEU:C	1:A:1911:VAL:HG12	2.42	0.40
1:A:2458:VAL:HG13	1:A:2459:GLU:H	1.87	0.40
1:C:157:ILE:CG1	1:C:172:ARG:HH22	2.31	0.40
1:C:216:ARG:HD2	1:C:234:LYS:HZ3	1.86	0.40
1:C:309:LEU:HA	1:C:346:LYS:NZ	2.35	0.40
1:C:577:PHE:CG	1:C:592:PHE:HB2	2.57	0.40
1:C:818:ARG:HB2	1:C:818:ARG:NH1	2.37	0.40
1:C:1431:VAL:HG13	1:C:1466:ALA:CB	2.52	0.40
1:C:1682:ALA:HB2	1:C:1717:ARG:HH22	1.87	0.40
1:C:1742:LEU:O	1:C:1746:LEU:HD13	2.21	0.40
1:C:1762:TRP:CE3	1:C:1763:ALA:HA	2.56	0.40
1:C:1913:VAL:O	1:C:1917:MET:N	2.52	0.40
1:C:2023:GLU:HA	1:C:2026:MET:HG2	2.02	0.40
3:E:371:UNK:C	3:E:373:UNK:N	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1309/2474 (53%)	872 (67%)	313 (24%)	124 (10%)	0	10
1	C	1267/2474 (51%)	849 (67%)	290 (23%)	128 (10%)	0	9
2	B	178/303 (59%)	122 (68%)	45 (25%)	11 (6%)	1	17
2	D	173/303 (57%)	113 (65%)	44 (25%)	16 (9%)	1	11
4	G	75/426 (18%)	57 (76%)	12 (16%)	6 (8%)	1	12
4	H	80/426 (19%)	43 (54%)	22 (28%)	15 (19%)	0	2
5	I	95/1176 (8%)	52 (55%)	29 (30%)	14 (15%)	0	4
5	J	88/1176 (8%)	52 (59%)	23 (26%)	13 (15%)	0	3
All	All	3265/8758 (37%)	2160 (66%)	778 (24%)	327 (10%)	1	9

All (327) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	ASP
1	A	112	SER
1	A	224	THR
1	A	257	TYR
1	A	342	LEU
1	A	348	ASP
1	A	402	ILE
1	A	490	PRO
1	A	582	ILE
1	A	583	HIS
1	A	586	TYR
1	A	650	ASP
1	A	767	CYS
1	A	769	ASP
1	A	771	SER
1	A	791	LYS
1	A	854	THR
1	A	1083	MET
1	A	1135	GLU
1	A	1192	ASN
1	A	1342	GLN
1	A	1428	GLU
1	A	1447	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1477	GLU
1	A	1583	GLN
1	A	1732	ARG
1	A	1750	ASP
1	A	1753	TRP
1	A	1871	GLY
1	A	1977	PHE
1	A	1978	GLY
1	A	2089	ILE
1	A	2247	ARG
1	A	2248	SER
1	A	2288	ILE
1	A	2328	VAL
1	A	2334	SER
1	A	2391	ASN
1	A	2392	GLU
1	A	2426	ARG
1	A	2436	ILE
1	A	2440	ASN
1	A	2441	ASP
1	A	2442	LEU
1	A	2453	GLN
2	B	106	SER
2	B	107	PRO
2	B	213	ILE
1	C	167	PRO
1	C	233	SER
1	C	273	ARG
1	C	409	ASN
1	C	425	PHE
1	C	473	PRO
1	C	490	CYS
1	C	491	PRO
1	C	530	LYS
1	C	534	SER
1	C	673	ALA
1	C	838	PRO
1	C	861	ILE
1	C	1085	PRO
1	C	1152	LEU
1	C	1193	ASN
1	C	1286	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1287	GLU
1	C	1293	GLN
1	C	1585	GLN
1	C	1586	LYS
1	C	1588	ILE
1	C	1750	HIS
1	C	1857	PRO
1	C	1878	VAL
1	C	1985	GLU
1	C	1997	MET
1	C	2090	PRO
1	C	2241	TYR
1	C	2330	VAL
1	C	2355	LEU
1	C	2378	LYS
1	C	2394	GLU
2	D	5	LEU
2	D	33	SER
2	D	56	ARG
2	D	298	VAL
4	H	121	TYR
4	H	140	THR
4	H	141	ASN
5	I	687	LYS
5	I	764	ILE
5	J	692	SER
5	J	741	LEU
5	J	764	ILE
1	A	178	VAL
1	A	261	ASN
1	A	341	TYR
1	A	359	TYR
1	A	395	TYR
1	A	493	ASP
1	A	539	ASN
1	A	600	ILE
1	A	669	PRO
1	A	743	THR
1	A	751	VAL
1	A	838	LEU
1	A	1022	SER
1	A	1091	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1590	GLN
1	A	1628	VAL
1	A	1731	TRP
1	A	1733	LEU
1	A	1868	ILE
1	A	1942	VAL
1	A	1979	GLU
1	A	2298	GLY
1	A	2390	ALA
2	B	245	THR
2	B	296	VAL
1	C	97	PRO
1	C	177	LEU
1	C	184	SER
1	C	234	LYS
1	C	235	LEU
1	C	324	SER
1	C	338	LEU
1	C	416	ILE
1	C	601	ILE
1	C	603	HIS
1	C	656	ILE
1	C	748	SER
1	C	925	LEU
1	C	1176	VAL
1	C	1477	GLY
1	C	1519	ILE
1	C	1541	ALA
1	C	1602	ILE
1	C	1612	ILE
1	C	1873	GLY
1	C	1913	VAL
1	C	2087	GLY
1	C	2091	ILE
1	C	2146	VAL
1	C	2184	SER
1	C	2185	ASP
1	C	2279	ASP
1	C	2308	LEU
1	C	2332	GLY
2	D	6	VAL
4	G	66	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	G	77	THR
4	H	72	THR
4	H	77	THR
4	H	78	CYS
4	H	131	VAL
5	I	686	LYS
5	I	716	THR
5	J	653	THR
5	J	702	THR
5	J	730	VAL
5	J	747	ASP
5	J	755	PHE
5	J	790	PRO
1	A	304	TRP
1	A	377	ALA
1	A	450	LYS
1	A	555	PHE
1	A	568	ASP
1	A	602	HIS
1	A	766	LYS
1	A	778	ALA
1	A	1233	LYS
1	A	1523	LEU
1	A	1593	LEU
1	A	1736	PRO
1	A	1813	ASN
1	A	2083	ALA
1	A	2122	LYS
1	A	2326	MET
1	A	2382	GLY
1	A	2443	ASP
2	B	177	ALA
1	C	122	GLN
1	C	176	TYR
1	C	224	LEU
1	C	259	PRO
1	C	267	ASN
1	C	275	ALA
1	C	341	PRO
1	C	683	MET
1	C	712	VAL
1	C	772	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1013	PRO
1	C	1197	ASP
1	C	1839	SER
1	C	2063	LEU
1	C	2097	PHE
1	C	2116	LYS
1	C	2154	ALA
1	C	2302	CYS
1	C	2374	LEU
2	D	193	ASP
2	D	195	SER
2	D	238	ASP
4	G	131	VAL
4	H	112	PRO
4	H	120	ASP
4	H	177	GLY
4	H	183	ASP
5	I	663	SER
5	I	668	ASP
1	A	519	ASN
1	A	717	THR
1	A	720	GLU
1	A	1076	GLU
1	A	1248	GLN
1	A	1333	PRO
1	A	1539	ALA
1	A	1597	SER
1	A	1602	PRO
1	A	1711	LYS
1	A	1751	ASN
1	A	1870	ILE
1	A	2304	ALA
2	B	73	GLY
2	B	277	TRP
1	C	116	ARG
1	C	139	HIS
1	C	339	LYS
1	C	340	ALA
1	C	370	TYR
1	C	493	SER
1	C	592	PHE
1	C	1084	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1216	LYS
1	C	1733	TRP
1	C	2111	ARG
2	D	206	HIS
2	D	242	LEU
4	G	145	PRO
4	H	44	LEU
4	H	74	LYS
5	I	698	ARG
5	I	708	GLY
5	I	730	VAL
1	A	269	VAL
1	A	580	GLN
1	A	1584	LYS
1	A	1599	VAL
1	A	1820	ILE
1	A	2085	GLY
2	B	219	VAL
1	C	96	VAL
1	C	995	GLN
1	C	1510	ASN
1	C	1599	SER
1	C	1611	ARG
1	C	1848	THR
1	C	2083	THR
1	C	2110	PRO
1	C	2419	ASN
2	D	272	HIS
4	G	137	VAL
4	G	149	CYS
5	I	670	VAL
5	I	715	SER
5	I	736	PRO
5	J	736	PRO
1	A	122	PHE
1	A	842	PRO
1	A	994	GLN
1	A	1106	GLY
1	A	1205	LYS
1	A	1348	ALA
1	A	2470	PRO
2	B	183	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	143	SER
1	C	298	ASP
1	C	1248	ILE
1	C	1388	ILE
1	C	2379	ILE
2	D	22	GLY
2	D	91	VAL
2	D	277	TRP
4	H	145	PRO
5	J	699	LYS
1	A	1242	ILE
1	A	1890	ILE
1	A	1940	SER
1	A	2305	ILE
1	C	299	PRO
1	C	528	GLY
1	C	561	GLY
1	C	1019	ILE
1	C	1563	LEU
1	C	1601	VAL
1	C	2300	GLY
1	C	2312	PHE
1	C	2347	VAL
1	C	2469	GLY
2	D	219	VAL
4	H	130	GLY
5	I	749	GLU
1	A	707	PRO
1	A	1334	ILE
1	A	1458	LYS
1	A	2013	GLY
1	C	166	LEU
1	C	508	PRO
1	C	752	VAL
1	C	1630	VAL
1	C	2446	VAL
5	I	682	ILE
1	A	930	ASP
1	C	1364	PRO
1	C	1727	VAL
1	C	1942	SER
1	C	2115	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	23	VAL
1	A	1517	ILE
1	A	2265	VAL
2	B	65	PRO
1	C	1468	ALA
1	C	2082	GLY
1	C	2333	ILE
5	J	703	ILE
5	J	756	GLY
1	A	2310	PHE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2029/2219 (91%)	1734 (86%)	295 (14%)	3 15
1	C	2029/2219 (91%)	1722 (85%)	307 (15%)	3 14
2	B	264/267 (99%)	229 (87%)	35 (13%)	4 18
2	D	264/267 (99%)	230 (87%)	34 (13%)	4 18
5	I	137/1066 (13%)	113 (82%)	24 (18%)	2 11
5	J	137/1066 (13%)	108 (79%)	29 (21%)	1 6
All	All	4860/7104 (68%)	4136 (85%)	724 (15%)	6 15

All (724) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	88	PHE
1	A	89	ASP
1	A	90	LYS
1	A	92	LYS
1	A	93	SER
1	A	111	THR
1	A	112	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	115	ARG
1	A	120	GLU
1	A	121	GLN
1	A	124	ARG
1	A	128	SER
1	A	133	ILE
1	A	150	LEU
1	A	152	VAL
1	A	153	ASP
1	A	179	LEU
1	A	180	ILE
1	A	187	VAL
1	A	212	PHE
1	A	216	THR
1	A	222	THR
1	A	224	THR
1	A	228	ASN
1	A	229	SER
1	A	230	SER
1	A	234	LEU
1	A	238	ARG
1	A	243	LEU
1	A	244	ILE
1	A	245	ILE
1	A	252	SER
1	A	255	LEU
1	A	256	LEU
1	A	257	TYR
1	A	265	ASP
1	A	269	VAL
1	A	273	ASP
1	A	276	LEU
1	A	290	LEU
1	A	302	LYS
1	A	304	TRP
1	A	307	ARG
1	A	320	THR
1	A	324	VAL
1	A	329	LEU
1	A	330	VAL
1	A	334	LEU
1	A	338	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	341	TYR
1	A	342	LEU
1	A	343	ARG
1	A	354	MET
1	A	378	PHE
1	A	384	THR
1	A	386	LYS
1	A	388	LEU
1	A	395	TYR
1	A	401	ASN
1	A	402	ILE
1	A	409	ASN
1	A	419	ILE
1	A	421	ASP
1	A	422	ILE
1	A	431	SER
1	A	439	ASP
1	A	441	ILE
1	A	449	PHE
1	A	452	ARG
1	A	453	LYS
1	A	466	LEU
1	A	474	PHE
1	A	480	LYS
1	A	487	LEU
1	A	489	CYS
1	A	493	ASP
1	A	511	SER
1	A	520	LEU
1	A	534	ASN
1	A	549	LYS
1	A	554	SER
1	A	562	SER
1	A	583	HIS
1	A	592	VAL
1	A	616	CYS
1	A	622	ASP
1	A	623	ASP
1	A	630	VAL
1	A	633	LEU
1	A	636	VAL
1	A	660	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	662	HIS
1	A	670	GLN
1	A	677	LEU
1	A	680	LEU
1	A	685	ASN
1	A	698	ILE
1	A	699	ILE
1	A	701	ARG
1	A	703	SER
1	A	709	TYR
1	A	719	LEU
1	A	723	THR
1	A	725	LEU
1	A	739	THR
1	A	743	THR
1	A	751	VAL
1	A	759	ILE
1	A	760	LEU
1	A	761	ASP
1	A	772	SER
1	A	777	THR
1	A	779	LEU
1	A	793	MET
1	A	805	ILE
1	A	817	ARG
1	A	824	LEU
1	A	848	LEU
1	A	849	ILE
1	A	860	ILE
1	A	921	ILE
1	A	927	ILE
1	A	944	ILE
1	A	951	LEU
1	A	954	ARG
1	A	957	SER
1	A	958	PHE
1	A	962	ILE
1	A	968	LEU
1	A	970	MET
1	A	982	PHE
1	A	985	LEU
1	A	997	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1003	ILE
1	A	1013	ILE
1	A	1015	LYS
1	A	1019	THR
1	A	1020	ILE
1	A	1027	ILE
1	A	1043	LEU
1	A	1050	LEU
1	A	1054	GLN
1	A	1067	SER
1	A	1068	LEU
1	A	1069	VAL
1	A	1083	MET
1	A	1086	VAL
1	A	1087	VAL
1	A	1090	THR
1	A	1102	ILE
1	A	1107	ARG
1	A	1111	ASN
1	A	1116	GLU
1	A	1117	MET
1	A	1127	ARG
1	A	1137	THR
1	A	1140	THR
1	A	1144	LEU
1	A	1153	THR
1	A	1170	ARG
1	A	1173	HIS
1	A	1175	VAL
1	A	1178	GLN
1	A	1182	LYS
1	A	1201	VAL
1	A	1207	TYR
1	A	1209	ASP
1	A	1212	GLN
1	A	1214	THR
1	A	1228	TYR
1	A	1229	CYS
1	A	1230	SER
1	A	1236	GLU
1	A	1243	ARG
1	A	1249	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1267	VAL
1	A	1287	LEU
1	A	1290	SER
1	A	1326	ASP
1	A	1332	ILE
1	A	1353	TYR
1	A	1354	LYS
1	A	1357	GLU
1	A	1366	THR
1	A	1370	LEU
1	A	1379	GLN
1	A	1380	THR
1	A	1384	ILE
1	A	1402	TRP
1	A	1404	GLU
1	A	1408	ARG
1	A	1425	ASP
1	A	1426	SER
1	A	1430	MET
1	A	1433	LYS
1	A	1434	LEU
1	A	1476	LEU
1	A	1477	GLU
1	A	1480	ASP
1	A	1491	SER
1	A	1493	SER
1	A	1504	CYS
1	A	1515	VAL
1	A	1523	LEU
1	A	1524	LEU
1	A	1527	GLU
1	A	1534	GLU
1	A	1557	LYS
1	A	1569	LEU
1	A	1570	THR
1	A	1585	ASN
1	A	1587	ASP
1	A	1612	PHE
1	A	1626	LYS
1	A	1648	SER
1	A	1669	LEU
1	A	1682	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1723	TRP
1	A	1731	TRP
1	A	1742	SER
1	A	1745	LEU
1	A	1811	SER
1	A	1820	ILE
1	A	1823	ILE
1	A	1824	LYS
1	A	1830	ILE
1	A	1832	LEU
1	A	1837	SER
1	A	1839	GLN
1	A	1844	LEU
1	A	1856	GLU
1	A	1868	ILE
1	A	1870	ILE
1	A	1875	GLU
1	A	1876	VAL
1	A	1884	ILE
1	A	1911	VAL
1	A	1921	GLU
1	A	1930	LEU
1	A	1965	TRP
1	A	1969	LEU
1	A	1976	PHE
1	A	1977	PHE
1	A	1998	ARG
1	A	2014	ARG
1	A	2017	ASN
1	A	2043	TYR
1	A	2049	ILE
1	A	2059	LEU
1	A	2070	SER
1	A	2081	THR
1	A	2090	VAL
1	A	2092	ILE
1	A	2093	SER
1	A	2095	PHE
1	A	2105	LYS
1	A	2109	ARG
1	A	2111	PHE
1	A	2125	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2134	ASP
1	A	2151	ASP
1	A	2159	LEU
1	A	2191	GLU
1	A	2219	LEU
1	A	2230	LEU
1	A	2231	ASN
1	A	2234	GLU
1	A	2250	GLU
1	A	2253	LEU
1	A	2263	LEU
1	A	2272	ILE
1	A	2275	LEU
1	A	2283	LEU
1	A	2285	LEU
1	A	2291	LYS
1	A	2299	ASP
1	A	2308	GLU
1	A	2335	PHE
1	A	2336	ARG
1	A	2338	THR
1	A	2353	LEU
1	A	2357	LEU
1	A	2360	PHE
1	A	2367	ASN
1	A	2372	LEU
1	A	2385	LEU
1	A	2387	VAL
1	A	2416	ARG
1	A	2425	LYS
1	A	2426	ARG
1	A	2428	THR
1	A	2431	LEU
1	A	2437	ARG
1	A	2462	CYS
2	B	4	ILE
2	B	10	TYR
2	B	24	CYS
2	B	28	ILE
2	B	39	GLU
2	B	40	ILE
2	B	55	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	56	ARG
2	B	68	VAL
2	B	78	VAL
2	B	79	THR
2	B	80	SER
2	B	85	GLN
2	B	86	ASP
2	B	103	ASP
2	B	122	VAL
2	B	155	THR
2	B	162	LEU
2	B	170	ASP
2	B	182	ASN
2	B	200	VAL
2	B	203	PHE
2	B	213	ILE
2	B	219	VAL
2	B	230	THR
2	B	233	VAL
2	B	244	THR
2	B	255	ASP
2	B	256	CYS
2	B	259	SER
2	B	270	SER
2	B	281	THR
2	B	286	ARG
2	B	292	HIS
2	B	302	ASP
1	C	82	PHE
1	C	87	LEU
1	C	91	LYS
1	C	96	VAL
1	C	110	THR
1	C	123	PHE
1	C	124	GLN
1	C	129	SER
1	C	150	ILE
1	C	151	LEU
1	C	153	VAL
1	C	156	LEU
1	C	157	ILE
1	C	176	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	179	VAL
1	C	188	VAL
1	C	191	LEU
1	C	196	LEU
1	C	206	LEU
1	C	207	THR
1	C	210	PHE
1	C	213	PHE
1	C	216	ARG
1	C	219	ILE
1	C	222	LEU
1	C	223	THR
1	C	225	THR
1	C	231	SER
1	C	234	LYS
1	C	235	LEU
1	C	236	GLU
1	C	237	TYR
1	C	243	LEU
1	C	260	TYR
1	C	263	SER
1	C	264	ILE
1	C	268	ILE
1	C	273	ARG
1	C	278	ILE
1	C	287	LEU
1	C	298	ASP
1	C	301	LEU
1	C	303	LYS
1	C	304	GLN
1	C	305	TRP
1	C	314	THR
1	C	321	THR
1	C	323	ASP
1	C	330	LEU
1	C	331	VAL
1	C	332	PHE
1	C	339	LYS
1	C	342	TYR
1	C	344	ARG
1	C	349	ASP
1	C	355	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	357	TYR
1	C	361	LYS
1	C	363	ASP
1	C	366	ARG
1	C	379	PHE
1	C	380	ASP
1	C	385	THR
1	C	387	LYS
1	C	389	LEU
1	C	397	LEU
1	C	402	ASN
1	C	404	ASP
1	C	412	ASP
1	C	419	SER
1	C	423	ILE
1	C	425	PHE
1	C	438	ILE
1	C	440	ASP
1	C	450	PHE
1	C	453	ARG
1	C	467	LEU
1	C	469	CYS
1	C	494	ASP
1	C	517	ARG
1	C	523	SER
1	C	526	LEU
1	C	541	ASN
1	C	566	ASP
1	C	568	THR
1	C	572	ILE
1	C	586	GLN
1	C	587	TYR
1	C	601	ILE
1	C	616	SER
1	C	617	CYS
1	C	630	SER
1	C	641	LEU
1	C	644	LEU
1	C	651	ASP
1	C	653	VAL
1	C	664	LEU
1	C	676	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	678	LEU
1	C	712	VAL
1	C	720	LEU
1	C	722	LEU
1	C	724	THR
1	C	730	ASN
1	C	762	ASP
1	C	764	ILE
1	C	765	LEU
1	C	767	LYS
1	C	768	CYS
1	C	785	GLU
1	C	794	MET
1	C	795	THR
1	C	801	LEU
1	C	806	ILE
1	C	816	PHE
1	C	818	ARG
1	C	842	TYR
1	C	850	ILE
1	C	852	ILE
1	C	854	LYS
1	C	856	GLU
1	C	860	HIS
1	C	861	ILE
1	C	862	ARG
1	C	865	THR
1	C	922	ILE
1	C	934	LEU
1	C	946	MET
1	C	950	GLN
1	C	971	MET
1	C	986	LEU
1	C	992	ILE
1	C	1004	ILE
1	C	1007	VAL
1	C	1010	GLU
1	C	1014	ILE
1	C	1017	LEU
1	C	1019	ILE
1	C	1029	SER
1	C	1063	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1066	LEU
1	C	1068	SER
1	C	1069	LEU
1	C	1080	SER
1	C	1087	VAL
1	C	1094	SER
1	C	1108	ARG
1	C	1117	GLU
1	C	1118	MET
1	C	1126	LEU
1	C	1128	ARG
1	C	1130	LEU
1	C	1134	ASP
1	C	1141	THR
1	C	1151	GLN
1	C	1154	THR
1	C	1173	GLN
1	C	1174	HIS
1	C	1175	SER
1	C	1183	LYS
1	C	1213	GLN
1	C	1219	VAL
1	C	1220	ASN
1	C	1230	CYS
1	C	1231	SER
1	C	1240	GLN
1	C	1241	GLU
1	C	1244	ARG
1	C	1245	ARG
1	C	1264	SER
1	C	1268	VAL
1	C	1291	SER
1	C	1334	ILE
1	C	1368	THR
1	C	1372	LEU
1	C	1382	THR
1	C	1386	ILE
1	C	1398	LEU
1	C	1399	GLN
1	C	1401	LYS
1	C	1403	THR
1	C	1406	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1427	ASP
1	C	1432	MET
1	C	1435	LYS
1	C	1451	LEU
1	C	1460	LYS
1	C	1478	LEU
1	C	1491	MET
1	C	1499	GLU
1	C	1504	ILE
1	C	1505	LEU
1	C	1506	CYS
1	C	1517	VAL
1	C	1530	LEU
1	C	1533	LEU
1	C	1536	GLU
1	C	1540	ARG
1	C	1542	TYR
1	C	1572	THR
1	C	1587	ASN
1	C	1598	ARG
1	C	1600	LEU
1	C	1603	LYS
1	C	1605	LYS
1	C	1611	ARG
1	C	1619	ARG
1	C	1626	LEU
1	C	1650	SER
1	C	1658	LEU
1	C	1678	THR
1	C	1709	GLU
1	C	1710	ASP
1	C	1725	TRP
1	C	1728	CYS
1	C	1730	GLN
1	C	1741	ILE
1	C	1746	LEU
1	C	1753	ASN
1	C	1757	LYS
1	C	1825	ILE
1	C	1834	LEU
1	C	1846	LEU
1	C	1849	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1872	ILE
1	C	1881	GLN
1	C	1900	LEU
1	C	1913	VAL
1	C	1927	ARG
1	C	1936	GLU
1	C	1946	VAL
1	C	1965	GLU
1	C	1967	TRP
1	C	1971	LEU
1	C	1978	PHE
1	C	1981	GLU
1	C	1996	GLU
1	C	1997	MET
1	C	2005	LEU
1	C	2007	GLU
1	C	2022	TYR
1	C	2027	ASN
1	C	2028	TYR
1	C	2041	TRP
1	C	2049	ARG
1	C	2059	GLN
1	C	2063	LEU
1	C	2078	LEU
1	C	2080	VAL
1	C	2097	PHE
1	C	2102	SER
1	C	2105	SER
1	C	2111	ARG
1	C	2113	PHE
1	C	2121	LYS
1	C	2127	LEU
1	C	2136	ASP
1	C	2141	GLN
1	C	2150	LEU
1	C	2153	ASP
1	C	2156	CYS
1	C	2161	LEU
1	C	2184	SER
1	C	2193	GLU
1	C	2198	LYS
1	C	2206	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2209	MET
1	C	2220	THR
1	C	2221	LEU
1	C	2240	LEU
1	C	2242	LYS
1	C	2244	LEU
1	C	2245	TRP
1	C	2248	SER
1	C	2256	GLU
1	C	2262	THR
1	C	2265	LEU
1	C	2286	MET
1	C	2293	LYS
1	C	2294	VAL
1	C	2297	ILE
1	C	2301	ASP
1	C	2308	LEU
1	C	2319	ARG
1	C	2336	SER
1	C	2343	ASN
1	C	2355	LEU
1	C	2362	PHE
1	C	2364	PHE
1	C	2372	PHE
1	C	2374	LEU
1	C	2382	GLU
1	C	2383	THR
1	C	2386	GLN
1	C	2387	LEU
1	C	2398	ASN
1	C	2402	THR
1	C	2425	VAL
1	C	2428	ARG
1	C	2430	THR
1	C	2433	LEU
1	C	2437	ASP
1	C	2439	ARG
1	C	2443	ASP
1	C	2450	VAL
1	C	2462	ASN
1	C	2468	ILE
2	D	3	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	5	LEU
2	D	6	VAL
2	D	10	TYR
2	D	20	LEU
2	D	21	THR
2	D	28	ILE
2	D	31	SER
2	D	40	ILE
2	D	66	ASN
2	D	90	MET
2	D	101	VAL
2	D	106	SER
2	D	116	ASN
2	D	119	VAL
2	D	122	VAL
2	D	133	SER
2	D	135	ASP
2	D	139	ASN
2	D	155	THR
2	D	167	MET
2	D	174	LEU
2	D	210	ILE
2	D	212	ARG
2	D	219	VAL
2	D	230	THR
2	D	236	ILE
2	D	256	CYS
2	D	273	TYR
2	D	278	ASP
2	D	286	ARG
2	D	297	CYS
2	D	298	VAL
2	D	302	ASP
5	I	658	VAL
5	I	666	CYS
5	I	672	ASN
5	I	680	ILE
5	I	681	TYR
5	I	682	ILE
5	I	685	SER
5	I	692	SER
5	I	694	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	I	695	THR
5	I	697	VAL
5	I	703	ILE
5	I	707	ILE
5	I	716	THR
5	I	728	LEU
5	I	730	VAL
5	I	731	GLU
5	I	744	VAL
5	I	758	LEU
5	I	759	ASP
5	I	760	ARG
5	I	768	SER
5	I	770	SER
5	I	775	CYS
5	J	660	GLU
5	J	675	SER
5	J	681	TYR
5	J	685	SER
5	J	690	ARG
5	J	692	SER
5	J	697	VAL
5	J	702	THR
5	J	709	PHE
5	J	711	LEU
5	J	712	PHE
5	J	713	LEU
5	J	716	THR
5	J	721	ASP
5	J	728	LEU
5	J	729	THR
5	J	730	VAL
5	J	731	GLU
5	J	740	SER
5	J	743	ILE
5	J	758	LEU
5	J	759	ASP
5	J	760	ARG
5	J	764	ILE
5	J	768	SER
5	J	770	SER
5	J	775	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	J	783	SER
5	J	787	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	ASN
1	A	303	GLN
1	A	310	GLN
1	A	319	ASN
1	A	454	GLN
1	A	484	ASN
1	A	539	ASN
1	A	540	ASN
1	A	553	GLN
1	A	574	GLN
1	A	583	HIS
1	A	661	GLN
1	A	706	ASN
1	A	813	ASN
1	A	923	ASN
1	A	937	HIS
1	A	950	ASN
1	A	977	GLN
1	A	1054	GLN
1	A	1113	ASN
1	A	1173	HIS
1	A	1185	ASN
1	A	1231	GLN
1	A	1277	ASN
1	A	1379	GLN
1	A	1547	GLN
1	A	1728	GLN
1	A	1759	ASN
1	A	1981	ASN
1	A	2010	ASN
1	A	2036	ASN
1	A	2057	GLN
1	A	2145	ASN
1	A	2204	HIS
1	A	2209	GLN
1	A	2231	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2279	HIS
1	A	2282	ASN
1	A	2341	ASN
1	A	2447	GLN
1	A	2454	GLN
2	B	12	HIS
2	B	29	GLN
2	B	53	GLN
2	B	127	ASN
2	B	152	HIS
2	B	229	HIS
1	C	86	ASN
1	C	124	GLN
1	C	128	ASN
1	C	131	ASN
1	C	132	ASN
1	C	168	ASN
1	C	228	ASN
1	C	252	ASN
1	C	307	GLN
1	C	311	GLN
1	C	320	ASN
1	C	395	HIS
1	C	402	ASN
1	C	485	ASN
1	C	540	ASN
1	C	553	ASN
1	C	585	HIS
1	C	662	GLN
1	C	667	ASN
1	C	671	GLN
1	C	693	GLN
1	C	725	GLN
1	C	814	ASN
1	C	827	GLN
1	C	858	ASN
1	C	924	ASN
1	C	938	HIS
1	C	943	GLN
1	C	1000	HIS
1	C	1226	ASN
1	C	1232	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1233	GLN
1	C	1249	GLN
1	C	1289	GLN
1	C	1293	GLN
1	C	1510	ASN
1	C	1521	ASN
1	C	1543	ASN
1	C	1722	GLN
1	C	1761	ASN
1	C	1871	GLN
1	C	1977	GLN
1	C	1983	ASN
1	C	2011	GLN
1	C	2012	ASN
1	C	2038	ASN
1	C	2064	GLN
1	C	2065	HIS
1	C	2108	GLN
1	C	2135	GLN
1	C	2194	HIS
1	C	2281	HIS
1	C	2284	ASN
1	C	2343	ASN
1	C	2407	GLN
1	C	2436	ASN
1	C	2449	GLN
1	C	2456	GLN
2	D	12	HIS
2	D	77	ASN
2	D	120	ASN
2	D	149	GLN
2	D	152	HIS
2	D	229	HIS
2	D	301	ASN
5	I	691	ASN
5	I	735	ASN
5	I	754	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
1	C	567
1	A	534
3	E	90
3	F	87
2	D	75
2	B	66
4	G	45
4	H	42
5	J	31
5	I	26

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	416:UNK	C	450:UNK	N	40.12
1	F	416:UNK	C	450:UNK	N	39.07
1	E	512:UNK	C	550:UNK	N	33.98
1	F	717:UNK	C	750:UNK	N	33.97
1	E	717:UNK	C	750:UNK	N	33.43
1	F	512:UNK	C	550:UNK	N	33.24
1	F	118:UNK	C	150:UNK	N	32.46

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	118:UNK	C	150:UNK	N	32.20
1	F	867:UNK	C	900:UNK	N	31.99
1	E	867:UNK	C	900:UNK	N	30.60
1	F	318:UNK	C	350:UNK	N	27.65
1	E	318:UNK	C	350:UNK	N	27.26
1	E	381:UNK	C	400:UNK	N	25.02
1	F	381:UNK	C	400:UNK	N	24.83
1	E	468:UNK	C	500:UNK	N	24.07
1	F	468:UNK	C	500:UNK	N	23.91
1	F	567:UNK	C	600:UNK	N	23.32
1	E	567:UNK	C	600:UNK	N	22.55
1	F	169:UNK	C	200:UNK	N	22.46
1	E	169:UNK	C	200:UNK	N	22.15
1	F	665:UNK	C	700:UNK	N	17.20
1	E	665:UNK	C	700:UNK	N	16.83
1	E	813:UNK	C	850:UNK	N	13.94
1	F	218:UNK	C	250:UNK	N	13.04
1	F	813:UNK	C	850:UNK	N	13.02
1	E	218:UNK	C	250:UNK	N	12.00
1	A	1811:SER	C	1812:SER	N	10.40
1	E	761:UNK	C	800:UNK	N	10.32
1	A	1637:ASP	C	1638:ASP	N	9.38
1	F	761:UNK	C	800:UNK	N	9.33
1	C	1639:ASP	C	1640:ASP	N	9.18
1	F	612:UNK	C	650:UNK	N	8.93
1	C	668:PHE	C	669:ASP	N	8.41
1	E	612:UNK	C	650:UNK	N	8.32
1	A	667:PHE	C	668:ASP	N	8.25
1	A	225:ALA	C	226:ASP	N	7.67
1	A	1422:ALA	C	1423:GLY	N	7.39
1	C	226:ALA	C	227:ASP	N	7.36
1	J	721:ASP	C	722:ASN	N	7.31
1	I	779:ASP	C	780:ALA	N	6.42
1	C	123:PHE	C	124:GLN	N	6.40
1	C	1202:VAL	C	1203:PRO	N	6.36
1	A	1018:ILE	C	1019:THR	N	6.23
1	A	1202:PRO	C	1203:GLU	N	6.23
1	J	791:LEU	C	792:PRO	N	6.20
1	C	814:ASN	C	815:SER	N	6.18
1	A	2400:THR	C	2401:GLU	N	6.14
1	I	720:PRO	C	721:ASP	N	6.09
1	A	710:VAL	C	711:VAL	N	6.07

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	653:THR	C	654:ASN	N	6.02
1	C	242:ALA	C	243:LEU	N	5.89
1	C	1472:ALA	C	1473:GLY	N	5.86
1	C	2386:GLN	C	2387:LEU	N	5.84
1	A	2376:LYS	C	2377:ILE	N	5.81
1	C	118:VAL	C	119:SER	N	5.81
1	A	813:ASN	C	814:SER	N	5.77
1	C	209:ASP	C	210:PHE	N	5.76
1	A	1633:LEU	C	1634:GLU	N	5.74
1	J	733:ILE	C	734:SER	N	5.73
1	A	84:LEU	C	85:ASN	N	5.67
1	C	2375:PRO	C	2376:THR	N	5.65
1	B	3:VAL	C	4:ILE	N	5.55
1	C	1017:LEU	C	1018:GLN	N	5.55
1	A	1014:ILE	C	1015:LYS	N	5.49
1	A	116:GLU	C	117:VAL	N	5.48
1	E	808:UNK	C	809:UNK	N	5.48
1	D	165:LEU	C	166:SER	N	5.44
1	C	2243:VAL	C	2244:LEU	N	5.43
1	A	2377:ILE	C	2378:GLU	N	5.42
1	C	265:LEU	C	266:ASP	N	5.40
1	A	1169:ASN	C	1170:ARG	N	5.39
1	C	104:ALA	C	105:ASN	N	5.34
1	A	1133:ASP	C	1134:ARG	N	5.32
1	C	294:ILE	C	295:GLN	N	5.31
1	C	468:ALA	C	469:CYS	N	5.31
1	A	315:GLY	C	316:LEU	N	5.29
1	A	106:LEU	C	107:SER	N	5.28
1	I	787:ILE	C	788:GLU	N	5.27
1	A	219:ASP	C	220:TRP	N	5.26
1	I	747:ASP	C	748:GLY	N	5.26
1	C	2388:PRO	C	2389:VAL	N	5.24
1	A	1144:LEU	C	1145:SER	N	5.22
1	C	2395:LEU	C	2396:LEU	N	5.22
1	A	408:ASN	C	409:ASN	N	5.21
1	A	2387:VAL	C	2388:MET	N	5.18
1	C	287:LEU	C	288:GLY	N	5.18
1	J	708:GLY	C	709:PHE	N	5.17
1	A	307:ARG	C	308:LEU	N	5.15
1	A	318:LEU	C	319:ASN	N	5.15
1	C	1911:ALA	C	1912:LEU	N	5.12
1	A	1201:VAL	C	1202:PRO	N	5.11

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	508:SER	C	509:LEU	N	5.08
1	A	117:VAL	C	118:SER	N	5.07
1	C	1764:LEU	C	1765:ALA	N	5.05
1	A	1531:LEU	C	1532:VAL	N	5.02
1	C	1132:ASN	C	1133:GLY	N	5.02
1	J	668:ASP	C	669:LYS	N	5.02
1	J	775:CYS	C	776:LYS	N	5.02
1	A	120:GLU	C	121:GLN	N	5.00
1	A	2396:ASN	C	2397:GLY	N	5.00
1	A	286:LEU	C	287:GLY	N	4.99
1	D	59:ASP	C	60:ILE	N	4.97
1	C	430:SER	C	431:ILE	N	4.95
1	J	766:SER	C	767:ILE	N	4.91
1	A	521:LEU	C	522:SER	N	4.90
1	A	2095:PHE	C	2096:GLU	N	4.90
1	G	155:ILE	C	156:SER	N	4.89
1	A	590:GLU	C	591:PHE	N	4.87
1	G	197:VAL	C	198:LEU	N	4.87
1	A	1016:LEU	C	1017:GLN	N	4.86
1	J	648:LYS	C	649:LYS	N	4.85
1	C	130:LEU	C	131:ASN	N	4.84
1	C	703:LEU	C	704:SER	N	4.83
1	D	58:TYR	C	59:ASP	N	4.82
1	A	2205:TRP	C	2206:VAL	N	4.81
1	A	2450:LYS	C	2451:LEU	N	4.81
1	C	1497:ASP	C	1498:LYS	N	4.80
1	C	241:ALA	C	242:ALA	N	4.79
1	C	309:LEU	C	310:PHE	N	4.78
1	J	723:PHE	C	724:GLU	N	4.77
1	C	222:LEU	C	223:THR	N	4.75
1	A	2434:ASN	C	2435:ASP	N	4.74
1	C	1819:ARG	C	1820:HIS	N	4.72
1	B	38:LEU	C	39:GLU	N	4.71
1	C	1206:LYS	C	1207:ASN	N	4.71
1	C	1671:LEU	C	1672:LYS	N	4.69
1	A	95:VAL	C	96:PRO	N	4.68
1	A	1216:LEU	C	1217:PRO	N	4.68
1	B	69:ALA	C	70:SER	N	4.68
1	C	229:ASN	C	230:SER	N	4.68
1	C	869:ILE	C	870:GLY	N	4.68
1	A	772:SER	C	773:ALA	N	4.67
1	C	89:PHE	C	90:ASP	N	4.65

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	126:SER	C	127:ASN	N	4.64
1	C	216:ARG	C	217:THR	N	4.64
1	A	429:SER	C	430:ILE	N	4.62
1	C	817:LYS	C	818:ARG	N	4.62
1	D	38:LEU	C	39:GLU	N	4.62
1	I	743:ILE	C	744:VAL	N	4.62
1	C	467:LEU	C	468:ALA	N	4.60
1	C	1115:LEU	C	1116:SER	N	4.60
1	C	2309:ARG	C	2310:GLU	N	4.60
1	C	2408:ARG	C	2409:VAL	N	4.60
1	A	949:GLN	C	950:ASN	N	4.59
1	A	1970:ASP	C	1971:ASP	N	4.59
1	C	127:SER	C	128:ASN	N	4.59
1	E	465:UNK	C	466:UNK	N	4.57
1	I	775:CYS	C	776:LYS	N	4.57
1	G	51:GLY	C	52:ARG	N	4.56
1	F	913:UNK	C	914:UNK	N	4.55
1	A	230:SER	C	231:SER	N	4.54
1	A	1212:GLN	C	1213:VAL	N	4.54
1	C	194:ASN	C	195:THR	N	4.54
1	C	385:THR	C	386:LYS	N	4.54
1	C	1542:TYR	C	1543:ASN	N	4.54
1	A	2036:ASN	C	2037:GLN	N	4.53
1	H	63:GLY	C	64:HIS	N	4.53
1	A	193:ASN	C	194:THR	N	4.52
1	A	480:LYS	C	481:ASP	N	4.51
1	C	334:GLU	C	335:LEU	N	4.51
1	H	91:LEU	C	92:HIS	N	4.51
1	C	2249:ARG	C	2250:SER	N	4.50
1	A	168:GLN	C	169:THR	N	4.49
1	C	1516:GLU	C	1517:VAL	N	4.48
1	D	48:ALA	C	49:THR	N	4.48
1	A	417:VAL	C	418:SER	N	4.47
1	C	1534:VAL	C	1535:ASN	N	4.47
1	C	1961:VAL	C	1962:LEU	N	4.47
1	I	672:ASN	C	673:TYR	N	4.47
1	A	292:ILE	C	293:ILE	N	4.46
1	F	371:UNK	C	372:UNK	N	4.45
1	A	427:GLY	C	428:SER	N	4.44
1	A	1743:TYR	C	1744:LEU	N	4.44
1	C	307:GLN	C	308:ARG	N	4.43
1	C	150:ILE	C	151:LEU	N	4.41

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1455:GLY	C	1456:THR	N	4.40
1	A	1514:GLU	C	1515:VAL	N	4.40
1	A	142:SER	C	143:SER	N	4.39
1	A	335:LEU	C	336:SER	N	4.39
1	A	526:SER	C	527:GLY	N	4.39
1	C	1200:ASN	C	1201:GLU	N	4.39
1	E	711:UNK	C	712:UNK	N	4.39
1	I	651:THR	C	652:ASN	N	4.39
1	A	91:LEU	C	92:LYS	N	4.38
1	C	823:THR	C	824:THR	N	4.37
1	C	1919:ALA	C	1920:ILE	N	4.37
1	A	1524:LEU	C	1525:VAL	N	4.36
1	A	1581:GLY	C	1582:CYS	N	4.36
1	A	2126:LYS	C	2127:GLY	N	4.36
1	C	957:VAL	C	958:SER	N	4.36
1	A	1206:ASN	C	1207:TYR	N	4.35
1	C	2207:TRP	C	2208:VAL	N	4.35
1	A	404:MET	C	405:ASN	N	4.34
1	A	819:ALA	C	820:ALA	N	4.34
1	A	1114:LEU	C	1115:SER	N	4.34
1	D	199:PRO	C	200:VAL	N	4.34
1	A	1397:GLN	C	1398:LEU	N	4.33
1	C	2460:VAL	C	2461:GLU	N	4.33
1	I	680:ILE	C	681:TYR	N	4.33
1	A	502:LEU	C	503:ASN	N	4.32
1	C	1172:ILE	C	1173:GLN	N	4.32
1	C	1213:GLN	C	1214:VAL	N	4.31
1	A	1726:CYS	C	1727:LEU	N	4.30
1	A	2111:PHE	C	2112:CYS	N	4.30
1	B	290:GLY	C	291:HIS	N	4.30
1	C	1294:GLU	C	1295:ASP	N	4.30
1	C	2434:THR	C	2435:GLY	N	4.30
1	A	816:LYS	C	817:ARG	N	4.29
1	C	250:ALA	C	251:ASP	N	4.29
1	C	990:ILE	C	991:SER	N	4.29
1	F	710:UNK	C	711:UNK	N	4.29
1	I	732:ASP	C	733:ILE	N	4.29
1	B	88:ARG	C	89:TRP	N	4.28
1	C	767:LYS	C	768:CYS	N	4.28
1	C	950:GLN	C	951:ASN	N	4.28
1	D	83:PHE	C	84:GLN	N	4.28
1	G	133:ALA	C	134:ASP	N	4.28

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	700:SER	C	701:SER	N	4.28
1	A	203:GLY	C	204:THR	N	4.27
1	A	277:ILE	C	278:ILE	N	4.27
1	A	1851:PHE	C	1852:GLY	N	4.26
1	B	55:VAL	C	56:ARG	N	4.26
1	C	181:ILE	C	182:PRO	N	4.26
1	C	706:VAL	C	707:ASN	N	4.26
1	C	1607:ASP	C	1608:ALA	N	4.25
1	A	2116:SER	C	2117:ASP	N	4.24
1	A	1957:MET	C	1958:ALA	N	4.23
1	A	2401:GLU	C	2402:GLU	N	4.22
1	A	1960:LEU	C	1961:TRP	N	4.21
1	A	1343:LYS	C	1344:CYS	N	4.20
1	B	54:ASN	C	55:VAL	N	4.20
1	C	151:LEU	C	152:ALA	N	4.20
1	C	205:THR	C	206:LEU	N	4.20
1	E	458:UNK	C	459:UNK	N	4.20
1	C	1221:GLN	C	1222:ASN	N	4.19
1	C	845:LEU	C	846:LEU	N	4.18
1	G	113:ILE	C	114:HIS	N	4.18
1	A	467:ALA	C	468:CYS	N	4.17
1	A	2008:PHE	C	2009:GLN	N	4.17
1	B	59:ASP	C	60:ILE	N	4.17
1	C	1405:TYR	C	1406:GLU	N	4.17
1	A	200:VAL	C	201:PRO	N	4.16
1	D	256:CYS	C	257:ALA	N	4.16
1	B	293:LYS	C	294:GLY	N	4.15
1	D	80:SER	C	81:VAL	N	4.15
1	G	70:ILE	C	71:LYS	N	4.15
1	C	293:ILE	C	294:ILE	N	4.14
1	C	1350:ALA	C	1351:LYS	N	4.14
1	E	552:UNK	C	553:UNK	N	4.13
1	A	1575:TRP	C	1576:ASN	N	4.12
1	C	454:LYS	C	455:GLN	N	4.12
1	C	1713:LYS	C	1714:LEU	N	4.12
1	C	2404:GLU	C	2405:GLU	N	4.12
1	F	309:UNK	C	310:UNK	N	4.12
1	J	649:LYS	C	650:ARG	N	4.12
1	A	810:ASP	C	811:GLN	N	4.11
1	A	2151:ASP	C	2152:ALA	N	4.11
1	A	2330:GLY	C	2331:ILE	N	4.11
1	C	709:ALA	C	710:TYR	N	4.11

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	1051:LEU	C	1052:GLU	N	4.11
1	G	91:LEU	C	92:HIS	N	4.11
1	A	2332:GLU	C	2333:GLY	N	4.10
1	C	295:GLN	C	296:ASP	N	4.10
1	C	317:LEU	C	318:SER	N	4.10
1	J	718:LYS	C	719:LYS	N	4.10
1	A	1030:ALA	C	1031:LEU	N	4.09
1	C	811:ASP	C	812:GLN	N	4.09
1	C	2181:VAL	C	2182:PRO	N	4.09
1	D	81:VAL	C	82:SER	N	4.08
1	D	269:SER	C	270:SER	N	4.08
1	H	93:LEU	C	94:LEU	N	4.08
1	B	256:CYS	C	257:ALA	N	4.07
1	C	382:ALA	C	383:ILE	N	4.07
1	A	1553:GLU	C	1554:GLU	N	4.06
1	C	1282:SER	C	1283:SER	N	4.06
1	D	87:ASN	C	88:ARG	N	4.06
1	E	268:UNK	C	300:UNK	N	4.06
1	H	79:VAL	C	80:HIS	N	4.06
1	C	1846:LEU	C	1847:LEU	N	4.05
1	F	557:UNK	C	558:UNK	N	4.05
1	H	97:GLN	C	98:PHE	N	4.05
1	A	171:ARG	C	172:LEU	N	4.04
1	C	84:THR	C	85:LEU	N	4.04
1	C	332:PHE	C	333:ARG	N	4.04
1	A	301:GLY	C	302:LYS	N	4.03
1	A	2054:PRO	C	2055:GLN	N	4.03
1	C	243:LEU	C	244:LEU	N	4.03
1	C	617:CYS	C	618:ASP	N	4.03
1	I	758:LEU	C	759:ASP	N	4.03
1	J	655:SER	C	656:VAL	N	4.03
1	A	1966:TYR	C	1967:GLU	N	4.02
1	D	121:GLU	C	122:VAL	N	4.02
1	D	183:CYS	C	184:TYR	N	4.01
1	A	1997:LYS	C	1998:ARG	N	4.00
1	C	568:THR	C	569:ASP	N	4.00
1	C	2135:GLN	C	2136:ASP	N	4.00
1	A	2004:ARG	C	2005:GLU	N	3.99
1	B	145:LEU	C	146:GLY	N	3.99
1	F	466:UNK	C	467:UNK	N	3.99
1	A	664:GLY	C	665:SER	N	3.98
1	C	414:PRO	C	415:PHE	N	3.98

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	991:SER	C	992:ILE	N	3.98
1	A	703:SER	C	704:SER	N	3.97
1	A	954:ARG	C	955:CYS	N	3.97
1	C	1755:TRP	C	1756:TYR	N	3.97
1	J	682:ILE	C	683:GLN	N	3.97
1	A	262:SER	C	263:ILE	N	3.96
1	A	1339:LYS	C	1340:TYR	N	3.96
1	E	262:UNK	C	263:UNK	N	3.96
1	A	505:LYS	C	506:ILE	N	3.95
1	A	2460:ASN	C	2461:LEU	N	3.95
1	F	611:UNK	C	612:UNK	N	3.95
1	H	134:ASP	C	135:LEU	N	3.95
1	J	732:ASP	C	733:ILE	N	3.95
1	A	166:PRO	C	167:ASN	N	3.94
1	A	594:LEU	C	595:ILE	N	3.94
1	A	645:MET	C	646:ILE	N	3.94
1	B	257:ALA	C	258:PHE	N	3.94
1	C	2049:ARG	C	2050:LYS	N	3.94
1	C	2433:LEU	C	2434:THR	N	3.94
1	D	66:ASN	C	67:PRO	N	3.94
1	E	466:UNK	C	467:UNK	N	3.94
1	C	667:ASN	C	668:PHE	N	3.93
1	A	687:GLU	C	688:ILE	N	3.92
1	C	2088:GLY	C	2089:LYS	N	3.92
1	H	157:CYS	C	158:MET	N	3.92
1	H	178:ASN	C	179:TRP	N	3.92
1	J	715:SER	C	716:THR	N	3.92
1	A	857:ASN	C	858:PRO	N	3.91
1	A	2105:LYS	C	2106:GLN	N	3.91
1	A	2466:ILE	C	2467:GLY	N	3.91
1	C	1427:ASP	C	1428:SER	N	3.91
1	D	65:PRO	C	66:ASN	N	3.91
1	A	1551:GLU	C	1552:LEU	N	3.90
1	C	1444:GLU	C	1445:TRP	N	3.90
1	C	1545:VAL	C	1546:VAL	N	3.90
1	C	1623:ARG	C	1624:MET	N	3.90
1	E	156:UNK	C	157:UNK	N	3.90
1	A	2324:TYR	C	2325:ALA	N	3.89
1	C	2428:ARG	C	2429:ILE	N	3.89
1	G	67:HIS	C	68:GLU	N	3.89
1	A	2130:ASP	C	2131:ILE	N	3.88
1	B	221:HIS	C	222:LEU	N	3.88

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2410:GLU	C	2411:ASN	N	3.88
1	C	984:GLN	C	985:GLN	N	3.87
1	C	1583:GLY	C	1584:CYS	N	3.87
1	J	739:PHE	C	740:SER	N	3.87
1	C	989:LEU	C	990:ILE	N	3.86
1	A	811:GLN	C	812:SER	N	3.85
1	A	1566:ASP	C	1567:LYS	N	3.85
1	C	81:THR	C	82:PHE	N	3.85
1	C	371:ALA	C	372:ILE	N	3.85
1	C	952:LEU	C	953:GLY	N	3.85
1	C	1341:LYS	C	1342:TYR	N	3.85
1	C	1442:LEU	C	1443:GLY	N	3.85
1	E	709:UNK	C	710:UNK	N	3.85
1	E	753:UNK	C	754:UNK	N	3.85
1	G	99:PRO	C	100:ARG	N	3.85
1	I	765:GLN	C	766:SER	N	3.85
1	C	1889:PRO	C	1890:ASN	N	3.84
1	C	1959:MET	C	1960:ALA	N	3.84
1	C	2422:ALA	C	2423:MET	N	3.84
1	E	603:UNK	C	604:UNK	N	3.84
1	G	110:ARG	C	111:ALA	N	3.84
1	A	622:ASP	C	623:ASP	N	3.83
1	A	1965:TRP	C	1966:TYR	N	3.83
1	A	2444:VAL	C	2445:PRO	N	3.83
1	C	840:LEU	C	841:ASP	N	3.83
1	F	563:UNK	C	564:UNK	N	3.83
1	C	1114:ASN	C	1115:LEU	N	3.82
1	C	1119:SER	C	1120:SER	N	3.82
1	C	1833:SER	C	1834:LEU	N	3.82
1	F	313:UNK	C	314:UNK	N	3.82
1	F	910:UNK	C	911:UNK	N	3.82
1	J	706:VAL	C	707:ILE	N	3.82
1	A	302:LYS	C	303:GLN	N	3.81
1	A	589:THR	C	590:GLU	N	3.81
1	C	1073:GLY	C	1074:PRO	N	3.81
1	A	1504:CYS	C	1505:LEU	N	3.80
1	C	1182:ASN	C	1183:LYS	N	3.80
1	E	150:UNK	C	151:UNK	N	3.80
1	F	250:UNK	C	251:UNK	N	3.80
1	G	87:HIS	C	88:GLU	N	3.80
1	J	781:GLU	C	782:LYS	N	3.80
1	C	366:ARG	C	367:ARG	N	3.79

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	402:ASN	C	403:ILE	N	3.79
1	C	1178:ASP	C	1179:GLN	N	3.79
1	C	1684:ASP	C	1685:LEU	N	3.79
1	D	132:ILE	C	133:SER	N	3.79
1	A	143:SER	C	144:GLU	N	3.78
1	A	852:LEU	C	853:LYS	N	3.78
1	C	729:SER	C	730:ASN	N	3.78
1	C	851:ASN	C	852:ILE	N	3.78
1	C	1075:ASN	C	1076:LEU	N	3.78
1	G	63:GLY	C	64:HIS	N	3.78
1	H	115:ILE	C	116:ALA	N	3.78
1	A	1625:ALA	C	1626:LYS	N	3.77
1	B	89:TRP	C	90:MET	N	3.77
1	C	276:LYS	C	277:LEU	N	3.77
1	C	364:VAL	C	365:ILE	N	3.77
1	E	554:UNK	C	555:UNK	N	3.77
1	A	279:ARG	C	280:LEU	N	3.76
1	A	1032:GLU	C	1033:GLY	N	3.76
1	A	1638:ASP	C	1639:PRO	N	3.76
1	A	2421:MET	C	2422:LEU	N	3.76
1	A	324:VAL	C	325:HIS	N	3.75
1	A	973:CYS	C	974:PRO	N	3.75
1	C	1531:SER	C	1532:ALA	N	3.75
1	C	2113:PHE	C	2114:CYS	N	3.75
1	C	2380:GLU	C	2381:GLU	N	3.75
1	F	310:UNK	C	311:UNK	N	3.75
1	C	1822:ILE	C	1823:PRO	N	3.74
1	C	2383:THR	C	2384:GLY	N	3.74
1	H	149:CYS	C	150:LEU	N	3.74
1	J	670:VAL	C	671:PRO	N	3.74
1	A	1045:PHE	C	1046:PHE	N	3.73
1	A	2081:THR	C	2082:ARG	N	3.73
1	C	256:LEU	C	257:LEU	N	3.73
1	C	1647:ALA	C	1648:LYS	N	3.73
1	C	2208:VAL	C	2209:MET	N	3.73
1	D	166:SER	C	167:MET	N	3.73
1	A	856:ASN	C	857:ASN	N	3.72
1	A	1903:GLY	C	1904:LYS	N	3.72
1	C	113:SER	C	114:LEU	N	3.72
1	C	135:PHE	C	136:GLU	N	3.72
1	C	710:TYR	C	711:VAL	N	3.72
1	C	1171:ARG	C	1172:ILE	N	3.72

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	1460:LYS	C	1461:PRO	N	3.72
1	D	101:VAL	C	102:TRP	N	3.72
1	A	757:ASP	C	758:PRO	N	3.71
1	A	2341:ASN	C	2342:VAL	N	3.71
1	C	134:ILE	C	135:PHE	N	3.71
1	C	2360:GLU	C	2361:ALA	N	3.71
1	E	809:UNK	C	810:UNK	N	3.71
1	A	2077:ALA	C	2078:VAL	N	3.70
1	C	1256:SER	C	1257:ALA	N	3.70
1	E	464:UNK	C	465:UNK	N	3.70
1	E	502:UNK	C	503:UNK	N	3.70
1	F	859:UNK	C	860:UNK	N	3.70
1	A	1430:MET	C	1431:MET	N	3.69
1	A	2010:ASN	C	2011:SER	N	3.69
1	A	2312:GLU	C	2313:LYS	N	3.69
1	C	103:GLY	C	104:ALA	N	3.69
1	C	632:HIS	C	633:ALA	N	3.69
1	C	2072:SER	C	2073:ALA	N	3.69
1	C	2224:LYS	C	2225:VAL	N	3.69
1	D	273:TYR	C	274:VAL	N	3.69
1	H	80:HIS	C	81:LEU	N	3.69
1	I	780:ALA	C	781:GLU	N	3.69
1	J	711:LEU	C	712:PHE	N	3.69
1	A	1902:LEU	C	1903:GLY	N	3.68
1	A	2217:LEU	C	2218:THR	N	3.68
1	A	1077:ASP	C	1078:TYR	N	3.67
1	A	1488:VAL	C	1489:MET	N	3.67
1	A	1619:SER	C	1620:GLY	N	3.67
1	A	2339:CYS	C	2340:GLU	N	3.67
1	D	128:GLN	C	129:GLY	N	3.67
1	H	90:THR	C	91:LEU	N	3.67
1	A	280:LEU	C	281:ASP	N	3.66
1	A	1892:SER	C	1893:ARG	N	3.66
1	B	181:GLY	C	182:ASN	N	3.66
1	C	1235:THR	C	1236:LYS	N	3.66
1	C	1392:ALA	C	1393:GLN	N	3.66
1	A	297:ASP	C	298:PRO	N	3.65
1	A	944:ILE	C	945:MET	N	3.65
1	C	547:LYS	C	548:ALA	N	3.65
1	C	642:SER	C	643:LYS	N	3.65
1	C	2314:GLU	C	2315:LYS	N	3.65
1	D	127:ASN	C	128:GLN	N	3.65

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	151:UNK	C	152:UNK	N	3.65
1	E	905:UNK	C	906:UNK	N	3.65
1	A	560:GLY	C	561:GLU	N	3.64
1	A	1050:LEU	C	1051:GLU	N	3.64
1	A	1891:VAL	C	1892:SER	N	3.64
1	C	659:GLU	C	660:ILE	N	3.64
1	C	698:LYS	C	699:ILE	N	3.64
1	D	45:LYS	C	46:LEU	N	3.64
1	F	900:UNK	C	901:UNK	N	3.64
1	H	100:ARG	C	101:PHE	N	3.64
1	A	167:ASN	C	168:GLN	N	3.63
1	A	963:ILE	C	964:PRO	N	3.63
1	A	1915:MET	C	1916:VAL	N	3.63
1	A	2313:LYS	C	2314:VAL	N	3.63
1	C	1447:GLU	C	1448:LEU	N	3.63
1	C	2119:ASP	C	2120:GLY	N	3.63
1	E	754:UNK	C	755:UNK	N	3.63
1	F	107:UNK	C	108:UNK	N	3.63
1	G	43:SER	C	44:LEU	N	3.63
1	G	157:CYS	C	158:MET	N	3.63
1	A	231:SER	C	232:SER	N	3.62
1	A	293:ILE	C	294:GLN	N	3.62
1	B	130:GLU	C	131:LEU	N	3.62
1	C	236:GLU	C	237:TYR	N	3.62
1	C	570:ALA	C	571:GLN	N	3.62
1	C	939:THR	C	940:ALA	N	3.62
1	C	2131:GLU	C	2132:ASP	N	3.62
1	D	253:VAL	C	254:TRP	N	3.62
1	A	1285:VAL	C	1286:GLU	N	3.61
1	A	1860:ALA	C	1861:MET	N	3.61
1	A	1907:PRO	C	1908:GLN	N	3.61
1	C	423:ILE	C	424:ALA	N	3.61
1	C	736:GLU	C	737:GLU	N	3.61
1	C	1348:ALA	C	1349:PHE	N	3.60
1	C	2084:ARG	C	2085:ALA	N	3.60
1	E	909:UNK	C	910:UNK	N	3.60
1	A	623:ASP	C	624:ILE	N	3.59
1	A	2242:LEU	C	2243:TRP	N	3.59
1	C	442:ILE	C	443:ARG	N	3.59
1	C	1222:ASN	C	1223:ILE	N	3.59
1	C	1330:LYS	C	1331:PRO	N	3.59
1	C	1432:MET	C	1433:MET	N	3.59

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	69:ALA	C	70:SER	N	3.59
1	E	716:UNK	C	717:UNK	N	3.59
1	A	2256:ARG	C	2257:THR	N	3.58
1	A	2368:TRP	C	2369:GLY	N	3.58
1	B	175:ALA	C	176:ALA	N	3.58
1	C	1473:GLY	C	1474:ALA	N	3.58
1	E	451:UNK	C	452:UNK	N	3.58
1	F	511:UNK	C	512:UNK	N	3.58
1	F	564:UNK	C	565:UNK	N	3.58
1	A	271:LEU	C	272:ARG	N	3.57
1	A	435:THR	C	436:LEU	N	3.57
1	A	1094:ALA	C	1095:GLY	N	3.57
1	A	1132:GLY	C	1133:ASP	N	3.57
1	A	1486:THR	C	1487:SER	N	3.57
1	C	618:ASP	C	619:LEU	N	3.57
1	C	1254:SER	C	1255:PRO	N	3.57
1	C	1625:ALA	C	1626:LEU	N	3.57
1	C	1905:GLY	C	1906:LYS	N	3.57
1	A	1434:LEU	C	1435:ARG	N	3.56
1	A	1565:SER	C	1566:ASP	N	3.56
1	D	118:PRO	C	119:VAL	N	3.56
1	E	112:UNK	C	113:UNK	N	3.56
1	G	196:LYS	C	197:VAL	N	3.56
1	A	779:LEU	C	780:LYS	N	3.55
1	A	2372:LEU	C	2373:PRO	N	3.55
1	C	499:THR	C	500:LEU	N	3.55
1	C	1924:SER	C	1925:LEU	N	3.55
1	C	2213:ALA	C	2214:PRO	N	3.55
1	D	125:HIS	C	126:PRO	N	3.55
1	D	188:MET	C	189:PRO	N	3.55
1	F	102:UNK	C	103:UNK	N	3.55
1	H	70:ILE	C	71:LYS	N	3.55
1	A	234:LEU	C	235:GLU	N	3.54
1	A	345:LYS	C	346:TYR	N	3.54
1	A	1765:PHE	C	1766:GLU	N	3.54
1	A	1917:ALA	C	1918:ILE	N	3.54
1	B	80:SER	C	81:VAL	N	3.54
1	B	189:PRO	C	190:ASN	N	3.54
1	C	161:LEU	C	162:SER	N	3.54
1	C	604:GLU	C	605:ASP	N	3.54
1	C	1344:GLN	C	1345:LYS	N	3.54
1	C	1413:ASP	C	1414:ALA	N	3.54

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	1978:PHE	C	1979:PHE	N	3.54
1	D	196:HIS	C	197:LEU	N	3.54
1	E	702:UNK	C	703:UNK	N	3.54
1	J	704:PHE	C	705:GLU	N	3.54
1	A	1034:GLU	C	1035:PHE	N	3.53
1	A	1508:ASN	C	1509:ASN	N	3.53
1	C	178:ARG	C	179:VAL	N	3.53
1	C	206:LEU	C	207:THR	N	3.53
1	C	2262:THR	C	2263:ARG	N	3.53
1	E	812:UNK	C	813:UNK	N	3.53
1	I	659:LEU	C	660:GLU	N	3.53
1	A	598:SER	C	599:TYR	N	3.52
1	A	1728:GLN	C	1729:PRO	N	3.52
1	A	1967:GLU	C	1968:GLY	N	3.52
1	C	418:VAL	C	419:SER	N	3.52
1	C	1963:TRP	C	1964:HIS	N	3.52
1	C	2318:PHE	C	2319:ARG	N	3.52
1	D	114:LYS	C	115:HIS	N	3.52
1	F	862:UNK	C	863:UNK	N	3.52
1	A	1532:VAL	C	1533:ASN	N	3.51
1	A	2302:GLU	C	2303:ALA	N	3.51
1	A	2438:ARG	C	2439:PHE	N	3.51
1	C	536:GLN	C	537:TYR	N	3.51
1	C	688:GLU	C	689:ILE	N	3.51
1	C	956:CYS	C	957:VAL	N	3.51
1	C	1217:LEU	C	1218:PRO	N	3.51
1	E	165:UNK	C	166:UNK	N	3.51
1	A	1006:VAL	C	1007:ILE	N	3.50
1	A	1956:ARG	C	1957:MET	N	3.50
1	C	707:ASN	C	708:PRO	N	3.50
1	C	2150:LEU	C	2151:GLN	N	3.50
1	C	2411:ASN	C	2412:GLU	N	3.50
1	F	610:UNK	C	611:UNK	N	3.50
1	G	183:ASP	C	184:VAL	N	3.50
1	I	648:LYS	C	649:LYS	N	3.50
1	A	104:ASN	C	105:GLU	N	3.49
1	A	609:LYS	C	610:LEU	N	3.49
1	A	1000:VAL	C	1001:GLU	N	3.49
1	A	1194:ILE	C	1195:PHE	N	3.49
1	A	1755:LYS	C	1756:ALA	N	3.49
1	A	2364:PRO	C	2365:LEU	N	3.49
1	C	1836:GLU	C	1837:SER	N	3.49

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2033:ASP	C	2034:VAL	N	3.49
1	F	350:UNK	C	351:UNK	N	3.49
1	F	414:UNK	C	415:UNK	N	3.49
1	A	249:ALA	C	250:ASP	N	3.48
1	A	346:TYR	C	347:ASP	N	3.48
1	A	441:ILE	C	442:ARG	N	3.48
1	A	485:LEU	C	486:MET	N	3.48
1	C	1212:MET	C	1213:GLN	N	3.48
1	C	1524:ASP	C	1525:LEU	N	3.48
1	C	2437:ASP	C	2438:ILE	N	3.48
1	E	202:UNK	C	203:UNK	N	3.48
1	E	258:UNK	C	259:UNK	N	3.48
1	H	135:LEU	C	136:TRP	N	3.48
1	A	1326:ASP	C	1327:ASP	N	3.47
1	A	1496:LYS	C	1497:GLU	N	3.47
1	A	1629:LEU	C	1630:ASN	N	3.47
1	C	1737:ASN	C	1738:PRO	N	3.47
1	D	102:TRP	C	103:ASP	N	3.47
1	F	658:UNK	C	659:UNK	N	3.47
1	G	94:LEU	C	95:LEU	N	3.47
1	H	196:LYS	C	197:VAL	N	3.47
1	I	756:GLY	C	757:LYS	N	3.47
1	A	499:LEU	C	500:MET	N	3.46
1	A	1762:LEU	C	1763:ALA	N	3.46
1	A	1182:LYS	C	1183:LEU	N	3.45
1	A	1591:ARG	C	1592:ILE	N	3.45
1	C	2457:ALA	C	2458:THR	N	3.45
1	E	306:UNK	C	307:UNK	N	3.45
1	E	309:UNK	C	310:UNK	N	3.45
1	G	186:GLN	C	187:THR	N	3.45
1	H	175:ASP	C	176:LYS	N	3.45
1	A	185:ILE	C	186:GLU	N	3.44
1	A	282:ALA	C	283:ALA	N	3.44
1	A	1586:ILE	C	1587:ASP	N	3.44
1	C	329:LEU	C	330:LEU	N	3.44
1	C	692:ILE	C	693:GLN	N	3.44
1	C	2001:GLY	C	2002:PRO	N	3.44
1	C	2321:THR	C	2322:ARG	N	3.44
1	E	560:UNK	C	561:UNK	N	3.44
1	F	914:UNK	C	915:UNK	N	3.44
1	A	975:PRO	C	976:SER	N	3.43
1	A	2041:ILE	C	2042:TYR	N	3.43

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	365:ILE	C	366:ARG	N	3.43
1	C	569:ASP	C	570:ALA	N	3.43
1	C	608:VAL	C	609:ARG	N	3.43
1	C	850:ILE	C	851:ASN	N	3.43
1	C	1081:HIS	C	1082:LEU	N	3.43
1	C	1338:THR	C	1339:LEU	N	3.43
1	C	1491:MET	C	1492:LYS	N	3.43
1	D	151:THR	C	152:HIS	N	3.43
1	A	1157:VAL	C	1158:PHE	N	3.42
1	A	1363:LYS	C	1364:ASN	N	3.42
1	A	1622:MET	C	1623:ALA	N	3.42
1	C	697:ILE	C	698:LYS	N	3.42
1	E	406:UNK	C	407:UNK	N	3.42
1	E	904:UNK	C	905:UNK	N	3.42
1	F	214:UNK	C	215:UNK	N	3.42
1	A	1546:ALA	C	1547:GLN	N	3.41
1	B	155:THR	C	156:PRO	N	3.41
1	C	88:ILE	C	89:PHE	N	3.41
1	C	335:LEU	C	336:LEU	N	3.41
1	C	1057:ASN	C	1058:LYS	N	3.41
1	A	1130:ASN	C	1131:ASN	N	3.40
1	A	1152:GLY	C	1153:THR	N	3.40
1	B	200:VAL	C	201:THR	N	3.40
1	C	2223:GLN	C	2224:LYS	N	3.40
1	C	2473:PHE	C	2474:TRP	N	3.40
1	E	203:UNK	C	204:UNK	N	3.40
1	F	909:UNK	C	910:UNK	N	3.40
1	A	666:ASN	C	667:PHE	N	3.39
1	C	2365:ASP	C	2366:PRO	N	3.39
1	D	19:ALA	C	20:LEU	N	3.39
1	A	500:MET	C	501:ILE	N	3.38
1	A	2144:VAL	C	2145:ASN	N	3.38
1	A	2260:THR	C	2261:ARG	N	3.38
1	C	1054:ASP	C	1055:GLN	N	3.38
1	A	1848:TRP	C	1849:PHE	N	3.37
1	A	2048:LYS	C	2049:ILE	N	3.37
1	C	270:VAL	C	271:PRO	N	3.37
1	C	1104:ILE	C	1105:THR	N	3.37
1	C	1849:LEU	C	1850:TRP	N	3.37
1	C	2219:LEU	C	2220:THR	N	3.37
1	D	12:HIS	C	13:THR	N	3.37
1	H	127:LEU	C	128:LEU	N	3.37

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	164:GLU	C	165:LEU	N	3.36
1	A	691:ILE	C	692:GLN	N	3.36
1	A	731:PRO	C	732:LYS	N	3.36
1	A	1950:VAL	C	1951:SER	N	3.36
1	A	2047:ARG	C	2048:LYS	N	3.36
1	A	2379:GLU	C	2380:GLU	N	3.36
1	C	815:SER	C	816:PHE	N	3.36
1	C	853:LEU	C	854:LYS	N	3.36
1	C	936:ILE	C	937:HIS	N	3.36
1	C	1489:SER	C	1490:VAL	N	3.36
1	C	1525:LEU	C	1526:LEU	N	3.36
1	C	2231:ALA	C	2232:LEU	N	3.36
1	D	42:ASN	C	43:ASP	N	3.36
1	D	189:PRO	C	190:ASN	N	3.36
1	D	288:TYR	C	289:GLY	N	3.36
1	D	300:LEU	C	301:ASN	N	3.36
1	F	655:UNK	C	656:UNK	N	3.36
1	A	80:THR	C	81:PHE	N	3.35
1	A	337:LEU	C	338:LYS	N	3.35
1	A	507:PRO	C	508:SER	N	3.35
1	A	517:ILE	C	518:LEU	N	3.35
1	A	569:ALA	C	570:GLN	N	3.35
1	A	629:SER	C	630:VAL	N	3.35
1	A	679:LEU	C	680:LEU	N	3.35
1	A	1344:CYS	C	1345:HIS	N	3.35
1	A	1723:TRP	C	1724:ARG	N	3.35
1	A	1885:HIS	C	1886:GLN	N	3.35
1	A	1923:LEU	C	1924:SER	N	3.35
1	A	1999:GLY	C	2000:PRO	N	3.35
1	A	2080:GLY	C	2081:THR	N	3.35
1	A	2192:HIS	C	2193:ARG	N	3.35
1	B	300:LEU	C	301:ASN	N	3.35
1	C	1091:THR	C	1092:GLU	N	3.35
1	C	1130:LEU	C	1131:ASN	N	3.35
1	C	1533:LEU	C	1534:VAL	N	3.35
1	C	1606:GLU	C	1607:ASP	N	3.35
1	C	1753:ASN	C	1754:THR	N	3.35
1	C	2412:GLU	C	2413:HIS	N	3.35
1	E	503:UNK	C	504:UNK	N	3.35
1	H	101:PHE	C	102:ILE	N	3.35
1	H	113:ILE	C	114:HIS	N	3.35
1	H	133:ALA	C	134:ASP	N	3.35

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	162:LEU	C	163:ASN	N	3.35
1	A	715:ARG	C	716:LYS	N	3.34
1	A	935:ILE	C	936:HIS	N	3.34
1	A	1763:ALA	C	1764:ASN	N	3.34
1	A	1859:GLN	C	1860:ALA	N	3.34
1	A	1872:THR	C	1873:TRP	N	3.34
1	A	2212:PRO	C	2213:ASP	N	3.34
1	A	2416:ARG	C	2417:ASN	N	3.34
1	B	167:MET	C	168:ALA	N	3.34
1	C	1380:HIS	C	1381:GLN	N	3.34
1	C	1414:ALA	C	1415:LEU	N	3.34
1	C	1430:GLU	C	1431:VAL	N	3.34
1	C	1530:LEU	C	1531:SER	N	3.34
1	C	1709:GLU	C	1710:ASP	N	3.34
1	C	2242:LYS	C	2243:VAL	N	3.34
1	C	2452:LYS	C	2453:LEU	N	3.34
1	E	380:UNK	C	381:UNK	N	3.34
1	E	450:UNK	C	451:UNK	N	3.34
1	E	601:UNK	C	602:UNK	N	3.34
1	E	864:UNK	C	865:UNK	N	3.34
1	F	268:UNK	C	300:UNK	N	3.34
1	F	453:UNK	C	454:UNK	N	3.34
1	F	903:UNK	C	904:UNK	N	3.34
1	G	53:TYR	C	54:LEU	N	3.34
1	H	124:CYS	C	125:LEU	N	3.34
1	H	161:LEU	C	162:LEU	N	3.34
1	A	834:VAL	C	835:VAL	N	3.33
1	A	1084:PRO	C	1085:ILE	N	3.33
1	A	1117:MET	C	1118:SER	N	3.33
1	A	1350:ALA	C	1351:LEU	N	3.33
1	A	1734:SER	C	1735:ASN	N	3.33
1	A	2067:LYS	C	2068:LEU	N	3.33
1	A	2091:LYS	C	2092:ILE	N	3.33
1	A	2181:ASN	C	2182:SER	N	3.33
1	A	2237:ASP	C	2238:LEU	N	3.33
1	A	2412:LYS	C	2413:ASN	N	3.33
1	B	195:SER	C	196:HIS	N	3.33
1	C	495:HIS	C	496:MET	N	3.33
1	C	541:ASN	C	542:GLN	N	3.33
1	C	639:GLU	C	640:VAL	N	3.33
1	C	760:ILE	C	761:LEU	N	3.33
1	C	1393:GLN	C	1394:GLN	N	3.33

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	1526:LEU	C	1527:VAL	N	3.33
1	C	1708:VAL	C	1709:GLU	N	3.33
1	C	2148:THR	C	2149:LEU	N	3.33
1	D	163:GLN	C	164:SER	N	3.33
1	F	560:UNK	C	561:UNK	N	3.33
1	F	908:UNK	C	909:UNK	N	3.33
1	G	81:LEU	C	82:ALA	N	3.33
1	G	151:GLU	C	152:TYR	N	3.33
1	G	198:LEU	C	199:LYS	N	3.33
1	H	57:VAL	C	58:TYR	N	3.33
1	H	191:GLY	C	192:ASN	N	3.33
1	A	343:ARG	C	344:ASP	N	3.32
1	A	472:PRO	C	473:ALA	N	3.32
1	A	850:ASN	C	851:ILE	N	3.32
1	A	1277:ASN	C	1278:ALA	N	3.32
1	A	1910:LEU	C	1911:VAL	N	3.32
1	A	2058:THR	C	2059:LEU	N	3.32
1	A	2399:ILE	C	2400:THR	N	3.32
1	A	2423:VAL	C	2424:LEU	N	3.32
1	C	318:SER	C	319:LEU	N	3.32
1	C	496:MET	C	497:GLN	N	3.32
1	C	865:THR	C	866:VAL	N	3.32
1	C	1232:GLN	C	1233:GLN	N	3.32
1	C	1557:ILE	C	1558:ILE	N	3.32
1	C	1664:THR	C	1665:GLY	N	3.32
1	C	1680:ARG	C	1681:MET	N	3.32
1	C	1748:ALA	C	1749:THR	N	3.32
1	C	1766:ASN	C	1767:PHE	N	3.32
1	C	1888:GLN	C	1889:PRO	N	3.32
1	E	462:UNK	C	463:UNK	N	3.32
1	E	756:UNK	C	757:UNK	N	3.32
1	F	902:UNK	C	903:UNK	N	3.32
1	G	88:GLU	C	89:GLN	N	3.32
1	G	184:VAL	C	185:ALA	N	3.32
1	H	106:GLY	C	107:GLU	N	3.32
1	J	687:LYS	C	688:TYR	N	3.32
1	A	471:GLY	C	472:PRO	N	3.31
1	A	725:LEU	C	726:LYS	N	3.31
1	A	860:ILE	C	861:ARG	N	3.31
1	A	1215:LYS	C	1216:LEU	N	3.31
1	A	1558:TYR	C	1559:LYS	N	3.31
1	A	1574:THR	C	1575:TRP	N	3.31

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1655:GLN	C	1656:LEU	N	3.31
1	A	1721:GLY	C	1722:GLU	N	3.31
1	A	1930:LEU	C	1931:SER	N	3.31
1	A	1962:HIS	C	1963:GLU	N	3.31
1	A	1990:GLU	C	1991:PRO	N	3.31
1	A	2187:VAL	C	2188:LEU	N	3.31
1	A	2457:SER	C	2458:VAL	N	3.31
1	B	216:SER	C	217:SER	N	3.31
1	C	326:HIS	C	327:ALA	N	3.31
1	C	406:ASN	C	407:ALA	N	3.31
1	C	695:GLU	C	696:ALA	N	3.31
1	C	940:ALA	C	941:ALA	N	3.31
1	C	1056:SER	C	1057:ASN	N	3.31
1	C	1281:PHE	C	1282:SER	N	3.31
1	C	1440:TYR	C	1441:ALA	N	3.31
1	C	1944:VAL	C	1945:LEU	N	3.31
1	C	2239:ASP	C	2240:LEU	N	3.31
1	D	96:ASP	C	97:GLY	N	3.31
1	E	163:UNK	C	164:UNK	N	3.31
1	F	114:UNK	C	115:UNK	N	3.31
1	F	166:UNK	C	167:UNK	N	3.31
1	F	701:UNK	C	702:UNK	N	3.31
1	G	59:LEU	C	60:ILE	N	3.31
1	G	72:THR	C	73:PHE	N	3.31
1	G	97:GLN	C	98:PHE	N	3.31
1	G	173:VAL	C	174:ARG	N	3.31
1	A	351:LYS	C	352:SER	N	3.30
1	A	1540:TYR	C	1541:ASN	N	3.30
1	A	1669:LEU	C	1670:LYS	N	3.30
1	A	1764:ASN	C	1765:PHE	N	3.30
1	A	2179:VAL	C	2180:PRO	N	3.30
1	A	2210:MET	C	2211:ALA	N	3.30
1	C	91:LYS	C	92:LEU	N	3.30
1	C	147:ILE	C	148:GLY	N	3.30
1	C	498:GLU	C	499:THR	N	3.30
1	C	574:ILE	C	575:GLN	N	3.30
1	C	663:HIS	C	664:LEU	N	3.30
1	C	1080:SER	C	1081:HIS	N	3.30
1	C	1146:SER	C	1147:LEU	N	3.30
1	C	1667:GLN	C	1668:ASP	N	3.30
1	C	1716:ALA	C	1717:ARG	N	3.30
1	C	2182:PRO	C	2183:ASN	N	3.30

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2432:LYS	C	2433:LEU	N	3.30
1	D	88:ARG	C	89:TRP	N	3.30
1	D	117:ALA	C	118:PRO	N	3.30
1	E	256:UNK	C	257:UNK	N	3.30
1	E	308:UNK	C	309:UNK	N	3.30
1	E	559:UNK	C	560:UNK	N	3.30
1	F	304:UNK	C	305:UNK	N	3.30
1	F	375:UNK	C	376:UNK	N	3.30
1	F	410:UNK	C	411:UNK	N	3.30
1	G	90:THR	C	91:LEU	N	3.30
1	G	172:ASN	C	173:VAL	N	3.30
1	H	85:LYS	C	86:GLY	N	3.30
1	J	694:THR	C	695:THR	N	3.30
1	J	750:PRO	C	751:PHE	N	3.30
1	J	767:ILE	C	768:SER	N	3.30
1	A	762:VAL	C	763:ILE	N	3.29
1	A	1438:TYR	C	1439:ALA	N	3.29
1	A	1460:GLU	C	1461:VAL	N	3.29
1	A	1816:HIS	C	1817:ARG	N	3.29
1	A	2006:ILE	C	2007:SER	N	3.29
1	A	2043:TYR	C	2044:ASN	N	3.29
1	B	217:SER	C	218:ASP	N	3.29
1	C	159:PHE	C	160:TYR	N	3.29
1	C	204:GLY	C	205:THR	N	3.29
1	C	554:GLN	C	555:SER	N	3.29
1	C	614:LEU	C	615:THR	N	3.29
1	C	774:ALA	C	775:VAL	N	3.29
1	C	780:LEU	C	781:LYS	N	3.29
1	C	856:GLU	C	857:ASN	N	3.29
1	C	1869:LEU	C	1870:ILE	N	3.29
1	C	1967:TRP	C	1968:TYR	N	3.29
1	C	2187:PHE	C	2188:HIS	N	3.29
1	C	2369:ASN	C	2370:TRP	N	3.29
1	C	2385:ILE	C	2386:GLN	N	3.29
1	D	73:GLY	C	74:HIS	N	3.29
1	F	707:UNK	C	708:UNK	N	3.29
1	F	864:UNK	C	865:UNK	N	3.29
1	G	71:LYS	C	72:THR	N	3.29
1	H	92:HIS	C	93:LEU	N	3.29
1	I	701:SER	C	702:THR	N	3.29
1	A	155:LEU	C	156:ILE	N	3.28
1	A	528:GLU	C	529:LYS	N	3.28

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	749:ASP	C	750:GLU	N	3.28
1	A	943:ALA	C	944:ILE	N	3.28
1	A	1253:SER	C	1254:PRO	N	3.28
1	A	1360:GLU	C	1361:GLU	N	3.28
1	A	1972:ALA	C	1973:SER	N	3.28
1	A	2128:HIS	C	2129:GLU	N	3.28
1	A	2459:GLU	C	2460:ASN	N	3.28
1	B	234:TRP	C	235:SER	N	3.28
1	C	93:LYS	C	94:SER	N	3.28
1	C	735:LYS	C	736:GLU	N	3.28
1	C	980:ASP	C	981:PHE	N	3.28
1	C	1211:GLU	C	1212:MET	N	3.28
1	C	2067:SER	C	2068:PRO	N	3.28
1	C	2216:TYR	C	2217:ASP	N	3.28
1	C	2264:SER	C	2265:LEU	N	3.28
1	C	2282:PRO	C	2283:SER	N	3.28
1	C	2363:ALA	C	2364:PHE	N	3.28
1	C	2424:LEU	C	2425:VAL	N	3.28
1	D	13:THR	C	14:ILE	N	3.28
1	E	369:UNK	C	370:UNK	N	3.28
1	E	911:UNK	C	912:UNK	N	3.28
1	F	756:UNK	C	757:UNK	N	3.28
1	H	54:LEU	C	55:ILE	N	3.28
1	H	143:ASP	C	144:THR	N	3.28
1	A	156:ILE	C	157:SER	N	3.27
1	A	197:ARG	C	198:LEU	N	3.27
1	A	291:THR	C	292:ILE	N	3.27
1	A	818:ASP	C	819:ALA	N	3.27
1	A	1373:ILE	C	1374:ASN	N	3.27
1	A	1876:VAL	C	1877:LEU	N	3.27
1	A	2160:ASP	C	2161:ILE	N	3.27
1	A	2395:SER	C	2396:ASN	N	3.27
1	B	237:ASP	C	238:ASP	N	3.27
1	C	531:PHE	C	532:ILE	N	3.27
1	C	803:PRO	C	804:LEU	N	3.27
1	C	1065:ILE	C	1066:LEU	N	3.27
1	C	1125:ALA	C	1126:LEU	N	3.27
1	C	1335:PRO	C	1336:ILE	N	3.27
1	C	1412:GLU	C	1413:ASP	N	3.27
1	C	1744:SER	C	1745:TYR	N	3.27
1	C	2095:SER	C	2096:LYS	N	3.27
1	C	2141:GLN	C	2142:LEU	N	3.27

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2366:PRO	C	2367:LEU	N	3.27
1	D	84:GLN	C	85:GLN	N	3.27
1	E	155:UNK	C	156:UNK	N	3.27
1	E	206:UNK	C	207:UNK	N	3.27
1	E	317:UNK	C	318:UNK	N	3.27
1	F	558:UNK	C	559:UNK	N	3.27
1	F	850:UNK	C	851:UNK	N	3.27
1	G	103:ASN	C	104:HIS	N	3.27
1	I	654:ASN	C	655:SER	N	3.27
1	A	332:ARG	C	333:GLU	N	3.26
1	A	985:LEU	C	986:GLY	N	3.26
1	A	1007:ILE	C	1008:ARG	N	3.26
1	A	1178:GLN	C	1179:LEU	N	3.26
1	A	1328:LYS	C	1329:PRO	N	3.26
1	A	1844:LEU	C	1845:LEU	N	3.26
1	A	2079:PRO	C	2080:GLY	N	3.26
1	A	2224:GLU	C	2225:VAL	N	3.26
1	A	2295:ILE	C	2296:ASP	N	3.26
1	A	2420:ALA	C	2421:MET	N	3.26
1	C	581:GLN	C	582:LEU	N	3.26
1	C	586:GLN	C	587:TYR	N	3.26
1	C	689:ILE	C	690:PHE	N	3.26
1	C	733:LYS	C	734:LYS	N	3.26
1	C	744:THR	C	745:LEU	N	3.26
1	C	812:GLN	C	813:SER	N	3.26
1	C	816:PHE	C	817:LYS	N	3.26
1	C	852:ILE	C	853:LEU	N	3.26
1	C	1376:ASN	C	1377:ASN	N	3.26
1	C	1830:HIS	C	1831:SER	N	3.26
1	C	1892:ILE	C	1893:VAL	N	3.26
1	C	2007:GLU	C	2008:ILE	N	3.26
1	C	2290:ILE	C	2291:THR	N	3.26
1	F	255:UNK	C	256:UNK	N	3.26
1	F	316:UNK	C	317:UNK	N	3.26
1	G	62:LEU	C	63:GLY	N	3.26
1	G	106:GLY	C	107:GLU	N	3.26
1	H	45:HIS	C	46:TYR	N	3.26
1	I	693:PHE	C	694:THR	N	3.26
1	I	741:LEU	C	742:LYS	N	3.26
1	J	765:GLN	C	766:SER	N	3.26
1	A	822:THR	C	823:THR	N	3.25
1	A	825:GLY	C	826:GLN	N	3.25

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	914:GLU	C	915:TYR	N	3.25
1	A	924:LEU	C	925:MET	N	3.25
1	A	1028:SER	C	1029:LYS	N	3.25
1	A	1053:ASP	C	1054:GLN	N	3.25
1	A	1207:TYR	C	1208:GLU	N	3.25
1	A	1542:VAL	C	1543:VAL	N	3.25
1	A	1719:LYS	C	1720:GLN	N	3.25
1	A	1742:SER	C	1743:TYR	N	3.25
1	A	1964:GLN	C	1965:TRP	N	3.25
1	A	2314:VAL	C	2315:PRO	N	3.25
1	B	193:ASP	C	194:ALA	N	3.25
1	C	654:ALA	C	655:GLU	N	3.25
1	C	970:VAL	C	971:MET	N	3.25
1	C	972:ARG	C	973:SER	N	3.25
1	C	1262:CYS	C	1263:SER	N	3.25
1	C	1366:ASN	C	1367:SER	N	3.25
1	C	1950:GLU	C	1951:LEU	N	3.25
1	C	2030:LYS	C	2031:SER	N	3.25
1	C	2055:LEU	C	2056:PRO	N	3.25
1	C	2277:LEU	C	2278:GLY	N	3.25
1	D	41:THR	C	42:ASN	N	3.25
1	D	49:THR	C	50:ALA	N	3.25
1	D	82:SER	C	83:PHE	N	3.25
1	E	310:UNK	C	311:UNK	N	3.25
1	E	566:UNK	C	567:UNK	N	3.25
1	E	858:UNK	C	859:UNK	N	3.25
1	F	262:UNK	C	263:UNK	N	3.25
1	F	303:UNK	C	304:UNK	N	3.25
1	F	463:UNK	C	464:UNK	N	3.25
1	F	805:UNK	C	806:UNK	N	3.25
1	H	171:ASP	C	172:ASN	N	3.25
1	A	162:THR	C	163:GLU	N	3.24
1	A	744:LEU	C	745:ILE	N	3.24
1	A	754:PRO	C	755:TYR	N	3.24
1	A	824:LEU	C	825:GLY	N	3.24
1	A	849:ILE	C	850:ASN	N	3.24
1	A	940:ALA	C	941:ILE	N	3.24
1	A	1138:LYS	C	1139:ALA	N	3.24
1	A	1527:GLU	C	1528:LEU	N	3.24
1	A	1580:LEU	C	1581:GLY	N	3.24
1	A	1959:VAL	C	1960:LEU	N	3.24
1	A	2204:HIS	C	2205:TRP	N	3.24

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2383:ILE	C	2384:GLN	N	3.24
1	B	22:GLY	C	23:VAL	N	3.24
1	C	846:LEU	C	847:GLY	N	3.24
1	C	981:PHE	C	982:TYR	N	3.24
1	C	1106:LEU	C	1107:GLY	N	3.24
1	C	1112:ASN	C	1113:ILE	N	3.24
1	C	1156:PHE	C	1157:VAL	N	3.24
1	C	1236:LYS	C	1237:GLU	N	3.24
1	C	1661:LEU	C	1662:TRP	N	3.24
1	C	1665:GLY	C	1666:LEU	N	3.24
1	C	1908:HIS	C	1909:PRO	N	3.24
1	D	37:ARG	C	38:LEU	N	3.24
1	F	159:UNK	C	160:UNK	N	3.24
1	A	383:PHE	C	384:THR	N	3.23
1	A	532:GLN	C	533:SER	N	3.23
1	A	1042:THR	C	1043:LEU	N	3.23
1	A	1056:ASN	C	1057:LYS	N	3.23
1	A	1131:ASN	C	1132:GLY	N	3.23
1	A	1352:HIS	C	1353:TYR	N	3.23
1	A	1612:PHE	C	1613:ALA	N	3.23
1	A	2203:GLU	C	2204:HIS	N	3.23
1	A	2234:GLU	C	2235:GLY	N	3.23
1	C	422:ASP	C	423:ILE	N	3.23
1	C	643:LYS	C	644:LEU	N	3.23
1	C	1043:THR	C	1044:LEU	N	3.23
1	C	1214:VAL	C	1215:THR	N	3.23
1	C	1492:LYS	C	1493:SER	N	3.23
1	C	1852:THR	C	1853:PHE	N	3.23
1	C	1894:SER	C	1895:ARG	N	3.23
1	C	1952:VAL	C	1953:SER	N	3.23
1	C	1970:GLY	C	1971:LEU	N	3.23
1	C	2031:SER	C	2032:LYS	N	3.23
1	C	2149:LEU	C	2150:LEU	N	3.23
1	D	149:GLN	C	150:CYS	N	3.23
1	G	49:TYR	C	50:HIS	N	3.23
1	G	82:ALA	C	83:LEU	N	3.23
1	G	182:ILE	C	183:ASP	N	3.23
1	H	88:GLU	C	89:GLN	N	3.23
1	H	159:LYS	C	160:MET	N	3.23
1	A	181:PRO	C	182:SER	N	3.22
1	A	245:ILE	C	246:LYS	N	3.22
1	A	728:SER	C	729:ASN	N	3.22

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	729:ASN	C	730:MET	N	3.22
1	A	836:GLY	C	837:PRO	N	3.22
1	A	1070:THR	C	1071:PHE	N	3.22
1	A	1530:ALA	C	1531:LEU	N	3.22
1	A	1550:ALA	C	1551:GLU	N	3.22
1	A	1838:LEU	C	1839:GLN	N	3.22
1	A	2206:VAL	C	2207:MET	N	3.22
1	A	2259:TYR	C	2260:THR	N	3.22
1	A	2300:CYS	C	2301:PHE	N	3.22
1	B	5:LEU	C	6:VAL	N	3.22
1	B	82:SER	C	83:PHE	N	3.22
1	C	153:VAL	C	154:ASP	N	3.22
1	C	1025:ILE	C	1026:GLU	N	3.22
1	C	1186:ASN	C	1187:ASN	N	3.22
1	C	1715:LEU	C	1716:ALA	N	3.22
1	C	1767:PHE	C	1768:GLU	N	3.22
1	C	2075:ASP	C	2076:LEU	N	3.22
1	C	2454:ILE	C	2455:GLN	N	3.22
1	D	86:ASP	C	87:ASN	N	3.22
1	D	281:THR	C	282:ARG	N	3.22
1	E	859:UNK	C	860:UNK	N	3.22
1	F	264:UNK	C	265:UNK	N	3.22
1	F	806:UNK	C	807:UNK	N	3.22
1	G	195:SER	C	196:LYS	N	3.22
1	H	102:ILE	C	103:ASN	N	3.22
1	I	726:ASP	C	727:GLY	N	3.22
1	A	1003:ILE	C	1004:TYR	N	3.21
1	A	1026:SER	C	1027:ILE	N	3.21
1	A	1494:PRO	C	1495:ASP	N	3.21
1	A	2149:GLN	C	2150:ASN	N	3.21
1	A	2350:LYS	C	2351:GLY	N	3.21
1	A	2397:GLY	C	2398:ALA	N	3.21
1	B	41:THR	C	42:ASN	N	3.21
1	B	90:MET	C	91:VAL	N	3.21
1	B	172:SER	C	173:MET	N	3.21
1	B	273:TYR	C	274:VAL	N	3.21
1	C	635:HIS	C	636:SER	N	3.21
1	C	699:ILE	C	700:ILE	N	3.21
1	C	1038:ARG	C	1039:PHE	N	3.21
1	C	1155:ASP	C	1156:PHE	N	3.21
1	C	1160:VAL	C	1161:PRO	N	3.21
1	C	1843:ALA	C	1844:LEU	N	3.21

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2164:GLN	C	2165:GLN	N	3.21
1	C	2295:ILE	C	2296:HIS	N	3.21
1	C	2342:GLU	C	2343:ASN	N	3.21
1	C	2467:TYR	C	2468:ILE	N	3.21
1	D	74:HIS	C	75:ARG	N	3.21
1	D	135:ASP	C	136:ARG	N	3.21
1	F	153:UNK	C	154:UNK	N	3.21
1	F	307:UNK	C	308:UNK	N	3.21
1	A	148:GLY	C	149:ILE	N	3.20
1	A	1604:GLU	C	1605:ASP	N	3.20
1	A	1829:SER	C	1830:ILE	N	3.20
1	A	2227:THR	C	2228:TYR	N	3.20
1	B	39:GLU	C	40:ILE	N	3.20
1	B	169:SER	C	170:ASP	N	3.20
1	C	257:LEU	C	258:TYR	N	3.20
1	C	1064:ARG	C	1065:ILE	N	3.20
1	C	1245:ARG	C	1246:LEU	N	3.20
1	C	1508:HIS	C	1509:ARG	N	3.20
1	C	1826:LYS	C	1827:GLY	N	3.20
1	C	1831:SER	C	1832:ILE	N	3.20
1	E	215:UNK	C	216:UNK	N	3.20
1	E	217:UNK	C	218:UNK	N	3.20
1	H	151:GLU	C	152:TYR	N	3.20
1	A	683:ALA	C	684:LEU	N	3.19
1	A	782:LEU	C	783:GLY	N	3.19
1	A	1107:ARG	C	1108:LEU	N	3.19
1	A	2343:MET	C	2344:LYS	N	3.19
1	B	68:VAL	C	69:ALA	N	3.19
1	B	94:SER	C	95:GLU	N	3.19
1	C	1110:ALA	C	1111:LYS	N	3.19
1	C	1251:LEU	C	1252:LYS	N	3.19
1	C	1645:ASN	C	1646:THR	N	3.19
1	C	1762:TRP	C	1763:ALA	N	3.19
1	C	2204:ILE	C	2205:GLU	N	3.19
1	D	234:TRP	C	235:SER	N	3.19
1	D	260:ALA	C	261:ASP	N	3.19
1	D	287:GLN	C	288:TYR	N	3.19
1	E	856:UNK	C	857:UNK	N	3.19
1	E	866:UNK	C	867:UNK	N	3.19
1	F	377:UNK	C	378:UNK	N	3.19
1	F	412:UNK	C	413:UNK	N	3.19
1	F	608:UNK	C	609:UNK	N	3.19

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	675:SER	C	676:MET	N	3.19
1	J	714:TYR	C	715:SER	N	3.19
1	A	497:GLU	C	498:THR	N	3.18
1	A	611:ALA	C	612:ALA	N	3.18
1	A	948:PHE	C	949:GLN	N	3.18
1	A	1059:ILE	C	1060:VAL	N	3.18
1	A	1284:TRP	C	1285:VAL	N	3.18
1	A	1981:ASN	C	1982:THR	N	3.18
1	A	2101:VAL	C	2102:ILE	N	3.18
1	A	2369:GLY	C	2370:PHE	N	3.18
1	A	2429:ASP	C	2430:LYS	N	3.18
1	B	188:MET	C	189:PRO	N	3.18
1	B	211:THR	C	212:ARG	N	3.18
1	C	268:ILE	C	269:TRP	N	3.18
1	C	717:LYS	C	718:THR	N	3.18
1	C	1163:ILE	C	1164:ASN	N	3.18
1	C	1180:LEU	C	1181:VAL	N	3.18
1	C	1231:SER	C	1232:GLN	N	3.18
1	C	1765:ALA	C	1766:ASN	N	3.18
1	C	1885:ARG	C	1886:ILE	N	3.18
1	C	1886:ILE	C	1887:HIS	N	3.18
1	C	1955:GLU	C	1956:LEU	N	3.18
1	E	608:UNK	C	609:UNK	N	3.18
1	F	252:UNK	C	253:UNK	N	3.18
1	F	364:UNK	C	365:UNK	N	3.18
1	F	510:UNK	C	511:UNK	N	3.18
1	F	758:UNK	C	759:UNK	N	3.18
1	H	49:TYR	C	50:HIS	N	3.18
1	H	107:GLU	C	108:ASN	N	3.18
1	A	566:ILE	C	567:THR	N	3.17
1	A	662:HIS	C	663:LEU	N	3.17
1	A	738:ALA	C	739:THR	N	3.17
1	A	798:LYS	C	799:GLU	N	3.17
1	A	814:SER	C	815:PHE	N	3.17
1	A	971:ARG	C	972:SER	N	3.17
1	A	1020:ILE	C	1021:ILE	N	3.17
1	A	1642:PRO	C	1643:ASN	N	3.17
1	A	2195:ALA	C	2196:LYS	N	3.17
1	A	2340:GLU	C	2341:ASN	N	3.17
1	C	480:ASN	C	481:LYS	N	3.17
1	C	670:PRO	C	671:GLN	N	3.17
1	C	719:LEU	C	720:LEU	N	3.17

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	834:TYR	C	835:VAL	N	3.17
1	C	1124:GLN	C	1125:ALA	N	3.17
1	C	1475:ALA	C	1476:TRP	N	3.17
1	C	2179:GLY	C	2180:TRP	N	3.17
1	C	2349:ARG	C	2350:ASP	N	3.17
1	E	109:UNK	C	110:UNK	N	3.17
1	E	204:UNK	C	205:UNK	N	3.17
1	E	401:UNK	C	402:UNK	N	3.17
1	E	706:UNK	C	707:UNK	N	3.17
1	G	96:GLN	C	97:GLN	N	3.17
1	I	674:GLU	C	675:SER	N	3.17
1	J	727:GLY	C	728:LEU	N	3.17
1	A	457:LYS	C	458:ASP	N	3.16
1	A	545:GLU	C	546:LYS	N	3.16
1	A	596:THR	C	597:ILE	N	3.16
1	A	639:VAL	C	640:LEU	N	3.16
1	A	711:VAL	C	712:PRO	N	3.16
1	A	1569:LEU	C	1570:THR	N	3.16
1	A	2039:TRP	C	2040:ASP	N	3.16
1	A	2145:ASN	C	2146:THR	N	3.16
1	A	2156:ARG	C	2157:ARG	N	3.16
1	C	179:VAL	C	180:LEU	N	3.16
1	C	239:ARG	C	240:HIS	N	3.16
1	C	513:THR	C	514:VAL	N	3.16
1	C	716:ARG	C	717:LYS	N	3.16
1	C	758:ASP	C	759:PRO	N	3.16
1	C	765:LEU	C	766:PRO	N	3.16
1	C	769:GLN	C	770:ASP	N	3.16
1	C	1161:PRO	C	1162:VAL	N	3.16
1	C	1331:PRO	C	1332:LEU	N	3.16
1	C	1428:SER	C	1429:VAL	N	3.16
1	C	1494:GLN	C	1495:SER	N	3.16
1	C	1622:GLY	C	1623:ARG	N	3.16
1	C	2168:ALA	C	2169:ILE	N	3.16
1	C	2180:TRP	C	2181:VAL	N	3.16
1	C	2429:ILE	C	2430:THR	N	3.16
1	C	2439:ARG	C	2440:ARG	N	3.16
1	C	2456:GLN	C	2457:ALA	N	3.16
1	D	78:VAL	C	79:THR	N	3.16
1	F	551:UNK	C	552:UNK	N	3.16
1	I	690:ARG	C	691:ASN	N	3.16
1	A	397:ARG	C	398:TYR	N	3.15

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1469:ALA	C	1470:ALA	N	3.15
1	A	1492:GLN	C	1493:SER	N	3.15
1	A	1552:LEU	C	1553:GLU	N	3.15
1	A	1656:LEU	C	1657:LYS	N	3.15
1	A	1831:SER	C	1832:LEU	N	3.15
1	A	1858:THR	C	1859:GLN	N	3.15
1	A	2215:ASP	C	2216:ASN	N	3.15
1	A	2220:LEU	C	2221:GLN	N	3.15
1	A	2352:SER	C	2353:LEU	N	3.15
1	A	2465:TYR	C	2466:ILE	N	3.15
1	B	228:ASP	C	229:HIS	N	3.15
1	B	236:ILE	C	237:ASP	N	3.15
1	C	200:THR	C	201:VAL	N	3.15
1	C	360:TYR	C	361:LYS	N	3.15
1	C	713:PRO	C	714:SER	N	3.15
1	C	915:GLU	C	916:TYR	N	3.15
1	C	1567:SER	C	1568:ASP	N	3.15
1	C	2465:GLN	C	2466:HIS	N	3.15
1	D	142:ILE	C	143:TRP	N	3.15
1	E	208:UNK	C	209:UNK	N	3.15
1	F	507:UNK	C	508:UNK	N	3.15
1	H	186:GLN	C	187:THR	N	3.15
1	A	1727:LEU	C	1728:GLN	N	3.14
1	A	2106:GLN	C	2107:ARG	N	3.14
1	A	2447:GLN	C	2448:VAL	N	3.14
1	B	140:ILE	C	141:ARG	N	3.14
1	B	192:THR	C	193:ASP	N	3.14
1	C	510:LEU	C	511:GLU	N	3.14
1	C	1226:ASN	C	1227:ALA	N	3.14
1	C	1410:ARG	C	1411:TRP	N	3.14
1	C	1832:ILE	C	1833:SER	N	3.14
1	C	2019:ASN	C	2020:ASP	N	3.14
1	C	2259:THR	C	2260:THR	N	3.14
1	D	246:LEU	C	247:ASP	N	3.14
1	A	459:LEU	C	460:PHE	N	3.13
1	A	678:ARG	C	679:LEU	N	3.13
1	A	1266:SER	C	1267:VAL	N	3.13
1	A	1709:TYR	C	1710:THR	N	3.13
1	A	1747:THR	C	1748:HIS	N	3.13
1	A	2049:ILE	C	2050:GLY	N	3.13
1	B	220:LYS	C	221:HIS	N	3.13
1	C	458:LYS	C	459:ASP	N	3.13

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	476:ALA	C	477:LYS	N	3.13
1	C	775:VAL	C	776:ALA	N	3.13
1	C	790:GLY	C	791:GLY	N	3.13
1	C	1060:ILE	C	1061:VAL	N	3.13
1	C	1188:GLU	C	1189:CYS	N	3.13
1	C	1228:TRP	C	1229:TYR	N	3.13
1	C	1964:HIS	C	1965:GLU	N	3.13
1	D	129:GLY	C	130:GLU	N	3.13
1	D	201:THR	C	202:LYS	N	3.13
1	E	565:UNK	C	566:UNK	N	3.13
1	G	101:PHE	C	102:ILE	N	3.13
1	A	709:TYR	C	710:VAL	N	3.12
1	A	806:ASN	C	807:THR	N	3.12
1	A	1568:ARG	C	1569:LEU	N	3.12
1	A	1946:GLN	C	1947:ALA	N	3.12
1	A	2059:LEU	C	2060:GLU	N	3.12
1	A	2097:PRO	C	2098:VAL	N	3.12
1	A	2226:PHE	C	2227:THR	N	3.12
1	A	2331:ILE	C	2332:GLU	N	3.12
1	C	352:LYS	C	353:SER	N	3.12
1	C	802:MET	C	803:PRO	N	3.12
1	C	926:MET	C	927:LYS	N	3.12
1	C	932:PRO	C	933:SER	N	3.12
1	C	1027:SER	C	1028:ILE	N	3.12
1	C	1321:LEU	C	1322:VAL	N	3.12
1	C	1983:ASN	C	1984:THR	N	3.12
1	C	2173:PRO	C	2174:LYS	N	3.12
1	C	2350:ASP	C	2351:ASN	N	3.12
1	D	220:LYS	C	221:HIS	N	3.12
1	E	758:UNK	C	759:UNK	N	3.12
1	F	704:UNK	C	705:UNK	N	3.12
1	H	150:LEU	C	151:GLU	N	3.12
1	A	398:TYR	C	399:LEU	N	3.11
1	A	477:HIS	C	478:LEU	N	3.11
1	A	688:ILE	C	689:PHE	N	3.11
1	A	1980:HIS	C	1981:ASN	N	3.11
1	A	2197:LYS	C	2198:ILE	N	3.11
1	B	246:LEU	C	247:ASP	N	3.11
1	C	245:ILE	C	246:ILE	N	3.11
1	C	700:ILE	C	701:GLY	N	3.11
1	C	1347:HIS	C	1348:ALA	N	3.11
1	C	1966:GLN	C	1967:TRP	N	3.11

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2002:PRO	C	2003:GLU	N	3.11
1	D	223:ALA	C	224:THR	N	3.11
1	A	760:LEU	C	761:ASP	N	3.10
1	A	785:LEU	C	786:SER	N	3.10
1	A	1754:TYR	C	1755:LYS	N	3.10
1	A	2344:LYS	C	2345:VAL	N	3.10
1	B	127:ASN	C	128:GLN	N	3.10
1	C	946:MET	C	947:HIS	N	3.10
1	C	1093:TYR	C	1094:SER	N	3.10
1	C	1646:THR	C	1647:ALA	N	3.10
1	D	252:TRP	C	253:VAL	N	3.10
1	G	181:PRO	C	182:ILE	N	3.10
1	A	440:ASN	C	441:ILE	N	3.09
1	A	549:LYS	C	550:SER	N	3.09
1	A	807:THR	C	808:PHE	N	3.09
1	A	1184:LEU	C	1185:ASN	N	3.09
1	A	2271:TYR	C	2272:ILE	N	3.09
1	A	2419:ARG	C	2420:ALA	N	3.09
1	B	185:VAL	C	186:TRP	N	3.09
1	B	284:ILE	C	285:VAL	N	3.09
1	C	315:HIS	C	316:GLY	N	3.09
1	C	1723:GLY	C	1724:GLU	N	3.09
1	C	2008:ILE	C	2009:SER	N	3.09
1	C	2036:ASN	C	2037:LEU	N	3.09
1	C	2316:VAL	C	2317:PRO	N	3.09
1	D	274:VAL	C	275:ARG	N	3.09
1	F	105:UNK	C	106:UNK	N	3.09
1	F	211:UNK	C	212:UNK	N	3.09
1	G	159:LYS	C	160:MET	N	3.09
1	J	672:ASN	C	673:TYR	N	3.09
1	A	559:THR	C	560:GLY	N	3.08
1	A	722:LEU	C	723:THR	N	3.08
1	B	33:SER	C	34:GLN	N	3.08
1	C	384:PHE	C	385:THR	N	3.08
1	C	1042:GLU	C	1043:THR	N	3.08
1	C	1225:LYS	C	1226:ASN	N	3.08
1	C	1603:LYS	C	1604:PRO	N	3.08
1	C	1658:LEU	C	1659:LYS	N	3.08
1	C	2048:PHE	C	2049:ARG	N	3.08
1	C	2186:THR	C	2187:PHE	N	3.08
1	D	286:ARG	C	287:GLN	N	3.08
1	E	357:UNK	C	358:UNK	N	3.08

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	407:UNK	C	408:UNK	N	3.08
1	F	216:UNK	C	217:UNK	N	3.08
1	A	980:PHE	C	981:TYR	N	3.07
1	A	1213:VAL	C	1214:THR	N	3.07
1	A	1706:VAL	C	1707:GLU	N	3.07
1	A	2273:LEU	C	2274:GLY	N	3.07
1	C	1063:ILE	C	1064:ARG	N	3.07
1	C	1107:GLY	C	1108:ARG	N	3.07
1	C	2054:GLN	C	2055:LEU	N	3.07
1	C	2117:GLY	C	2118:SER	N	3.07
1	E	505:UNK	C	506:UNK	N	3.07
1	G	147:HIS	C	148:VAL	N	3.07
1	A	1064:ILE	C	1065:LEU	N	3.06
1	A	1240:GLU	C	1241:TRP	N	3.06
1	A	1286:GLU	C	1287:LEU	N	3.06
1	A	1464:ALA	C	1465:MET	N	3.06
1	A	1614:ASN	C	1615:LEU	N	3.06
1	A	1938:ILE	C	1939:HIS	N	3.06
1	A	2462:CYS	C	2463:GLN	N	3.06
1	B	13:THR	C	14:ILE	N	3.06
1	B	118:PRO	C	119:VAL	N	3.06
1	B	214:LEU	C	215:LEU	N	3.06
1	C	732:PRO	C	733:LYS	N	3.06
1	C	1039:PHE	C	1040:VAL	N	3.06
1	C	2221:LEU	C	2222:LEU	N	3.06
1	D	77:ASN	C	78:VAL	N	3.06
1	J	660:GLU	C	661:TYR	N	3.06
1	A	1576:ASN	C	1577:THR	N	3.05
1	A	2094:LYS	C	2095:PHE	N	3.05
1	A	2154:CYS	C	2155:PHE	N	3.05
1	B	252:TRP	C	253:VAL	N	3.05
1	C	469:CYS	C	470:ALA	N	3.05
1	C	801:LEU	C	802:MET	N	3.05
1	C	923:HIS	C	924:ASN	N	3.05
1	C	1482:ASP	C	1483:GLU	N	3.05
1	C	1736:SER	C	1737:ASN	N	3.05
1	E	403:UNK	C	404:UNK	N	3.05
1	F	116:UNK	C	117:UNK	N	3.05
1	A	543:SER	C	544:ILE	N	3.04
1	A	642:LYS	C	643:LEU	N	3.04
1	A	1567:LYS	C	1568:ARG	N	3.04
1	A	1651:VAL	C	1652:VAL	N	3.04

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1818:HIS	C	1819:VAL	N	3.04
1	A	1899:LEU	C	1900:SER	N	3.04
1	A	2042:TYR	C	2043:TYR	N	3.04
1	B	85:GLN	C	86:ASP	N	3.04
1	C	1267:SER	C	1268:VAL	N	3.04
1	C	1383:ASP	C	1384:SER	N	3.04
1	C	1815:ASN	C	1816:LEU	N	3.04
1	C	2053:LYS	C	2054:GLN	N	3.04
1	C	2291:THR	C	2292:GLY	N	3.04
1	E	113:UNK	C	114:UNK	N	3.04
1	F	208:UNK	C	209:UNK	N	3.04
1	G	56:CYS	C	57:VAL	N	3.04
1	A	922:HIS	C	923:ASN	N	3.03
1	A	1281:SER	C	1282:SER	N	3.03
1	A	1519:ASN	C	1520:ALA	N	3.03
1	A	1988:ALA	C	1989:LEU	N	3.03
1	C	1580:ARG	C	1581:LEU	N	3.03
1	C	2043:ILE	C	2044:TYR	N	3.03
1	H	181:PRO	C	182:ILE	N	3.03
1	I	767:ILE	C	768:SER	N	3.03
1	C	1517:VAL	C	1518:HIS	N	3.02
1	C	1881:GLN	C	1882:LEU	N	3.02
1	D	213:ILE	C	214:LEU	N	3.02
1	A	221:LEU	C	222:THR	N	3.01
1	A	756:ILE	C	757:ASP	N	3.01
1	A	967:ILE	C	968:LEU	N	3.01
1	A	1380:THR	C	1381:ASP	N	3.01
1	C	938:HIS	C	939:THR	N	3.01
1	C	1486:GLN	C	1487:TYR	N	3.01
1	E	604:UNK	C	605:UNK	N	3.01
1	B	148:ASN	C	149:GLN	N	3.00
1	C	1224:LEU	C	1225:LYS	N	3.00
1	C	1561:LYS	C	1562:LYS	N	3.00
1	D	216:SER	C	217:SER	N	3.00
1	D	265:LEU	C	266:VAL	N	3.00
1	A	364:ILE	C	365:ARG	N	2.99
1	A	968:LEU	C	969:VAL	N	2.99
1	A	1526:THR	C	1527:GLU	N	2.99
1	A	2315:PRO	C	2316:PHE	N	2.99
1	C	462:TYR	C	463:CYS	N	2.99
1	C	494:ASP	C	495:HIS	N	2.99
1	C	1014:ILE	C	1015:ILE	N	2.99

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	1677:PHE	C	1678:THR	N	2.99
1	C	2126:VAL	C	2127:LEU	N	2.99
1	C	2229:THR	C	2230:TYR	N	2.99
1	C	2413:HIS	C	2414:LYS	N	2.99
1	F	407:UNK	C	408:UNK	N	2.99
1	G	142:GLY	C	143:ASP	N	2.99
1	A	253:PRO	C	254:TYR	N	2.98
1	A	718:LEU	C	719:LEU	N	2.98
1	A	2014:ARG	C	2015:ASP	N	2.98
1	A	2045:VAL	C	2046:PHE	N	2.98
1	A	2184:THR	C	2185:PHE	N	2.98
1	B	16:PHE	C	17:TRP	N	2.98
1	C	1158:VAL	C	1159:PHE	N	2.98
1	C	2233:ASN	C	2234:ASN	N	2.98
1	D	28:ILE	C	29:GLN	N	2.98
1	D	89:TRP	C	90:MET	N	2.98
1	A	797:LEU	C	798:LYS	N	2.97
1	A	1219:ASN	C	1220:GLN	N	2.97
1	C	516:SER	C	517:ARG	N	2.97
1	C	974:CYS	C	975:PRO	N	2.97
1	C	1514:LYS	C	1515:ALA	N	2.97
1	C	1641:PRO	C	1642:ASP	N	2.97
1	C	1747:LEU	C	1748:ALA	N	2.97
1	C	1871:GLN	C	1872:ILE	N	2.97
1	C	2069:LYS	C	2070:LEU	N	2.97
1	D	25:SER	C	26:ARG	N	2.97
1	E	361:UNK	C	362:UNK	N	2.97
1	A	928:LEU	C	929:ASN	N	2.96
1	A	1061:PRO	C	1062:ILE	N	2.96
1	A	1265:VAL	C	1266:SER	N	2.96
1	A	1537:ASN	C	1538:ARG	N	2.96
1	A	1933:ILE	C	1934:GLU	N	2.96
1	C	778:THR	C	779:ALA	N	2.96
1	C	969:LEU	C	970:VAL	N	2.96
1	C	2108:GLN	C	2109:ARG	N	2.96
1	C	2471:CYS	C	2472:PRO	N	2.96
1	B	43:ASP	C	44:LYS	N	2.95
1	B	164:SER	C	165:LEU	N	2.95
1	C	550:LYS	C	551:SER	N	2.95
1	C	661:LEU	C	662:GLN	N	2.95
1	F	353:UNK	C	354:UNK	N	2.95
1	A	1069:VAL	C	1070:THR	N	2.94

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2284:MET	C	2285:LEU	N	2.94
1	A	326:ALA	C	327:THR	N	2.93
1	A	371:ILE	C	372:LEU	N	2.93
1	A	414:PHE	C	415:ILE	N	2.93
1	A	1228:TYR	C	1229:CYS	N	2.93
1	B	260:ALA	C	261:ASP	N	2.93
1	B	275:ARG	C	276:LEU	N	2.93
1	C	1993:PRO	C	1994:LEU	N	2.93
1	A	1346:ALA	C	1347:PHE	N	2.92
1	A	1947:ALA	C	1948:GLU	N	2.92
1	C	455:GLN	C	456:PHE	N	2.92
1	C	847:GLY	C	848:ILE	N	2.92
1	C	2251:SER	C	2252:GLU	N	2.92
1	A	1119:SER	C	1120:ARG	N	2.91
1	C	1277:PHE	C	1278:ASN	N	2.91
1	C	1591:TRP	C	1592:GLN	N	2.91
1	A	780:LYS	C	781:VAL	N	2.90
1	A	1062:ILE	C	1063:ARG	N	2.90
1	A	1680:ALA	C	1681:HIS	N	2.90
1	C	378:ALA	C	379:PHE	N	2.90
1	C	793:GLU	C	794:MET	N	2.90
1	C	948:ILE	C	949:PHE	N	2.90
1	C	1483:GLU	C	1484:ILE	N	2.90
1	A	218:ILE	C	219:ASP	N	2.89
1	A	1855:PRO	C	1856:GLU	N	2.89
1	B	66:ASN	C	67:PRO	N	2.89
1	C	1618:CYS	C	1619:ARG	N	2.89
1	C	1840:LEU	C	1841:GLN	N	2.89
1	C	2123:TYR	C	2124:LYS	N	2.89
1	C	2133:ILE	C	2134:ARG	N	2.89
1	A	270:PRO	C	271:LEU	N	2.88
1	A	1079:SER	C	1080:HIS	N	2.88
1	B	241:LYS	C	242:LEU	N	2.88
1	C	1469:PRO	C	1470:LEU	N	2.88
1	C	1943:PRO	C	1944:VAL	N	2.88
1	A	424:PHE	C	425:GLU	N	2.86
1	A	1001:GLU	C	1002:LYS	N	2.86
1	C	1122:ILE	C	1123:VAL	N	2.86
1	C	1520:PHE	C	1521:ASN	N	2.86
1	C	2100:VAL	C	2101:PHE	N	2.86
1	A	1291:TYR	C	1292:GLN	N	2.85
1	A	2291:LYS	C	2292:VAL	N	2.85

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	753:ALA	C	754:LYS	N	2.85
1	C	1446:GLU	C	1447:GLU	N	2.85
1	C	556:PHE	C	557:MET	N	2.84
1	C	966:GLY	C	967:ILE	N	2.84
1	C	1898:LEU	C	1899:SER	N	2.84
1	C	2156:CYS	C	2157:PHE	N	2.84
1	C	2337:PHE	C	2338:ARG	N	2.84
1	E	214:UNK	C	215:UNK	N	2.84
1	A	723:THR	C	724:GLN	N	2.83
1	A	957:SER	C	958:PHE	N	2.83
1	A	1824:LYS	C	1825:GLY	N	2.83
1	C	566:ASP	C	567:ILE	N	2.83
1	C	1240:GLN	C	1241:GLU	N	2.83
1	C	2098:GLU	C	2099:PRO	N	2.83
1	A	2137:VAL	C	2138:MET	N	2.82
1	A	2320:ARG	C	2321:MET	N	2.82
1	A	2322:LEU	C	2323:THR	N	2.82
1	C	2139:VAL	C	2140:MET	N	2.82
1	C	804:LEU	C	805:ILE	N	2.81
1	C	2287:LEU	C	2288:ASP	N	2.81
1	C	392:ILE	C	393:MET	N	2.80
1	D	249:HIS	C	250:GLN	N	2.80
1	C	1097:SER	C	1098:LEU	N	2.79
1	C	1652:PRO	C	1653:VAL	N	2.79
1	A	671:LEU	C	672:ALA	N	2.78
1	C	2021:ALA	C	2022:TYR	N	2.78
1	B	136:ARG	C	137:ASP	N	2.77
1	C	964:ILE	C	965:PRO	N	2.77
1	A	2019:ALA	C	2020:TYR	N	2.76
1	A	673:GLN	C	674:PRO	N	2.75
1	A	946:HIS	C	947:ILE	N	2.73
1	C	1478:LEU	C	1479:GLU	N	2.73
1	C	1574:ARG	C	1575:GLU	N	2.73
1	C	2112:LYS	C	2113:PHE	N	2.73
1	A	461:TYR	C	462:CYS	N	2.72
1	A	534:ASN	C	535:GLN	N	2.71
1	C	2227:VAL	C	2228:PHE	N	2.71
1	C	799:LYS	C	800:GLU	N	2.70
1	C	998:ARG	C	999:PRO	N	2.68
1	A	1609:ARG	C	1610:ILE	N	2.65
1	A	960:ASP	C	961:GLN	N	2.61
1	C	542:GLN	C	543:PHE	N	2.61

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2448:GLU	C	2449:GLN	N	2.59
1	C	1578:ASN	C	1579:THR	N	2.55

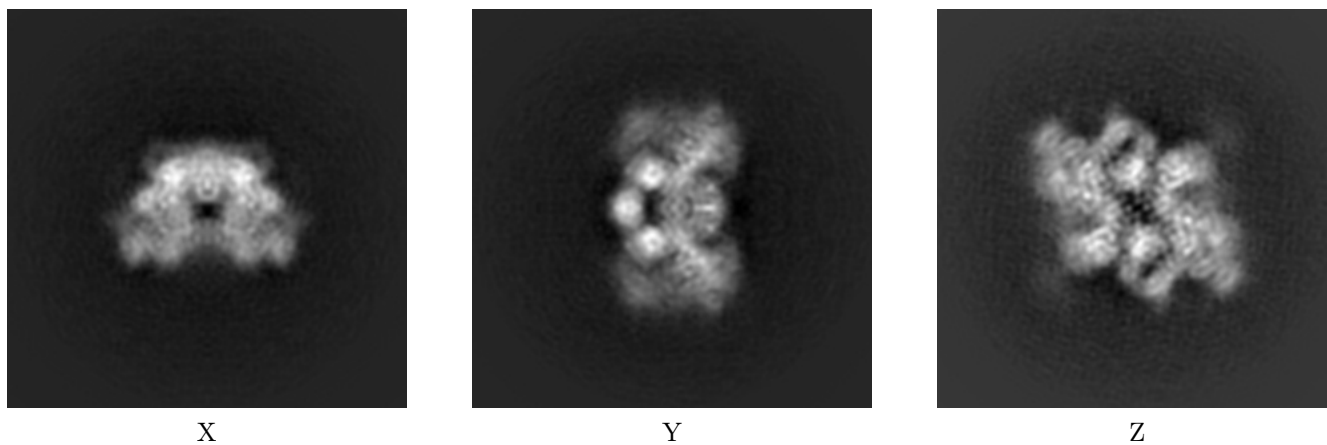
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3896. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

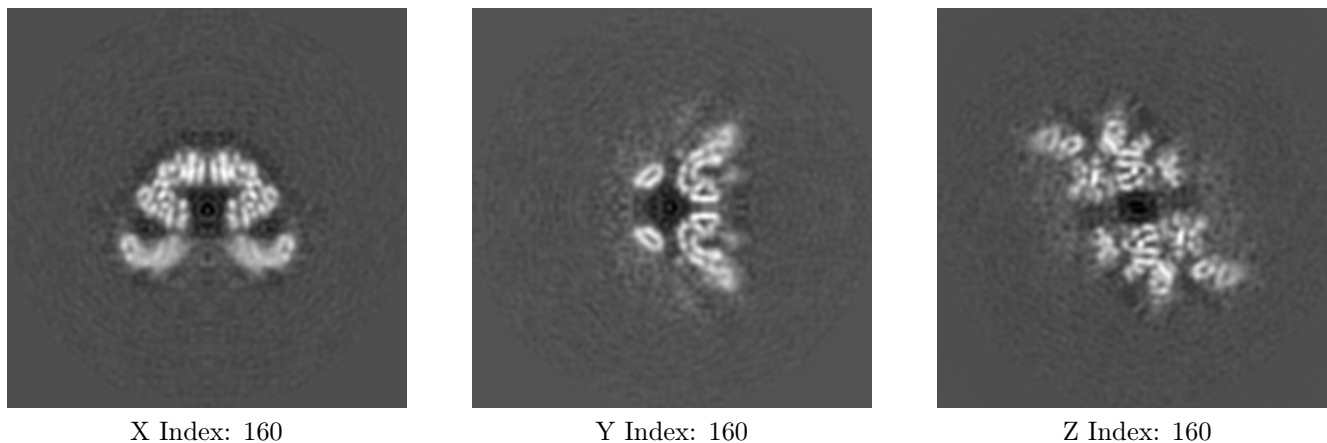
6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

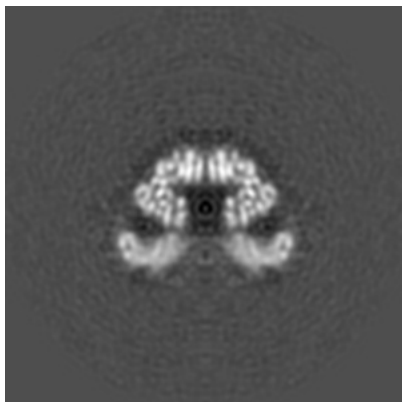
6.2.1 Primary map



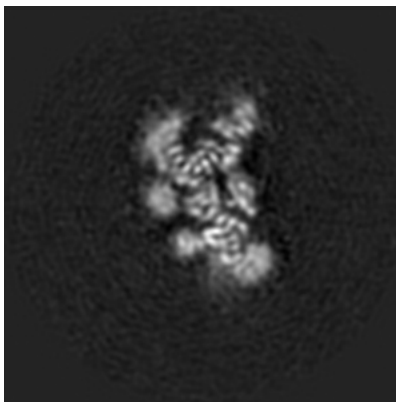
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

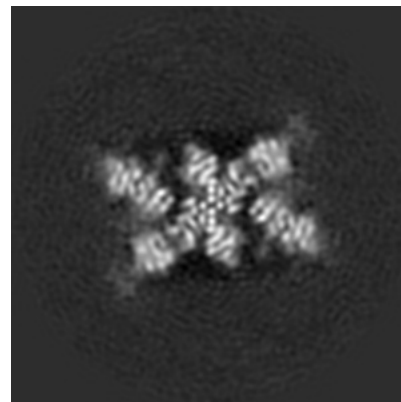
6.3.1 Primary map



X Index: 160



Y Index: 133

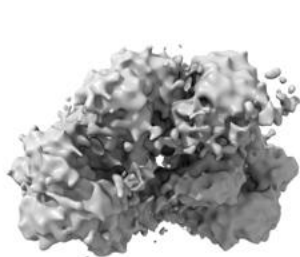


Z Index: 190

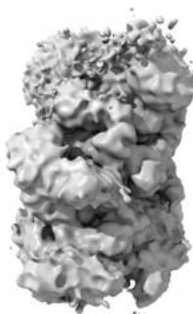
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

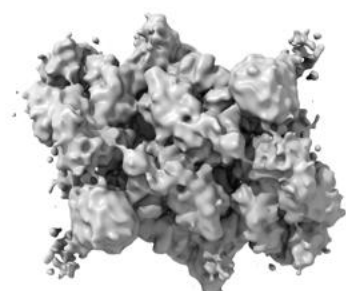
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0147. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

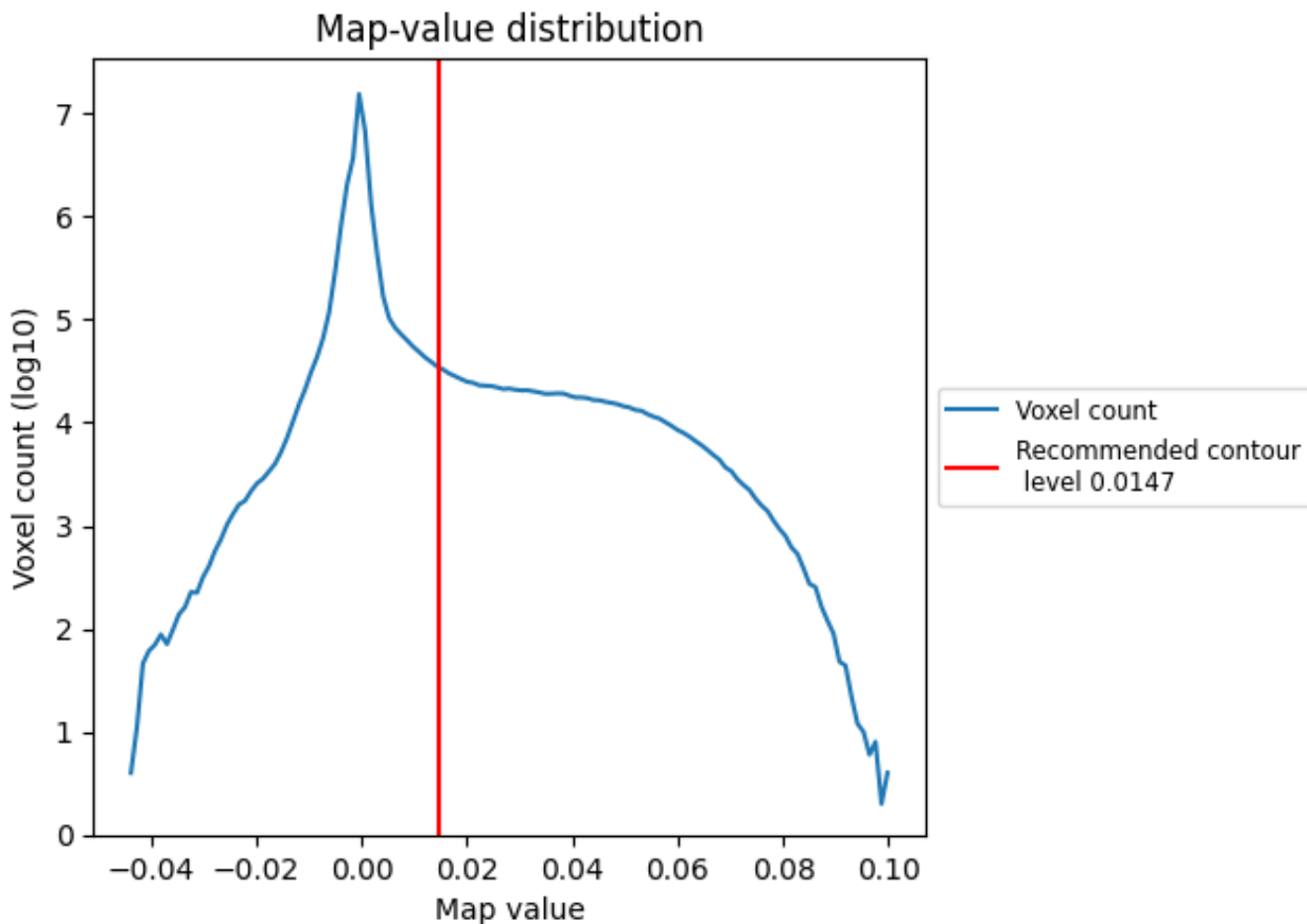
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

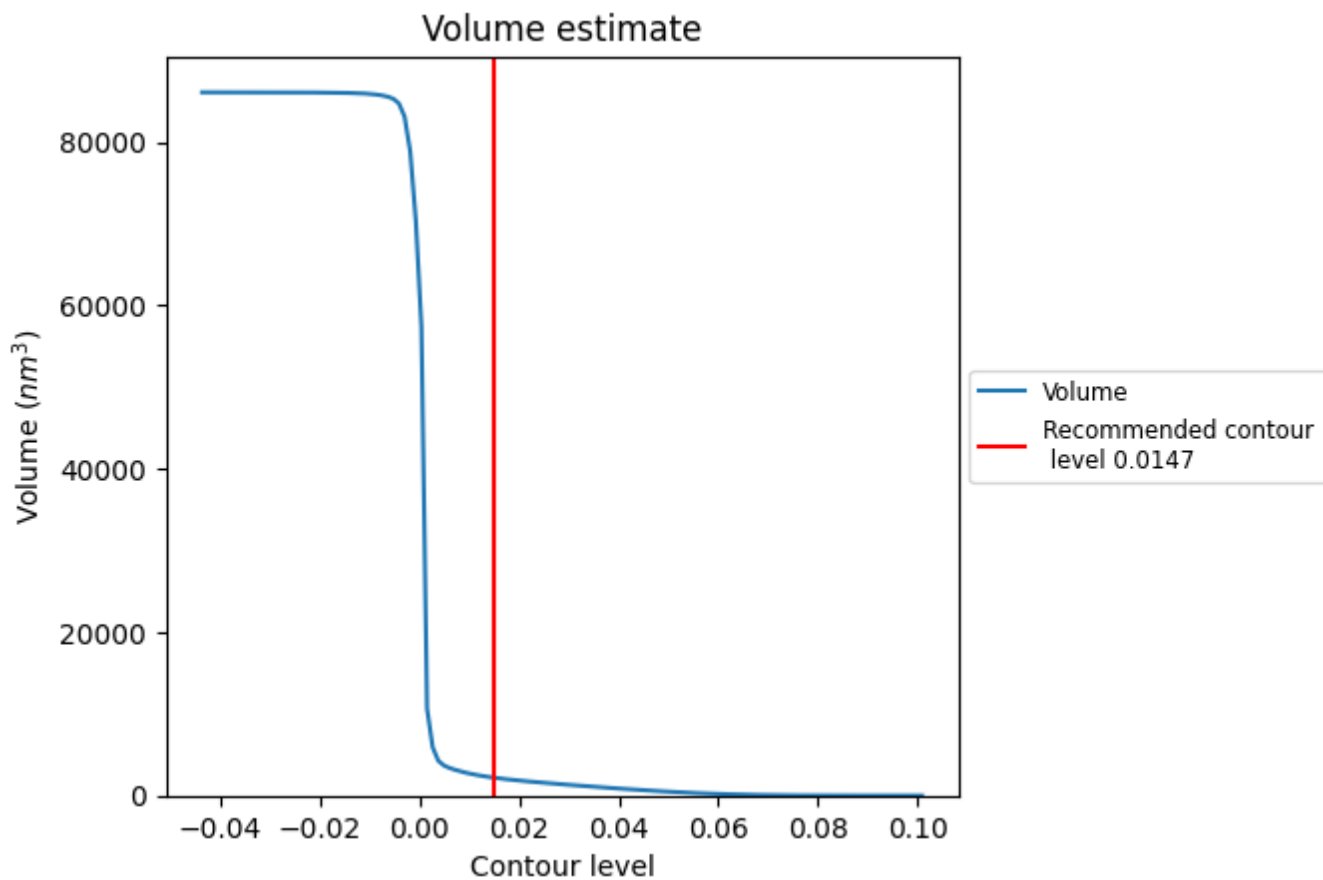
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

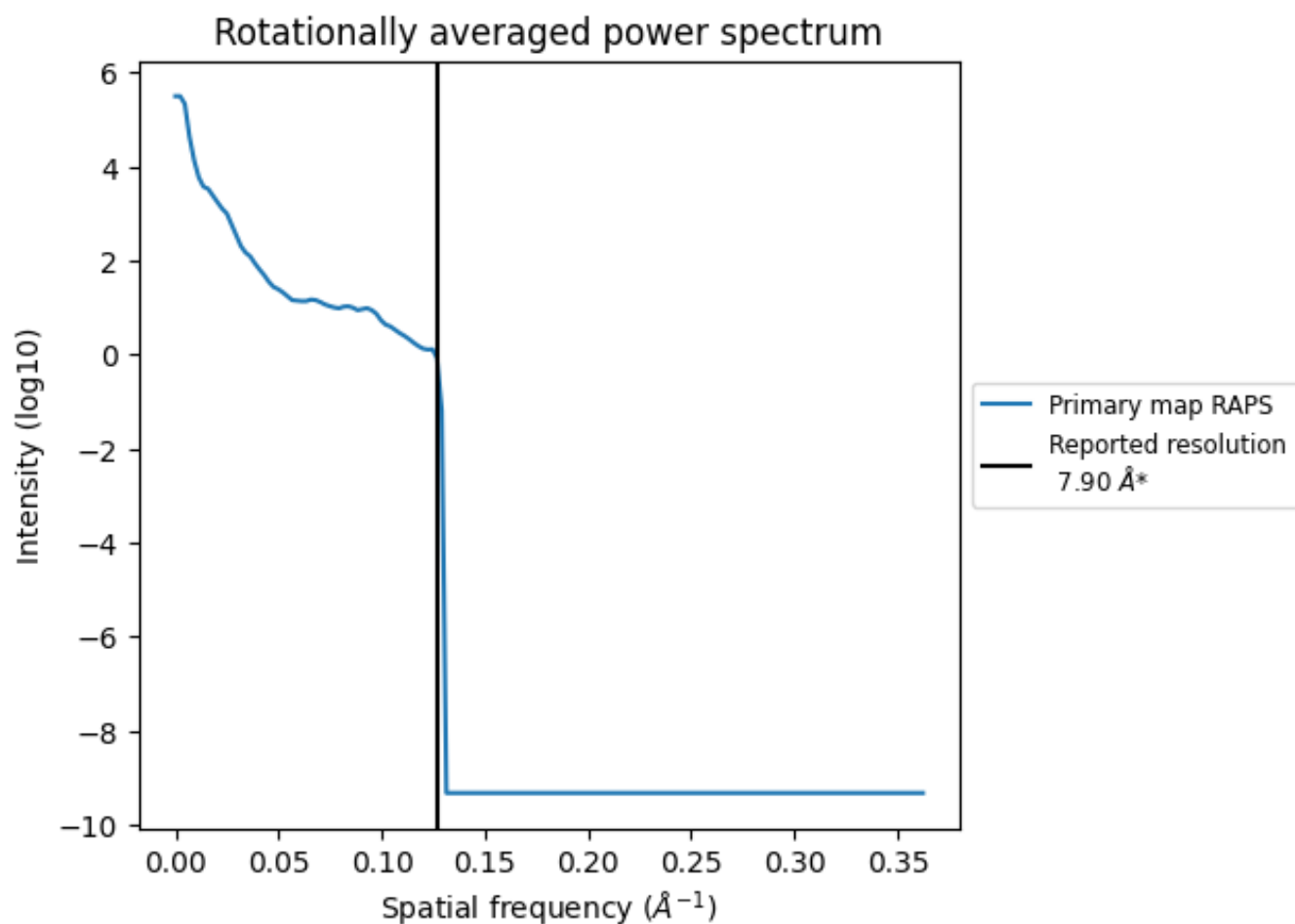
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2205 nm^3 ; this corresponds to an approximate mass of 1992 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.127 Å⁻¹

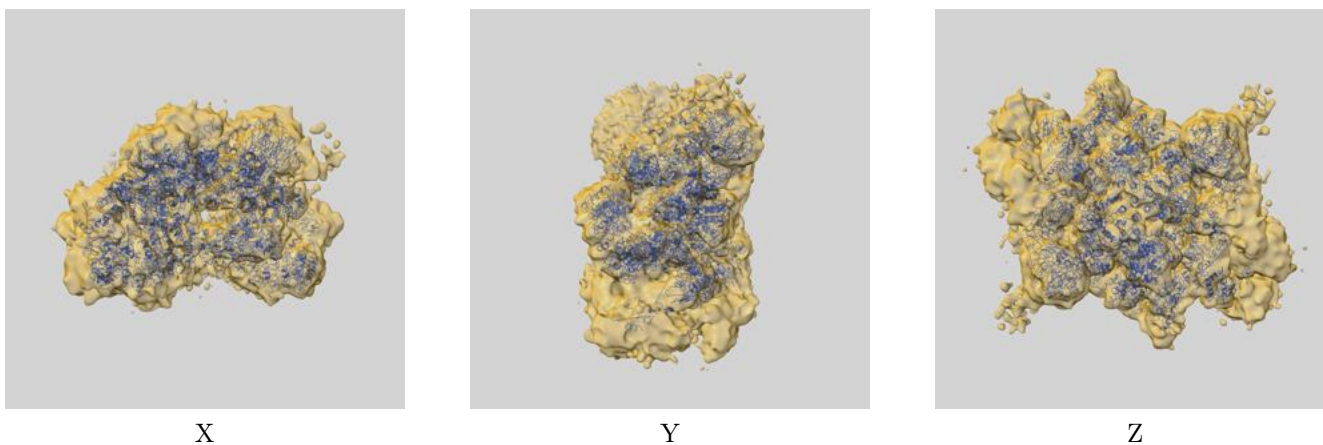
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

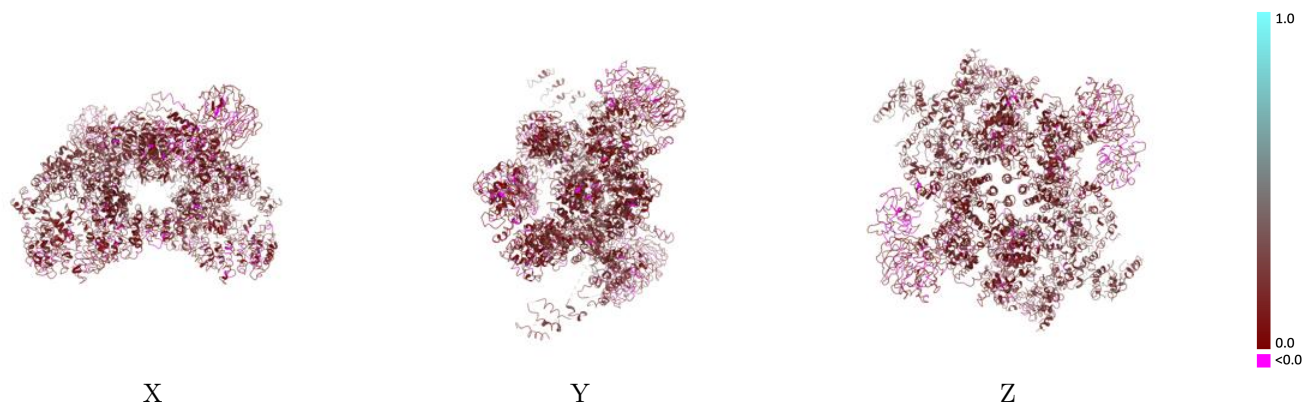
This section contains information regarding the fit between EMDB map EMD-3896 and PDB model 6EMK. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



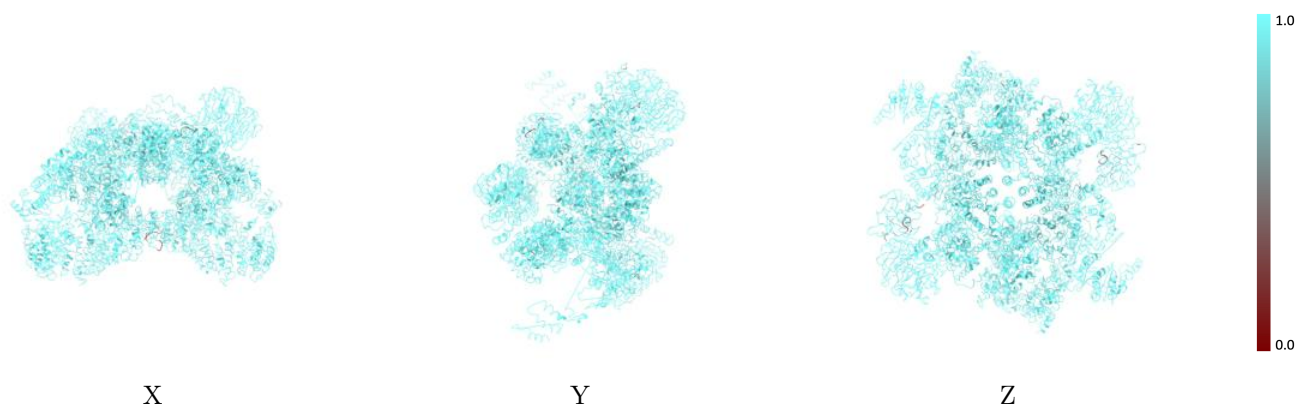
The images above show the 3D surface view of the map at the recommended contour level 0.0147 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



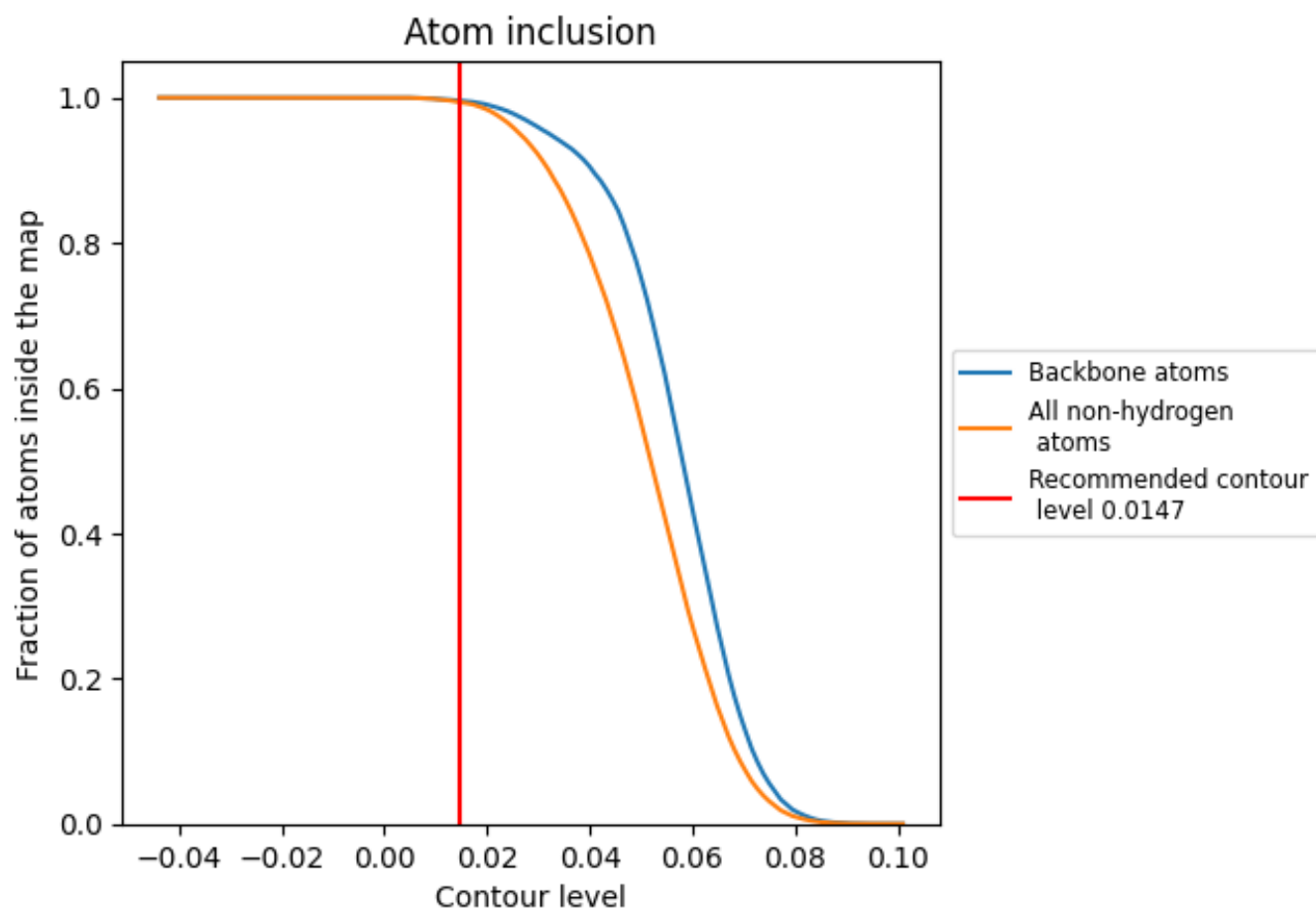
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0147).























9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0147) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9939	 0.1450
A	 0.9954	 0.1430
B	 1.0000	 0.1080
C	 0.9955	 0.1410
D	 1.0000	 0.1070
E	 1.0000	 0.2680
F	 1.0000	 0.2690
G	 1.0000	 0.2330
H	 1.0000	 0.2340
I	 0.9344	 0.0480
J	 0.9568	 0.0550

